Semiclassical localization in phase space

Dissertation
zur Erlangung des Doktorgrades Dr. rer. nat.
der Fakultät für Naturwissenschaften
der Universität Ulm

vorgelegt von

Roman Schubert
aus Hamburg

Ulm 2001

Amtierender Dekan:	Prof. Dr. W. Witschel
Erstgutachter:	Prof. Dr. F. Steiner
Zweitgutachter:	Prof. Dr. W. Arend
Drittgutachter:	Prof. Dr. A. Knauf
Tag der Promotion:	9.7.2001

Contents

Chapter 1

Introduction

Nowadays quantum mechanics is considered as the fundamental theory of physics which aims to describe phenomena at a microscopic level, e.g., systems like atoms and molecules are described by it. In this role it has replaced classical mechanics in the beginning of the 20'th century. Nevertheless classical mechanics kept its importance for the description of macroscopic systems, e.g., the solar system. Furthermore, it saw many developments since then, together with the general theory of dynamical systems. Beginning with Poincaré and Birkhoff the emphasis shifted from quantitative to more qualitative methods. The advent of KAM theory led to an understanding of sufficiently small perturbations of integrable systems, and showed more generally how intricate and rich the dynamical behavior of a Hamiltonian system in the neighborhood of an elliptic orbit can be. The term chaos was introduced to describe the extreme sensitivity to small variations of the initial conditions, which some systems show. Further concepts and properties, like ergodicity, mixing, positive entropy have been developed and studied in detail. Also the route from integrability to chaos was investigated, where a special role is played by the bifurcations of periodic orbits which occur along this route. So despite the fact that quantum mechanics has replaced classical mechanics as the fundamental microscopic description of nature, there has been a very vivid and fruitful development of classical mechanics.

These new concepts and results have even influenced quantum mechanics. Since classical mechanics is an approximation to quantum mechanics in certain situations, it is natural to ask how the dynamical properties of the classical approximation of a quantum mechanical system are reflected in the quantum mechanical system itself. This question has many facets and there are many different ways to approach it. The earliest approaches, such as WKB theory, have aimed at explicit computations, based on classical quantities, of quantum mechanical objects such as eigenvalues, eigenfunctions, time evolution, transition amplitudes and so on. Here it has turned out that in general this is only possible if the classical system possesses stable or marginally stable structures such as invariant tori or elliptic orbits. This means that the classical localization of the motion on a certain part of phase space is reflected in the quantum mechanical system: To certain regions in phase space one can associate, say, approximate eigenvalues and eigenfunctions which depend only on the dynamics in this part of phase space. The classical example is torus quantization, also called EBK quantization, but there are related methods which apply to elliptic periodic orbits, and we will spend a considerable amount of space to the discussion of these methods. But these methods are not applicable if the classical dynamics lacks such structures, which is for instance the case for chaotic systems. Then more qualitative methods are needed. Considerable progress in this direction was made by Gutzwiller with the invention of the trace formula, [Gut71, BB72]. The trace formula gives an asymptotic approximation of the quantum mechanical spectral density in terms of the periodic orbits of the classical system and their stabilities. Due to the exponential proliferation of periodic orbits in chaotic systems, this formula can usually not be used to determine individual eigenvalues, but one can study the distribution of eigenvalues. Rigorous proofs of similar trace formulae appeared shortly afterwards in the mathematical community using the newly developed tool of Fourier integral operators, [Col73, Cha74, DG75].

A number of hypotheses concerning the behavior of eigenfunctions were formulated, [Ber77b, Vor77], culminating in two main ones: first, eigenfunctions should condense semiclassically on ergodic subsets of phase space, the semiclassical eigenfunction hypothesis, and second that for classically chaotic systems the eigenfunctions should asymptotically behave like a random superposition of plane waves. Both are rather qualitative statements. With the methods from microlocal analysis it was possible to prove a strong theorem on the behavior of eigenfunctions of a system with ergodic classical limit, the quantum ergodicity theorem, [Shn74, Zel87, Col85]. It says that almost all eigenfunctions become equidistributed in the semiclassical limit if the classical system is ergodic. So for ergodic systems the semiclassical eigenfunction hypothesis is proven for almost all eigenfunctions.

Similar qualitative conjectures concerning the behavior of the eigenvalues have been formulated, e.g. the Bohigas-Giannoni-Schmit conjecture, [BGS84], which says that the statistical properties of the suitably rescaled eigenvalues are, for generic chaotic systems, the same as for those of random matrices. This random matrix conjecture has been tested numerically to a great extent, and some analytical arguments based on the trace formula supporting this conjecture are known [Ber85], but no proof has been found so far.

In this work we will concentrate mainly on the behavior of eigenfunctions. But first we have to say what the semiclassical limit is, and how the classical system which corresponds to a given quantum mechanical system is defined. The field of microlocal analysis provides a setup to discuss the semiclassical limit on a rigorous basis. One of our particular aims is to get rid of the usual interpretation of the semiclassical limit as the limit $\hbar \to 0$, since this appears to be unphysical. Physically, the semiclassical limit is the limit of highly oscillating states, i.e., the Hamiltonian and all the observables are fixed and do not depend on a parameter, but the de Broglie wavelength of the states governs the degree to which the systems behave classically. We will show that in many situations one can shift the semiclassical limit from the states to the observables by introducing a parameter λ, which plays the role of $1/\hbar$ then, but whose limit $\lambda \to \infty$ has a more concrete physical interpretation.

A fundamental problem which one has to cope with when one tries to construct approximate eigenfunctions and eigenvalues is the quasimode problem. Assume $\mathcal{H}$ is the

Hamiltonian of our system and that we have a pair (ψ, E) such that

$$\mathcal{H}\psi = E\psi + r$$

with $||r|| \leq \delta$, then one can show that, if the spectrum of $\mathcal{H}$ is discrete, there is an eigenvalue of $\mathcal{H}$ in the interval $[E-\delta, E+\delta]$. So E is close to an eigenvalue, but in contrast it turns out that ψ doesn't need not be close to an eigenfunction. Roughly speaking, if there is more that one eigenvalue in the interval $[E-\delta, E+\delta]$, then ψ can be a superposition of the corresponding eigenfunctions. This is the reason why such approximate solutions of the Schrödinger equation have been called quasimodes.

A good example to illustrate the situation is provided by a symmetric double well potential, e.g. $V(x) = (1-x^2)^2$. Here one can construct two approximate solutions of the Schrödinger equation to the same energy, one concentrated in the left well and one concentrated in the right well, which are transformed into each other by reflection on the y-axis,

$$\psi_L(x) \qquad \text{and} \qquad \psi_R(x) = \psi_L(-x) \ ,$$

see e.g. [HS96]. They satisfy

$$\mathcal{H}\psi_L = E\psi_L + O(\mathrm{e}^{-d/\hbar})$$
$$\mathcal{H}\psi_R = E\psi_R + O(\mathrm{e}^{-d/\hbar})$$

with exponentially small errors in $\hbar$. But the true eigenfunctions $\psi^{\pm}(x)$ are symmetric or antisymmetric under reflection, and we have approximately

$$\psi^{\pm}(x) \cong \frac{1}{\sqrt{2}}(\psi_L(x) \pm \psi_R(x)) \ ,$$

and for the eigenvalues $E^{\pm}$ of $\psi^{\pm}$ one has

$$|E^- - E^+| = O(\mathrm{e}^{-d/\hbar}) \ ,$$

so they are quasi-degenerate.

Hence we see that the quasimodes $\psi_L(x)$ and $\psi_R(x)$ are linear combinations of the two eigenfunctions $\psi^{\pm}(x)$ which have approximately the same eigenenergy. It seems to be quite probable that the presence of symmetries is the main reason in most cases where a sequence of quasimodes does not become close to a sequence of eigenfunctions. However, nothing rigorous is known in this direction. But if this would be the case, then a small perturbation of the system, which destroys the symmetry, would lead to eigenfunctions which are concentrated on a connected domain, and hence to quasimodes close to eigenfunctions.

In the above example of a symmetric double well potential, Simon [Sim85], has shown that an arbitrarily small perturbation which destroys the symmetry but which can be supported far outside the semiclassical support of the eigenfunction, has the effect that the true eigenfunctions become close to ψ_L and ψ_R, hence are concentrated in one of the wells.

We will argue that this example is typical, i.e., we believe that for generic perturbations of an arbitrary system quasimodes are close to eigenfunctions. The perturbations we study are of a semiclassically small type, which means that they do not change the classical system. E.g., one can think of the perturbed systems as being a family of quantizations of the same classical system. In physical terms these perturbations can represent the influence of an environment. No system is completely isolated, and the environment acts as a fluctuating perturbation, which has the effect that the quantities which are observable in nature are the generic ones. This interpretation of the influence of generic perturbations is quite close to the ideas in the field of decoherence, see e.g. [Omn94, GJK⁺96].

The notion of stability with respect to small perturbations, which emerges from the previous discussion, is interesting in its own right. We examine the usual quasimode constructions with respect to stability, and it turns out that not all quasimodes are stable. For instance in the case of torus quantizations it turns out that stability requires that the torus satisfies a KAM condition. Surprisingly, although we subject the system to a perturbation which does not affect the classical limit, the condition for stability is the same as in classical mechanics for the perturbation of an integrable system. The classical result, due to von Neuman and Wigner, that avoided crossings of eigenvalues are generic can also be interpreted as saying that almost degeneracies of eigenvalues are unstable under small perturbations.

The main tools we use in the study of these questions are a class of approximate projection operators which we can associate with every open domain in phase space. If the domain is invariant under the classical flow one can furthermore choose an approximate projection operator which commutes with the Hamilton operator up to a semiclassically small remainder. More precisely, to an open domain

$$D \subset T^*M$$

we associate a class of operators

$$\pi_D := \left(\frac{\lambda}{2\pi}\right)^d \int_D |z\rangle\langle z| \, \mathrm{d}z \ ,$$

where $|z\rangle$ denotes a family of coherent states on M. Here λ is a semiclassical parameter and $\lambda \to \infty$ corresponds to the semiclassical limit. These operators can be thought of as approximate projection operators, and if D is invariant under the classical flow one furthermore has

$$[\mathcal{H}, \pi_D] = O(\lambda^{-1/2}) \ . \tag{1.1}$$

If the domain D is moreover stably invariant, in the sense that for all sufficiently small perturbations of the classical Hamilton function there is an invariant domain D' close to D, then by choosing the family of coherent states carefully, one can achieve that

$$[\mathcal{H}, \pi_D] = O(\lambda^{-N})$$

quantum mechanics	**classical mechanics**
Hilbert space	phase space
Hamilton operator	Hamilton function
operators	functions
commutator	Poisson bracket

Table 1.1: Basic objects in quantum and classical mechanics which correspond to each other.

for every $N \in \mathbb{N}$. Such operators are a good tool to study localization properties of eigenfunctions in phase space.

We will now give a more detailed description of the contents of this work. In the Chapter 2 we give a presentation of the main features of microlocal analysis from the point of view of semiclassics. The adjective microlocal means localization in phase space, and in mathematics microlocal analysis is, roughly speaking, the qualitative theory of linear partial differential equations which uses the cotangentbundle of the manifold where the equations live on (which is nothing but phase space), to study it. So it is no surprise that there are close relations to semiclassics. The main elements of the theory are pseudodifferential and Fourier integral operators and some basic relations connecting them.

The microlocal point of view emphasizes the algebras of observables in contrast to the standard point of view in textbooks on quantum mechanics where more emphasis is put on the states. In many respects the transition from quantum mechanics to classical mechanics is much simpler if one studies it for the algebras of observables. The states are then viewed as positive linear forms on the algebras.

Given an algebra of operators on some function space, the basic principle in microlocal analysis is to classify these operators by their action on highly oscillating test functions, which means in physical terms, by testing their semiclassical limit. A pseudodifferential operator is an operator which satisfies two requirements: first it does not change the frequency of the highly oscillatory test function, and secondly it changes the amplitude of this test function in a way depending smoothly on the position and frequency. In order to express this in formulas we take the simplest type of an oscillating function, a plane wave

$$\mathrm{e}_\xi := \mathrm{e}^{\mathrm{i}\langle x,\xi\rangle} ,$$

where $\xi \in \mathbb{R}^d$ is the frequency vector and $|\xi| \to \infty$ corresponds to the semiclassical limit. Then we require that the operator $\mathcal{A}$ satisfies

$$\mathcal{A}\mathrm{e}_\xi = a(\xi, x)\mathrm{e}_\xi$$

where $a(\xi, x)$ is a smooth function, called the symbol of the operator $\mathcal{A}$, which satisfies suitable estimates. The precise estimates which the symbol has to satisfy, define the class of pseudodifferential operators to which $\mathcal{A}$ belongs. The simplest class is given by the so called polyhomogeneous symbols, where one requires that the symbols have an asymptotic expansion in homogeneous functions of ξ for large $|\xi|$,

$$a(\xi, x) \sim \sum_{k=0}^{\infty} a_{m-k}(\xi, x) ,$$

where $a_{m-k}(\lambda\xi, x) = \lambda^{m-k} a_{m-k}(\xi, x)$ for $\lambda > 0$. The last condition means essentially that a does not oscillate for large ξ, and hence adds no contribution to the oscillations of e_ξ. The degree of homogeneity of the leading term m is called the order of the operator and the leading part itself is called the principal symbol,

$$\sigma(\mathcal{A})(\xi, x) := a_m(\xi, x) ,$$

which plays an important role in the theory since it turns out to be the classical limit of the quantum observable $\mathcal{A}$

Operators of this type can be multiplied and the products are of the same type, hence they form an algebra, and explicit formulas for the products in terms of the symbols are known. In particular, the principal symbols show a simple behavior,

$$\sigma(\mathcal{A}\mathcal{B}) = \sigma(\mathcal{A})\sigma(\mathcal{B}) , \qquad \sigma([\mathcal{A}, \mathcal{B}]) = \frac{1}{\mathrm{i}}\{\sigma(\mathcal{A}), \sigma(\mathcal{B})\} ,$$

where $\{\sigma(\mathcal{A}), \sigma(\mathcal{B})\}$ denotes the Poisson bracket of $\sigma(\mathcal{A})$ and $\sigma(\mathcal{B})$. Hence the principal symbol defines an algebra morphism from the algebra of quantum mechanical observables to the algebra of classical observables. In physical terms these relations mean that $\sigma(\mathcal{A})$ is really the classical observable corresponding to $\mathcal{A}$.

As an application we will discuss complex powers of an elliptic differential operator and the corresponding trace, which is the so-called MP-zeta function. From this Weyl's law can be deduced and, furthermore, the Szegö limit theorem, an important result which shows how the high energy limit acts on pseudodifferential operators as a semiclassical limit. Let the Hamiltonian $\mathcal{H}$ be an elliptic pseudodifferential operator on some compact manifold, and let ψ_n be the eigenfunctions and $N(E)$ be the spectral counting function, counting the number of eigenvalues of $\mathcal{H}$ below E. Then the Szegö limit theorem says that

$$\lim_{E\to\infty} \frac{1}{N(E)} \sum_{E_n \leq E} \langle \psi_n, \mathcal{A}\psi_n \rangle = \frac{1}{\mathrm{vol}(\Sigma_1)} \int_{\Sigma_1} \sigma(\mathcal{A}) \, \mathrm{d}\mu ,$$

where $\Sigma_1 := \{(\xi, x) \, ; \, \sigma(\mathcal{H})(\xi, x) = 1\}$ denotes the equienergy shell at energy 1 and $\mathrm{d}\mu$ denotes the canonical Liouville measure on Σ_1. Hence the high energy behavior of expectation values of pseudodifferential operators does only depend on the principal symbol.

A further important class of operators can be characterized by demanding that they change the oscillations of a highly oscillating function in a well defined way. Since ξ and

x are identified as coordinates on phase space, we expect that a change of them is related to a canonical transformation. Indeed, if one requires that an operator $\mathcal{U}$ acts on a plane wave as

$$\mathcal{U}\mathrm{e}_\xi = b(\xi, x)\mathrm{e}^{\mathrm{i}\varphi(\xi,x)}$$

where b is a smooth symbol and φ is realvalued, smooth and homogeneous of degree one in ξ, then $\mathcal{U}$ is called a Fourier integral operator, and can be viewed as a quantization of the canonical transformation Φ whose generating function is φ. The main relation connecting Fourier integral operators and pseudodifferential operators is the Theorem of Egorov, which in a simplified version means that one can find for each canonical transformation Φ a Fourier integral operator $\mathcal{U}(\Phi)$ with

$$\sigma(\mathcal{U}(\Phi)\mathcal{A}\mathcal{U}(\Phi)^*) = \sigma(\mathcal{A}) \circ \Phi \ .$$

The canonical transformations can also be characterized by their action on the Poisson algebra of the classical observables, they are the algebra automorphisms, and there is a beautiful theorem, due to Duistermaat and Singer [DS76], that conjugation with Fourier integral operators gives exactly the order preserving automorphisms of the algebra of pseudodifferential operators.

We next turn to some applications of the concepts developed so far in quantum chaos, in order to illustrate their use. The first one is the quantum ergodicity theorem which can be proven using the Szegö limit theorem and Egorov's theorem. It gives a characterization of the semiclassical behavior of almost all eigenfunctions of a system whose classical limit is ergodic. It says that they become equi-distributed in the high energy limit, mimicking the behavior of the classical Liouville probability density. E.g., for a billiard this means that in position space

$$\lim_{j\to\infty} |\psi_{n_j}|^2 = \frac{1}{\operatorname{vol} M}$$

in the weak sense, where $\{\psi_n\}_{n\in\mathbb{N}}$ denotes the set of eigenfunctions. This is the strongest rigorous result of a general nature obtained so far in quantum chaos, since it makes a prediction under well defined and rather weak conditions. In the following we show examples and discuss further questions related to quantum ergodicity.

The second application is the trace formula, which is based on the observation that the time evolution operator is a Fourier integral operator associated with the classical flow. Using methods from the theory of Fourier integral operators one can determine its trace, which can be expressed in terms of the periodic orbits of the classical system. This is the famous formula which connects the quantum mechanical spectrum with the classical periodic orbits, and is at the heart of most attempts to prove results about the dependence of the statistical properties of the eigenvalues on the hyperbolic properties of the flow. We then give some applications to spectral asymptotics which we illustrate with examples.

Up to now we have only dealt with systems on compact manifolds to which the usual methods of microlocal analysis are perfectly applicable, since the semiclassical limit is realized as the limit of large energies. Many systems are not of this type, for instance an atom has a non-compact configuration space, and a finite ionization energy. Here we expect semiclassical behavior for highly excited states close to the ionization energy, so here the limit $E \to \infty$ is not the limit we want to study. In the literature the semiclassical limit is typically performed as the limit $\hbar \to 0$, and this can be applied perfectly to this situation. There exists a theory analogous to the theory of pseudodifferential and Fourier integral operators described before, which contains $\hbar$ and where the classical structures appear in the limit $\hbar \to 0$. We give a short review of the main ingredients, showing how the formulas are adapted. The main drawback of this approach, compared with the previous one, is that although the number of systems to which this can be applied is considerably larger, its physical meaning has to be clarified. In nature $\hbar$ is a constant, so a priori the limit $\hbar \to 0$ is purely formal from the physical point of view, and has to be justified further. This is attempted in Section 2.5 of Chapter 2, which departs from the general review character this chapter and contains some new ideas.

The overall picture of the semiclassical limit that emerges from the discussions in Chapter 2 is that quantum mechanical quantities become close to classical quantities, if

1. the states are highly oscillatory, meaning the de Broglie wavelength tends to 0 and, in the case of eigenstates, the quantum numbers become large,

2. the quantum mechanical spectrum becomes close to the classical spectrum, i.e. the spectrum of the generator of the classical time evolution, and since the classical spectrum is for most systems continuous, this means typically that the mean spectral density has to tend to ∞.

Guided by a simple embedding of the classical pseudodifferential operators into the λ-dependent operators (λ playing formally the role of $1/\hbar$), we construct for a large class of systems a map which maps these systems to λ-dependent systems, where the semiclassical limit is obtained as the limit $\lambda \to \infty$. This construction is illustrated with some examples. From thereon we will discuss only the λ-dependent calculus.

In Chapter 3 about Lagrangian states the main technical tools used in this work are developed. Here the necessary theory of Lagrangian states, which we will apply in the following chapters to construct quasimodes and approximate projection operators, is developed. A Lagrangian state is, generally speaking, a function which is locally given by an oscillating integral of the form

$$u(\lambda, x) = \int_{\mathbb{R}^\kappa} \mathrm{e}^{\mathrm{i}\lambda\varphi(\theta,x)} a(\lambda, \theta, x) \; \mathrm{d}\theta \; , \tag{1.2}$$

where φ and a are smooth functions satisfying suitable conditions which we omit for the moment. Semiclassically, i.e. in the limit $\lambda \to \infty$, such a function is concentrated on the set

$$L := \{(\varphi'_x(\theta, x), x) \, , \; \varphi'_\theta(\theta, x) = 0\} \; , \tag{1.3}$$

i.e. , we have $\mathcal{A}u(\lambda) = O(\lambda^{-\infty})$ for every $\mathcal{A}$ whose symbol vanishes in a neighborhood of L. If φ is real valued, as we have tacitly assumed, then, under some non-degeneracy conditions on φ, L will be a Lagrangian submanifold of phase space. This is the reason why such states are called Lagrangian. They have been studied thoroughly and their theory is well developed; their main use in quantum mechanics is the quantization of tori in integrable and KAM systems, see, e.g., [Mas72, Dui74, Laz93]. Furthermore the kernels of Fourier integral operators are of this type.

But if one wants to study quasimodes concentrated on lower dimensional submanifolds, e.g., on elliptic periodic orbits, one is naturally led to states of the form (1.2) with complex valued phase functions. The theory of these states is less completely developed, although there exist some treatments [MS73, MSS90]. Our aim is to develop a general theory of such states, along the lines of the development of the theory of Fourier integral operators with complex phase functions in [Hör85b], in the same way as the theory with real valued phase functions was developed in [Dui74].

In the first sections of Chapter 3 we treat some local questions and two special classes of such Lagrangian states, the one with real valued phase functions and the so-called coherent states which are concentrated semiclassically in one point of phase space. As an introduction and motivation we give a review of how the classical WKB ansatz leads to a construction of quasimodes as Lagrangian states with real valued phase functions for classically integrable systems in Section 3.1. Special emphasis is put on the symplectic geometry underlying this construction and a geometrical interpretation of the Maslov index appearing in the quantization condition. If we try to apply the same procedure to an elliptic orbit, we see that we are forced to consider complex valued phase functions. In Section 3.2 we study some local questions related to oscillatory integrals with complex valued phase functions, especially the damping induced by the imaginary part. We present a theorem due to [MS75] on the action of a pseudodifferential operator on oscillatory integrals with complex valued phase function. This makes the introduction of almost analytic extensions necessary. In order to illustrate the problem, assume that $\mathcal{P} = \sum_{|\alpha|\leq m} p_\alpha(x) D^\alpha$, with $D := \frac{1}{\mathrm{i}\lambda}\partial_x$, is a partial differential operator, and $\varphi(x)$ is smooth and complex valued with $\operatorname{Im}\varphi \geq 0$, then we have

$$\mathcal{P}\mathrm{e}^{\mathrm{i}\lambda\varphi}(x) = P(\varphi'(x), x)\mathrm{e}^{\mathrm{i}\lambda\varphi(x)}$$

where $P(\xi, x) = \sum_{|\alpha|\leq m} p_\alpha(x)\xi^\alpha$ is the symbol of $\mathcal{P}$. Now for a general pseudodifferential operator we expect in leading order a similar formula, but since the symbol will no longer be polynomial in ξ, but just a smooth function on phase space, it is a priory not clear how to evaluate it at complex arguments $(\varphi'(x), x)$. The method of almost analytic extensions provides now a way to extend a smooth function to complex arguments, which we can use for our case.

The simplest type of Lagrangian states with complex phase function are, in a sense, the coherent states, which we will study in detail in Section 3.3. Since they are concentrated in one point it is sufficient to study them on $\mathbb{R}^d$. The term coherent state has been used in the literature for a particular type of states with a more or less precisely defined range of properties, see e.g. [Per86, CR95, Pau97]. We will denote by this an oscillatory function with quadratic phase function which is concentrated in one point in phase space. Explicitly, a coherent state is given by

$$u^B_{p,q}(\lambda, x) := \left(\frac{\lambda}{\pi}\right)^{d/4} (\det \operatorname{Im} B)^{1/4} \mathrm{e}^{\mathrm{i}\lambda[\langle p, x-q\rangle + \frac{1}{2}\langle x-q, B(x-q)\rangle]} , \tag{1.4}$$

where $(p,q) \in T^*\mathbb{R}^d$ denotes a point in phase space and B is a complex symmetric matrix with $\operatorname{Im} B > 0$. The pre-factor ensures that the state is normalized. What we are interested in is the dependence on B and (p,q). There is a rich geometrical structure associated with B, which we study in detail. If we use the formula (1.3) to associate a Lagrangian manifold with it, we obtain

$$L_B = \{(p + Bx, q + x)\}$$

which we interpret, by allowing $x \in \mathbb{C}^d$, as a complex Lagrangian plane in the complexified tangent space $T^{\mathbb{C}}_{(p,q)}T^*\mathbb{R}^d$ to $T^*\mathbb{R}^d$ at (p,q). From complex linear symplectic geometry it is known that such a Lagrangian plane defines a complex structure and a metric $\mathbf{g}_L$ on $T_{(p,q)}T^*\mathbb{R}^d$. These structures play an important role in the theory of coherent states: for instance, the Wigner function of a coherent state is given by

$$W(\xi, x) = \left(\frac{\lambda}{\pi}\right)^d \mathrm{e}^{-\lambda\langle(\xi-p, x-q), \mathbf{g}_L(\xi-p, x-q)\rangle}$$

where $\langle(\xi - p, x - q), \mathbf{g}_L(\xi - p, x - q)\rangle$ is the squared distance between (p,q) and (ξ, x) measured in the metric $\mathbf{g}_L$.

For the later applications it will be useful to study families of coherent states. It is well known that the set of states defined by (1.4) forms a complete set of states in the sense that

$$\left(\frac{\lambda}{2\pi}\right)^d \iint |u^B_{p,q}\rangle\langle u^B_{p,q}| \; \mathrm{d}p\mathrm{d}q = 1 \; .$$

It will turn out to be useful to let B vary with (p,q). This means that we have an almost complex structure and a non-constant metric on phase space. The states are still normalized then, but the completeness relation is no longer true. Instead we get

$$\left(\frac{\lambda}{2\pi}\right)^d \iint |u^B_{p,q}\rangle\langle u^B_{p,q}| \; \mathrm{d}p\mathrm{d}q = 1 - \frac{1}{12\lambda}\mathbf{s} \; ,$$

where $\mathbf{s}$ is a symmetric pseudodifferential operator whose principal symbol is given by the scalar curvature $s(p,q)$ of the metric $\mathbf{g}_L$. The calculus of pseudodifferential operators shows that $\mathcal{P} := (1 - \frac{1}{12\lambda}\mathbf{s})^{-1/2}$ is well defined for sufficiently large λ, and is a pseudodifferential operator then. Then the modified family of coherent states

$$\tilde{u}^B_{p,q} := \mathcal{P} u^B_{p,q}$$

satisfies the completeness relation

$$\left(\frac{\lambda}{2\pi}\right)^d \iint |\tilde{u}^B_{p,q}\rangle\langle\tilde{u}^B_{p,q}| \, \mathrm{d}p\mathrm{d}q = 1 \ .$$

But now the states are generally no longer normalized, instead we have

$$||\tilde{u}^B_{p,q}||^2 = 1 + \frac{1}{12\lambda}s(p,q) + O(\lambda^{-2}) \ ,$$

so the scalar curvature of $\mathbf{g}$ is the leading order obstruction for a family of coherent states to be simultaneously normalized and complete.

In Section 3.4 we turn to the general theory of Lagrangian states with complex phase functions on manifolds. We develop the theory along the lines of Lagrangian distributions with complex valued phase functions [Hör85b]. The first task is to define the complex Lagrangian submanifold of phase space which acts as a classical support of the state. In the first treatments of the theory, [MS73, MS75, MSS90], this was done using the machinery of almost analytic extensions, which is quite technical. We will therefore follow Hörmander, who has replaced the almost analytic machinery by Lagrangian ideals. The idea can be thought of as shifting the attention from the states to the algebras of observables, which has already been proven to be fruitful in Chapter 2. Let Λ be a real Lagrangian submanifold of phase space, then we can associate the vanishing ideal

$$J_\Lambda := \{f \in C^\infty(T^*M) \ , \ f|_\Lambda = 0\}$$

with it. It is easy to see that J_Λ is closed under Poisson brackets and can be locally generated by $d = \dim M$ functions. One can show conversely that for every ideal with these properties the set of common zeros of the functions in the ideal form a Lagrangian submanifold. Hence we have a one-to-one correspondence between Lagrangian submanifolds and a certain type of ideals in the space of smooth functions, which are called Lagrangian ideals. Now one just removes the condition that the functions should be real valued, and arrives at complex Lagrangian ideals, which play the role of the (non-existent) complex Lagrangian submanifolds.

This idea of determining a distinguished subset of the set of classical observables as the "complex Lagrangian submanifold" suggests a natural intrinsic definition of the set of Lagrangian states associated with this complex Lagrangian ideal J. Namely, if we have a classical state ν concentrated on the zero set of J, then $\nu(f) = 0$ for all $f \in J$, and this condition characterizes the set of classical states concentrated on J. Now we demand for the quantum mechanical states that the same condition holds asymptotically. We say that $\psi(\lambda)$ is a Lagrangian state associated with the complex Lagrangian ideal J if, roughly speaking,

$$\mathcal{A}_1 \cdots \mathcal{A}_N \psi = O(\lambda^{m-N})$$

for every $N \in \mathbb{N}$ and for all $\mathcal{A}_i$ whose principal symbols are in J,

$$\sigma(\mathcal{A}_i) \in J \ .$$

Here $m \in \mathbb{R}$ is called the order of ψ. So classically a set of states is defined by requiring that they should vanish on the Lagrangian ideal, and the corresponding set of quantum states is defined by requiring that the quantized Lagrangian ideal should vanish asymptotically on them.

The quantized Lagrangian ideal can as well be thought of as a set of annihilation operators. In the simplest case that the Lagrangian ideal is generated by a set of linear complex functions, the Lagrangian states are given by the coherent states, and the quantizations of the generators are exactly the annihilation operators known from the harmonic oscillator. The adjoint operators then give the corresponding creation operators.

We then turn to discuss local representations of such states. Exactly as for the real valued case there exist generating functions for complex Lagrangian ideals, and the Lagrangian states have local representations as oscillatory integrals with this generating function as exponent. This means that we have found a general global invariant characterization of the states of the form (1.2).

Our next aim is to define a principal symbol, and here unfortunately we cannot follow anymore the treatise of Hörmander, since he does not discuss this point. As a preparation a careful study of the linear case is necessary. By this we mean Lagrangian states defined by complex Lagrangian planes, but in contrast to the coherent states we only require the Lagrangian planes to be non-negative. The set of all such planes is called the complex Lagrangian Grassmannian and we show that the set of Lagrangian states associated with them form a line bundle over the Lagrangian Grassmannian which is a half density bundle tensored with the so-called complex Maslov bundle.

Given a complex Lagrangian ideal J, then at each point of the zero set of it a unique complex Lagrangian plane in the complexification of the tangent space is defined by requiring that the differentials of all elements of the ideal should vanish on the plane at that point,

$$L_z := \{\hat{z} \in T_z^{\mathbb{C}} T^* M \;,\; \langle df(z), \hat{z}\rangle = 0 \text{ for all } f \in J\} \;.$$

This family of Lagrangian planes can be used to define a Maslov bundle on the zero set of J by a pull back from the complex Lagrangian Grassmannian. If the complex Lagrangian ideal satisfies certain non-degeneracy conditions one can split this bundle into two parts, one real part to which all the known results from the real case can be applied, and a purely complex one which is then studied separately.

The principal symbol of a general Lagrangian state is then defined by testing against coherent states. It turns out that in addition to the Maslov phase another phase appears, connected with the Liouville class. So the principal symbol can be defined as a section in a line bundle which is the tensor product of the half-density bundle, the Maslov bundle and the Liouville bundle.

In the last sections of Chapter 3 we discuss the time evolution of Lagrangian states. This can be reduced to the case of a coherent state, for which we give a simplified presentation of a proof due to Combescure and Robert [CR97] on the time evolution that allows estimates for large times.

In Chapter 4 we apply the results on families of coherent states to the construction of localized operators via the so-called Anti-Wick quantization. An Anti-Wick operator is a superposition of projection operators onto coherent states with a relative weight given by a function on phase space. To a function a on phase space one associates the operator

$$\mathrm{Op}_B^{AW}[a] := \left(\frac{\lambda}{2\pi}\right)^d \iint a(p,q)|\tilde{u}_{p,q}^B\rangle\langle\tilde{u}_{p,q}^B| \, \mathrm{d}p\mathrm{d}q \ ,$$

which is called the Anti-Wick quantization of a. The use of the modified coherent states $\tilde{u}_{p,q}^B$ is important, since it ensures the completeness relation

$$\mathrm{Op}_B^{AW}[1] = 1 \ .$$

The Anti-Wick quantization has some nice properties. It maps real valued functions to symmetric operators and it maps positive functions to positive operators. But most importantly, it can be used to quantize non-smooth functions or even distributions. The most severe drawback is that the Anti-Wick operators do not form an algebra, i.e. the product of two Anti-Wick operators is in general not an Anti-Wick operator.

After collecting some general properties of these operators in Section 4.1, we discuss estimates in the case of quantizations of measures. It turns out that Cotlar's Lemma allows very precise estimates of the norm of such operators in terms of the Hausdorff dimension of the measure one quantizes. In Section 4.3 we then turn to our main application of Anti-Wick quantization, the construction of approximate projection operators. Given a domain D in phase space, the Anti-Wick quantization allows us to quantize the characteristic function of D,

$$\pi_D := \left(\frac{\lambda}{2\pi}\right)^d \iint_D |\tilde{u}_{p,q}^B\rangle\langle\tilde{u}_{p,q}^B| \, \mathrm{d}p\mathrm{d}q \ .$$

Such operators indeed form approximate projection operators since they satisfy

$$\pi_D^2 - \pi_D = O(\lambda^{-\infty}) \ ,$$

microlocally away from the boundary of D.

In the applications we want to associate such approximate projection operators to domains in phase space which are invariant under the classical flow, in order to study localization of eigenfunctions on these domains. We expect that for an invariant domain D, π_D approximately commutes with the Hamilton operator $\mathcal{H}$, and indeed we show that

$$[\mathcal{H}, \pi_D] = O(\lambda^{-1/2})$$

if D is invariant. In order to improve the remainder estimate it turns out that further requirements on D are needed. As already mentioned, if D is stably invariant, then one can choose the metric $\mathbf{g}$ in such a way that for every $N \in \mathbb{N}$

$$[\mathcal{H}, \pi_D] = O(\lambda^{-N}) \ . \tag{1.5}$$

Two immediate applications are discussed then, which are among the main results of this work.

First, using Duhamels principle, (1.5) immediately implies that

$$||\mathcal{U}(t)^*\pi_D\mathcal{U}(t) - \pi_D|| \leq C|t|\lambda^{-N}$$

where $\mathcal{U}(t)$ is the time evolution operator generated by $\mathcal{H}$. Hence the image and the kernel of π_D form an approximate decomposition of the Hilbert space into two approximately invariant subspaces. So the strict decomposition of the classical phase space into D and its complement can be lifted in an approximate way to the quantum mechanical Hilbert space.

Secondly, if the flow restricted to D is ergodic one can carry over the proof of the quantum ergodicity theorem to this situation, which gives that for almost all eigenfunctions

$$\lim_{j\to\infty}\left[\langle\psi_{n_j},\pi_D\mathcal{A}\psi_{n_j}\rangle - \langle\psi_{n_j},\pi_D\psi_{n_j}\rangle\overline{\sigma(\mathcal{A})}^D\right] = 0 \ ,$$

where $\overline{\sigma(\mathcal{A})}^D$ denotes the classical mean over D. The quantity $\langle\psi_{n_j},\pi_D\psi_{n_j}\rangle$ measures the fraction of ψ_{n_j} which lives on D. So this result tells us that the part of ψ_{n_j} living on D becomes equidistributed on D.

In Chapter 5 we now finally turn to apply the considerably large technical apparatus developed so far to the questions of semiclassical localization of eigenfunctions we are interested in. In Section 5.1 we review some general properties of quasimodes. As already mentioned, quasimodes are approximate solutions to the Schrödinger equation, and the main observation is that although the approximate eigenvalues are close to the real eigenvalues, the approximate eigenfunctions need not be close to real eigenfunctions, hence the name quasimodes. The main obstruction for a quasimode to be close to an eigenfunctions is the existence of more than one eigenvalue which is closer to the approximate eigenvalue than the error of the Schrödinger equation. We show how the classical work of von Neumann and Wigner on avoided level crossings [vNW29] can be interpreted as demonstrating that such near degeneracies of eigenvalues are unstable under small perturbations of the system.

In Section 5.2 we study the effect of perturbations more closely and conjecture that generically quasimodes are close to eigenfunctions in the semiclassical limit. The connection to some ideas in the field of decoherence is mentioned as well. Especially from (1.5) it follows that $\pi_D\psi_n$ is a sequence of quasimodes, and if quasimodes were generically close to eigenfunctions, then we could conclude, that the eigenfunctions are generically concentrated in D or the complement of D. So in this case the splitting of phase space would be directly visible in the eigenfunctions.

The tools from Chapter 3 are applied in Section 5.4 to construct quasimodes attached to stable or marginally stable invariant sets in phase space, especially to invariant tori and to elliptic orbits. Such constructions are well known in the literature, see, e.g., [MF81, Col77, Laz93, Ral76], and our emphasis is mainly on one new point. Inspired by the previous section, we study the question which quasimodes are stable under perturbations.

It turns out that not all quasimodes are stable under perturbations. And, although we study perturbations which leave the classical system invariant, the conditions on stability of the quasimodes on the classical support of them are the same as the conditions of stability of the classical structures under small perturbations of the classical system. So for invariant tori we obtain that they have to satisfy certain KAM conditions in order that the quasimodes supported by them are stable. Similarly, for elliptic orbits we show that these have to satisfy classical non-resonance conditions in order that the quasimodes concentrated on them are stable.

In the four appendices some technical tools are discussed. In Appendix A we recall the definition of densities and half-densities and collect their basic properties. When working on manifolds they are very useful objects to have at hand, and especially the definition of a principal symbol for Lagrangian functions is facilitated by them. Appendix B contains the basic results on the so-called Gauss transforms and their mapping properties on certain function spaces. These results are needed rather frequently when one works with symbols and wants to show that certain operations on them again give symbols. In Appendix C the Malgrange preparation theorem and some of its applications are discussed. This theorem and its consequences are needed when we discuss Lagrangian ideals and how they are generated. Finally Appendix D gives a discussion of the method of stationary phase and some of the basic theorems. We have to go beyond most standard treatments in that we have to include the case of complex valued phase functions, which can be done using the machinery of almost analytic extensions, or, more elegantly, by using the Malgrange preparation theorem from Appendix C.

Since some parts of this work have the character of an review while other parts contain new results, and these two are not always clearly distinguished, I finally would like to point out where the results are new. Chapter 2 is of an review character with the only exception of Section 2.5 which contains some new results. Chapter 3 is of an intermediate type, the results on the families of coherent states in Section 3.3 are new and Section 3.4 consists of extensions of known results and ideas. Chapter 4 is in a sense the heart of the work and almost all results presented there are new. Finally in Chapter 5 the Sections 5.3 and 5.5 contain new results, while the remaining part is mainly a discussion of known results in the light of two new conjectures from Section 5.2.

Chapter 2

Microlocal analysis and semiclassics

> *"... it seems to me that there has been in the literature entirely too much emphasis on quantization, (i.e. general methods for obtaining quantum mechanics from classical methods) as opposed to the converse problem of the classical limit of quantum mechanics. This is unfortunate since the latter is an important question for various areas of modern physics while the former is, in my opinion, a chimera."*
>
> Barry Simon [Sim80]

The aim of this chapter is to present some basic concepts of microlocal analysis from the point of view of quantum mechanics and the semiclassical limit. This will serve as a background for the following chapters, where we will use the mathematical language and methods from microlocal analysis. Since on the one hand we cannot assume that every reader is familiar with this part of mathematics, and on the other hand introducing all these concepts from the scratch would definitely go beyond the scope of this work, we have decided to give an informal introduction. We will describe the results which are important for the further development, and set up a kind of dictionary, which translates the mathematical terms into a more physical language. This will be illustrated by examples, and occasionally we will sketch some formal computations in more detail in order to make the reader familiar with the flair of the theory and the methods.

2.1 Quantum and classical mechanics

In this section the basic structures of quantum and classical mechanics, respectively, will be described for simple types of systems. The basic example, which the reader should keep in mind, is the motion of a free particle on a Riemannian manifold.

2.1.1 Quantum mechanics

Let (M, g) be a Riemannian manifold. The state space of the quantum system is the Hilbert space of square integrable functions on M,

$$L^2(M, g) = \left\{ \psi(x) \, ; \; ||\psi||^2 = \int_M |\psi(x)|^2 \, \mathrm{d}\nu_g(x) < \infty \right\} ,$$

where $\mathrm{d}\nu_g(x)$ denotes the Riemannian volume element on M. More precisely, the pure states are represented by the normalized functions in $L^2(M, g)$, i.e. $||\psi|| = 1$. If the particle is in the state ψ, then $|\psi(x)|^2$ is the probability distribution of the position, i.e., if $D \subset M$ is some domain, then the probability of finding the particle in the domain D is given by

$$\int_D |\psi(x)|^2 \, \mathrm{d}\nu_g(x) \; .$$

This can as well be written as $\langle \psi, \chi_D \psi \rangle$, where χ_D denotes the multiplication operator with the characteristic function of D, and $\langle \cdot, \cdot \rangle$ denotes the standard scalar-product in $L^2(M, g)$. More generally, observable quantities are represented by selfadjoint operators on $L^2(M, g)$ and the quantity

$$\omega_\psi(\mathcal{A}) := \langle \psi, \mathcal{A}\psi \rangle$$

for a selfadjoint operator $\mathcal{A}$ is the expectation value, i.e., the mean value which one finds when measuring the quantity $\mathcal{A}$ sufficiently often while the system is in the state ψ.

The bounded operators on $L^2(M, g)$ form an algebra, which by abuse of language is called the algebra of observables; the observable quantities correspond to the selfadjoint elements in this algebra. The states can be viewed as positive linear maps from the algebra of observables into the complex numbers. More precisely, for every normalized element $\psi \in L^2(M)$, i.e. , $||\psi|| = 1$, the map

$$\mathcal{A} \mapsto \omega_\psi(\mathcal{A}) = \langle \psi, \mathcal{A}\psi \rangle \tag{2.1}$$

is linear and in addition normalized, positive and maps selfadjoint operators to real numbers:

$$\omega_\psi(I) = 1 \tag{2.2}$$
$$\omega_\psi(\mathcal{A}\mathcal{A}^*) \geq 0 \tag{2.3}$$
$$\omega_\psi(\mathcal{A}^*) = \omega_\psi(\mathcal{A})^* \; , \tag{2.4}$$

here I denotes the identity operator. By generalization, any linear functional on the algebra of observables with these three properties, (2.2), (2.3) and (2.4), is called a state. E.g., every trace class operator $\boldsymbol{\rho}$ that is selfadjoint, positive and has trace one defines a state by

$$\mathcal{A} \mapsto \omega(\mathcal{A}) := \operatorname{tr} \mathcal{A}\boldsymbol{\rho} \; .$$

The set of states is a convex set, i.e., if ω_1 and ω_2 are states, then $\lambda\omega_1 + (1-\lambda)\omega_2$ is a state for $\lambda \in [0,1]$. The states which cannot be represented as a convex combination of other states are called pure states; e.g., the states defined by the elements of $L^2(M)$ according to (2.1) are pure.

Instead of the usual point of view in most textbooks on quantum mechanics, where the state space is the primary object, one can also start from the algebra of observables (assumed to be some C^*-algebra). Then every state defines via the GNS construction [BR79] a Hilbert space, and a representation of the algebra of observables as bounded operators on that Hilbert space. We will follow an intermediate point of view, because the semiclassical limit is more natural on the algebraic level, but we will always work with an explicit realization of the algebra of observables on a given Hilbert space. An account of quantum mechanics with emphasis on this algebraic point of view can be found, e.g., in [Thi79, Seg47].

The dynamics is defined by specifying a selfadjoint operator, the Hamilton operator, representing the energy. In case of a free particle this is just the Laplace-Beltrami operator on M, $\mathcal{H} = -\frac{\hbar^2}{2m}\Delta_g$. The Schrödinger equation, which determines the time-evolution of the states, then reads

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = \mathcal{H}\psi \ .$$

The solution of this equation with initial value $\psi(0,x) = \psi_0(x)$ is given by

$$\mathcal{U}(t)\psi_0 = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}t\mathcal{H}}\psi_0 \ , \tag{2.5}$$

where $\mathcal{U}(t)$ is called the time evolution operator. It is unitary, because $\mathcal{H}$ is selfadjoint. Since $\langle\mathcal{U}(t)\psi, \mathcal{A}_0\mathcal{U}(t)\psi\rangle = \langle\psi, \mathcal{U}(t)^*\mathcal{A}_0\mathcal{U}(t)\psi\rangle$, where $\mathcal{A}_0$ is an operator on $L^2(M,g)$ and ψ is assumed to be in the domain of $\mathcal{A}_0$, the time evolution can as well be shifted to the algebra of observables. The corresponding equation for the dynamics then is the Heisenberg equation, which, in the case that $\mathcal{A}_0$ is time independent, reads

$$-\mathrm{i}\hbar\frac{\mathrm{d}\mathcal{A}}{\mathrm{d}t} = [\mathcal{H}, \mathcal{A}] \ , \tag{2.6}$$

where $[\mathcal{H}, \mathcal{A}]$ denotes the commutator of $\mathcal{H}$ and $\mathcal{A}$. The solution of the Heisenberg equation with initial value $\mathcal{A}_0$ is given by conjugation of $\mathcal{A}_0$ with the time evolution operator

$$\mathcal{A}(t) = \mathcal{U}^*(t)\mathcal{A}_0\mathcal{U}(t) \ . \tag{2.7}$$

Therefore on the algebra of observables the time evolution is given by a one parameter group of automorphisms of this algebra. Generally, by conjugation any unitary operator gives rise to an automorphism of the algebra of observables. Hence, from the conventional point of view, the morphisms of the theory can be identified with the unitary operators, and from the algebraic point of view by the algebra-automorphisms. But the set of algebra-automorphisms can be larger than the set of unitary operators, because a priori not every algebra-automorphism has to be induced by a unitary operator. Especially the anti-unitary operators enter as further algebra-automorphisms.

This was a rather condensed and abstract description of the basic structure of quantum mechanics, for a more thorough treatment emphasizing the algebraic point of view see [Thi79], and for a classical treatment, e.g., [Dir58].

We are especially interested in the stationary states, i.e. the eigenfunctions of $\mathcal{H}$, which satisfy the stationary Schrödinger equation

$$\mathcal{H}\psi_n = \lambda_n \psi_n \ .$$

When M is compact and $\mathcal{H}$ satisfies certain natural conditions which we will specify later, the spectrum is discrete and has no finite accumulation point. We will assume that the eigenvalues are ordered increasingly, $\lambda_0 \leq \lambda_1 \leq \lambda_2 \cdots$. The information on the eigenvalues will often be encoded in certain spectral functions, the simplest one being the counting function

$$N(\lambda) := \#\{\lambda_n \leq \lambda\} \ , \tag{2.8}$$

which has a jump at each eigenvalue λ_n whose height is the multiplicity of the eigenvalue. In figure 2.1 the counting function is shown for three different systems which are described below.

Our aim is to obtain information on the behavior of the eigenvalues and eigenfunctions in the limit $n \to \infty$. The results in the next sections show that this limit depends in leading order only on the corresponding classical system, therefore this is called the semiclassical limit.

In quantum chaos one often studies billiards. A billiard is given by a compact (or sometimes finite-volume) domain $\Omega \subset \mathbb{R}^d$ with smooth or piecewise smooth boundary $\partial\Omega$. The Hamilton operator is given by the Laplace operator $-\Delta$ with suitable boundary conditions on $\partial\Omega$. We will in the following only meet the case of Dirichlet conditions. The advantage of billiards is that they are simple enough to allow for effective numerical computations, while on the other hand they encompass a great diversity of dynamical behavior. The examples which we will look at in the following are taken from the family of limaçon billiards in $\mathbb{R}^2$. In polar coordinates $(r, \varphi) \in \mathbb{R}^+ \times [-\pi, \pi]$ their boundary $\partial\Omega$ is parameterized by

$$r(\varphi) = 1 + \varepsilon \cos\varphi \tag{2.9}$$

with $\varepsilon \in [0, 1]$. For $\varepsilon = 0$ we have a circle, for $\varepsilon = 0.3$ the shape looks like a slightly deformed circle and for $\varepsilon = 1$ we get the cardioid, which has a cusp at the origin, see fig. 2.2. This family has been introduced as a family of quantum billiards by Robnik [Rob83, Rob84], and since then has been an object of frequent studies in classical and quantum chaos. The numerical data we present in the following have been kindly provided by Arnd Bäcker, whose Ph.D-thesis can be consulted for more details on these systems [Bäc98]. In order to illustrate the spectral quantities we have shown in fig. 2.1 $N(\lambda)$ for

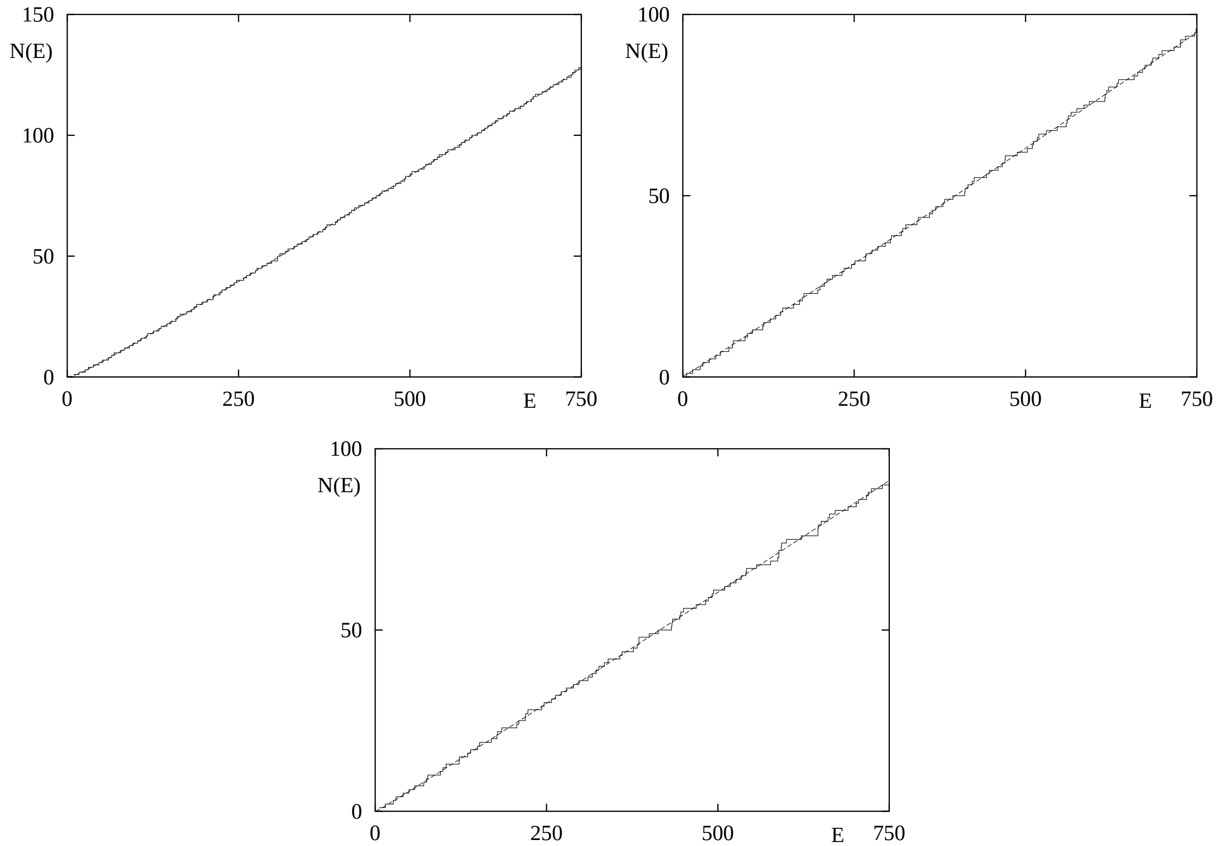

Figure 2.1: The spectral counting function (2.8) for three different systems, the cardioid billiard at the top left, the limaçon billiard, see (2.9), with parameter $\varepsilon = 0.3$ at the top right and the circle billiard at the bottom. See the text and (2.9) for a description of the systems. Note that the strength of the fluctuations about the mean behavior is strongest for the circle billiard followed by the limaçon billiard with parameter $\varepsilon = 0.3$ and weakest for the cardioid billiard. As dotted lines are plotted the mean behavior according to Weyl's law.

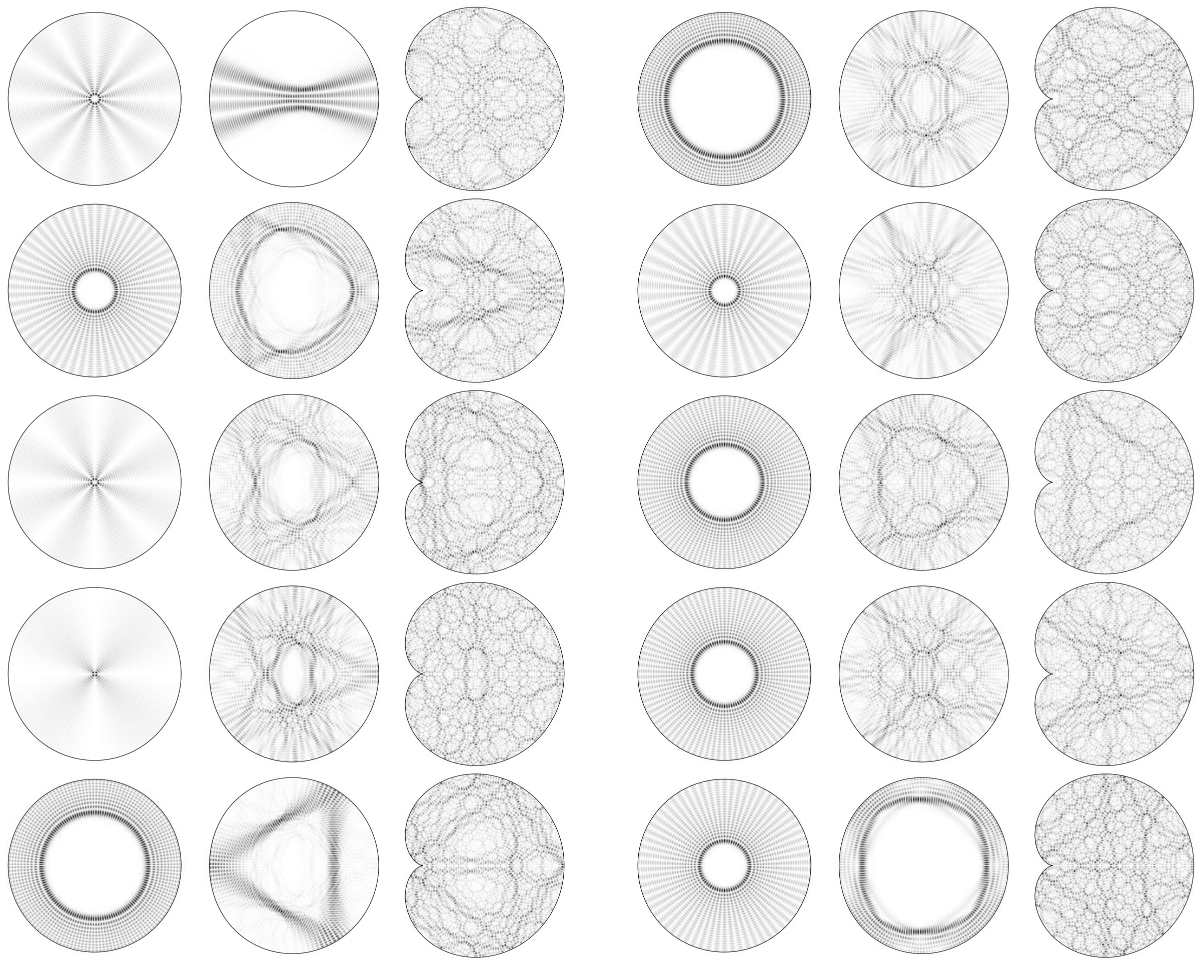

Figure 2.2: Density plots of $|\psi_n|^2$ for a consecutive sequence of Dirichlet eigenfunctions ψ_n of the circle billiard on the left, the limaçon billiard , see (2.9), with $\varepsilon = 0.3$ in the middle, and the cardioid billiard on the right, respectively. The upper left starts with $n = 1800$ down to the lower left with $n = 1804$ and the upper right with $n = 1805$ to the lower right with $n = 1809$. Note the different types of structures which appear in the eigenfunctions of the different systems. The eigenfunction densities of the circular billiard are of course all rotationally-symmetric and have pronounced structures, but all of a similar type. The eigenfunctions of the cardioid billiard are more or less all rather equidistributed in the billiard and possess only weak structures. In contrast to the other two billiards, the eigenfunctions of the limaçon billiard with $\varepsilon = 0.3$ display a variety of different structures, ranging from localization to almost equidistribution. This reflects the structures of the corresponding classical systems, as we will see later on.

the three different systems, the circle billiard, the cardioid billiard and the limaçon billiard (2.9) with $\varepsilon = 0.3$. Furthermore, in fig. 2.2 density plots of a couple of eigenfunctions of each billiard is shown.

2.1.2 Classical mechanics

We now describe some of the basic structures of classical mechanics, or more precisely of Hamiltonian mechanics, see, e.g. , [Arn78, AM78]. We will present Hamiltonian mechanics in a way that the structural similarities with quantum mechanics are pronounced, with a view towards our aim to describe how Hamiltonian mechanics is generated as a limit of quantum mechanics [Thi88].

The state space in Hamiltonian mechanics is given by a symplectic manifold and is usually called phase space. In our cases this will always be a cotangent bundle T^*M of some compact manifold M of dimension d. A symplectic manifold is a smooth manifold together with a nondegenerate closed two-form ω on it and necessarily is of even dimension $2d$. On a cotangent bundle there is a natural one-form given in local coordinates (ξ, x), where $x \in M$ denotes position and ξ momentum, by

$$\alpha = \xi \mathrm{d}x := \sum_{i=1}^{d} \xi_i \mathrm{d}x_i \ ,$$

and the usual symplectic two-form on T^*M is the differential of α

$$\omega := -\mathrm{d}\alpha = -\mathrm{d}\xi \wedge \mathrm{d}x = \sum_{i=1}^{d} \mathrm{d}x_i \wedge \mathrm{d}\xi_i \ .$$

A pure state of the system is given by a point (ξ, x) in phase space, e.g., for a one particle system x is the position of the particle and ξ is its momentum. An observable is given by a function a on phase space, and the value of the observable in a state (ξ, x) is the value of the function at that point. The set of observables form an algebra, e.g., $C^\infty(T^*M)$ if we allow only smooth functions. The evaluation of an observable at a given state is a linear map from the algebra of observables into the set of complex numbers. Therefore we can generalize the notion of a state by defining a general state as a smooth positive linear functional ν on the algebra of observables, i.e. a distribution, which is normalized, positive and takes real values on real observables, exactly as in quantum mechanics. Since positive distributions are measures, see e.g. [Hör83, Theorem 2.1.7.], which means

$$\nu(a) \leq C \sup(a) \ , \quad \text{for all } a \in C^\infty(T^*M) \ ,$$

the states are positive measures. The pure states are the ones which are concentrated in one point, i.e. delta functions.

An explicit system and its dynamics are defined by specifying a Hamilton function $H(\xi, x)$ on phase space, giving the energy of the system in the state (ξ, x). To each real valued smooth function H in phase space one can associate a vector-field, the so called Hamiltonian vector-field X_H, which is defined by

$$\omega(X_H, Y) = \mathrm{d}H(Y)$$

for all vector-fields Y. In local symplectic coordinates (ξ, x), the vector-field X_H is hence given by

$$X_H = \left(-\frac{\partial H}{\partial x}, \frac{\partial H}{\partial \xi}\right)^T ,$$

where we used the shorthand $\frac{\partial H}{\partial x} = (\frac{\partial H}{\partial x_1}, \cdots, \frac{\partial H}{\partial x_d})$ and similarly $\frac{\partial H}{\partial \xi} = (\frac{\partial H}{\partial \xi_1}, \cdots, \frac{\partial H}{\partial \xi_d})$. Hamilton's equations corresponding to H are then given by

$$\frac{\mathrm{d}}{\mathrm{d}t}(\xi, x) = X_H ,$$

and in local coordinates this is the usual set of Hamilton's equations

$$\frac{\mathrm{d}\xi}{\mathrm{d}t} = -\frac{\partial H}{\partial x} , \quad \frac{\mathrm{d}x}{\mathrm{d}t} = \frac{\partial H}{\partial \xi} .$$

So the specification of a function on phase space defines a dynamical system on phase space. For a free particle the Hamiltonian is just

$$H(\xi, x) = \frac{1}{2m}|\xi|_g^2 = \frac{1}{2m}\sum g^{ij}(x)\xi_i\xi_j ,$$

and the corresponding flow is the geodesic flow lifted to T^*M.

By duality the flow $\Phi^t = \exp(tX_H)$ on phase space defines an automorphism of the algebra of observables:

$$(\Phi^t)^* a(\xi, x) := a(\Phi^t(\xi, x)) , \tag{2.10}$$

for $a \in C^\infty(T^*M)$. Differentiating this equation with respect to time t leads to

$$\frac{\partial a}{\partial t} = -\{H, a\} ,$$

where $\{H, a\}$ denotes the Poisson bracket of h and a, defined by

$$\{H, a\} := \omega(X_H, X_a) = \frac{\partial H}{\partial x}\frac{\partial a}{\partial \xi} - \frac{\partial H}{\partial \xi}\frac{\partial a}{\partial x} .$$

With the help of the Jacobi identity for the Poisson bracket, see, e.g., [Arn78], one easily sees that the flow leaves the symplectic form and the Poisson-bracket invariant, so it is an example of a so-called canonical transformation, or symplectomorphism. Generally a canonical transformation is defined to be a smooth invertible map $\Phi : T^*M \to T^*M$, which leaves the symplectic form invariant,

$$\Phi^*\omega = \omega \ . \tag{2.11}$$

The group of canonical transformations are the morphisms of Hamiltonian mechanics. The d'th power of the two-form ω defines a volume element

$$\mu := \frac{(-1)^{[d/2]}}{d!}\omega \wedge \cdots \wedge \omega$$

on phase space, which is invariant under canonical transformations. Therefore the pullback of a canonical transformation is a unitary operator in the space $L^2(T^*M, \mu)$. One special example is given by the canonical transformations induced by the time evolution of a Hamiltonian system, $V(t) = \Phi^{t*}$, whose action on $L^2(T^*M, \mu)$ is given by (2.10),

$$(V(t)a)(\xi, x) = a(\Phi^t(\xi, x)) \ . \tag{2.12}$$

This operator is the analogue of the quantum mechanical time evolution operator $\mathcal{U}(t)$, and we will later see how it appears as the classical limit of $\mathcal{U}(t)$. The spectral properties of this operator contain information on the flow. This point of view in mechanics, using the spectral theory of $V(t)$ to study the flow, is sometimes called Koopmanism, see [AM78].

A further important class of objects in classical mechanics, or more precisely in symplectic geometry, are Lagrangian submanifolds. A submanifold $\Lambda \subset T^*M$ is called Lagrangian if it has half the dimension of T^*M, i.e., $\dim \Lambda = \dim M$, and if the symplectic two form vanishes on Λ, $\omega|_\Lambda = 0$. A simple example is given by the graph of the differential of some smooth function φ, that is in local coordinates $\Lambda = \{(\varphi'(x), x) \mid x \in M\}$. Then Λ is Lagrangian because $\omega|_\Lambda = \mathrm{d}\alpha|_\Lambda = \mathrm{d}(\varphi'(x)\mathrm{d}x) = \mathrm{d}^2\varphi = 0$. On the other hand, every Lagrangian manifold Λ whose projection to the base M is locally an diffeomorphism can locally be represented in this way. Since on Λ one has $\mathrm{d}\alpha = \omega = 0$ there is a function on Λ, which can be parameterized by a subset of M, with $\alpha = \mathrm{d}\varphi$. This function φ is called a generating function for Λ.

With similar arguments it can be shown [Hör85a] that for an arbitrary Lagrangian submanifold Λ there exists locally a generating function $\varphi(x, \theta)$, depending on some auxiliary variables $\theta \in \mathbb{R}^\kappa$, such that locally

$$\Lambda = \{(\varphi'_x(x, \theta), x) \mid x \in X \ , \ \varphi'_\theta(x, \theta) = 0\} \ . \tag{2.13}$$

According to the "symplectic creed" [Wei77] everything in symplectic geometry should be represented by Lagrangian submanifolds. What about symplectomorphisms? Consider a symplectomorphism $\Phi : T^*M \to T^*M$, then it follows from (2.11) that if we equip $T^*M \times T^*M$ with the symplectic form $\pi_1^*\omega_1 - \pi_2^*\omega_2$, where $\pi_1^*\omega_1$ is the pullback of the symplectic form on the first factor by the projection π_1 to the first factor and $\pi_2^*\omega_2$ the one on the second factor, then the graph of Φ, $\Lambda_\Phi = \{(\xi, x, \Phi(\xi, x)\} \subset T^*M \times T^*M$ is a

Lagrangian submanifold of $(T^*M \times T^*M, \omega_1 - \omega_2)$. So according to the previous paragraph, there exists a generating function as in (2.13) for this graph. The map

$$T^*M \times T^*M \ni (\xi, x; y, \eta) \mapsto (\xi, x; y, -\eta) \in T^*M \times T^*M$$

maps Λ to

$$\Lambda^- = \{(\xi, x; y, \eta) \mid (\xi, x; y, -\eta) \in \Lambda\} ,$$

which is a Lagrangian submanifold in $T^*(M \times M)$ with the symplectic form $\pi_1^*\omega_1 + \pi_2^*\omega_2$. Choosing $\eta \in \mathbb{R}^d$ as auxiliary variable we make an ansatz for a generating function of Λ^- as

$$\varphi(x, y, \eta) = \psi(x, \eta) - \langle y, \eta \rangle . \tag{2.14}$$

Then $\partial_x \varphi = \partial_x \psi$, $\partial_y \varphi = -\eta$, $\partial_\eta \varphi = \partial_\eta \psi - y$, so from (2.13) it follows that the Lagrangian submanifold generated by φ in $T^*(M \times M)$ is

$$\Lambda_\varphi = \{(\partial_x \psi, x, -\eta, \partial_\eta \psi)\} .$$

Therefore in order that $\Lambda_\varphi = \Lambda^-$, the function ψ has to satisfy the equation

$$\Phi(\partial_x \psi, x) = (\eta, \partial_\eta \psi) . \tag{2.15}$$

In classical mechanics such a function is called a generating function for the canonical transformation Φ. Under certain conditions on Φ, e.g., if Φ is homogeneous of degree one in ξ, a generating function of the type (2.15) locally always exists. Other types of generating functions are needed in addition if one wants to incorporate all canonical transformations, see [Arn78].

The previous discussion suggests a generalization of the concept of a canonical transformation. Given two manifolds M, N, one calls a Lagrangian submanifold

$$\Lambda \subset (T^*M \times T^*N, \omega_M - \omega_N) \tag{2.16}$$

a canonical relation from T^*M to T^*N [Wei77]. Relations can be composed, i.e., let M_1, M_2 and M_3 be three manifolds, then the composition of two relations $\Lambda_1 \subset T^*M_2 \times T^*M_1$ and $\Lambda_2 \subset T^*M_3 \times T^*M_2$ is defined as

$$\begin{aligned}\Lambda_2 \circ \Lambda_1 := \{(\zeta, z; \xi, x) \in T^*M_3 \times T^*M_1 \mid \\ \exists\, (\eta, y) \in T^*M_2 \text{ with } (\zeta, z; \eta, y) \in \Lambda_2 \text{ and } (\eta, y; \xi, x) \in \Lambda_1\} .\end{aligned}$$

Under some geometrical conditions on Λ_1 and Λ_2, [Wei77, Hör85a, chapter 21.2], the composition of two canonical relations is again a canonical relation. So in this sense they are generalizations of the group of canonical transformations.

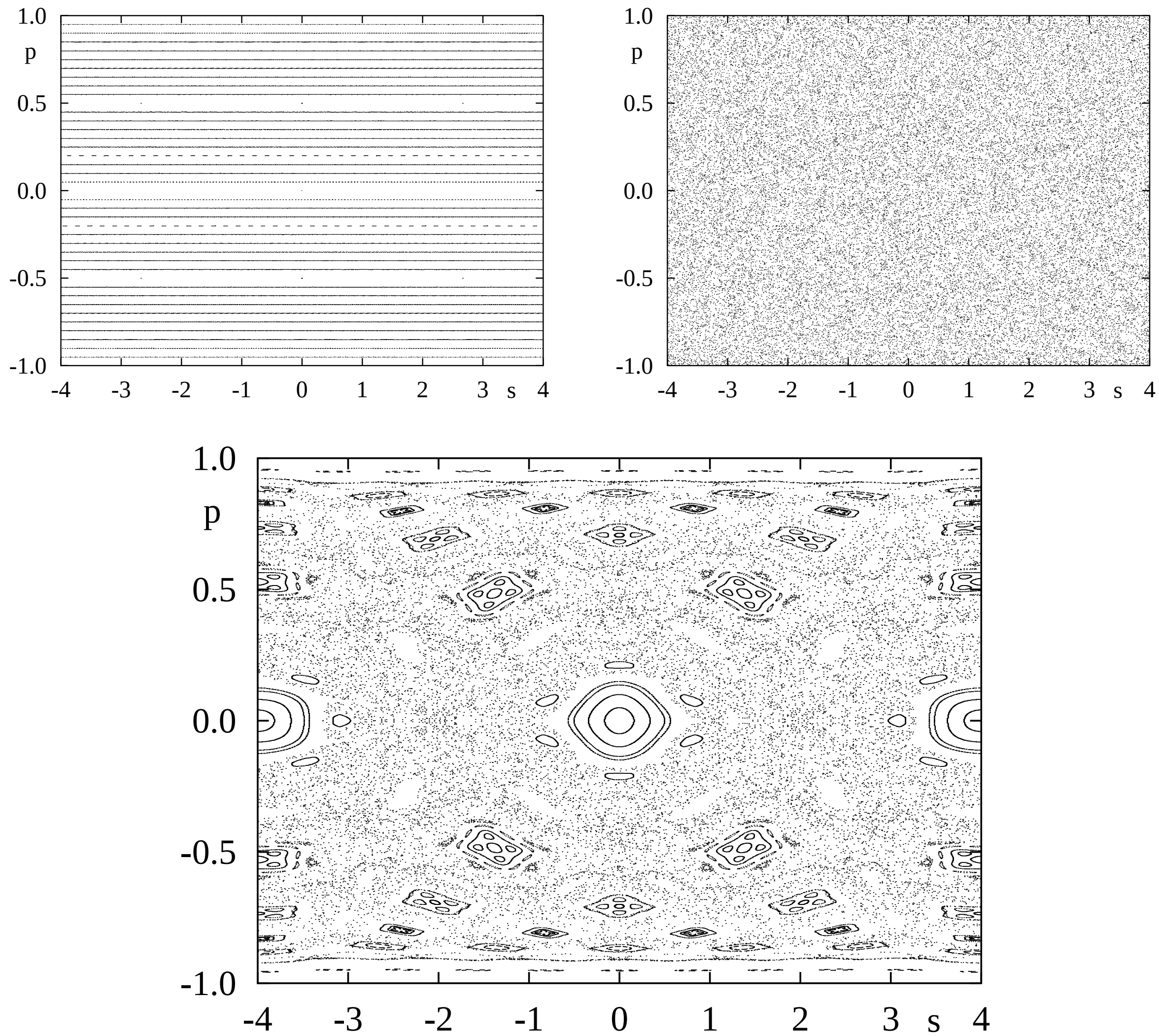

Figure 2.3: The Poincaré section (2.17) for three different billiards, [Bäc98]. Shown are the orbits of different initial points under the Poincaré map. They give a qualitative picture of the dynamics. The upper left system is the integrable circle billiard, the invariant tori are visible as straight lines. The upper right system is the ergodic cardioid billiard, and one sees that a typical orbit explores the whole phase space. The third system is the limaçon billiard (2.9) with parameter $\varepsilon = 0.3$, which has a mixed phase space.

The properties of the flow Φ^t generated by a Hamiltonian H depend of course on the properties of H. Denote by

$$\Sigma_\lambda := \{(\xi, x) \in T^*M \mid H(\xi, x) = \lambda\}$$

the energy shell with energy λ. Then $\Phi^t : \Sigma_\lambda \to \Sigma_\lambda$, and the invariant volume form μ on T^*M induces a measure on Σ_λ, the Liouville measure μ_λ, which is invariant under the flow Φ^t. If the Hamilton function is homogeneous of degree m in ξ and the manifold M is compact, then Σ_λ is compact too, and $\Sigma_\lambda = \lambda^{1/m} \cdot \Sigma_1 := \{(\lambda^{1/m}\xi, x) \mid (\xi, x) \in \Sigma_1\}$.

If there exist further conserved quantities g_i, i.e. $\{g_i, H\} = 0$, which are in involution $\{g_i, g_j\} = 0$, then the flow leaves the level-sets of $\{g_1, \cdots, g_k, H\}$, i.e. the sets in phase space on which the functions g_i and h are constant, invariant. In the case that the system has $d = \dim M$ such conserved quantities which are independent almost everywhere, it is called integrable, see e.g. [Arn78, AM78] for more details and precise statements. Then the theorem of Liouville-Arnold says that the $2d$-dimensional phase space is foliated into d-dimensional invariant Lagrangian tori on which the motion is quasi-periodic. A trajectory starting on a torus will always stay on it and will never explore any other part of the phase space.

A rather opposite behavior is characteristic for ergodic systems. A system is called ergodic if a typical trajectory comes arbitrarily close to every point in the energy shell. This can be expressed formally as the fact that the time mean of an observable equals the space mean for almost all trajectories,

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T a(\Phi^t(\xi, x))\, \mathrm{d}t = \frac{1}{\mu_\lambda(\Sigma_\lambda)} \int_{\Sigma_\lambda} a \, \mathrm{d}\mu_\lambda \ ,$$

for almost all $(\xi, x) \in \Sigma_\lambda$.

Integrability and ergodicity are on the two opposite ends of a variety of possible behaviors of Hamiltonian systems; typically the phase space structure is very complicated, with invariant sets on all scales. We will illustrate these different types of systems by the three billiards which we considered already in the last section, see (2.9): the circle billiard, a limaçon billiard with $\varepsilon = 0.3$ and the cardioid billiard, see also fig. 2.2.

By a classical billiard in two dimensions we mean a system consisting of a single point-particle moving freely in the interior of the billiard table. A particle on a billiard table will move on straight lines inside the billiard and will be elastically reflected at the billiard boundary, i.e. the component of the velocity vector normal to the boundary is multiplied by -1 at the point of reflection. This dynamics can be described by a special Poincaré section: denote by s the arclength of a given point on the boundary which is hit by the particle and denote by p the cosine of the angle between the tangent vector of the boundary at s and the trajectory of the particle immediately after the bounce with the boundary. By knowing (s, p) we can predict the position s' of the next bounce and the angle of reflection p'. The set

$$\mathcal{P} := \{(s, p) \ ; \ s \in \partial\Omega \ , \ p \in [-1, 1]\} \tag{2.17}$$

defines a complete Poincaré section, and the map $(s, p) \mapsto (s', p')$ which we just described is called the billiard map. The billiard map determines the flow uniquely, and the ergodic properties of the flow are the same as the ones of the billiard map. In figure 2.3 the Poincaré section for the three billiards is shown, which illustrates the different possible behaviors. The circle billiard is integrable, and the invariant tori are visible as parallel lines in the Poincaré section. The limaçon with $\varepsilon = 0.3$ has a mixed phase space, there are elliptic islands, invariant tori and unstable orbits; finally the cardioid is ergodic which leads to a uniform and rather boring Poincaré section. As a further illustration in figure 2.4 some orbits of the different billiards are shown.

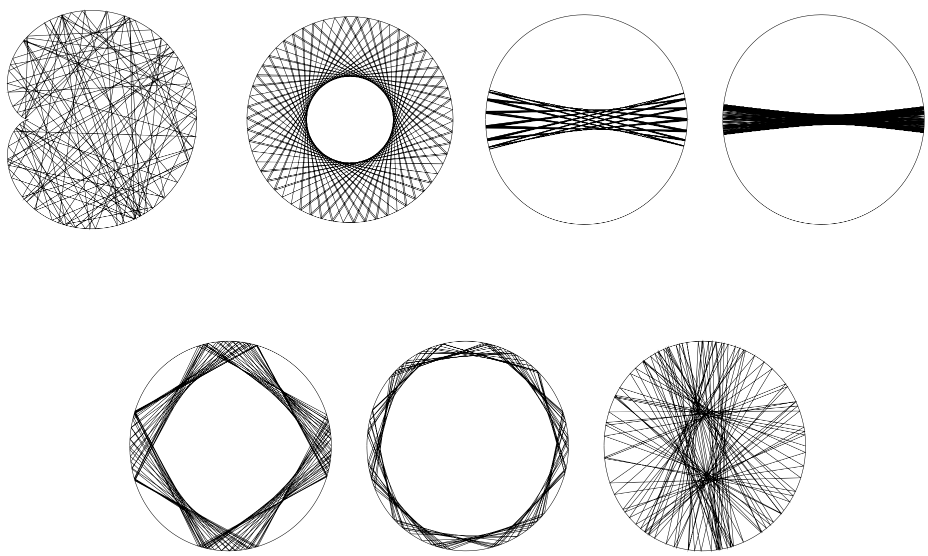

Figure 2.4: Examples of orbits in the three different billiards. The upper left one is the cardioid billiard, the next to the right the circle billiard, and all others are in the limaçon with $\varepsilon = 0.3$. Compare with the structures of the eigenfunctions of the quantized systems, fig. 2.2.

2.1.3 Quantum mechanics versus classical mechanics

Now we want to summarize the contents of the last two sections, and compare the structures of quantum and classical mechanics; an overview is provided in Table 2.1.

In both theories the observables form an algebra, in quantum mechanics it is an algebra of operators, and in classical mechanics it is an algebra of functions. The basic difference is that the algebra in quantum mechanics is non-commutative, whereas the one in classical mechanics is commutative.

Furthermore, in both cases there is an additional structure on the algebra which enters in the equation governing the dynamics. In quantum mechanics it is the commutator, and the dynamics, defined by a given operator $\mathcal{H}$, on the algebra of observables is governed by the Heisenberg equation

$$-\mathrm{i}\hbar\frac{\partial}{\partial t}\mathcal{A} = [\mathcal{H}, \mathcal{A}] \ .$$

In classical mechanics it is the Poisson bracket, defined by the symplectic structure. And the equations of motion on the algebra of observables for a given Hamilton function H are

$$\frac{\partial a}{\partial t} = \{H, a\} \ .$$

quantum mechanics		**classical mechanics**
	observables	
An algebra of operators on the Hilbert space $L^2(X, g)$.	$\overset{?}{\longrightarrow}$	An algebra of functions on T^*X.
	states	
Continuous positive linear functionals on the algebra of observables:		
Density operators	$\overset{?}{\longrightarrow}$	Measures
	morphisms	
unitary operators	$\overset{?}{\longrightarrow}$	symplectomorphisms (canonical transformations)

Table 2.1: Comparison of the structures of quantum and classical mechanics.

The states can in both cases be described as continuous positive linear functionals on the algebra of observables. Depending on the topology one gets different state spaces, but typically one expects the states to be representable as density operators in quantum mechanics, and as measures in classical mechanics.

Finally one has the group of morphisms, which are unitary and anti-unitary operators in quantum mechanics, respectively, and canonical and anti-canonical transformations in classical mechanics.

Our aim in the next sections is to describe the relation between these two structures. Since quantum mechanics is more fundamental than classical mechanics, one expects that there are maps, indicated by arrows in Table 2.1, which associate at least to a subclass of the quantum mechanical objects a class of classical objects. One might not expect that every quantum object has a sensible classical limit, and therefore we do not aim at a most complete description, but we will instead be satisfied if we find a suitable subalgebra of observables which have a nice classical limit.

Finally we will return to the comparison of quantum and classical mechanics, and present some examples to show how the technical apparatus developed can be used then.

2.2 Microlocal analysis

Partial differential operators are local operators, this means that they do not increase the support of a function. This allows one to localize certain problems in space, e.g. , by using cutoff functions and partitions of unity. Microlocalisation means to go one step further and to localize in phase space. The term microlocal analysis refers to a set of methods for the study of partial differential equations which uses the phase space structure of T^*M. For general references to this subject see, e.g., [Hör85, Tay81, GS94].

The point of view from which we will approach the theory is by classifying the operators according to their action on oscillating functions [Hör71, Dui73, Dui74, Gui94]. The simplest oscillating function is a plane wave in $\mathbb{R}^d$, given by

$$\mathrm{e}_\xi(x) := \mathrm{e}^{\mathrm{i}\langle x,\xi\rangle} \ . \tag{2.18}$$

Physically the plane wave corresponds to a current of particles moving with momentum $\xi \in \mathbb{R}^d$, and the semiclassical limit corresponds to the limit $|\xi| \to \infty$. This will be our heuristic guiding principle. This strategy is completely analogous to the short wavelength limit in optics, and the corresponding transition from wave optics to geometrical optics.

2.2.1 Pseudodifferential operators

Following the principles formulated in the introduction to Section 2.2 we will look for a classical counterpart of an operator. Let $\mathcal{A}$ be an operator $\mathcal{A} : \mathcal{S}'(\mathbb{R}^d) \to \mathcal{S}'(\mathbb{R}^d)$, we look at the action of $\mathcal{A}$ on a plane wave $\mathrm{e}_\xi(x) = \mathrm{e}^{\mathrm{i}\langle x,\xi\rangle}$, where $\xi \in \mathbb{R}^d$ is the "momentum" of the wave. This action defines a distribution $a(\xi, x) \in \mathcal{S}'(\mathbb{R}^d \times \mathbb{R}^d)$ by

$$\mathcal{A}\mathrm{e}_\xi(x) = a(\xi, x)\, \mathrm{e}^{\mathrm{i}\langle x,\xi\rangle} = a(\xi, x)\mathrm{e}_\xi(x) \ , \tag{2.19}$$

which describes how $\mathcal{A}$ alters a plane wave (2.18) with momentum ξ. By expanding a function u in plane waves, i.e. representing it as the inverse Fourier transformation of its Fourier transform $\hat{u}$, one can recover $\mathcal{A}$ from a,

$$\mathcal{A}u(x) = \frac{1}{(2\pi)^d} \int \mathrm{e}^{\mathrm{i}\langle x,\xi\rangle} a(\xi, x)\hat{u}(\xi)\, \mathrm{d}\xi \ . \tag{2.20}$$

In the literature a is usually called the symbol of the operator $\mathcal{A}$. We will sometimes call this a right-symbol in order to distinguish it from the Weyl-symbol which will appear later on, see (2.26).

Example 2.2.1. Let $\mathcal{A}$ be a differential operator,

$$\mathcal{A} = \sum_{|\alpha| \leq m} a_\alpha(x) \mathrm{D}_x^\alpha \ ,$$

where $\mathrm{D}_x = \frac{1}{\mathrm{i}} \frac{\partial}{\partial x}$, and the standard multi-index notation is used. Then the symbol of $\mathcal{A}$ is given by

$$a(\xi, x) = \sum_{|\alpha| \leq m} a_\alpha(x) \xi^\alpha \ .$$

Example 2.2.2. Let Δ be the Laplace operator on $\mathbb{R}^d$, and consider its resolvent

$$\mathcal{R}(\lambda) := (-\Delta - \lambda)^{-1} \ ,$$

for $\lambda \in \mathbb{C} \backslash \mathbb{R}^+$. Then it follows from (2.20) that the operator $\mathcal{A}$ with symbol $(\xi^2 - \lambda)^{-1}$ satisfies $(-\Delta - \lambda)\mathcal{A} = 1$ and therefore $\mathcal{A} = \mathcal{R}(\lambda)$. Hence the resolvent $\mathcal{R}(\lambda)$ has the symbol

$$r(\lambda) = (\xi^2 - \lambda)^{-1} \ .$$

The first example explains why $a(\xi, x)$ will sometimes be called the right-symbol of $\mathcal{A}$, because if $A(\xi, x)$ is a polynomial in ξ one gets the corresponding operator (2.20) by writing all powers of ξ to the right of the functions of x and substituting then D_x for ξ.

Our heuristic guiding principle is that $|\xi| \to \infty$ corresponds to the semiclassical limit, so in order that $\mathcal{A}$ has a nice semiclassical limit one has to impose some condition on the symbol a for large ξ. A suitable space of symbols is given by the set of smooth functions $a(\xi, x) \in C^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ which satisfy

$$|\partial_x^\alpha \partial_\xi^\beta a(\xi, x)| \leq C_{\alpha\beta}(1 + |\xi|)^{m - |\beta|} \quad \text{for all } \alpha, \beta \in \mathbb{Z}_+^d \ , \tag{2.21}$$

for some real number m. The space of these functions is denoted by $S^m(\mathbb{R}^d \times \mathbb{R}^d)$, and m is called the order of the symbol. Roughly speaking the condition (2.21) means that the symbols behave very much like polynomials in ξ, or more general like sums of homogeneous functions in ξ. The smallest constants $C_{\alpha\beta}$ in (2.21) define a family of semi-norms on $S^m(\mathbb{R}^d \times \mathbb{R}^d)$ with respect to which it is a Fréchet space, see [Hör85a].

A subclass of the space of symbols of order m is given by the symbols which have an asymptotic expansion in homogeneous functions,

$$a(\xi, x) \sim \sum_{k=0}^\infty a_{m-k}(\xi, x) \ , \tag{2.22}$$

with

$$a_{m-k}(\lambda\xi, x) = \lambda^{m-k} a_{m-k}(\xi, x) \ ,$$

for all $\lambda > 1$ and $|\xi| > 1$. Since homogeneity is only assumed for $|\xi| > 1$, this allows the $a_{m-k}(\xi, x)$ to be smooth around $\xi = 0$. The definition of the asymptotic expansion (2.22) is

$$a(\xi, x) - \sum_{k=0}^{N-1} a_{m-k}(\xi, x) \in S^{m-N}(\mathbb{R}^d \times \mathbb{R}^d) \ , \tag{2.23}$$

for all $N \in \mathbb{N}$. These symbols are called classical or polyhomogeneous, and the space of them is denoted by $S^m_{\mathrm{phg}}(\mathbb{R}^d \times \mathbb{R}^d)$. The leading term in the asymptotic series, i.e. $a_m(\xi, x)$, is called the principal symbol of $a(\xi, x)$.

We will denote the class of operators with symbols in $S^m_{\mathrm{phg}}(\mathbb{R}^d \times \mathbb{R}^d)$ by $\Psi^m_{\mathrm{phg}}(\mathbb{R}^d)$, and the one with symbols in $S^m(\mathbb{R}^d \times \mathbb{R}^d)$ by $\Psi^m(\mathbb{R}^d)$. For an operator $\mathcal{A}$ in $\Psi^m_{\mathrm{phg}}(\mathbb{R}^d)$ one denotes the principal symbol often by

$$\sigma(\mathcal{A})(\xi, x) := a_m(\xi, x) \ .$$

In order to clarify the nature and meaning of the symbol and the principal symbol, respectively, we apply $\mathcal{A} \in \Psi^m_{\mathrm{phg}}(\mathbb{R}^d)$ to a function of the form $\mathrm{e}^{\mathrm{i}\lambda\varphi(x)}$ with $\varphi \in C^\infty(\mathbb{R}^d)$ and $\lambda \in \mathbb{R}$, and consider the limit $\lambda \to \infty$, i.e. , the highly oscillating or semiclassical limit,

$$\begin{aligned} \mathcal{A}\mathrm{e}^{\mathrm{i}\lambda\varphi}(x) &= \frac{1}{(2\pi)^d} \iint \mathrm{e}^{\mathrm{i}\langle x-y,\xi\rangle + \mathrm{i}\lambda\varphi(y)} a(\xi, x) \ \mathrm{d}y \mathrm{d}\xi \\ &= \frac{\lambda^d}{(2\pi)^d} \iint \mathrm{e}^{\mathrm{i}\lambda[\langle x-y,\xi\rangle + \varphi(y)]} a(\lambda\xi, x) \ \mathrm{d}y \mathrm{d}\xi \ . \end{aligned}$$

Applying the method of stationary phase, see Appendix D, to this integral gives

$$\mathcal{A}\mathrm{e}^{\mathrm{i}\lambda\varphi}(x) = \lambda^m \sigma(\mathcal{A})(\varphi'(x), x)\mathrm{e}^{\mathrm{i}\lambda\varphi(x)} + O(\lambda^{m-1}) \ . \tag{2.24}$$

But $(\varphi'(x), x)$ is a point in $T^*\mathbb{R}^d$, because $\varphi'(x)$ is just the vector of coefficients of the one-form $\mathrm{d}\varphi$, so the principal symbol is a function on phase space $T^*\mathbb{R}^d$. In contrast the full symbol is not a function on phase space, and is only defined locally. Therefore the principal symbol defines a map from the space of polyhomogeneous operators $\Psi_{\mathrm{phg}}(\mathbb{R}^d) = \bigcup_{m\in\mathbb{R}} \Psi^m_{\mathrm{phg}}(\mathbb{R}^d)$ to the smooth homogeneous functions on phase space,[1]

$$\begin{aligned} \sigma : \Psi_{\mathrm{phg}}(\mathbb{R}^d) &\longrightarrow C^\infty(T^*\mathbb{R}^d \backslash 0) \\ \mathcal{A} \quad &\longmapsto \quad \sigma(\mathcal{A}) \ . \end{aligned}$$

Hence the principal symbol $\sigma(\mathcal{A})$ is the natural candidate for the classical observable corresponding to $\mathcal{A}$; it is a function on phase space, and it determines the "semiclassical limit" (2.24) of $\mathcal{A}$.

[1] Note that a homogeneous function $p(\xi, x)$ is usually not smooth at $\xi = 0$, so it can only be in $C^\infty(T^*\mathbb{R}^d \backslash 0)$, where $T^*\mathbb{R}^d \backslash 0$ means that the zero section is removed.

We now want to discuss the algebraic properties of Ψ_{phg}. Recall that we want the observables to form an algebra, and therefore in order to be acceptable as observables Ψ_{phg} has to be an algebra. Before doing so we want to make a remark on the full symbols. Although the most important part is generally the principal symbol, it is often useful to consider the full symbol and to ask how well it reflects properties of the operator. E.g., it would be nice if a selfadjoint operator had a real valued symbol. But this is only true for the principal symbol, not for the full symbol. A different convention for associating a function to an operator is given by the Weyl convention [Wey28], see, e.g., [Fol89] for a nice presentation. Weyl considered the converse problem of quantization, i.e. of associating an operator to a function on phase space. His basic postulate was that to the function $\mathrm{e}^{\mathrm{i}(\langle\alpha,x\rangle+\langle\beta,\xi\rangle)}$ one should associate the operator $\mathrm{e}^{\mathrm{i}(\langle\alpha,x\rangle+\langle\beta,\mathrm{D}_x\rangle)}$. By Fourier transformation one then obtains for a function $A(\xi,x)$ the quantization

$$\mathcal{A}=\frac{1}{(2\pi)^{2d}}\iint \hat{A}(\alpha,\beta)\mathrm{e}^{\mathrm{i}(\langle\alpha,x\rangle+\langle\beta,\mathrm{D}_x\rangle)}\,\mathrm{d}\alpha\mathrm{d}\beta\ , \tag{2.25}$$

where $\hat{A}(\alpha,\beta)$ denotes the Fourier transform of A in both variables. The action of $\mathcal{A}$ defined by (2.25) on a function $u\in\mathcal{S}(\mathbb{R}^d)$ can be written as an integral operator of the form

$$\mathcal{A}u(x)=\frac{1}{(2\pi)^{d}}\iint \mathrm{e}^{\mathrm{i}\langle x-y,\xi\rangle}A(\xi,(x+y)/2)u(y)\ \mathrm{d}y\mathrm{d}\xi\ , \tag{2.26}$$

and A is called the Weyl symbol of $\mathcal{A}$. Let $K(x,y)$ be the Schwartz kernel of a given operator $\mathcal{A}$, then conversely the Weyl symbol of $\mathcal{A}$ is

$$A(\xi,x):=\int \mathrm{e}^{-\mathrm{i}\langle y,\xi\rangle}K(x+y/2,x-y/2)\,\mathrm{d}y\ , \tag{2.27}$$

i.e. the operator $\mathcal{A}$ can be written in the form (2.26) with A given by (2.27). From the definition it follows easily that the adjoint operator $\mathcal{A}^*$ has as a Weyl symbol the complex conjugate of the Weyl symbol of $\mathcal{A}$. In particular, one sees that a selfadjoint operator has a real valued Weyl symbol.

The expression (2.27) looks more complicated than the simple one for the right-symbol (2.19), but it turns out that computations with Weyl symbols are often simpler than with the symbol (2.19). Therefore we will in the following mainly work with the Weyl symbol, and refer to it sometimes simply as the symbol.

A further interesting aspect of the Weyl convention is that the Weyl symbol of the projection operator onto a state ψ is the Wigner function [Wig32] of that state [Moy49]. The kernel of the projection operator onto the state ψ is simply $K(x,y)=\overline{\psi}(x)\psi(y)$, and therefore (2.27) gives

$$\int \mathrm{e}^{-\mathrm{i}\langle y,\xi\rangle}\,\overline{\psi}(x+y/2)\psi(x-y/2)\,\mathrm{d}y=:W[\psi](\xi,x)\ . \tag{2.28}$$

From (2.27) it is simple to obtain the relation between the two types of symbols. If $\mathcal{A}$ has right-symbol a, then its Weyl symbol is given by

$$A(\xi, x) = \mathrm{e}^{-\mathrm{i}\langle \mathrm{D}_x, \mathrm{D}_\xi\rangle/2} a(\xi, x) \ , \tag{2.29}$$

where the operator $\mathrm{e}^{-\mathrm{i}\langle \mathrm{D}_x, \mathrm{D}_\xi\rangle/2}$ is defined by $\mathrm{e}^{-\mathrm{i}\langle \mathrm{D}_x, \mathrm{D}_\xi\rangle/2}\mathrm{e}^{\mathrm{i}(\langle x,\eta\rangle+\langle \xi,y\rangle)} = \mathrm{e}^{-\mathrm{i}\langle \eta,y\rangle/2}\mathrm{e}^{\mathrm{i}(\langle x,\eta\rangle+\langle \xi,y\rangle)}$. Operators of the form $\mathrm{e}^{\mathrm{i}Q(\mathrm{D}_x,\mathrm{D}_\xi)/2}$, where Q is a quadratic form, are called Gauss operators and occur quite frequently in the theory of pseudodifferential operators. Their properties are for instance studied in [Hör85a], where it is shown that they map symbols to symbols, more precisely one has

$$\mathrm{e}^{-\mathrm{i}\langle \mathrm{D}_x, \mathrm{D}_\xi\rangle/2} : S^m(\mathbb{R}^d) \to S^m(\mathbb{R}^d)$$

for all $m \in \mathbb{R}$, and for $a \in S^m(\mathbb{R}^d \times \mathbb{R}^d)$ one can expand the exponential in (2.29) to get an asymptotic expansion in the sense of (2.23),

$$A(\xi, x) \sim \sum_k^\infty \frac{1}{k!}(-\mathrm{i}\langle \mathrm{D}_x, \mathrm{D}_\xi\rangle/2)^k a(\xi, x) \ . \tag{2.30}$$

Note that $(-\mathrm{i}\langle \mathrm{D}_x, \mathrm{D}_\xi\rangle/2)^k a(\xi, x) \in S^{m-k}(\mathbb{R}^d \times \mathbb{R}^d)$ by the definition of $S^m(\mathbb{R}^d \times \mathbb{R}^d)$ in (2.21), and therefore the asymptotic series is well defined. A similar expression exists for a in terms of A, and therefore the class $\Psi^m(\mathbb{R}^d)$ and $\Psi^m_{\mathrm{phg}}(\mathbb{R}^d)$ can as well be characterized as the operators with Weyl symbols in $S^m(\mathbb{R}^d \times \mathbb{R}^d)$ and $S^m_{\mathrm{phg}}(\mathbb{R}^d \times \mathbb{R}^d)$. Furthermore, it follows from (2.30) that if a is polyhomogeneous with $a \sim a_m + a_{m-1} \cdots$, then A is polyhomogeneous with the same leading term $A \sim a_m + a_{m-1} + \mathrm{i}\langle \partial_x, \partial_\xi\rangle a_m/2 \cdots$, and vice versa. Therefore the principal symbol of $\mathcal{A}$ is given by the leading term of its Weyl symbol, $a_m = \sigma(\mathcal{A})$. The next-to-leading term in the asymptotic expansion of the Weyl symbol is called the subprincipal symbol,

$$\mathrm{sub}(\mathcal{A})(\xi, x) := A_{m-1}(\xi, x) \ .$$

We come now to one of the principal tools in the theory of pseudodifferential operators, the product-formula. The main point in the theory of pseudodifferential operators is to shift the computations from operators to symbols, and to express properties of the operators through the symbols.

Theorem 2.2.3. *Let $\mathcal{A} \in \Psi^m(\mathbb{R}^d)$ with Weyl symbol A and $\mathcal{B} \in \Psi^{m'}(\mathbb{R}^d)$ with Weyl symbol B, then $\mathcal{AB} \in \Psi^{m+m'}(\mathbb{R}^d)$ with Weyl symbol $A\#B$ given by*

$$\begin{aligned} A\#B(\xi, x) &= \mathrm{e}^{\frac{\mathrm{i}}{2}(\langle \mathrm{D}_y, \mathrm{D}_\xi\rangle - \langle \mathrm{D}_x, \mathrm{D}_\eta\rangle)} A(\xi, x)B(\eta, y)|_{(\xi,x)=(\eta,y)} \\ &\sim \sum_{k=0}^\infty \frac{1}{k!}\left[\frac{\mathrm{i}}{2}(\langle \mathrm{D}_y, \mathrm{D}_\xi\rangle - \langle \mathrm{D}_x, \mathrm{D}_\eta\rangle)\right]^k A(\xi, x)B(\eta, y)|_{(\xi,x)=(\eta,y)} \\ &= A(\xi, x)B(\xi, x) - \frac{\mathrm{i}}{2}\{A, B\}(\xi, x) \mod S^{m+m'-3}(\mathbb{R}^d \times \mathbb{R}^d) \ , \end{aligned} \tag{2.31}$$

where $\{A, B\} = \langle \partial_x A, \partial_\xi B\rangle - \langle \partial_\xi A, \partial_x B\rangle$ denotes the Poisson bracket.

This is a basic theorem in the theory of pseudodifferential operators. A formula similar to this one in the context of $\hbar \to 0$ asymptotics has been derived by Moyal [Moy49], who also noted for the first time the relation between the Weyl symbol and the Wigner function. Most applications use the algebraic properties of these operators. As a corollary we get for the principal symbols of products and commutators:

Corollary 2.2.4. *If $\mathcal{A} \in \Psi^m_{\mathrm{phg}}(\mathbb{R}^d)$ and $\mathcal{B} \in \Psi^{m'}_{\mathrm{phg}}(\mathbb{R}^d)$, then*

$$\begin{aligned}\sigma(\mathcal{A}\mathcal{B}) &= \sigma(\mathcal{A})\sigma(\mathcal{B})\\ \mathrm{sub}(\mathcal{A}\mathcal{B}) &= \mathrm{sub}(\mathcal{A})\sigma(\mathcal{B}) + \mathrm{sub}(\mathcal{B})\sigma(\mathcal{A}) - 2\mathrm{i}\{\sigma(\mathcal{A}), \sigma(\mathcal{B})\}\\ \sigma([\mathcal{A},\mathcal{B}]) &= \frac{1}{\mathrm{i}}\{\sigma(\mathcal{A}), \sigma(\mathcal{B})\}\ .\end{aligned}$$

Therefore the principal symbol map is an algebra and a Lie algebra morphism (if we consider $\frac{1}{\mathrm{i}}\{\cdot,\cdot\}$ as the Lie algebra structure of the classical observables) between the algebras of quantum mechanical and classical observables.

Let us sketch a first application of Theorem 2.2.3, which was one of the motivations for developing the calculus of pseudodifferential operators. Let $\mathcal{A} \in \Psi^m$ and assume that $\sigma(\mathcal{A})(\xi, x) \neq 0$ for all (ξ, x) with $\xi \neq 0$: such an operator is called elliptic.

Theorem 2.2.5. *Assume $\mathcal{A} \in \Psi^m$ is elliptic, then there exist operators $\mathcal{R}, \mathcal{L} \in \Psi^{-m}$, called a right and a left parametrix, respectively, such that*

$$\begin{aligned}\mathcal{A}\mathcal{R} - I &\in \Psi^{-\infty}\ ,\\ \mathcal{L}\mathcal{A} - I &\in \Psi^{-\infty}\ ,\end{aligned}$$

and $\sigma(\mathcal{R}) = \sigma(\mathcal{L}) = 1/\sigma(\mathcal{A})$. Here I denotes the identity operator and $\Psi^{-\infty} := \bigcap_{m\in\mathbb{R}} \Psi^m$ is the algebra of operators whose symbols decay faster than any power in ξ for $|\xi| \to \infty$.

A parametrix can be viewed as an approximate inverse, but it exists as well in the case when the operator is not invertible. We will sketch the proof for the left parametrix $\mathcal{L}$. Choose an operator $\mathcal{L}_1 \in \Psi^{-m}$ with $\sigma(\mathcal{L}) = 1/\sigma(\mathcal{A})$, then by Theorem 2.2.3 one has

$$\mathcal{L}_1\mathcal{A} = I + \mathcal{S}$$

with $\mathcal{S} \in \Psi^{-1}$. Now choose $\mathcal{L}_2 \in \Psi^0$ with

$$\mathcal{L}_2 \sim \sum_{k=0}^{\infty} (-1)^k \mathcal{S}^k$$

where the asymptotic summation is understood on the symbolic level. Since $(1+x)^{-1} = \sum(-1)^k x^k$ for $|x| < 1$ we get with $\mathcal{L} = \mathcal{L}_2\mathcal{L}_1$ the result $\mathcal{L}\mathcal{A} - I \in \Psi^{-\infty}$, and the result on the principal symbol follows from Corollary 2.2.4, $\sigma(\mathcal{L}_2) = 1$ and $\sigma(\mathcal{L}) = 1/\sigma(\mathcal{A})$.

If $\mathcal{A}$ is polyhomogeneous, then it follows that the parametrices are polyhomogeneous too. The algebra of polyhomogeneous pseudodifferential operators is basically the smallest extension of the algebra of partial differential operators in which elliptic differential operators possess a parametrix. This was one of the motivations for mathematicians to introduce this algebra [KN65].

As can be seen from Theorem 2.2.3 and Theorem 2.2.5 computations with symbols based on asymptotic expansions lead to results modulo $\Psi^{-\infty}$. In this sense $\Psi^{-\infty}$ is the residual set in Ψ^{∞}. The operators in $\Psi^{-\infty}$ are the smoothing ones in Ψ^{∞}, which means that they map distributions to smooth (C^{∞}) functions, which is equivalent to the fact that their kernels are C^{∞}-functions.

Example 2.2.6. As a further consequence of Theorem 2.2.3 we note an important class of operators that do not belong to Ψ^{∞}, the orthogonal projection operators P on $L^2(M)$, for compact M, with $\dim \operatorname{Im} P = \dim \operatorname{Ker} P = \infty$. A projection operator satisfies the relation

$$P^2 = P \, . \tag{2.32}$$

Now assume that such an operator belongs to Ψ^m for some $m \in \mathbb{R}$, then by Theorem 2.2.3 one gets $2m = m$, so $m \in \{-\infty, 0\}$. If $m = 0$ then the principal symbol has to satisfy

$$\sigma(P)^2 = \sigma(P) \, ,$$

so it can only take the values 0 and 1, and since it is assumed to be smooth it can only be a constant equal to 1 or 0. Therefore P is the identity plus some smoothing operator, or it is in $\Psi^{-\infty}$. But the operators in $\Psi^{-\infty}$ are all of trace class if M is a compact manifold, therefore any projection operator in $\Psi^{-\infty}$ is of finite rank.

The set of points where a pseudodifferential operator $\mathcal{A} \in \Psi^m_{\mathrm{phg}}$ is not elliptic is called the characteristic set of $\mathcal{A}$,

$$\operatorname{char}(\mathcal{A}) := \{(\xi, x) \,|\, \sigma(\mathcal{A})(\xi, x) = 0\,\} \, . \tag{2.33}$$

It is clear from the definition that pseudodifferential operators map $\mathcal{A} : \mathcal{S}(\mathbb{R}^d) \to \mathcal{S}(\mathbb{R}^d)$ and by duality we have $\mathcal{A} : \mathcal{S}'(\mathbb{R}^d) \to \mathcal{S}'(\mathbb{R}^d)$. The characteristic sets can be used to define a very useful set describing the singularities of a distribution, the wave front set. Intuitively the wave front set of a distribution consists of the points where the distribution is singular, together with the directions in which it is singular.

Definition 2.2.7. *Let $u \in \mathcal{S}'(\mathbb{R}^d)$, then the* ***wave front set*** $\mathrm{WF}(u)$ *is defined as*

$$\mathrm{WF}(u) := \bigcap \operatorname{char}(\mathcal{A}) \, , \tag{2.34}$$

where the intersection is taken over all $\mathcal{A} \in \Psi^m_{\mathrm{phg}}$ with $\mathcal{A}u \in C^{\infty}(\mathbb{R}^d)$. This set is independent of m.

The wave front set is a closed conic subset of $T^*\mathbb{R}^d \backslash 0$, and the projection of $\mathrm{WF}(u)$ to $\mathbb{R}^d$ is the singular support of u. A more direct characterization of the wave front set of u can be given as follows. $\mathrm{WF}(u)$ is the complement of the set of all $(\xi, x) \in \mathbb{R}^d \times \mathbb{R}^d$ for which there is a neighborhood $U \subset \mathbb{R}^d$ of x and a conical neighborhood[2] $V \subset \mathbb{R}^d$ of ξ such that for all $\varphi \in C_0^\infty(U)$

$$\widehat{\varphi u}(\xi) = O(|\xi|^{-N}) \ , \tag{2.35}$$

for $\xi \in V$ and each $N \in \mathbb{N}$. Thus the wave front set consists of the points where the distribution is singular, together with the rays in which its local Fourier transform is not rapidly decreasing.

Examples 2.2.8:

- For the delta distribution centered at x_0 one has $\mathrm{WF}(\delta_{x_0}) = \{(x_0, \xi) \mid \xi \in \mathbb{R}^d \backslash 0\}$.
- Let $u^\pm(x) = \lim_{\varepsilon \to 0}(x \pm \mathrm{i}\varepsilon)^{-1}$, for $x \in \mathbb{R}$, and where the limit is taken in $\mathcal{D}'$, then $\mathrm{WF}(u^\pm) = \{0\} \times \mathbb{R}^\pm$.
- Let $u(x) = \delta(f(x))$ where f is smooth. Then u is concentrated on the submanifold $S_f := \{x \in \mathbb{R}^d \mid f(x) = 0\}$, and the wave front set of u is the conormal bundle of S_f, see fig. 2.5,

$$\mathrm{WF}(u) = N^* S_f := \{(\xi, x) \mid f(x) = 0, \xi = \lambda f'(x) \,\text{for}\, \lambda \in \mathbb{R}\backslash 0\} \ . \tag{2.36}$$

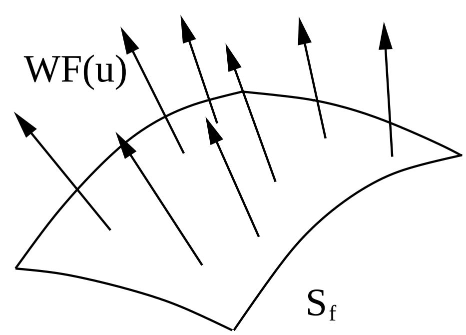

Figure 2.5: Visualization of the wave front set (2.36) of a delta-function on a submanifold $S_f \subset \mathbb{R}^2$. It consists of the manifold S_f together with the rays perpendicular to it. This set is called the conormal-bundle $N^* S_f$ of S_f.

The projection of the wave front set to the x-space is the singular support, and it follows immediately from the definition of the wave front set, that for all $\mathcal{A} \in \Psi(M)$

$$\begin{aligned} \mathrm{WF}(\mathcal{A}u) &\subset \mathrm{WF}(u) \\ \mathrm{singsupp}(\mathcal{A}u) &\subset \mathrm{singsupp}(u) \\ \mathrm{WF}(u) &\subset \mathrm{WF}(\mathcal{A}u) \cup \mathrm{char}(\mathcal{A}) \ . \end{aligned}$$

The first and second property are called microlocality and pseudolocality, respectively. From the first and third property it follows that $\mathrm{WF}(\mathcal{A}u) = \mathrm{WF}(u)$ for an elliptic operator $\mathcal{A}$.

The notion of the wave front set suggests to define an analogous set for operators, which characterizes the set in phase space on which the operator is not smoothing:

[2]A conical neighborhood of ξ is a set $V \ni \xi$ which is conical, i.e. with $\eta \in V$ one has $\lambda\eta \in V$ for all $\lambda > 0$, and the set of $\eta \in V$ with $|\eta| = 1$ is open in the unit sphere in $\mathbb{R}^d$.

Definition 2.2.9. *For an operator $\mathcal{A} : \mathcal{S}'(\mathbb{R}^d) \to \mathcal{S}'(\mathbb{R}^d)$ the* ***wave front set****, also called essential support, is defined as*

$$\mathrm{WF}(\mathcal{A}) := \{(\xi, x) \,|\, \textit{there exists } u \in \mathcal{S}'(\mathbb{R}^d) \textit{ with } (\xi, x) \in \mathrm{WF}(u) \textit{ and } (\xi, x) \in \mathrm{WF}(\mathcal{A}u) \ \} \ .$$

It is clear from the definition that

$$\mathrm{WF}(\mathcal{A}u) \subset \mathrm{WF}(\mathcal{A}) \cap \mathrm{WF}(u) \ .$$

For pseudodifferential operators the wave front set can be characterized easily through the symbol. It consists of the points where the symbol is not in $S^{-\infty}(\mathbb{R}^d \times \mathbb{R}^d) := \bigcap_{m\in\mathbb{R}} S^m(\mathbb{R}^d \times \mathbb{R}^d)$,

$$(\xi_0, x_0) \notin \mathrm{WF}(\mathcal{A}) \quad \text{iff} \quad a(\xi, x) \in S^{-\infty}(\mathbb{R}^d \times \mathbb{R}^d) \quad \text{in a conical neighbourhood of } (\xi_0, x_0) \ .$$

A further operation which can be transferred from the operator level to the symbol level is the trace. Assume that $\mathcal{A}$ is of trace class, then the trace can be expressed through the kernel $K(x, y)$ of $\mathcal{A}$ as

$$\operatorname{tr} \mathcal{A} = \int K(x, x) \, \mathrm{d}x \ .$$

The kernel can be deduced from (2.26) and if we insert it into this expression, we get

$$\operatorname{tr} \mathcal{A} = \frac{1}{(2\pi)^d} \iint a(\xi, x) \, \mathrm{d}x\mathrm{d}\xi \ ,$$

where a is the Weyl symbol of $\mathcal{A}$. A similar formula is valid for the trace of a product. Let a and b be the Weyl symbols of $\mathcal{A}$ and $\mathcal{B}$, then

$$\operatorname{tr} \mathcal{A}\mathcal{B} = \frac{1}{(2\pi)^d} \iint a(\xi, x) b(\xi, x) \, \mathrm{d}x\mathrm{d}\xi \ .$$

A special case of this relation is the well known expression for the expectation value of an operator $\mathcal{A}$ with Weyl-symbol a in a state $\psi \in L^2(M)$ through the Wigner-function (2.28) of ψ,

$$\langle \psi, \mathcal{A}\psi \rangle = \frac{1}{(2\pi)^d} \iint a(\xi, x) W[\psi](\xi, x) \, \mathrm{d}x\mathrm{d}\xi \ .$$

Finally, before turning to applications, we want to discuss L^2-estimates of pseudodifferential operators. From the classical-to-quantum correspondence one might expect that operators which are mapped to bounded functions are bounded operators. For the algebra Ψ^∞ this is true.

Theorem 2.2.10. *The operators in Ψ^0 are bounded and their L^2-norm is a continuous seminorm in S^0 (see (2.21)).*

Furthermore, if the symbol is positive one expects that this is reflected in the properties of the operator. This is the content of the Gårding inequality:

Theorem 2.2.11. *Let $\mathcal{A}$ be an operator with Weyl symbol $a \in S^{2m+1}$ and $\operatorname{Re} a \geq 0$, then*

$$\operatorname{Re}\langle \mathcal{A}u, u\rangle \geq -C||u||^2_{(m)} ,$$

where $||u||_{(m)}$ denotes the Sobolev norm with index m, see e.g. [Hör85a].

Pseudodifferential operators can be defined on manifolds basically in the same way as on $\mathbb{R}^d$. The symbols are defined in local charts, which makes a slight modification of their definition necessary. Let $U \subset \mathbb{R}^d$ be an open set, we will from now on say that $a \in S^m(U \times \mathbb{R}^d)$, if for each compact subset $K \in U$ there exists constants $C_{\alpha\beta,K}$ such that

$$|\partial_x^\alpha \partial_\xi^\beta a(\xi, x)| \leq C_{\alpha\beta,K}(1 + |\xi|)^{m-|\beta|} \quad \text{for all } x \in K , \tag{2.37}$$

and for all $\alpha, \beta \in \mathbb{Z}^d_+$.

It turns out that the transformation formula under coordinate changes is quite complicated. But the principal symbols can be glued together to give a function on the cotangent bundle, and the formula (2.24) applies globally to give an invariant characterization of the principal symbol. Therefore the notion of a wave front set for distributions and operators can be transferred directly. And all the further results mentioned so far are valid on manifolds, too. We refer to [Hör85a] for more precise statements and a detailed discussion.

2.2.2 An application: complex powers and the MP-zeta function

We want to discuss an application of the apparatus developed so far to spectral problems, which is due to Seely [See67]. Let M be a compact manifold, and $\mathcal{H}$ be an elliptic polyhomogeneous pseudodifferential operator of order m on M with Weyl symbol H. We want to study the complex powers of $\mathcal{H}$,

$$\mathcal{H}^z , \qquad z \in \mathbb{C} ,$$

and the Minakshisundaram-Plejel, or MP-zeta function [MP49], which is the trace of $\mathcal{H}^z$,

$$\zeta(z) := \operatorname{tr} \mathcal{H}^z .$$

If $\mathcal{H}$ is selfadjoint and positive, the complex powers can be defined by the spectral theorem,

$$\mathcal{H}^z = \sum_n \lambda_n^z |\psi_n\rangle\langle\psi_n| , \tag{2.38}$$

where λ_n and ψ_n are the eigenvalues and eigenfunctions of $\mathcal{H}$, and $|\psi_n\rangle\langle\psi_n|$ is the projector on the eigenspace spanned by ψ_n. We have used in the representation (2.38) that the spectrum is discrete, which follows from the compactness of M, see, e.g., [Hör85b]. For the trace we then get

$$\zeta(z) = \sum_n \lambda_n^z \ , \tag{2.39}$$

so it only depends on the eigenvalues of $\mathcal{H}$. Since the eigenvalues tend to ∞ the sum will be absolutely convergent for $-\operatorname{Re} z$ large enough, and therefore (2.39) defines a holomorphic function in a half space. The aim is to find a meromorphic continuation to the whole complex plane, and to use information on the analytic properties and poles of $\zeta(z)$ to obtain information about the spectrum of $\mathcal{H}$.

Using the counting function (2.8), the zeta function can be expressed as

$$\zeta(z) = \int_0^\infty \lambda^z \, \mathrm{d}N(\lambda) \ . \tag{2.40}$$

Assume now that $N(\lambda)$ has an asymptotic expansion for $\lambda \to \infty$,

$$N(\lambda) = \frac{a}{\alpha}\lambda^\alpha + O(\lambda^\beta) \ ,$$

with $\beta < \alpha$, then by (2.40) $\zeta(z)$ is holomorphic for $\operatorname{Re} z < -\alpha$. Since we have assumed that $\mathcal{H}$ is positive, the spectrum is positive and the lower limit of the integral (2.40) can be shifted from 0 to some $\varepsilon > 0$. Then we get

$$\begin{aligned} \zeta(z) &= \int_\varepsilon^\infty a\lambda^{z+\alpha-1} \, \mathrm{d}\lambda + f_1(z) \\ &= -\frac{a}{z+\alpha}\varepsilon^{z+\alpha} + f_1(z) = -\frac{a}{z+\alpha} + f_2(z) \ , \end{aligned}$$

where $f_1(z)$ and $f_2(z)$ are holomorphic for $\operatorname{Re} z < -\beta$. So the first pole of the zeta function gives the exponent of the leading term of $N(\lambda)$ for $\lambda \to \infty$, and the residue determines the pre-factor. The converse is the content of the Tauberian theorem of Ikehara [Wie32].

Theorem 2.2.12. *Let $N(\lambda)$ be a non-decreasing function equal to 0 for $\lambda \leq 1$ and such that the integral $\zeta(z) = \int_1^\infty \lambda^z \mathrm{d}N(\lambda)$ converges for $\operatorname{Re} z < -\alpha$ and the function*

$$\zeta(z) + \frac{a}{z+\alpha}$$

is continuous for $\operatorname{Re} z \leq -\alpha$. Then one has for $\lambda \to \infty$

$$N(\lambda) = \frac{a}{\alpha}\lambda^\alpha + o(\lambda^\alpha) \ .$$

Unfortunately, more information on the analytic behavior of the zeta function does not lead to a better remainder estimate for $N(\lambda)$. The reason for this is that possible oscillating contributions to $N(\lambda)$, for instance of the form $\lambda^\beta \cos(\lambda^\gamma)$, give a holomorphic contribution to the zeta function. But nevertheless, we see that from a study of the analytic properties of the zeta function we can determine the leading asymptotic behavior of the spectral counting function.

Now the analytic properties of the zeta function can be determined with the help of the calculus of pseudodifferential operators.

Theorem 2.2.13. *Let $\mathcal{H}$ be an elliptic polyhomogeneous pseudodifferential operator of order m, then $\mathcal{H}^z$ is a polyhomogeneous pseudodifferential operator of order $m\,\mathrm{Re}\,z$ with principal and subprincipal symbol given by*

$$\sigma(\mathcal{H}^z) = \sigma(\mathcal{H})^z$$
$$\mathrm{sub}(\mathcal{H}^z) = z\,\mathrm{sub}(\mathcal{H})\sigma(\mathcal{H})^{z-1} ,$$

respectively. If M is compact, then the zeta function $\zeta(z) := \mathrm{tr}\,\mathcal{H}^z$ has a meromorphic continuation to the whole complex plane with possible simple poles at the points $z = (k-d)/m$ for $k = 0, 1, 2, 3, \cdots$, but no pole at $z = 0$. The residues at the first two poles are given by

$$\mathrm{res}_{z=-\frac{d}{m}}\,\zeta = -m \int \delta\big(\sigma(\mathcal{H})(\xi, x) - 1\big)\;\mathrm{d}x\mathrm{d}\xi$$
$$\mathrm{res}_{z=\frac{1-d}{m}}\,\zeta = (d-1) \int \mathrm{sub}(\mathcal{H})(\xi, x)\delta\big(\sigma(\mathcal{H})(\xi, x) - 1\big)\;\mathrm{d}x\mathrm{d}\xi\ .$$

The starting point for the derivation of this result is the following representation of $\mathcal{H}^z$ through the resolvent of $\mathcal{H}$ by a Dunford integral

$$\mathcal{H}^z = \frac{\mathrm{i}}{2\pi} \int_\Gamma \lambda^z (\mathcal{H} - \lambda)^{-1}\;\mathrm{d}\lambda\ , \tag{2.41}$$

for $\mathrm{Re}\,z < 0$, where Γ is a path in $\mathbb{C}$ starting at $-\infty + \mathrm{i}\epsilon$ surrounding the origin clockwise, and tending to $-\infty - \mathrm{i}\epsilon$, see fig. 2.6.

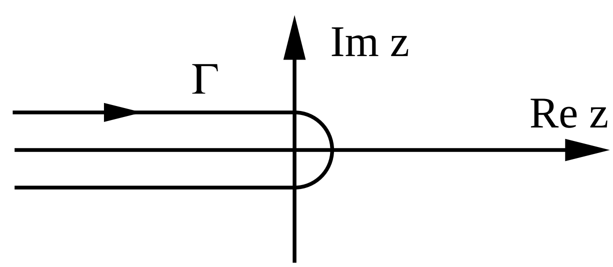

Figure 2.6: The path of integration Γ in the complex domain for the integral (2.41), by which the complex powers $\mathcal{H}^z$ are represented.

Furthermore we assume that $\mathcal{H}$ is positive. The expression (2.41) for $\mathcal{H}^z$ can be continued to $\mathrm{Re}\,z \geq 0$ by multiplication with integer powers of $\mathcal{H}$, which are already known to be pseudodifferential operators by Theorem 2.2.3. In order to use (2.41) we have to construct the resolvent for $\mathcal{H}$,

$$\mathcal{R}(\lambda) = \frac{1}{\mathcal{H} - \lambda}\ ,$$

for λ away from the spectrum of $\mathcal{H}$. We have already discussed a similar problem in Theorem 2.2.5, i.e. the construction of a parametrix for an elliptic operator. The only drawback of this construction is that it is not uniform in the parameter λ. In order to achieve this we will make an ansatz for the symbol of $\mathcal{R}(\lambda)$ which is an asymptotic sum of functions which are jointly homogeneous in ξ and λ;

$$R(\xi, x, \lambda) \sim \sum_{k=0}^{\infty} R_{-m-k}(\xi, x, \lambda) \ , \tag{2.42}$$

with

$$R_k(t\xi, x, t^m\lambda) = t^k R_k(\xi, x, \lambda) \ , \tag{2.43}$$

for $t > 0$. We have already seen in the simple Example 2.2.2 that the symbol of the resolvent of the Laplacian in $\mathbb{R}^d$ was of this form. Note that $\mathcal{H} - \lambda$ is of the same type, since

$$H - \lambda \sim \sum_{k=0}^{\infty} (H_{m-k} - \lambda\delta_{0,k}) \tag{2.44}$$

and the terms in the sum are jointly homogeneous in (ξ, λ) of degree $m - k$ in the sense of (2.43). The symbol of $\mathcal{H}^z$ will then be given by

$$H(z; \xi, x) \sim \sum_{k=0}^{\infty} H_{m-k}(z; \xi, x) \tag{2.45}$$

with

$$H_{m-k}(z; \xi, x) = \frac{\mathrm{i}}{2\pi} \int_\Gamma \lambda^z R_{-m-k}(\xi, x, \lambda) \, \mathrm{d}\lambda \ . \tag{2.46}$$

Now the defining equation for the resolvent, $\mathcal{R}(\lambda)(\mathcal{H} - \lambda) = I$, reads on the symbolic level

$$R(\xi, x, \lambda) \# (H(\xi, x) - \lambda) = 1 \ ,$$

and inserting the product formula for pseudodifferential operators, eq. (2.31), gives

$$\sum_{l=0}^{\infty} \frac{1}{l!} \left[\frac{\mathrm{i}}{2} (\langle \mathrm{D}_y, \mathrm{D}_\xi \rangle - \langle \mathrm{D}_x, \mathrm{D}_\eta \rangle) \right]^l R(\xi, x, \lambda)(H(\eta, y) - \lambda)|_{(\xi,x)=(\eta,y)} = 1 \ .$$

Inserting the asymptotic series for $H - \lambda$, and R, (2.44) and (2.42), and ordering by homogeneity gives the set of equations

$$R_{-m}(\xi, x, \lambda)(H_m(\xi, x) - \lambda) = 1$$

and

$$\sum_{k+j+n=p} \frac{1}{n!}\left[\frac{\mathrm{i}}{2}(\langle \mathrm{D}_y, \mathrm{D}_\xi\rangle - \langle \mathrm{D}_x, \mathrm{D}_\eta\rangle)\right]^n R_{-m-k}(\xi,x,\lambda)(H_{m-j}(\eta,y)-\lambda\delta_{j,0})\bigg|_{(\xi,x)=(\eta,y)} = 0 \ , \tag{2.47}$$

for $p = 1, 2, \ldots$. Since the sum contains no derivatives of $R_{-m-p}(\xi, x, \lambda)$ and only terms $R_{-m-k}(\xi, x, \lambda)$ with $k \le p$, this set of equations can be solved recursively to get the functions $R_{-m-k}(\xi, x, \lambda)$. The first two terms in the asymptotic expansion (2.42) of R follow to be

$$R_{-m}(\xi,x,\lambda) = \frac{1}{H_m(\xi,x)-\lambda} \tag{2.48}$$

$$R_{-m-1}(\xi,x,\lambda) = -\frac{H_{m-1}(\xi,x)}{(H_m(\xi,x)-\lambda)^2} \ . \tag{2.49}$$

The next terms become considerably more complicated, but can in principle be computed by elementary algebraic manipulations. From (2.47) it can be deduced by induction that they are of the general form

$$R_{-m-k}(\xi,x,\lambda) = \sum_{l=1}^{k} \frac{\gamma_{l,k}(\xi,x)}{(H_m(\xi,x)-\lambda)^{l+1}} \ , \tag{2.50}$$

where the functions $\gamma_{l,k}(\xi, x)$ are homogeneous of degree $ml - k$ in ξ and do not depend on λ.

Since the dependence on λ is explicitly known for all R_{-m-k}, one can compute, with the help of the formula

$$\frac{\mathrm{i}}{2\pi}\int_\Gamma \frac{\lambda^z}{(t-\lambda)^{l+1}}\,\mathrm{d}\lambda = (-1)^l \frac{z(z-1)\cdots(z-l+1)}{l!} t^{z-l} \ ,$$

the terms in the asymptotic expansion (2.45) for the symbol of $\mathcal{H}^z$. The first two terms follow from (2.48) and (2.49) to be

$$H_m(z;\xi,x) = H_m(\xi,x)^z$$
$$H_{m-1}(z;\xi,x) = zH_{m-1}(\xi,x)H_m(\xi,x)^{z-1} \ ,$$

and for $k \ge 2$ the terms are given by

$$H_{m-k}(z;\xi,x) = \sum_{l=1}^{k} \gamma_{l,k}(\xi,x)(-1)^l \frac{z(z-1)\cdots(z-l+1)}{l!} H_m(\xi,x)^{z-l} \ . \tag{2.51}$$

Notice that

$$H_{m-k}(z;t\xi,x) = t^{mz-k} H_{m-k}(z;\xi,x) \ , \tag{2.52}$$

for $t > 0$. Hence $\mathcal{H}^z$ is a classical pseudodifferential operator of order $m \operatorname{Re} z$, with principal symbol $\sigma(\mathcal{H}^z) = \sigma(\mathcal{H})^z$ and subprincipal symbol $\operatorname{sub}(\mathcal{H}^z) = z \operatorname{sub}(\mathcal{H})\sigma(\mathcal{H})^{z-1}$, as claimed in the first part of Theorem 2.2.13.

From (2.52) it follows that for $m \operatorname{Re} z < -d$ the operator $\mathcal{H}^z$ is of trace class with trace given by

$$\operatorname{tr} \mathcal{H}^z = \iint H(z;\xi,x)\ \mathrm{d}x\mathrm{d}\xi\ ,$$

and this function is holomorphic in the half plane $\operatorname{Re} z < -d/m$. In order to obtain an analytic extension to $\operatorname{Re} z \geq -d/m$ we write $H(z;\xi,x) = \sum_{k=0}^{N} H_{m-k}(z;\xi,x) + [H(z;\xi,x) - \sum_{k=0}^{N} H_{m-k}(z;\xi,x)]$, and note that $[H(z;\xi,x) - \sum_{k=0}^{N} H_{m-k}(z;\xi,x)] \in S^{m \operatorname{Re} z - N - 1}$. Therefore the second term in

$$\operatorname{tr} \mathcal{H}^z = \iint \sum_{k=0}^{N} H_{m-k}(z;\xi,x)\ \mathrm{d}x\mathrm{d}\xi + \iint H(z;\xi,x) - \sum_{k=0}^{N} H_{m-k}(z;\xi,x)\ \mathrm{d}x\mathrm{d}\xi$$

is holomorphic in the half plane $\operatorname{Re} z < -(d+N+1)/m$. Hence we only have to find the analytic continuation of the first term,

$$\iint \sum_{k=0}^{N} H_{m-k}(z;\xi,x)\ \mathrm{d}x\mathrm{d}\xi\ ,$$

which can be done for each summand separately. The function $H_{m-k}(z;\xi,x)$ is homogeneous of degree $m \operatorname{Re} z - k$ for $|\xi| \geq 1$ and smooth everywhere. Choose a smooth cutoff function $\chi(\lambda)$ which is 0 for $\lambda \leq 1/2$, and 1 for $\lambda \geq 1$. Then we get

$$\begin{aligned}\iint H_{m-k}(z;\xi,x)\ \mathrm{d}x\mathrm{d}\xi &= \iint \chi(H_m(\xi,x))H_{m-k}(z;\xi,x)\ \mathrm{d}x\mathrm{d}\xi \\ &\quad + \iint (1-\chi(H_m(\xi,x)))H_{m-k}(z;\xi,x)\ \mathrm{d}x\mathrm{d}\xi\ ,\end{aligned}$$

where the second term is holomorphic in $\mathbb{C}$. The first term gives, by introducing $s = H_m(\xi,x)$ as new coordinate,

$$\begin{aligned}\iint \chi(H_m(\xi,x))H_{m-k}(z;\xi,x)\ \mathrm{d}x\mathrm{d}\xi &= \int_0^\infty \chi(s) \int_{\Sigma_1} H_{m-k}(z;s\xi,x)\ \mathrm{d}\mu_1(\xi,x)\, s^{d-1}\ \mathrm{d}s \\ &= \int_{\Sigma_1} H_{m-k}(z;\xi,x)\ \mathrm{d}\mu(\xi,x) \int_0^\infty \chi(s)s^{mz-k+d-1}\ \mathrm{d}s\ ,\end{aligned}$$

where $\mathrm{d}\mu_1(\xi,x)$ is the Liouville measure on $\Sigma_1 := \{(\xi,x)\,;\, H_m(\xi,x) = 1\}$. The integral over s defines for $mz - k + d < 0$ a holomorphic function of z, which by partial integration can be written as

$$\int_0^\infty \chi(s)s^{mz-k+d-1}\ \mathrm{d}s = -\frac{1}{mz-k+d}\int_0^\infty \chi'(s)\, s^{mz-k+d}\ \mathrm{d}s\ .$$

Since $\chi'(s)$ has compact support the integral defines a holomorphic function of z, and we have found the meromorphic continuation we were looking for; $\iint H_{m-k}(z;\xi,x)\;\mathrm{d}x\mathrm{d}\xi$ is meromorphic with exactly one pole at $z=(k-d)/m$ and its residue there is

$$-m\int_{\Sigma_1} H_{m-k}((k-d)/m;x,\xi)\;\mathrm{d}\mu(\xi,x)\;.$$

Notice that because of (2.46) $H_{m-d}(0;\xi,x)=0$ and therefore the residue at $z=0$ vanishes.

Hence we have found that $\zeta(z)$ is a meromorphic function on $\mathbb{C}$ with possible simple poles located at the points $z=(k-d)/m$ for $k=0,1,2,3,\cdots$ and $k\neq d$. The residues at these poles can be computed explicitly from the symbol of $\mathcal{H}$, and the first two are given by

$$\begin{aligned}\operatorname{res}_{z=-d/m}\zeta(z)&=-m\int_{\Sigma_1}\mathrm{d}\mu(\xi,x)=-m\operatorname{vol}(\Sigma_1)\\ \operatorname{res}_{z=(1-d)/m}\zeta(z)&=(d-1)\int_{\Sigma_1}H_{m-1}(\xi,x)\;\mathrm{d}\mu(\xi,x)\;.\end{aligned}$$

By a closer inspection of (2.51) and the functions $\gamma_{l,k}(\xi,x)$ one can say more about the residues; e.g., the residues at $z=1,2,\ldots$ vanish, and if $\mathcal{H}$ is a second order differential operator, then there are no poles at $z=-d/2+k$, $k=0,1,2\ldots.$ For more information on this subject we refer to the literature [See67, DG75, Shu87].

Example 2.2.14. Consider as an example $M=S^1$ and

$$\mathcal{H}=-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+P\;,$$

where P is the projection operator onto the constant functions. The eigenvalues of $\mathcal{H}$ are the squares of the natural numbers; n^2, $n\in\mathbb{N}$, with multiplicity 2 except for the first one which has multiplicity 3. So the zeta function is given by

$$\zeta(z)=3+\sum_{n=1}^{\infty}2n^{2z}=3+2\zeta_R(-2z)\;,$$

where $\zeta_R(s)=\sum_{n=1}^{\infty}n^{-s}$ denotes the Riemann zeta function. The symbol of $\mathcal{H}$ is

$$H(\xi,x)=\xi^2$$

modulo the smoothing part coming from P. The symbol of $\mathcal{H}^z$ turns out to be ξ^{2z} modulo $S^{-\infty}$ and so $\zeta(z)$ has only one pole at $z=-1/2$ with residue equal to -1. Therefore one can conclude that the Riemann zeta function has only one pole at $s=1$ with residue 1.

2.2.3 Functions of pseudodifferential operators and applications to spectral asymptotics

The Tauberian Theorem of Ikehara, Theorem 2.2.12, together with the results on the analytic structure of the zeta function and its residues in Theorem 2.2.13 give an asymptotic formula for $N(\lambda)$.

Theorem 2.2.15. *Let M be a compact manifold of dimension d, and $\mathcal{H}$ be an elliptic selfadjoint classical pseudodifferential operator of order $m > 0$, then*

$$N(\lambda) = \frac{1}{d}\,\mathrm{vol}(\Sigma_1)\,\lambda^{d/m} + o(\lambda^{d/m})\;, \quad \lambda \to \infty\;, \tag{2.53}$$

where $\mathrm{vol}(\Sigma_1) = \iint \delta(\sigma(\mathcal{H})(\xi,x) - 1)\,\mathrm{d}x\mathrm{d}\xi$ *is the volume of the energy shell at energy* $\lambda = 1$.

The method used in the last section to construct powers of $\mathcal{H}$ can be extended to construct more general functions of an operator. Let $f(z)$ be holomorphic in a domain containing the spectrum of $\mathcal{H}$, then by the spectral theorem

$$f(\mathcal{H}) = \frac{\mathrm{i}}{2\pi}\int_\Gamma \frac{f(\lambda)}{\mathcal{H}-\lambda}\,\mathrm{d}\lambda\;, \tag{2.54}$$

where Γ is a path surrounding the spectrum anticlockwise, and the function f should satisfy the additional assumption $|f(z)| = o(1)$ for $z \in \Gamma$, in order that the integral converges. Going through the calculations for $f(\lambda) = \lambda^z$, one sees that $f(\mathcal{H})$ is a pseudodifferential operator with symbol

$$q(\xi,x) \sim \sum_{k=0}^{\infty} q_{m-k}(\xi,x)\;,$$

where

$$q_{m-k}(\xi,x) = \sum_{l=0}^{k} \gamma_{l,k}(\xi,x) f^{(k)}(H_m(\xi,x))\;, \tag{2.55}$$

and the summation starts at $l = 1$ for $k \geq 1$. The functions $\gamma_{l,k}(\xi,x)$ are identical to the ones in (2.50). This implies that if f satisfies a symbol condition of order κ, like

$$|f^{(l)}(z)| \leq C_l(1+|z|)^{\kappa-l}$$

for $z \in \mathbb{R}$, then $f(\mathcal{H})$ is a pseudodifferential operator in $\Psi^{\kappa m}(M)$. For $\kappa < 0$ this follows from (2.54) and (2.55), and for $\kappa \geq 0$ one uses the family $\mathcal{H}^z$ to define the family of functions $f_s(z) := z^s f(z)$. For $\mathrm{Re}\, s < \kappa$, $f_s(\mathcal{H})$ is already defined, and can be extended analytically to $\operatorname{Re} s \geq \kappa$, and in particular to $s = 0$. The principal symbol and the subprincipal symbol of $f(\mathcal{H})$ are given by

$$\sigma(f(\mathcal{H})) = f(\sigma(\mathcal{H})) \tag{2.56}$$
$$\operatorname{sub}(f(\mathcal{H})) = \operatorname{sub}(\mathcal{H}) f'(\sigma(\mathcal{H})) \ . \tag{2.57}$$

The formula (2.54) is only one possibility to define and study functions of pseudodifferential operators. Other methods use integral transformations, like the Fourier transformation,

$$f(\mathcal{H}) = \frac{1}{2\pi} \int \hat{f}(t)\, \mathrm{e}^{\mathrm{i}t\mathcal{H}}\, \mathrm{d}t \ ,$$

where $\hat{f}(t)$ is the Fourier transform of f. Instead of a construction of the resolvent, a functional calculus using this representation has to be based on a construction of $\mathrm{e}^{-\mathrm{i}t\mathcal{H}}$. But these operators are generally not pseudodifferential operators. For a first order operator $\mathcal{H}$, $\mathrm{e}^{-\mathrm{i}t\mathcal{H}}$ is a Fourier integral operator, a type of operator which we will discuss in the next section. A further, more recent, powerful method of defining functions of operators is via the method of almost analytic extensions, see [DS99].

The advantage of having other ways of defining functions of operators available is that one can allow larger classes of functions, e.g., functions which are not analytic, like smooth functions with compact support. They can be used for a different approach to the asymptotic behavior of $N(\lambda)$, which is based on the representation

$$N(\lambda) = \operatorname{tr} \Theta(\lambda - \mathcal{H}) \ ,$$

where Θ is the Heaviside step function, which is 0 on the negative half-axis, and 1 on the positive half axis. By approximating Θ with smooth functions for which a functional calculus is available, Tulovskii and Shubin [TS73], and Hörmander [Hör79], have proven asymptotic expansions for $N(\lambda)$ with better remainder estimates than the one obtained with the zeta function method. To illustrate the idea we proceed as if the functional calculus would be valid for $\Theta(\lambda - \mathcal{H})$, and get by using (2.56) and (2.57) that

$$\begin{aligned} \operatorname{tr} \Theta(\lambda - \mathcal{H}) &= \frac{1}{(2\pi)^d} \iint \big[\Theta(\lambda - \sigma(\mathcal{H})(\xi, x)) - \operatorname{sub}(\mathcal{H})(\xi, x)\Theta'(\lambda - \sigma(\mathcal{H})(\xi, x))\big] \mathrm{d}x\mathrm{d}\xi + \dots \\ &= \frac{1}{(2\pi)^d} \iint_{\sigma(\mathcal{H})(\xi,x) \leq \lambda} \mathrm{d}x\mathrm{d}\xi \\ &\qquad - \frac{1}{(2\pi)^d} \iint_{\sigma(\mathcal{H})(\xi,x) = \lambda} \operatorname{sub}(\mathcal{H})(\xi, x)\ \mathrm{d}\mu(\xi, x) + \dots \ . \end{aligned} \tag{2.58}$$

The first term is the same as in (2.53) as can be seen by the theorem of Stokes. In this form it admits a nice interpretation: It is approximately equal to the number of Planck cells of side-length 2π which fit into the ball $\{(\xi, x) \in T^*M \mid \sigma(\mathcal{H})(\xi, x) \leq \lambda\}$. This is what one expects heuristically from the uncertainty principle, see [Fef83] for a beautiful discussion of this point and much more. Under some mild additional conditions on the flow generated by $\sigma(\mathcal{H})$ the second term is as well correct [DG75], i.e. the corrections to (2.58) are of lower order in λ. In the semiclassical context, which we will study in more detail in Section 2.5, a similar result has been proven in [PR85].

In [TS73, Hör79] operators on $\mathbb{R}^d$ are considered, instead of operators on compact manifolds, as we do here. They show that, for a large class of operators $\mathcal{H}$, (2.58) is true with a remainder $O(\lambda^{2(d-2/3)/m+\epsilon})$ for every $\epsilon > 0$.

2.2.4 The Szegö limit theorem and quantum limits

We continue to assume in this whole subsection that $\mathcal{H}$ is a first order elliptic selfadjoint pseudodifferential operator on some compact manifold M, and we will study some general properties of eigenfunctions of this operator.

Powers of $\mathcal{H}$ can be used as well to draw certain conclusions on how the high energy behavior of expectation values $\langle\psi_n, \mathcal{A}\psi_n\rangle$ depends on the principal symbol $\sigma(\mathcal{A})$. Since the operators in $\Psi^0(M)$ are bounded, and $\mathcal{H}^{-m}\mathcal{A} \in \Psi^0(M)$ for $\mathcal{A} \in \Psi^m(M)$, one has

$$|\langle\psi_n, \mathcal{A}\psi_n\rangle| \leq C_{\mathcal{A}}\lambda_n^m$$

for $\mathcal{A} \in \Psi^m(M)$. Now assume that $\mathcal{A}, \mathcal{A}' \in \Psi^m_{\mathrm{phg}}(M)$ have the same principal symbol, then $\mathcal{A} - \mathcal{A}' \in \Psi^{m-1}_{\mathrm{phg}}(M)$, and therefore

$$|\langle\psi_n, \mathcal{A}\psi_n\rangle - \langle\psi_n, \mathcal{A}'\psi_n\rangle| \leq C\lambda_n^{m-1} \ . \tag{2.59}$$

So the leading asymptotic behavior of the sequence $\langle\psi_n, \mathcal{A}\psi_n\rangle$ depends only on the principal symbol of $\mathcal{A}$. This is a further support for the interpretation of $\sigma(\mathcal{A})$ as the classical limit of $\mathcal{A}$, and the interpretation of the high energy limit as the semiclassical limit.

We can view the eigenstates as a sequence of bounded maps $\Psi^0(M) \to \mathbb{C}$,

$$\Psi^0(M) \ni \mathcal{A} \mapsto \langle\psi_n, \mathcal{A}\psi_n\rangle \in \mathbb{C} \ ,$$

and by (2.59) the limit points of this sequence do only depend on the principal symbol. Hence they define a classical state $\nu : C^\infty(S^*X) \to \mathbb{C}$; these states are called diagonal quantum limits. More generally, sequences of pairs of eigenfunctions can define classical states.

Definition 2.2.16. *A linear map $\nu : C^\infty(S^*X) \to \mathbb{C}$ is called a **quantum limit** of $\mathcal{H}$, if there exists a sequence of pairs of eigenfunctions $\{\psi_{n_j}, \psi_{m_j}\}$ such that*

$$\lim_{j\to\infty} \langle\psi_{n_j}, \mathcal{A}\psi_{m_j}\rangle = \nu(\sigma(\mathcal{A})) \ ,$$

*for all $\mathcal{A} \in \Psi^0(M)$. If $m_j = n_j$ for all j, ν is called a **diagonal quantum limit**.*

The notion of a quantum limit is due to Zelditch [Zel90], who also has shown that these are measures, i.e. they extend to continuous maps $\nu : C(\Sigma_1) \to \mathbb{C}$.

Proposition 2.2.17 ([Zel90]). *Assume ν is a quantum limit defined by a sequence of pairs of eigenfunctions $\{\psi_{n_j}, \psi_{m_j}\}_{j\in\mathbb{N}}$ of $\mathcal{H} \in \Psi^m$. Then the sequence of the differences of the corresponding eigenvalues of $\mathcal{H}^{1/m}$ is convergent*

$$\lim_{j\to\infty} \left((\lambda_{n_j})^{1/m} - (\lambda_{m_j})^{1/m}\right) = s \ ,$$

and the measure ν is an eigenmeasure of the classical time evolution operator (2.12)*, $V_t = \exp tX_{\sigma(\mathcal{H})}$, with eigenvalue determined by s*

$$\nu(V_t a) = \mathrm{e}^{\mathrm{i}ts}\nu(a) \ .$$

In particular, the diagonal quantum limits are invariant measures.

The same techniques which lead to asymptotics of $N(\lambda)$ can be used to determine the asymptotic behavior of sums of expectation values,

$$N_{\mathcal{A}}(\lambda) := \sum_{\lambda_n \leq \lambda} \langle \psi_n, \mathcal{A}\psi_n\rangle \ , \tag{2.60}$$

for $\mathcal{A} \in \Psi^0_{\mathrm{phg}}(M)$. A zeta function adapted to this sum is given by

$$\zeta_{\mathcal{A}}(z) := \operatorname{tr} \mathcal{A}\mathcal{H}^z = \sum_n \langle \psi_n, \mathcal{A}\psi_n\rangle \lambda_n^z \ .$$

Since $\mathcal{A}\mathcal{H}^z$ has principal symbol

$$\sigma(\mathcal{A}\mathcal{H}^z) = \sigma(\mathcal{A})\sigma(\mathcal{H})^z \ ,$$

the zeta function $\zeta_{\mathcal{A}}(z)$ has its first pole at the same point as $\zeta(z)$, with residue given by

$$\mathrm{res}_{z=-d/m}\, \zeta_{\mathcal{A}}(z) = -m \int_{\Sigma_1} \sigma(\mathcal{A})(\xi, x)\mathrm{d}\mu(\xi, x) \ .$$

We would now like to apply the Tauberian theorem, Theorem 2.2.12, but this requires $N_{\mathcal{A}}(\lambda)$ to be real valued and non-decreasing. This is not the case for general $\mathcal{A}$, but by noting that $N_{\mathcal{A}}(\lambda)$ is linear in $\mathcal{A}$, we can easily reduce the general case to the special case of positive $\mathcal{A}$. By splitting $\mathcal{A}$ first into its selfadjoint and anti-selfadjoint part we are reduced to real valued expectation values, and since $\mathcal{A}$ is bounded we can split $\mathcal{A} = (\mathcal{A}+||\mathcal{A}||)-||\mathcal{A}||$. The first term is positive, whereas $N_{-||\mathcal{A}||}(\lambda) = -||\mathcal{A}||N(\lambda)$ is known for the second term. So an application of the Ikehara theorem leads to the following theorem which is called the Szegö limit theorem [Gui79, Hör85b].

Theorem 2.2.18. *Let $\mathcal{H}$ be a selfadjoint classical pseudodifferential operator of positive order with eigenvalues and eigenfunctions λ_n and ψ_n, then*

$$\lim_{\lambda\to\infty} \frac{1}{N(\lambda)} \sum_{\lambda_n\leq\lambda} \langle \psi_n, \mathcal{A}\psi_n\rangle = \frac{1}{\mathrm{vol}(\Sigma_1)} \int_{\Sigma_1} \sigma(\mathcal{A}) \ \mathrm{d}\mu \ , \tag{2.61}$$

for all $\mathcal{A} \in \Psi^0_{\mathrm{phg}}(M)$.

This is an important semiclassical result. It means that quantum mechanical mean values approach the classical mean value of an observable in the high energy limit. In view of the notion of quantum limits, the Szegö limit theorem implies that the mean of all diagonal quantum limits is given by the Liouville measure on Σ_1.

In fact Guillemin [Gui79] gave a more general statement which can be deduced from (2.61). Let $E(\lambda) = \sum_{\lambda_j \leq \lambda} |\psi_j\rangle\langle\psi_j|$ be the projection onto all eigenstates with energy smaller than λ, then one has for all $f \in C(\mathbb{R})$ and all self-adjoint $\mathcal{A} \in \Psi^0_{\mathrm{phg}}(M)$

$$\lim_{\lambda\to\infty} \frac{1}{N(\lambda)} \operatorname{tr} f(E(\lambda)\mathcal{A}E(\lambda)) = \frac{1}{\mathrm{vol}(\Sigma_1)} \int f(\sigma(\mathcal{A}))\, \mathrm{d}\mu \ . \tag{2.62}$$

This can be used to draw conclusions on the non-diagonal quantum limits also. Take, e.g., $f(t) = t^2$; in this case (2.62) leads to

$$\lim_{\lambda\to\infty} \frac{1}{N(\lambda)} \sum_{\lambda_n\lambda_m \leq \lambda} |\langle\psi_n, \mathcal{A}\psi_m\rangle|^2 = \frac{1}{\mathrm{vol}(\Sigma_1)} \int \sigma(\mathcal{A})^2\, \mathrm{d}\mu \ .$$

The preceeding constructions can be used to introduce a further interesting concept, the so-called residue trace, also called non-commutative residue or Wodzicki residue [Wod82, Gui85], see [Kas89, FGLS96] for overviews. The aim is to define a trace on the algebra of pseudodifferential operators, even if these are not of trace class in the usual sense. Let $\mathcal{H}$ be a positive elliptic selfadjoint pseudodifferential operator of first order, and $\mathcal{A} \in \Psi^m_{\mathrm{phg}}$, then, as we have seen, $\operatorname{tr} \mathcal{A}\mathcal{H}^z$ is well defined for $m + \operatorname{Re} z < -d$ and admits a meromorphic continuation to $\mathbb{C}$ with poles at the points $-m, -m+1, \dots$. One defines the residue trace of $\mathcal{A}$ to be the residue of $\operatorname{tr} \mathcal{A}\mathcal{H}^z$ at $z = 0$,

$$\operatorname{res} \mathcal{A} := \operatorname{res}_{z=0} \operatorname{tr} \mathcal{A}\mathcal{H}^z \ .$$

A remarkable property of this expression is that it is a trace, i.e. it vanishes on commutators,

$$\operatorname{res} [\mathcal{A}, \mathcal{B}] = 0 \ ,$$

and furthermore it is independent of the choice of $\mathcal{H}$. Additionally, it vanishes on trace class operators and $\operatorname{res} \mathcal{A}$ does only depend on the term of order $-d$ in the asymptotic expansion of the symbol of $\mathcal{A}$.

2.2.5 Fourier integral operators

Our characterization of pseudodifferential operators was based on their action on plane waves, see (2.19). Their characteristic feature is that they do not change the frequency of the wave, but only add a slowly varying amplitude. Now we are looking for a class of operators which can be interpreted as quantizations of canonical transformations, and for them one expects that they change the frequency of a plane wave according to the associated canonical transformation. So we make an ansatz similar to (2.19), with $e_\xi(x) = e^{i\langle x,\xi\rangle}$,

$$\mathcal{F}e_\xi(x) = a(\xi, x)e^{i\psi(\xi,x)} \ , \tag{2.63}$$

where we assume that $a(\xi, x)$ is a symbol in $S^m(\mathbb{R}^d \times \mathbb{R}^d)$ for some m, and $\psi(\xi, x)$ is a smooth function which is homogeneous of degree one in ξ for $|\xi| \geq 1$. By linear superposition the action of such an operator on an arbitrary distribution $u \in \mathcal{S}'(\mathbb{R}^d)$ is then given by

$$\mathcal{F}u(x) = \frac{1}{(2\pi)^d} \int e^{i\psi(\xi,x)} a(\xi, x)\hat{u}(\xi) \, d\xi \ . \tag{2.64}$$

Such an operator is called a (local) Fourier integral operator. They were introduced in this form by Hörmander [Hör68, Hör71], but they have many predecessors and roots in different areas of mathematics and physics, e.g., [Foc59, Mas72]. Some of their history is discussed in [Gui94].

Examples 2.2.19:

- For $\psi(\xi, x) = \langle x, \xi\rangle$, $\mathcal{F}$ is a pseudodifferential operator, so pseudodifferential operators can be considered as special cases of Fourier integral operators.

- Let $\psi(\xi, x) = \langle \varphi(x), \xi\rangle$, where $\varphi : \mathbb{R}^d \to \mathbb{R}^d$ is a diffeomorphism, and $a(\xi, x) = 1$. Then

$$\mathcal{F}u(x) = \frac{1}{(2\pi)^d} \int e^{i\langle\varphi(x),\xi\rangle} \hat{u}(\xi) \, d\xi = u(\varphi(x)) \ , \tag{2.65}$$

  so $\mathcal{F}$ transforms functions to new coordinates, $y = \varphi(x)$. If one chooses instead $a(\xi, x) = |\det \varphi'|^{1/2}$, then

$$\mathcal{F}u(x) = \frac{1}{(2\pi)^d} \int e^{i\langle\varphi(x),\xi\rangle} |\det \varphi'|^{1/2} \hat{u}(\xi) \, d\xi = |\det \varphi'|^{1/2} u(\varphi(x)) \ , \tag{2.66}$$

  so u is transformed as a half-density, see Appendix A.

In contrast to pseudodifferential operators, a Fourier integral operator $\mathcal{F}$ is characterized by two functions, the phase function ψ and the amplitude a. The question arises which significance they have, and if the operator determines them uniquely. It turns out that the most relevant object associated with $\mathcal{F}$ is the canonical transformation χ generated by the phase function ψ, see Section 2.1.2, eq. (2.15). This was defined as

$$\begin{aligned} \Phi : T^*M &\to T^*M \\ (\xi, x) &\mapsto \Phi(\xi, x) = (\eta, y) \end{aligned}$$

if and only if

$$\eta = \psi'_y(\xi, y) \ , \qquad x = \psi'_\xi(\xi, y) \ . \tag{2.67}$$

Notice that in order that a bijective map is defined by this prescription the matrix of mixed second derivatives $\psi''_{y\xi}(y,\xi)$ has to be nondegenerate.

The following theorem due to Egorov [Ego69], with a predecessor by Fock [Foc59], is one of the main reasons for the usefulness of Fourier integral operators.

Theorem 2.2.20. *Let $\mathcal{F}$ be given by (2.64) with $\psi''_{\xi,x} := \left\{\frac{\partial^2\psi}{\partial x_i \partial\xi_j}\right\}_{ij}$ nondegenerate, $a \in S^0_{\mathrm{phg}}(\mathbb{R}^d\times\mathbb{R}^d)$ with leading term $a_0 = |\det\psi''_{\xi,x}|^{1/2}$ and $\mathcal{B} \in \Psi^m_{\mathrm{phg}}(\mathbb{R}^d)$, then one has $\mathcal{F}^*\mathcal{B}\mathcal{F} \in \Psi^m_{\mathrm{phg}}(\mathbb{R}^d)$ and*

$$\sigma(\mathcal{F}^*\mathcal{B}\mathcal{F}) = \sigma(\mathcal{B}) \circ \Phi \ , \tag{2.68}$$

where Φ is the canonical transformation generated by the phase function ψ according to (2.67).

So indeed Fourier integral operators can be viewed as quantizations of canonical transformations. This theorem has a wide range of applications, a first one we note is that it contains the invariance of the algebra of pseudodifferential operators under coordinate transformations. This follows if we take F from the second example (2.65).

It might illuminate the basic methods of the theory if we indicate a formal proof of the result of Egorov on the principal symbol (2.68). According to (2.24) the principal symbol of $\mathcal{F}^*\mathcal{B}\mathcal{F}$ is given as the leading term in λ of

$$\mathrm{e}^{-\mathrm{i}\lambda\varphi(x)}(\mathcal{F}^*\mathcal{B}\mathcal{F}\mathrm{e}^{\mathrm{i}\lambda\varphi})(x) \ . \tag{2.69}$$

We will choose $\varphi(x) = \langle x, \xi_0\rangle$, and call the oscillating function $\mathrm{e}_{\lambda\xi_0}$,

$$\mathrm{e}_{\lambda\xi_0}(x) = \mathrm{e}^{\mathrm{i}\lambda\langle x,\xi_0\rangle} \ .$$

By (2.63) we have

$$\mathcal{F}\mathrm{e}_{\lambda\xi_0}(x) = \mathrm{e}^{\mathrm{i}\lambda\psi(\xi_0,x)}a(\lambda\xi_0, x) \ ,$$

and then (2.24) gives

$$\mathcal{B}\mathcal{F}\mathrm{e}_{\lambda\xi_0}(x) = \mathrm{e}^{\mathrm{i}\lambda\psi(\xi_0,x)}a_0(\lambda\xi_0,x)\sigma(\mathcal{B})(\lambda\psi'_x(\xi_0,x),x)(1+O(1/\lambda)) \ .$$

Now from (2.64) it follows by inserting the definition of the Fourier transform of u that the adjoint of $\mathcal{F}$ is given by

$$\mathcal{F}^*u(x) = \frac{1}{(2\pi)^d}\iint \mathrm{e}^{-\mathrm{i}(\psi(\eta,y)-\langle x,\eta\rangle)}a^*(\eta,y)u(y)\ \mathrm{d}y\mathrm{d}\eta \ ,$$

so modulo terms which are of lower order in λ we arrive at

$$\begin{aligned}
&\mathcal{F}^*\mathcal{B}\mathcal{F}\mathrm{e}_{\lambda\xi_0}(x) \\
&\qquad \equiv \frac{1}{(2\pi)^d}\iint \mathrm{e}^{-\mathrm{i}(\psi(\eta,y)-\langle x,\eta\rangle-\psi(\lambda\xi_0,y))}a^*(\eta,y)a_0(\lambda\xi_0,y)\sigma(\mathcal{B})(\lambda\psi'_x(\xi_0,y),y)\ \mathrm{d}y\mathrm{d}\eta \\
&\qquad = \frac{\lambda^d}{(2\pi)^d}\iint \mathrm{e}^{-\mathrm{i}\lambda(\psi(\eta,y)-\langle x,\eta\rangle-\psi(\xi_0,y))}a_0^*(\lambda\eta,y)a_0(\lambda\xi_0,y)\sigma(\mathcal{B})(\lambda\psi'_x(\xi_0,y),y)\ \mathrm{d}y\mathrm{d}\eta \ .
\end{aligned}$$

To evaluate these integrals further we use the method of stationary phase, see Appendix D. The stationary points of $\psi(\eta, y) - \langle x, \eta\rangle - \psi(\xi_0, y)$ are determined by the equations

$$\psi'_\eta(\eta, y) - x = 0$$
$$\psi'_y(\eta, y) - \psi'_y(\xi_0, y) = 0 \ .$$

Since $\psi''_{y,\eta}$ is nondegenerate, these equations determine an isolated nondegenerate stationary point $\eta = \xi_0$ and $y = y(\xi_0, x)$. Evaluating the stationary phase formula together with (2.69) gives

$$\sigma(\mathcal{F}^*\mathcal{B}\mathcal{F})(\xi_0, x) = \frac{|a_0(\xi_0, y)|^2}{|\det \psi''_{y,\eta}(\xi_0, y)|}\, \sigma(\mathcal{B})(\psi'_y(\xi_0, y), y) \ ,$$

and in view of (2.67) this gives the conclusion in the theorem of Egorov (2.68).

Definition 2.2.21. *The class of operators on a manifold M which are given locally as a sum of expressions of the form* (2.64)*, where ψ is a generating function for a canonical transformation $\Phi : T^*M \to T^*M$ and $a \in S^m(\mathbb{R}^d \times \mathbb{R}^d)$, will be denoted by*

$$I^m(M, \Phi) \ .$$

Since canonical transformations can be composed, one expects the same to be possible for the corresponding Fourier integral operators. Indeed, let $\mathcal{F}_1 \in I^{m_1}(M, \Phi_1)$ and $\mathcal{F}_2 \in I^{m_2}(M, \Phi_2)$ and assume for simplicity that M is compact, then the product is a Fourier integral operator associated with the composition $\Phi_1 \circ \Phi_2$ of Φ_1 and Φ_2,

$$\mathcal{F}_1\mathcal{F}_2 \in I^{m_1+m_2}(M, \Phi_1 \circ \Phi_2) \ .$$

Furthermore, if $\mathcal{F} \in I^m(M, \Phi)$ then its adjoint $\mathcal{F}^*$ is in $I^m(M, \Phi^{-1})$. As for pseudo-differential operators, Fourier integral operators of order zero on compact manifolds are L^2-bounded.

Due to the homogeneity of the phase functions ψ the canonical transformations are homogeneous too. They form the automorphisms of the classical algebra of observables, given by the smooth functions on Σ_1, or equivalently the functions on T^*M which are homogeneous of degree zero. So Fourier integral operators provide quantizations for the whole classical automorphism group. But the converse is true as well. This is the content of a beautiful theorem of Duistermaat and Singer [DS76].

Theorem 2.2.22. *Let $\alpha : \Psi^\infty_{\mathrm{phg}}(M) \to \Psi^\infty_{\mathrm{phg}}(M)$ be an order preserving continuous automorphism, i.e. $\alpha(\mathcal{AB}) = \alpha(\mathcal{A})\alpha(\mathcal{B})$ for all $\mathcal{A}, \mathcal{B} \in \Psi^\infty_{\mathrm{phg}}(M)$, and $\alpha(\mathcal{A}) \in \Psi^m_{\mathrm{phg}}(M)$ for $\mathcal{A} \in \Psi^m_{\mathrm{phg}}(M)$. Then there exists a unitary or anti-unitary[3] Fourier integral operator $\mathcal{U}$ such that $\alpha(\mathcal{A}) = \mathcal{U}^*\mathcal{A}\mathcal{U}$, for all $\mathcal{A} \in \Psi^\infty_{\mathrm{phg}}(M)$.*

[3] A anti-unitary operator is an anti-linear operator with $\mathcal{U}^*\mathcal{U} = I$.

We now want to discuss some consequences of the theorem of Egorov. First it follows directly from the definition of the wave front set (2.34), that for $F \in I^m(M, \Phi)$

$$\mathrm{WF}(\mathcal{F}u) \subset \Phi(\mathrm{WF}(u)) \ ,$$

so the wave front set is transformed with the symplectomorphism. In the theory of partial differential equations Fourier integral operators are used to transform equations to normal forms. By classifying the normal forms into which functions on phase space can be brought by conjugation with a canonical transformation, one gets a classification for the corresponding operators. As we have already noted, the theorem on the invariance of the class of pseudodifferential operators under coordinate transformations is as well a special case of the theorem of Egorov, because according to example (2.65) the pull back of a coordinate transformation on M to $C^\infty(M)$ is a Fourier integral operator.

Strictly speaking up to now we have only discussed the local theory of Fourier integral operators. The generating function which appears in the representation of a Fourier integral operator is only defined locally, as well as the amplitudes a. The global object corresponding to the phase function is the canonical transformation Φ, and one can define a principal symbol which is glued together in an invariant way from the amplitudes a for such operators too. But there one additionally has to take the freedom in the choice of the phase functions into account, which becomes rather technical at first sight, therefore we refer to the literature for this subject [Hör85b, Dui73].

A prominent example for a Fourier integral operator is given by

$$\mathcal{U}(t) := \mathrm{e}^{-\mathrm{i}t\mathcal{H}}$$

where $\mathcal{H}$ is a first order elliptic selfadjoint pseudodifferential operator, e.g., $\mathcal{H} = \sqrt{-\Delta}$. If we denote by Φ^t the classical flow generated by the principal symbol of $\mathcal{H}$, then

$$\mathcal{U}(t) \in I^0(M, \Phi^t) \ .$$

$\mathcal{U}(t)$ is the time evolution operator for a quantum mechanical system on M whose Hamilton operator is $\mathcal{H}$ in units where $\hbar = 1$.

Since this is an operator which one needs frequently we will describe its representation as a Fourier integral operator more closely. We will denote the kernel of $\mathcal{U}(t)$ by $K(t, x, y)$. It can be constructed from the Schrödinger equation,

$$(\mathrm{D}_t + \mathcal{H}_x) K(t, x, y) = 0 \tag{2.70}$$

together with the initial condition at $t = 0$,

$$K(0, x, y) = \delta(x - y) \ .$$

Because $\mathcal{H}$ is assumed to be of first order and elliptic, eq. (2.70) is a hyperbolic equation, and such equations can be solved with Lagrange distributions, which are the kernels of Fourier integral operators. Inserting in the equations an ansatz of the form of the kernel of a Fourier integral operator leads to a set of equations for the phase function and the terms in the asymptotic series of the amplitude. Solving these equations leads to the following form of the kernel,

$$K(t,x,y) = \frac{1}{(2\pi)^d} \int e^{i(\psi(t,\xi,x)-\langle y,\xi\rangle)}\, a(t,\xi,x)\; d\xi \;, \tag{2.71}$$

where $\psi(t,\xi,x)$ is a generating function for the Hamiltonian flow $\Phi^t = \exp(tX_{\sigma(\mathcal{H})})$ of the principal symbol of $\mathcal{H}$, and $a(t,\xi,x)$ is in $S^0_{\rm phg}(\mathbb{R}^{d+1}\times\mathbb{R}^d)$ with leading term

$$a_0(t,\xi,x) = e^{i\nu\pi/2}|\det\psi''_{x\xi}(t,\xi,x)|^{1/2} \;.$$

Here ν is an integer, called the Maslov index. It is related to the fact that the generating function $\psi(t,\xi,x)$ and the integral representation (2.71) are only defined locally. Recall that a necessary condition for $\psi(t,\xi,x)$ to be a generating function (2.67) was that $\det\psi''_{x\xi}(t,\xi,x)\neq 0$. At points where a generating function ψ_1 becomes degenerate the representation (2.71) breaks down, but one can always choose different local coordinates, in which again a nondegenerate generating function ψ_2, and therefore a representation (2.71), exists. It turns out that at these changes of the local representations the amplitude has to be multiplied by a constant phase factor

$$e^{i(\operatorname{sign}{\psi_1}''_{x\xi}-\operatorname{sign}{\psi_2}''_{x\xi})\pi/4} \tag{2.72}$$

in order that the kernels define the same operator. The number $(\operatorname{sign}{\psi_1}''_{x\xi}-\operatorname{sign}{\psi_2}''_{x\xi})$ is even because the signature will only change by an even number. The Maslov index ν is determined by the initial condition at $t=0$, together with the transition functions (2.72).

In case of the time evolution operator the theorem of Egorov implies that time evolution for finite times and quantization commute in the semiclassical limit. Since

$$\langle\psi_n, \mathcal{U}(t)^*\mathcal{A}\mathcal{U}(t)\psi_n\rangle = \langle\psi_n,\mathcal{A}\psi_n\rangle$$

for eigenfunctions ψ_n of $\mathcal{H}$, it follows from the theorem of Egorov that diagonal quantum-limits ν are invariant under the classical flow, i.e. they are eigenmeasures of the classical time evolution operator

$$V_t\nu = \nu \;.$$

The kernel of a Fourier integral operator in $I^m(M,\Phi)$ is a distribution given by the oscillatory integral

$$K(x,y) = \frac{1}{(2\pi)^d}\int e^{i(\psi(\xi,x)-\langle y,\xi\rangle)} a(\xi,x)\; d\xi \;.$$

According to the discussion after (2.14) the phase $\psi(\xi,x)-\langle y,\xi\rangle$ is a generating function for the Lagrangian submanifold in $T^*M\times T^*M$ given by the graph of Φ. Generalizing this expression, one calls a distribution of the form

$$u(x) = \frac{1}{(2\pi)^\kappa}\int e^{i\varphi(x,\theta)} a(x,\theta)\; d\theta$$

with $a(x, \theta) \in S^m(\mathbb{R}^d \times \mathbb{R}^\kappa)$ a Lagrangian distribution associated with the Lagrangian manifold Λ_φ generated by φ according to (2.13). Many of their properties are determined by Λ, e.g., $\mathrm{WF}(u) \subset \Lambda$.

The Lagrangian distributions associated to canonical relations between different manifolds according to (2.16) define a larger class of operators than the one associated with canonical transformations. An example is for instance the operator of restriction to a submanifold $N \subset M$. As a further example let us consider the case that there is a fibration of M by submanifolds N_α, $\alpha \in \Gamma$, and on each submanifold a density ρ_α is given such that the dependence on α is smooth. Then the operation consisting of first restricting to N_α and then integrating against ρ_α

$$u \mapsto \int u|_{N_\alpha} \ \rho_\alpha$$

defines a Fourier integral operator from M to Γ.

2.2.6 Microlocal analysis and the quantum-to-classical correspondence

We now come back to the problem posed at the end of the first section, i.e. how the classical and the quantum world are related to each other. We can now supply, with the help of what we have learned about microlocal analysis, the missing relations in table 2.1.

First we consider the algebras. If we choose as quantum mechanical observables an algebra of pseudodifferential operators $\Psi^m(M)$, then the map to the classical observables is given by the principal symbol. It maps commutators to Poisson brackets, and has therefore the desired algebraic properties. Furthermore, we have seen that in the high energy limit the behavior of observables in leading order only depends on the principal symbol, and the Szegö limit theorem told us that in the mean the quantum mechanical observables approach the classical mean. Further properties like boundedness, positivity or selfadjointness are preserved. But note that of course the principal symbol map is not an isomorphism, it is not injective. This is not a flaw of our methods, but it reflects the fundamental fact that there exists no quantization which exactly preserves the Lie-algebra structures induced by the Poisson bracket and the commutator. This is the content of the Gronewald-van Howe Theorems, see e.g. [AM78, Fol89].

A relation between the states on these algebras is given by the notion of quantum limits. Convergent sequences of quantum states define a classical state. But notice that pure states need not converge to pure states, even in the subclass of invariant states.

The automorphisms of the algebra of quantum mechanical observables are represented by Fourier integral operators. Through the theorem of Egorov they define a canonical transformation, i.e. an automorphism of the algebra of classical observables. For the case of a first-order Hamilton operator the one-parameter group of automorphisms defined by the Schrödinger equation is given by a family of Fourier integral operators, whose family of canonical transformations is the classical flow generated by the principal symbol of

quantum mechanics		**classical mechanics**
	observables	
An algebra of pseudodifferential operators $\Psi^0_{\text{phg}}(M)$	σ $\longrightarrow$ principal symbol	Homogeneous functions on T^*M: $C^\infty(\Sigma_1)$.
	states	
Continuous positive linear functionals on the algebra of observables:		
eigenfunctions	quantum limits $\longrightarrow$ Szegö limit theorem	eigenmeasures
	morphisms	
Fourier integral operators $I^0(M,\Phi)$	$\longrightarrow$ Egorov	symplectomorphisms Φ

Table 2.2: Comparison of the structures of quantum and classical mechanics with the relations provided by microlocal analysis.

the Hamiltonian. Furthermore, the quantum limits generated by the eigenfunctions are measures which are invariant under the classical flow.

2.3 Applications

In the last section we have described a considerable technical apparatus, and in order to show that this was not just “l'art pour l'art”, we will now describe two applications of this machinery to problems in semiclassical analysis. The first one is a theorem on the asymptotic behavior of eigenfunctions in the case that the classical flow is ergodic. The second one will be a discussion of the trace formula, a beautiful result which relates the eigenvalues of a quantum mechanical system to the periodic orbits of the corresponding classical system.

2.3.1 Quantum ergodicity

Let $\mathcal{H}$ be an elliptic selfadjoint positive pseudodifferential operator on a compact manifold M. We are interested in the asymptotic behavior of the eigenfunctions

$$\mathcal{H}\psi_n = \lambda_n\psi_n ,$$

for $\lambda_n \to \infty$. Since the eigenfunctions are the same for all powers of $\mathcal{H}$, it will be no loss of generality if we assume that $\mathcal{H}$ is of first order, e.g. , $\mathcal{H} = \sqrt{-\Delta}$. The corresponding classical system is defined by the principal symbol $\sigma(\mathcal{H})$, in case of $\mathcal{H} = \sqrt{-\Delta}$ it is conjugate to the geodesic flow on T^*M. We will study the case when the flow Φ^t is ergodic on Σ_1.

Ergodicity can be defined in a probabilistic way as follows: we start a trajectory at $t = 0$ at a point $(\xi, x) \in \Sigma_1$ and ask how often it will be in a given region $D \subset \Sigma_1$ of the phase space. Then the relative time the particle stays in D will tend to the relative volume of D, measured with the invariant measure μ, in the limit $t \to \infty$ for almost all starting-points $(\xi, x) \in \Sigma_1$. Or phrased in a different way, the probability of finding the particle in D is $\operatorname{vol}(D)/\operatorname{vol}(\Sigma_1)$, where $\operatorname{vol}(D) := \int_D \mathrm{d}\mu$, independent of the position or shape of D.

What could be the quantum mechanical analog of this behavior? The classical observable just studied was the characteristic function of D, χ_D. This is not smooth, so there is no pseudodifferential operator associated to it, but one might take a smoothing of it and proceed with that. For the sake of simplicity we will ignore this point for the moment, then the analog of classical ergodicity in the quantum mechanical system would be that the expectation values of the observable associated with χ_D tend to the relative volume of D, i.e., the classical expectation value. Generalizing this to all bounded observables gives the expectation

$$\langle \psi_n, \mathcal{A}\psi_n \rangle \to \overline{\sigma(\mathcal{A})}$$

for $n \to \infty$ and all $\mathcal{A} \in \Psi^0_{\mathrm{phg}}(M)$, where $\overline{\sigma(\mathcal{A})}$ denotes the mean value

$$\overline{\sigma(\mathcal{A})} = \frac{1}{\operatorname{vol}(\Sigma_1)} \int_{\Sigma_1} \sigma(\mathcal{A}) \, \mathrm{d}\mu \ .$$

The quantum ergodicity theorem states that this is true for almost all eigenfunctions ψ_n. More precisely, one says that a subsequence $\{n_j\}_{j \in \mathbb{N}} \subset \mathbb{N}$ has density $\alpha \in [0, 1]$, if

$$\lim_{N \to \infty} \frac{\#\{n_j \leq N\}}{N} = \alpha \ .$$

Theorem 2.3.1. *Let $\mathcal{H} \in \Psi^1_{\mathrm{phg}}$ be an elliptic selfadjoint positive operator on a compact manifold M, whose principal symbol generates an ergodic flow. Then there is a subsequence of eigenfunctions $\{\psi_{n_j}\}$ of density one with*

$$\lim_{j \to \infty} \langle \psi_{n_j}, \mathcal{A}\psi_{n_j} \rangle = \overline{\sigma(\mathcal{A})} \ , \tag{2.73}$$

for all $\mathcal{A} \in \Psi^0_{\mathrm{phg}}(M)$.

This property is called quantum ergodicity. In terms of quantum limits it means that the Liouville-measure is a diagonal quantum limit of a sequence of eigenfunctions of density one. It was first stated by Shnirelman [Shn74], and then proven for surfaces of constant negative curvature by Zelditch [Zel87] and in the general case by Colin de Verdière [Col85]. The theorem is also valid for manifolds with boundary, e.g. , Euclidean billiards, [GL93, ZZ96]. In the semiclassical ($\hbar \to 0$) context the analogous result was proven in [HMR87]. In order to avoid confusion one should note that the notion of quantum ergodicity is not related to the older notion of (von Neuman) ergodicity in statistical quantum mechanics [BR79]. The assumption that the order of the operator is one is not very restrictive, since by taking suitable powers we can reduce rather general operators to this case without changing the eigenfunctions.

We will present a sketch of the proof, using some simplifications invented by Sunada [Sun97]. Which tools we have to use is easy to see: first we have to implement the dynamics, because we have to bring ergodicity into play. This will be done using the theorem of Egorov. Secondly we need to take the high energy limit which we perform with the help of the Szegö limit theorem.

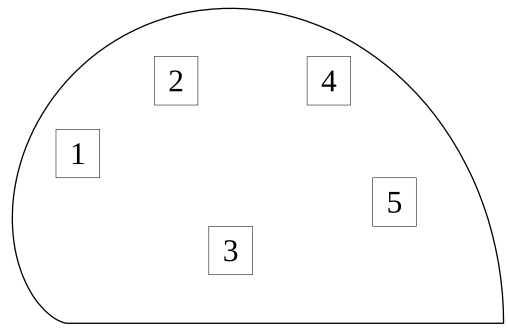

Figure 2.7: The desymmetrized cardioid billiard with the domains $D_1, \ldots, D_5$ for which the rate of quantum ergodicity is shown in the figures 2.8 and 2.9.

Let $\mathcal{A}$ be in $\Psi^0_{\mathrm{phg}}(M)$; we will study the asymptotic behavior for $\lambda \to \infty$ of

$$S_2(\mathcal{A},\lambda) := \frac{1}{N(\lambda)} \sum_{\lambda_n \le \lambda} |\langle \psi_n, \mathcal{A}\psi_n\rangle - \overline{\sigma(\mathcal{A})}|^2 ,$$

where $N(\lambda)$ denotes the spectral counting function. Define

$$\overline{\mathcal{A}}_T := \frac{1}{T} \int_0^T \mathcal{U}^*(t)[\mathcal{A} - \overline{\sigma(\mathcal{A})}]\mathcal{U}(t)\, \mathrm{d}t ,$$

and notice that because $\mathcal{U}(t)\psi_n = \mathrm{e}^{-\mathrm{i}t\lambda_n}\psi_n$ we have

$$\langle \psi_n, \overline{\mathcal{A}}_T \psi_n\rangle = \langle \psi_n, \mathcal{A}\psi_n\rangle - \overline{\sigma(\mathcal{A})} .$$

Using this and the Cauchy-Schwarz inequality we get

$$\begin{aligned} |\langle \psi_n, \mathcal{A}\psi_n\rangle - \overline{\sigma(\mathcal{A})}|^2 &= |\langle \psi_n, \overline{\mathcal{A}}_T\psi_n\rangle|^2 \\ &\le ||\overline{\mathcal{A}}_T\psi_n||^2 = \langle \psi_n, \overline{\mathcal{A}}_T^*\overline{\mathcal{A}}_T\psi_n\rangle , \end{aligned}$$

and therefore $S_2(\mathcal{A},\lambda)$ can be estimated as

$$S_2(\mathcal{A},\lambda) = \frac{1}{N(\lambda)} \sum_{\lambda_n \le \lambda} |\langle \psi_n, \overline{\mathcal{A}}_T\psi_n\rangle|^2 \le \frac{1}{N(\lambda)} \sum_{\lambda_n \le \lambda} \langle \psi_n, \overline{\mathcal{A}}_T^*\overline{\mathcal{A}}_T\psi_n\rangle .$$

Applying the Szegö limit theorem, Theorem 2.2.18, to the right hand side gives an upper bound for the limit of $S_2(\mathcal{A},\lambda)$

$$\lim_{\lambda\to\infty} S_2(\mathcal{A},\lambda) \leq \frac{1}{\mathrm{vol}(\Sigma_1)} \int_{\Sigma_1} \sigma(\overline{\mathcal{A}}_T)^* \, \sigma(\overline{\mathcal{A}}_T) \, \mathrm{d}\mu \ . \tag{2.74}$$

Now we have to estimate the right-hand side of (2.74). By the theorem of Egorov (2.68) we have

$$\sigma(\overline{\mathcal{A}}_T)(\xi,x) = \frac{1}{T}\int_0^T \sigma(\mathcal{A}) \circ \Phi^t(\xi,x) \, \mathrm{d}t - \overline{\sigma(\mathcal{A})} \ ,$$

and since the flow Φ^t is ergodic it follows that

$$\lim_{T\to\infty} \sigma(\overline{\mathcal{A}}_T)(\xi,x) = \overline{\sigma(\mathcal{A})} - \overline{\sigma(\mathcal{A})} = 0 \ ,$$

for μ-almost all $(\xi,x)\in\Sigma_1$. Therefore, the right-hand side of (2.74) can be made as small as one wishes by choosing T large enough, and so we arrive at the conclusion

$$\lim_{\lambda\to\infty} \frac{1}{N(\lambda)} \sum_{\lambda_n\leq\lambda} |\langle\psi_n, \mathcal{A}\psi_n\rangle - \overline{\sigma(\mathcal{A})}|^2 = 0 \ .$$

This is a mean value of a sequence of positive numbers, and it is a simple lemma [Wal82] that if this mean value is zero, then there exists a subsequence of density one which tends to zero.

So we have shown that for every $\mathcal{A}\in\Psi^0_{\mathrm{phg}}(M)$ there exists a subsequence ψ_{n_j} of density one which satisfies (2.73), and by a diagonal argument [Col85, Zel87] one arrives at a subsequence of density one which satisfies (2.73) for all $\mathcal{A}$.

The subject of quantum ergodicity is currently an active area of research. The two main open problems are the questions on the existence or non-existence of exceptional subsequences of eigenfunctions of density zero not tending to the quantum ergodic limit, and the rate by which the quantum ergodic limit is achieved. For $\mathcal{H}=\sqrt{-\Delta}$ on surfaces of constant negative curvature, Sarnak [Sar95] conjectured that unique quantum ergodicity holds, i.e. all eigenfunctions tend to the quantum ergodic limit, and furthermore that they approach this limit with a rate $\lambda^{-1/4}$,

$$|\langle\psi_n, \mathcal{A}\psi_n\rangle - \overline{\sigma(\mathcal{A})}| \leq C_\epsilon \lambda_n^{-1/2+\epsilon} \ , \tag{2.75}$$

for all $\epsilon > 0$.

For the Hecke eigenfunctions on the modular surface it was shown that

$$\frac{1}{N(\lambda)} \sum_{\lambda_n\leq\lambda} |\langle\psi_n, \chi_D\psi_n\rangle - \overline{\sigma(\mathcal{A})}|^2 \leq C_\varepsilon \lambda^{-1/2+\epsilon} \ , \tag{2.76}$$

see [LS95, Jak97], which is consistent with (2.75). A similar result was for more general systems derived from the so-called diagonal approximation in [Wil87, EFK+95], which is however not rigorous.

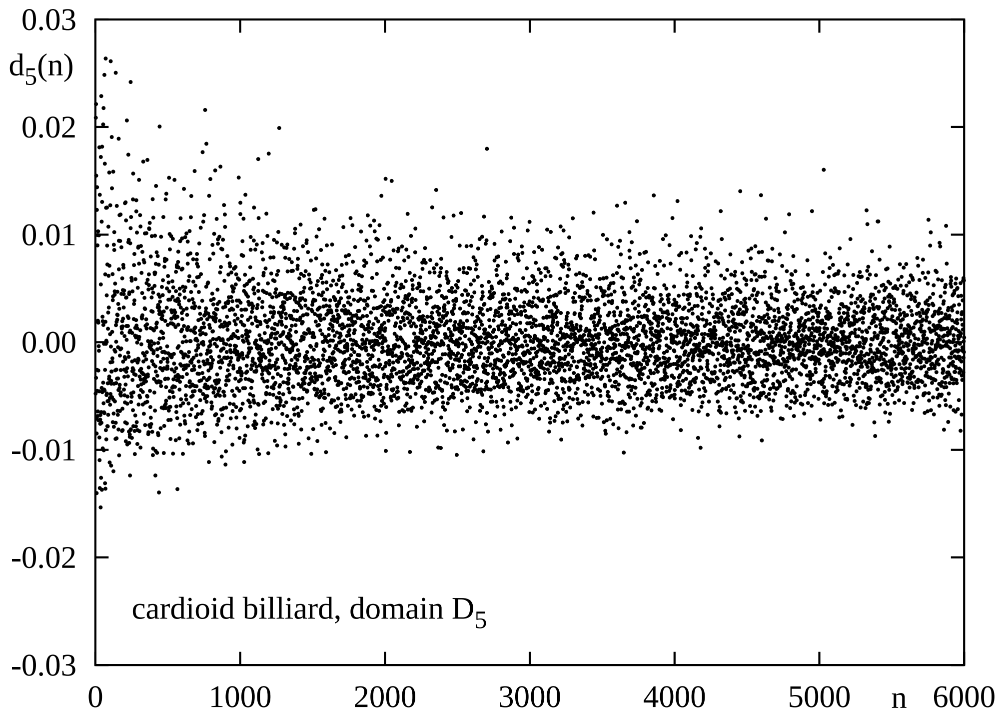

Figure 2.8: The expectation-values of χ_{D_5} minus the classical expectation value as a function of n, where D_5 is shown in fig. 2.7.

In fig. 2.8 we show the quantity $\langle\psi_n, \mathcal{A}\psi_n\rangle - \overline{\sigma(\mathcal{A})}$ for the cardioid billiard with an observable $\mathcal{A} = \chi_D$ where $D \subset M$ is a domain in position space. In order to see the rate of quantum ergodicity more clearly, in fig. 2.9

$$S_1(E, \chi_D) := \frac{1}{N(\sqrt{E})} \sum_{\lambda_n \leq \sqrt{E}} |\langle\psi_n, \chi_D\psi_n\rangle - \overline{\chi_D}| \ , \tag{2.77}$$

is plotted, taken from [BSS98], which is only partially consistent with the expected rate $E^{-1/4}$. A systematic study of the rate of quantum ergodicity for Euclidean and hyperbolic billiards can be found in [AT98, BSS98].

The question of unique quantum ergodicity is related to the existence of scars. Since quantum limits are invariant under the flow, for ergodic systems a quantum limit not equal to the Liouville measure has to be singular relative to the Liouville measure, and in particular has to have support of μ-measure zero. Candidates for such limits are measures concentrated on periodic orbits, the ones concentrated on unstable isolated orbits are called scars. Such states have been observed numerically, e.g., in the stadium and the cardioid billiard, but no proof of their existence up to arbitrary high energies exists currently.

A probably more accessible candidate for a non-quantum ergodic subsequence is provided by the so called bouncing-ball modes. They exist in billiards which possess two

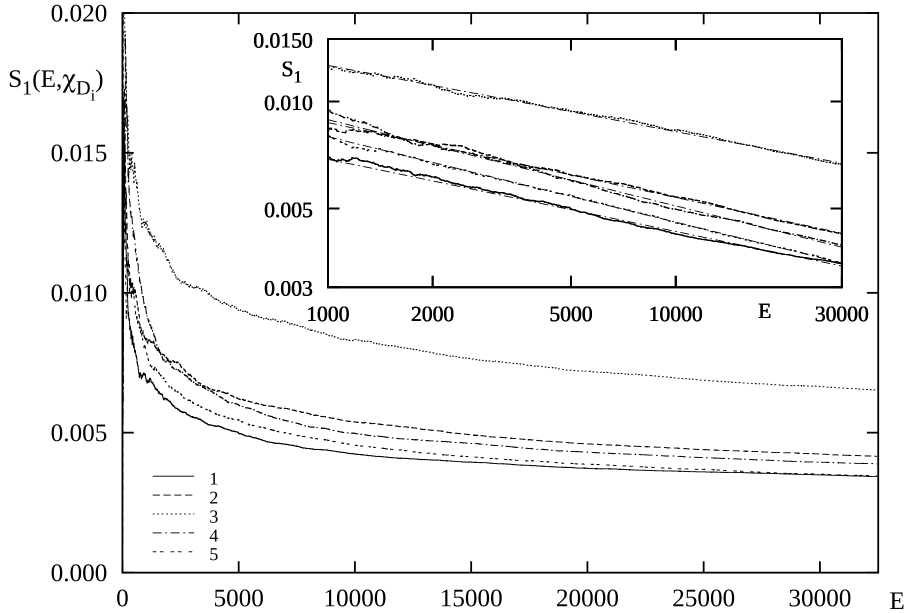

Figure 2.9: The quantity $S_1(E, \chi_D)$, see (2.77), for the different domains D_i shown in fig. 2.7. The inset shows a logarithmic plot together with the fits to $CE^{1/4+\epsilon}$, [BSS98].

opposite parallel sections of the boundary, like the stadium or the Sinai billiard. Some examples of them are shown in fig. 2.10. They are concentrated on the rectangular part of the billiard and have a structure close to eigenfunctions of a rectangle. In [BSS97] heuristic arguments were given that these non-quantum ergodic eigenfunctions survive the semiclassical limit, and furthermore an estimate for their number was obtained and numerically checked. It turned out that their number depends on the shape of the billiard, and that one can find ergodic billiards for which this number comes arbitrarily close to the upper limit given by the quantum ergodicity theorem. So the quantum ergodicity theorem appears to be sharp.

2.3.2 The trace formula

The second application of the methods from microlocal analysis we want to discuss is the trace formula. In physics it is called the Gutzwiller trace formula, and was derived by Gutzwiller and Balian Bloch [Gut71, BB72]. It is an important tool in quantum chaos, since it relates the quantum mechanical eigenvalues to the periodic orbits of the classical system. The formulation we want to discuss here is due to Duistermaat and Guillemin, [DG75], and applies to first order pseudodifferential operators on compact manifolds. The relation to Gutzwiller's formula will be discussed in Section 2.4.

Let $\mathcal{H}$ be an elliptic selfadjoint first order classical pseudodifferential operator on a compact manifold M, and $\mathcal{U}(t) = \mathrm{e}^{-\mathrm{i}t\mathcal{H}}$. The trace formula gives an expression for the

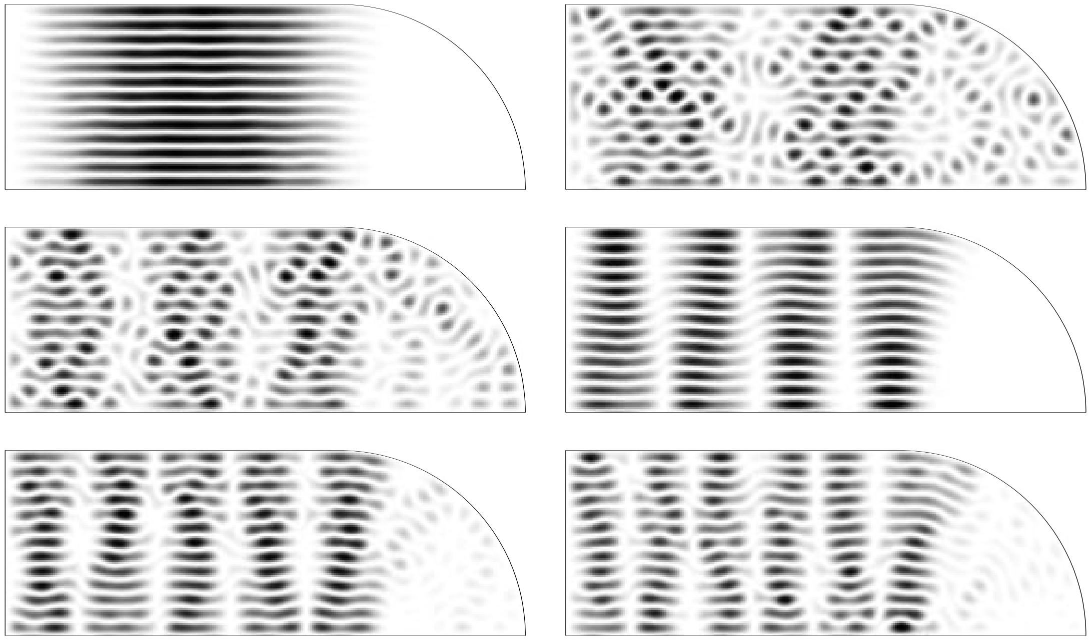

Figure 2.10: A series of bouncing-ball modes in the stadium billiard with Dirichlet boundary conditions [BSS97]. Such eigenfunctions are conjectured to exist for arbitrary energies, and therefore possibly form a non-quantum ergodic subsequence of eigenfunctions in the ergodic stadium billiard.

trace of $\mathcal{U}(t)$,

$$\mathrm{tr}\,\mathcal{U}(t) = \sum_n \mathrm{e}^{-\mathrm{i}t\lambda_n} \ .$$

Obviously $\mathcal{U}(t)$ is not of trace class, but since by Weyl's law, equation (2.53), $\lambda_n \sim Cn^{1/d}$ for $n \to \infty$, the trace can be viewed as a distribution on $\mathcal{S}(\mathbb{R})$,

$$\mathcal{S}(\mathbb{R}) \ni \rho \mapsto \int \rho(t)\,\mathrm{tr}\,\mathcal{U}(t)\ \mathrm{d}t = \sum_n \hat{\rho}(\lambda_n) \ .$$

The trace formula is concerned with the nature of the singularities of this distribution. A first beautiful result, called the Poisson relation, gives the position of the singularities of the wave-trace. Let Φ^t be the flow generated by the principal symbol of $\mathcal{H}$ on Σ_1. One calls T a period of Φ^t, if there is a point $(\xi, x) \in \Sigma_1$ with $\Phi^T(\xi, x) = (\xi, x)$. The orbit through (ξ, x) is then a periodic orbit with period T. The set of all periods is called the period spectrum and will be denoted by $\mathcal{T}$.

Theorem 2.3.2. *The singular support of the distribution* $\mathrm{tr}\,\mathcal{U}$ *is contained in* $\mathcal{T}$. *More generally*

$$\mathrm{WF}(\mathrm{tr}\,\mathcal{U}) \subset \mathcal{T} \times \mathbb{R}_+ \ . \tag{2.78}$$

This was proven by Chazarain [Cha74]. So the periodic orbits determine the possible positions of the singularities of this sum over eigenvalues. The original proof is based on the wave-front set calculus and needs a representation of $\mathcal{U}(t)$ as a Fourier-integral operator.

We will sketch a different proof, see [Wun99], which works via microlocalisation. Given an interval $[t_1, t_2]$ which contains no element of $\mathcal{T}$, we will show that $\operatorname{tr}\mathcal{U}(t) \in C^\infty([t_1, t_2])$, which is the first part of the theorem. That there is no element of $\mathcal{T}$ in $[t_1, t_2]$ means that there is no $(\xi, x) \in \Sigma_1$ with $\Phi^t(\xi, x) = (\xi, x)$ for $t \in [t_1, t_2]$. Because Σ_1 is compact we can therefore find a finite open covering $\{\Omega_j\}_{j\in J}$ with

$$\Omega_j \cap \Phi^t(\Omega_j) = \emptyset \ ,$$

for $t \in [t_1, t_2]$ and all $j \in J$. Now one can find operators $\mathcal{A}_j \in \Psi^0_{\mathrm{phg}}(M)$ such that $\{\mathcal{A}_j^2\}_{j\in J}$ form a microlocal partition of unity subordinate to $\{\Omega_j\}_{j\in J}$. This means that modulo smoothing operators

$$\sum_{j\in J} \mathcal{A}_j^2 = 1 \quad \text{and} \quad \mathrm{WF}(\mathcal{A}_j) \subset \Omega_j \ .$$

Therefore we get modulo smooth functions

$$\operatorname{tr}\mathcal{U}(t) = \sum_{j\in J} \operatorname{tr}\mathcal{U}(t)\mathcal{A}_j^2 = \sum_{j\in J} \operatorname{tr}\mathcal{A}_j\mathcal{U}(t)\mathcal{A}_j \ ,$$

but since by the theorem of Egorov $\mathrm{WF}(\mathcal{U}(t)\mathcal{A}_j) = \Phi^t(\mathrm{WF}(\mathcal{A}_j))$, we have

$$\mathrm{WF}(\mathcal{A}_j\mathcal{U}(t)\mathcal{A}_j) = \mathrm{WF}(\mathcal{A}_j) \cap \Phi^t(\mathrm{WF}(\mathcal{A}_j)) = \emptyset \ .$$

So $\mathcal{A}_j\mathcal{U}(t)\mathcal{A}_j$ is smoothing for $t \in [t_1, t_2]$, and therefore of trace class for all $j \in J$. But since J is finite $\operatorname{tr}\mathcal{U}(t)$ is smooth too for $t \in [t_1, t_2]$. The fact that the wave front set now contains only positive frequencies follows simply from the fact that the operator $\mathcal{H}$ is assumed to be positive. Let $\varphi \in \mathcal{S}(\mathbb{R})$, then

$$\widehat{\varphi \operatorname{tr}\mathcal{U}}(\lambda) = \sum_n \hat{\varphi}(\lambda - \lambda_n) \sim \lambda^{-N}$$

for all $N \in \mathbb{N}$.

Is there equality in the Poisson relation (2.78)? That means, is the period spectrum a spectral invariant? This question is not entirely solved, but for certain types of systems it has been shown that equality holds in (2.78). In order to answer this question one has to study the wave-trace $\operatorname{tr}\mathcal{U}(t)$ more closely near the periods T. The structure there depends only on the type of the periodic orbits with period T, and for a large class of periodic orbits it was studied by Duistermaat and Guillemin [DG75]. But before describing their result, we want to study some examples.

Example 2.3.3. Let $\mathbb{R}^2/\mathbb{Z}^2$ be the two dimensional torus, with Hamilton operator $\mathcal{H} = \sqrt{-\Delta}$. The eigenvalues of $\mathcal{H}$ can easily be computed. They are given by

$$2\pi|k| = 2\pi\sqrt{k_1^2 + k_2^2} \ , \quad \text{for } k = (k_1, k_2) \in \mathbb{Z}^2 \ .$$

The basic tool for the study of the wave-trace of $\sqrt{-\Delta}$ will be the Poisson summation formula,

$$\sum_{k\in\mathbb{Z}^2}\delta(x-k)=\sum_{k\in\mathbb{Z}^2}\mathrm{e}^{2\pi\mathrm{i}kx}\ , \tag{2.79}$$

for $x\in\mathbb{R}^2$, see e.g. [Hör83]. Using this formula one can express the wave-trace of $\sqrt{-\Delta}$ as

$$\begin{aligned}\operatorname{tr}\mathcal{U}(t)=\sum_{k\in\mathbb{Z}^2}\mathrm{e}^{-2\pi\mathrm{i}t|k|}&=\sum_{k\in\mathbb{Z}^2}\int\mathrm{e}^{-2\pi\mathrm{i}t|x|}\delta(x-k)\ \mathrm{d}x\\&=\sum_{k\in\mathbb{Z}^2}\int\mathrm{e}^{-2\pi\mathrm{i}t|x|}\mathrm{e}^{2\pi\mathrm{i}kx}\ \mathrm{d}x\ .\end{aligned}$$

But the integrals in last line can, upon introducing polar coordinates, easily seen to be

$$\int\mathrm{e}^{-2\pi\mathrm{i}t|x|}\mathrm{e}^{2\pi\mathrm{i}kx}\ \mathrm{d}x=\frac{1}{2\pi}\int_0^\infty\lambda J_0(|k|\lambda)\,\mathrm{e}^{\mathrm{i}\lambda t}\ \mathrm{d}\lambda\ , \tag{2.80}$$

where $J_0(z)$ denotes a Bessel function of the first kind. Hence we have arrived at the following expression for the wave-trace of $\sqrt{-\Delta}$

$$\operatorname{tr}\mathcal{U}(t)=\sum_{k\in\mathbb{Z}^2}\frac{1}{2\pi}\int_0^\infty\lambda J_0(|k|\lambda)\,\mathrm{e}^{\mathrm{i}\lambda t}\ \mathrm{d}\lambda\ ,$$

as an equality between distributions on $\mathcal{S}(\mathbb{R})$. Now the individual terms (2.80) have their singularities at $t=\pm|k|$, which are exactly the periods of the periodic orbits of the flow generated by the principal symbol $|\xi|$ of $\sqrt{-\Delta}$.

By taking the Fourier transformation of the wave-trace $\operatorname{tr}\mathcal{U}(t)=\sum_n\mathrm{e}^{-\mathrm{i}t\lambda_n}$ one arrives at a representation of the spectral density of $\mathcal{H}=\sqrt{-\Delta}$,

$$\sum_{n=0}^{\infty}\delta(\lambda-\lambda_n)=\frac{1}{2\pi}\lambda_+ +\frac{1}{2\pi}\sum_{k\in\mathbb{Z}^2\backslash\{0\}}\lambda_+\,J_0(|k|\lambda)\ , \tag{2.81}$$

where $\lambda_+=0$ for $\lambda\leq 0$ and $\lambda_+=\lambda$ for $\lambda>0$.

At first sight it might appear that the crucial fact which allowed the derivation of (2.81) in the preceeding example is that the eigenvalues are exactly known. But this is not quite right, the main point is that the torus is a homogeneous space, i.e. the quotient of $\mathbb{R}^2$ by a discrete group. A similar situation occurs for compact Riemannian surfaces of genus $g\geq 2$, they can be represented as the quotient of the upper half-plane $\mathbb{H}$ by a discrete subgroup $\Gamma\subset SL(2,\mathbb{R})$, $M=\mathbb{H}/\Gamma$. Here the eigenvalues of the Laplace-Beltrami operator are not known explicitly, but group theory allows to set up a similar formula as for the last example. Let $\mathcal{H}=\sqrt{-\Delta-1/4}$, and let λ_n be the eigenvalues of $\mathcal{H}$, then the famous Selberg trace formula [Sel56] reads

$$\sum_{n=0}^{\infty} h(\lambda_n) = \frac{\mathcal{A}_M}{4\pi}\int_{-\infty}^{\infty} \lambda h(\lambda)\tanh(\pi\lambda)\,\mathrm{d}\lambda + \frac{1}{2\pi}\sum_{T\in\mathcal{T}\setminus\{0\}} \frac{T^{\#}}{2|\sinh(T/2)|}\int_{-\infty}^{\infty} h(\lambda)\mathrm{e}^{-\mathrm{i}\lambda T}\,\mathrm{d}\lambda\ , \tag{2.82}$$

where h is assumed to be an even function which is analytic in a strip $|\operatorname{Im}\lambda|\leq 1/2+\delta$ for some $\delta>0$, and decays faster than $(1+|\lambda|)^{-2-\epsilon}$ for some $\epsilon>0$. Here $T^{\#}$ denotes the primitive period of T, and $\mathcal{A}_M$ denotes the area of M.

Now we turn to the description of the results of Duistermaat and Guillemin, which generalize the results of the previous two examples to a much larger class of systems, but only asymptotically in the high energy limit $\lambda\to\infty$. In order to describe their results one has to introduce some notions related to the periodic orbits. Let γ be a periodic orbit or a connected family of periodic orbits with period T, that means γ is a connected component of the set

$$\{(\xi,x)\in\Sigma_1\,|\,\Phi^T(\xi,x)=(\xi,x)\}\ .$$

Families of orbits appear for instance in integrable systems, where they are given by invariant tori with rational frequencies, whereas in chaotic systems isolated orbits are typical. We will denote the dimension of γ by d_γ.

Now choose a point $(\xi,x)\in\gamma$ and consider the linearized flow $\mathrm{d}\Phi^T(\xi,x): T_{(\xi,x)}(\Sigma_1)\to T_{(\xi,x)}(\Sigma_1)$. Since γ is invariant under Φ^T, the tangent space of γ at (ξ,x), $T_{(\xi,x)}\gamma$, is contained in the kernel of $\mathrm{d}\Phi^T(\xi,x)-I$. If it is equal to the kernel,

$$\operatorname{Ker}(\mathrm{d}\Phi^T(\xi,x)-I)=T_{(\xi,x)}\gamma\ , \tag{2.83}$$

then γ is called clean. The map $\mathrm{d}\Phi^T(\xi,x)$ has always one eigenvalue equal to 1 corresponding to the eigenvector $X_{\sigma(\mathcal{H})}$ along the flow. By dividing the subspace spanned by this vector out we get a reduced map $P_\gamma: T_{(\xi,x)}(\Sigma_1)/(\mathbb{R}\cdot X_{\sigma(\mathcal{H})})\to T_{(\xi,x)}(\Sigma_1)/(\mathbb{R}\cdot X_{\sigma(\mathcal{H})})$ called the Poincaré map of γ. If γ is one-dimensional, then the condition that γ is clean is equivalent to $I-P_\gamma$ being nondegenerate, i.e.

$$\det(I-P_\gamma)\neq 0\ .$$

For an integrable system whose Hamilton function is homogeneous, the radial coordinate can be chosen as one of the action variables. If we call the remaining action variables I', then the torus γ is clean if

$$b_\gamma := \det\left(T\frac{\partial^2 H}{\partial I'\partial I'}\right)(I)\neq 0$$

for I on γ.

Duistermaat and Guillemin have shown that on a clean γ a natural density $|\mathrm{d}\mu_\gamma|$ can be defined. For example, for an isolated nondegenerate orbit it is given by

$$|\mathrm{d}\mu_\gamma| = \frac{1}{|\det(I-P_\gamma)|^{1/2}}\,|\mathrm{d}t| \ , \tag{2.84}$$

and for a clean family in an integrable system with angle coordinates $(\varphi_1,\dots,\varphi_d)$ by

$$|\mathrm{d}\mu_\gamma| = \frac{1}{|b_\gamma|^{1/2}}\,|\mathrm{d}\varphi_1\cdots\mathrm{d}\varphi_d| \ . \tag{2.85}$$

Now the result of Duistermaat and Guillemin [DG75] is:

Theorem 2.3.4. *Assume $T\in\mathcal{T}$ and all orbits γ with period T are clean (c.f. (2.83)), then T is an isolated singularity of $\mathrm{tr}\,\mathcal{U}(t)$ and near $t=T$ one has*

$$\mathrm{tr}\,\mathcal{U}(t) = \frac{1}{2\pi}\sum_{|\gamma|=T}\int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}(t-T)\lambda}\,a_\gamma(\lambda)\,\mathrm{d}\lambda \ . \tag{2.86}$$

The sum is over all orbits with period T, and $a_\gamma(\lambda)$ is a smooth function with

$$a_\gamma(\lambda)\sim \mathrm{e}^{\mathrm{i}\nu_\gamma\pi/2}\left(\frac{\lambda}{2\pi}\right)^{\frac{d_\gamma-1}{2}}\sum_{k=0}^{\infty} a_\gamma^{(k)}\lambda^{-k} \ , \qquad \textit{for} \quad \lambda\to+\infty \ , \tag{2.87}$$

and $a_\gamma(\lambda)=O(|\lambda|^{-N})$ for $\lambda\to-\infty$ and every $N\in\mathbb{N}$, where $\nu_\gamma\in\mathbb{Z}/2$ is the so called Maslov index of γ. The leading term of $a_\gamma(\lambda)$ is given by

$$a_\gamma^{(0)} = \int_\gamma \mathrm{e}^{\mathrm{i}T\,\overline{\mathrm{sub}\,\mathcal{H}}^{\gamma}}\,|\mathrm{d}\mu_\gamma| \ ,$$

where $\overline{\mathrm{sub}\,\mathcal{H}}^{\gamma}(\xi,x)=\frac{1}{T}\int_0^T \mathrm{sub}\,\mathcal{H}\circ\Phi^t(\xi,x)\,\mathrm{d}t$ denotes the average of the subprincipal symbol over one period.

E.g., for an isolated nondegenerate orbit one has $d_\gamma=1$ and with (2.84)

$$a_\gamma^{(0)} = \frac{T^\#}{|\det(I-P_\gamma)|^{1/2}}\,\mathrm{e}^{\mathrm{i}\,T\,\overline{\mathrm{sub}\,\mathcal{H}}^{\gamma}} \ .$$

For a family of periodic orbits in an integrable system one has $d_\gamma=d$ and it follows from (2.85) that

$$a_\gamma^{(0)} = \frac{1}{|b_\gamma|^{1/2}}\int_\gamma \mathrm{e}^{\mathrm{i}\,T\,\overline{\mathrm{sub}\,\mathcal{H}}^{\gamma}}\,\mathrm{d}\varphi_1\cdots\mathrm{d}\varphi_d \ .$$

Since every point is periodic with period 0, $\mathrm{tr}\,\mathcal{U}(t)$ has always a singularity at $t=0$, which is called the "big" singularity. Here the "family of orbits" is given by Σ_1 which is always clean, so this singularity is isolated. The corresponding density is just the Liouville density μ on Σ_1, and the Maslov index is zero. For this singularity the first two terms in the asymptotic expansion of $a(\lambda)$ have been computed,

$$a_0^{(0)} = \int_{\Sigma_1} \mathrm{d}\mu =: \mathrm{vol}(\Sigma_1) \ , \qquad a_0^{(1)} = (d-1)\int_{\Sigma_1} \mathrm{sub}(\mathcal{H})\ \mathrm{d}\mu =: \overline{\mathrm{sub}\,\mathcal{H}}^{\Sigma_1} \ ,$$

and $d_\gamma = 2d-1$.

The informations on the singularities can be transformed by taking the Fourier transformation of $\mathrm{tr}\,\mathcal{U}$ into information on the asymptotic behavior of this Fourier transform for large λ. Take a function $\rho \in C^\infty(\mathbb{R})$ whose Fourier transform $\hat{\rho}$ has compact support, and assume that all orbits with periods in the support are clean. Then multiplying (2.86) with $\hat{\rho}$, and taking the inverse Fourier transform leads to

$$\sum_n \rho(\lambda-\lambda_n) = \frac{1}{2\pi}\sum_{T\in\mathcal{T}}\sum_{|\gamma|=T}\int_{\mathbb{R}} \rho(\lambda-\lambda')a_\gamma(\lambda')\mathrm{e}^{\mathrm{i}T\lambda'}\ \mathrm{d}\lambda' \ .$$

The individual terms in the sum give with (2.87)

$$\int_{\mathbb{R}} \rho(\lambda-\lambda')a_\gamma(\lambda')\mathrm{e}^{\mathrm{i}T\lambda'}\ \mathrm{d}\lambda' \sim \mathrm{e}^{\mathrm{i}\nu_\gamma\pi/2}\left(\frac{\lambda}{2\pi}\right)^{\frac{d_\gamma-1}{2}} \hat{\rho}(T)\,\mathrm{e}^{\mathrm{i}T\lambda}[a_\gamma^{(0)} + a_\gamma^{(1)}\frac{1}{\lambda} + \cdots] \ .$$

Let us consider as examples two types of two-dimensional systems, corresponding to the two examples discussed above. The first type of system is one where the flow has only isolated nondegenerate periodic orbits. This is for instance the case if the flow is hyperbolic, e.g., in the case of a geodesic flow on a manifold of strictly negative curvature. Then one has for $\hat{\rho} \in C_0^\infty(\mathbb{R})$

$$\begin{aligned}\sum_n \rho(\lambda-\lambda_n) =& \frac{\hat{\rho}(0)}{(2\pi)^2}\ \mathrm{vol}(\Sigma_1)\ \lambda + \frac{\hat{\rho}^{(1)}(0)}{(2\pi)^2}\,\overline{\mathrm{sub}\,\mathcal{H}}^{\Sigma_1} \\ &+ \frac{1}{2\pi}\sum_T \hat{\rho}(T)\sum_{|\gamma|=T}\frac{T^{\#}\mathrm{e}^{\mathrm{i}\nu_\gamma\pi/2}}{|\det(I-P_\gamma)|^{1/2}}\ \mathrm{e}^{\mathrm{i}\,T\,\overline{\mathrm{sub}\,\mathcal{H}}^\gamma}\ \mathrm{e}^{\mathrm{i}T\lambda} + O(1/\lambda) \ .\end{aligned} \tag{2.88}$$

How does this compare with the Selberg trace formula (2.82)? First of all in this case the subprincipal symbol vanishes. Furthermore $|\det(1-P_\gamma)|^{1/2} = 2|\sinh(T/2)|$ and the Maslov indices are zero. If one chooses then for h in (2.82) a function of the form $h(s) = \rho(\lambda - s)$, the formulas (2.82) and (2.88) almost coincide. All the remainder terms in the Duistermaat-Guillemin formula vanish, except an exponentially small contribution to the $T=0$ term, given by

$$\tanh(\pi\lambda) = 1 + O(\mathrm{e}^{-\pi\lambda}) \ ,$$

which has an interesting interpretation in terms of the dual to $\mathbb{H}$ as a symmetric space, when one allows λ to be complex, see [CV90, BO95].

The second type of systems we want to consider are integrable systems in two dimensions. Here the orbits come in two-dimensional families and the trace formula reads

$$\sum_n \rho(\lambda-\lambda_n) = \frac{\hat\rho(0)}{(2\pi)^2}\,\mathrm{vol}(\Sigma_1)\;\lambda + \frac{\hat\rho^{(1)}(0)}{(2\pi)^2}\,\overline{\mathrm{sub}\,\mathcal{H}}^{\Sigma_1} + \frac{\lambda^{1/2}}{(2\pi)^{3/2}}\sum_T \hat\rho(T)\sum_{|\gamma|=T}\int_\gamma \mathrm{e}^{\mathrm{i}\,T\,\overline{\mathrm{sub}\,\mathcal{H}}^\gamma}\,|\mathrm{d}\mu_\gamma|\;\mathrm{e}^{\mathrm{i}\nu_\gamma\pi/2}\,\mathrm{e}^{\mathrm{i}T\lambda} + O(\lambda^{-1/2})\;. \tag{2.89}$$

with the same conditions on ρ as before. We have furthermore assumed that there are no one-dimensional orbits, which can occur in systems where the tori have bifurcations. Let us compare this formula with the one obtained for the flat torus with the help of the Poisson summation formula, (2.81). Again the subprincipal symbol is zero, the term b_γ turns out to be equal to $|T|=|k|$ and the Maslov indices are ±1. Upon expanding the Bessel functions in (2.81) we get

$$J_0(|k|\lambda) = \frac{1}{(2\pi\lambda)^{1/2}}\,\frac{1}{\sqrt{|k|}}\left(\mathrm{e}^{-\mathrm{i}\pi/4}\mathrm{e}^{\mathrm{i}|k|\lambda} + \mathrm{e}^{\mathrm{i}\pi/4}\mathrm{e}^{-\mathrm{i}|k|\lambda}\right) + O(\lambda^{-3/2})\;,$$

giving the result (2.89). In contrast to the Selberg case the higher order corrections do not vanish in this case. On might be tempted to think that this is related to the integrability or chaoticity of the classical flow, but this does not seem to be the case. E.g., for the Laplace operator on the sphere S^2 or on a three-dimensional torus there are no higher order corrections, too.

The main difference between the two examples is that the oscillating contribution is stronger by a factor $\lambda^{1/2}$ in the integrable case. The consequences of this will be discussed in the next subsection.

One can use the trace formula to determine the periods and stabilities of the periodic orbits of the classical system from the quantum mechanical eigenvalues. By shifting the Fourier-transformed test function in the trace formula by $t\in\mathbb{R}$ one obtains

$$\sum_n \mathrm{e}^{\mathrm{i}t\lambda_n}\rho(\lambda-\lambda_n) = \frac{\hat\rho(t)}{(2\pi)^2}\,\mathrm{vol}(\Sigma_1)\;\lambda + \frac{\hat\rho^{(1)}(t)}{(2\pi)^2}\,\overline{\mathrm{sub}\,\mathcal{H}}^{\Sigma_1} + \frac{1}{2\pi}\sum_T \hat\rho(T-t)\sum_{|\gamma|=T}\frac{T^{\#}\mathrm{e}^{\mathrm{i}\nu_\gamma\pi/2}}{|\det(I-P_\gamma)|^{1/2}}\,\mathrm{e}^{\mathrm{i}\,T\,\overline{\mathrm{sub}\,\mathcal{H}}^\gamma}\;\mathrm{e}^{\mathrm{i}T\lambda} + O_t(1/\lambda)\;.$$

for a system with only isolated and nondegenerate orbits. So if $\hat\rho$ is concentrated around zero, the left hand side has peaks as a function of t at the periods of the periodic orbits. In practice it is hard to find a smooth function with compact support whose Fourier transform can be computed explicitly, therefore for numerical checks on relaxes this condition and takes, e.g., a Gaussian as test function.

The numbers $a_\gamma^{(k)}$ are called the wave trace invariants at γ. The question how much information they contain about the classical system has been studied recently in detail by Guillemin and Zelditch [Gui93, Gui96, Zel97, Zel98]. In a nutshell, they have shown that the wave trace invariants up to order N of a periodic orbit γ and all its iterates, determine the Birkhoff normal form of order N of the classical system. So already the eigenvalues alone of the quantum mechanical system determine the Birkhoff normal form at each periodic orbit.

The trace formula of Duistermaat and Guillemin was preceeded by a number of works in physics and mathematics. Gutzwiller was the first who derived a trace formula for general systems in a series of papers culminating in [Gut71], therefore the trace formula is in physics usually called Gutzwiller's trace formula. He worked in the semiclassical context, i.e. studied the limit $\hbar \to 0$, and we will discuss this approach in Section 2.4. Almost parallel to Gutzwiller's work Balian and Bloch developed their trace formula for billiards [BB72]. In mathematics, the first rigorous asymptotic trace formula was derived by Colin de Verdière [Col73]. The work of Duistermaat and Guillemin then was based on [Cha74]. They obtained the most complete result, in the sense that they obtained the contributions of large classes of periodic orbits, namely all the ones which satisfy the cleanness condition. The previous results covered mostly just the contribution of isolated nondegenerate orbits.

2.3.3 Spectral asymptotics

We have noted in the discussion of $N(\lambda)$ for the examples in Section 2.1.1, see figure 2.1, that the fluctuations of $N(\lambda)$ about the Weyl term are much larger in the integrable case than in the chaotic case. Can we use the trace formula to explain this behavior?

Already the Poisson relation gives a way for splitting spectral sums into two parts, one giving the mean behavior, and the other one describing the oscillations around the mean behavior. Let $\varphi \in C_0^\infty(\mathbb{R})$ be a cutoff function whose support contains only the singularity at zero of $\operatorname{tr}\mathcal{U}(t)$, and with $\varphi(t) \equiv 1$ for t in a neighborhood of 0. Then one can split the spectral density into two parts

$$d(\lambda) = \sum_n \delta(\lambda - \lambda_n) = \frac{1}{2\pi}\int \varphi(t)\operatorname{tr}\mathcal{U}(t)\mathrm{e}^{-it\lambda}\,\mathrm{d}t + \frac{1}{2\pi}\int [1-\varphi(t)]\operatorname{tr}\mathcal{U}(t)\mathrm{e}^{-it\lambda}\,\mathrm{d}t\ .$$

The first part will be called the mean part $d_0(\lambda)$, and by the trace formula we have

$$d_0(\lambda) = \frac{\operatorname{vol}(\Sigma_1)}{(2\pi)^d}\,\lambda^{d-1} + \frac{\overline{\operatorname{sub}\mathcal{H}}^{\Sigma_1}}{(2\pi)^d}\lambda^{d-2} + \cdots\ . \tag{2.90}$$

The second part is called the oscillatory part $d_{\text{osc}}(\lambda)$, because, according to the trace formula, it is of an oscillatory nature. Its high energy asymptotics are determined by the periodic orbits.

By integrating $d(\lambda)$ one gets a corresponding splitting of the counting functions into a mean part and an oscillatory part,

$$N(\lambda) = N_0(\lambda) + N_{\rm osc}(\lambda) \ .$$

The asymptotic behavior of the mean value follows directly from (2.90) to be

$$N_0(\lambda) = \frac{\mathrm{vol}(\Sigma_1)}{d(2\pi)^d}\,\lambda^d + \frac{\overline{\mathrm{sub}\,\mathcal{H}}^{\Sigma_1}}{(d-1)(2\pi)^d}\lambda^{d-1} + \cdots \ ,$$

so in order to determine the behavior of $N(\lambda)$ one has to estimate $N_{\rm osc}(\lambda)$. The trace formula gives an expression for a smoothed $N_{\rm osc}(\lambda)$, if $\hat{\rho}$ has compact support and all orbits with periods in that support are clean, then

$$\rho * N_{\rm osc}(\lambda) = \frac{1}{2\pi}\sum_{T\in\mathcal{T}}\frac{\hat{\rho}(T)}{\mathrm{i}T}\sum_{|\gamma|=T}\left(\frac{\lambda}{2\pi}\right)^{\frac{d_\gamma-1}{2}}\mathrm{e}^{\mathrm{i}\nu_\gamma\pi/2}\mathrm{e}^{\mathrm{i}T\,\overline{\mathrm{sub}\,\mathcal{H}}^\gamma}\,\mathrm{e}^{\mathrm{i}T\lambda}\left[a_\gamma^{(0)} + a_\gamma^{(1)}\frac{1}{\lambda} + \cdots\right] \ ,$$

where $\rho * N_{\rm osc}$ denotes the convolution of ρ with $N_{\rm osc}$. This formula allows easily to give a lower bound on $N_{\rm osc}(\lambda)$. Let $\kappa_{\max} := \sup_\gamma\{(d_\gamma-1)/2\}$ and define $F(\lambda) := \lambda^{-\kappa_{\max}}N_{\rm osc}(\lambda)$, then we get from the inequality $|\rho * F| \leq \sup|F|||\rho||_1$ that

$$\limsup N_{\rm osc}(\lambda)\lambda^{-\kappa_{\max}} \geq C \ , \qquad (2.91)$$

so we have a lower bound for the order of the oscillations.

Unfortunately it is much harder to get upper bounds for $N_{\rm osc}(\lambda)$. The best general upper bound is due to Hörmander [Hör68, Hör85b],

$$N_{\rm osc}(\lambda) = O(\lambda^{d-1}) \ .$$

This bound is sharp as can be seen from the example of the Laplace-Beltrami operator on the sphere. There all orbits are periodic with the same primitive period, hence it follows from (2.91) that their contribution is at least of order λ^{d-1} because $d_\gamma = 2d-1$. More generally the behavior of $N_{\rm osc}(\lambda)$ is rather well understood if the classical flow is periodic, as it is the case, e.g. , for Zoll-surfaces [Bes78], see [Hör85b, Sch95].

The reason that the general case is much harder is that one cannot take the limit $\hat{\rho} \to 1$ in the periodic orbit sum for $\rho * N_{\rm osc}(\lambda)$, because the resulting series is not convergent in general. Furthermore, one has no estimate on the remainder in the trace formula. The best result known for the case that the flow is not periodic is the one by Duistermaat and Guillemin [DG75],

$$N_{\rm osc}(\lambda) = o(\lambda^{d-1}) \ .$$

For a generic integrable system, where not all orbits are periodic, the individual periodic tori contribute a term of order $\lambda^{(d-1)/2}$. Hence one will naively expect a behavior

$$N_{\rm osc}(\lambda) = O(\lambda^{(d-1)/2+\varepsilon}) \ ,$$

for every $\varepsilon > 0$. This is in accordance with the Hardy Littlewood conjecture for the case of the Laplace-Beltrami operator on the flat two-dimensional torus. In this system $N(\lambda)$ is the number of lattice points on $\mathbb{Z}^2$ inside a circle of radius λ, therefore it is often called the circle problem. But the best general upper bound for a large class of integrable systems, due to Colin de Verdière [Col77], is

$$N_{\text{osc}}(\lambda) = O(\lambda^{d-2+2/(d+1)}) \ .$$

In two dimensions the exponent is 2/3 and corresponds to an old estimate by van der Corput for the circle problem. For the circle problem a rather recent result is $N_{\text{osc}}(\lambda) = O(\lambda^{43/73}(\ln \lambda)^{315/146})$, due to Huxley [Hux93].

Especially for chaotic systems the strong proliferation of periodic orbits makes the unsmoothed version of the periodic orbit sum highly divergent. Therefore, the best upper bound obtained so far for chaotic systems is probably far away from the real behavior. It is the one proven for the Laplace-Beltrami operator on manifolds with negative curvature,

$$N_{\text{osc}}(\lambda) = O(\lambda^{d-1}/\ln \lambda) \ ,$$

see [Hej76, Bér77a, Ran78, Don78, DKV79]. The naive conjecture based on the trace formula,

$$N_{\text{osc}}(\lambda) = O(\lambda^{\varepsilon}) \ , \tag{2.92}$$

for all $\varepsilon > 0$ can only be true for a subclass of hyperbolic systems. Because Selberg [Hej76] has proven a lower bound for a special type of system, a so-called arithmetical one, of the form

$$N_{\text{osc}}(\lambda) = \Omega(\lambda^{1/2}/\ln \lambda) \ ,$$

roughly the same behavior as one expects for integrable systems. The reason for this exceptional behavior is that the period spectrum is exponentially degenerate for arithmetic systems. This means that the number of orbits with the same period equal to $T \in \mathcal{T}$ grows exponentially with $|T|$. But for non-arithmetical systems on might expect the behavior (2.92) to be true. Lower bounds which strengthen (2.91) have as well been proven for certain other classes of systems. E.g., for the circle problem Hardy has already proven that $N_{\text{osc}}(\lambda) = \Omega(\lambda^{1/2}(\ln \lambda)^{1/4})$ and for surfaces of constant negative curvature one has $N_{\text{osc}}(\lambda) = \Omega((\ln \lambda/\ln\ln \lambda)^{1/2})$, see [Hej76].

Instead of searching for a pointwise upper bound on $N_{\text{osc}}(\lambda)$ it might be easier to study the quadratic mean of $N_{\text{osc}}(\lambda)$ and the value distribution of a suitably normalized $N_{\text{osc}}(\lambda)$. This direction of research has been initiated by Heath-Brown with a work on the circle problem [HB92], which was followed by a number of works by Bleher, Dyson, Lebowitz, Sinai and many others on integrable systems. A recent review can be found in [Ble99]. The results they obtain are of the following type: They show that for the two-dimensional systems which they consider, the normalized oscillating part of the spectral counting function is in a space of almost periodic functions,

$$\lambda^{-1/2} N_{\text{osc}}(\lambda) \in B^p(\mathbb{R}) \ ,$$

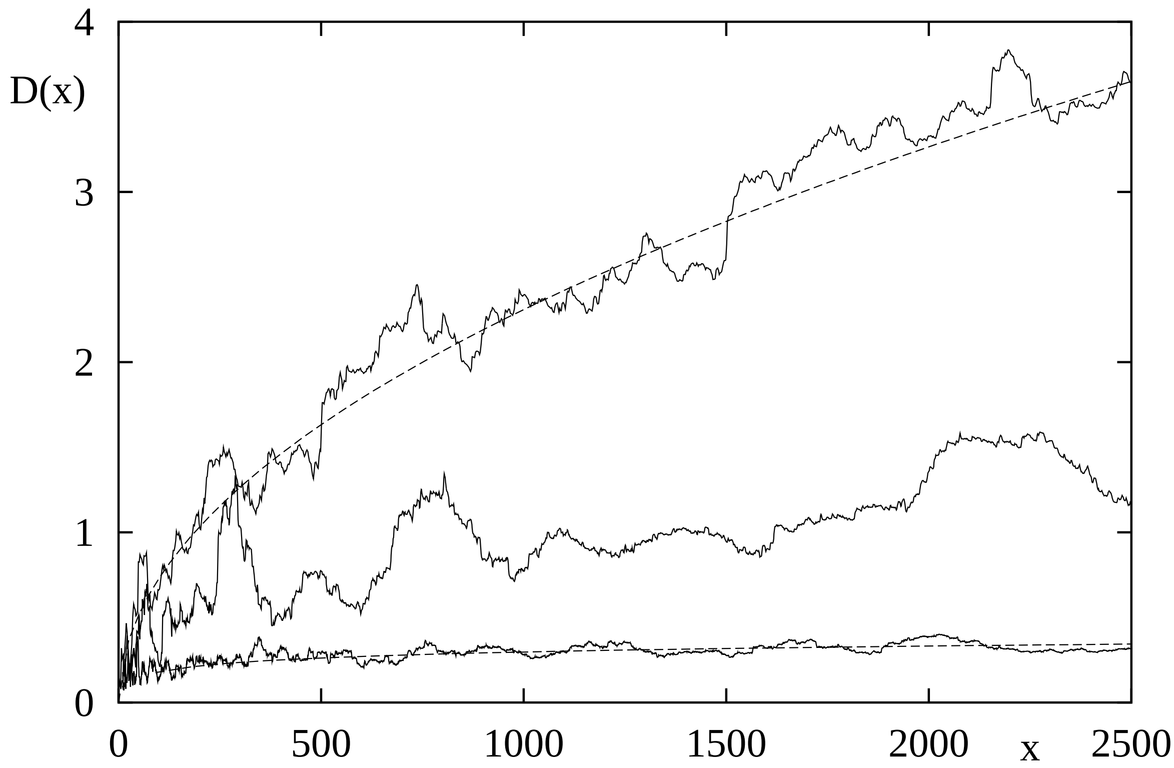

Figure 2.11: The second moment $D(x) = \left(\frac{1}{x}\int_0^x |N_{\rm osc}(\lambda(x'))|^2 \, {\rm d}x'\right)^{1/2}$ of $N_{\rm osc}(\lambda)$ for three different billiards. The quantity $\lambda(x')$, defined by $N_0(\lambda(x')) = x'$, is introduced to make the comparison between different systems possible, x' is a rescaled energy. The system with the largest fluctuations is the circle billiard, the one with the smallest ones is the cardioid billiard and the intermediate one is the limaçon with $\varepsilon = 0.3$. The data are from [Bäc98].

for $p = 1$ or $p = 2$. Here the spaces $B^p(\mathbb{R})$ are Besicovitch spaces, which consist of the functions $f(x)$ on the real line which satisfy

$$\lim_{T\to\infty} \frac{1}{2T}\int_T^T |f(x)|^p \, {\rm d}x \leq \infty \ .$$

So these results mean that $N_{\rm osc}(\lambda)$ is of the order $\lambda^{1/2}$ on average. Furthermore, for these systems estimates on the value distribution of $P = \lambda^{-1/2}N_{\rm osc}(\lambda)$ were obtained, which imply that it decays faster than $\exp(-P^4)$. This means that large values of $\lambda^{-1/2}N_{\rm osc}(\lambda)$ are rather rare.

For chaotic systems the question is much more difficult. Assume that one has a uniformly hyperbolic system with only isolated periodic orbits. Then heuristic arguments based on the trace formula lead for non-arithmetical systems to

$$\langle N_{\rm osc}^2\rangle(\lambda) \sim C \ln\lambda \ ,$$

where the brackets $\langle\ \rangle$ denotes an average over an interval around λ [Ber85]. Furthermore it has been conjectured [Ste94, ABS94] that the value distribution of the normalized fluctuations of the spectral staircase

$$W(\lambda) = \frac{N_{\text{osc}}(\lambda)}{\sqrt{\langle N_{\text{osc}}^2\rangle(\lambda)}} , \tag{2.93}$$

are Gaussian. This conjecture has been tested numerically, e.g., in [ABS97], and has been confirmed for all systems studied up today.

In fig. 2.11 the second moment of $N_{\text{osc}}(\lambda)$ is shown for three different systems, and in fig. 2.12 the corresponding value distributions of $W(\lambda)$ are shown, [Bäc98].

The preceeding discussion gives an impression of the possible applications of the trace formula. It should enable one in principle to compute spectral statistical measures in the high energy limit, which should depend only on properties of the classical system, more precisely on the periodic orbits. But doing such computations rigorously is a very hard job, and has only been accomplished in rare cases.

2.4 The limit $\hbar \to 0$

We have discussed the semiclassical limit of quantum mechanics in a way which is rather uncommon in physics. In the physical literature the semiclassical limit is usually worked out by taking the limit $\hbar \to 0$. In contrast to this we have interpreted the high energy limit, in the case of a system on a compact manifold, as the semiclassical limit. This has the advantage that its physical interpretation is clear, whereas in nature $\hbar$ is a constant and so taking the limit $\hbar \to 0$ has to be interpreted suitably . On the other hand, the class of systems we have considered does not contain all interesting types of systems one would like to consider. Although one often has quantum systems with symmetries, like the periodicities in crystals, which allow to reduce a system to one on a compact manifold, there are many important ones, e.g. , molecules, for which this is not possible.

In this section we therefore want to discuss the relation between these two limits and their justifications.

There exists a complete calculus for pseudodifferential and Fourier integral operators depending on a small parameter $\hbar$, analogous to the classical calculus described in the last sections. For introductions see [Rob87, Hel97]. A typical example for the operators which occur in this calculus is given by a one-particle Schrödinger operator

$$\mathcal{H}_\hbar = -\frac{\hbar^2}{2m}\Delta + V(x) \tag{2.94}$$

with smooth potential V. Here $\hbar$ is not treated as a constant, but the behavior of $\mathcal{H}_\hbar$ is studied in the limit $\hbar \to 0$. To a general symbol $a(\xi, x)$ one associates an $\hbar$ dependent operator

$$\mathcal{A}_\hbar u(x) := \frac{1}{(2\pi\hbar)^d}\iint \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\langle x-y,\xi\rangle} a((x+y)/2,\xi)u(y)\,\mathrm{d}y\mathrm{d}\xi , \tag{2.95}$$

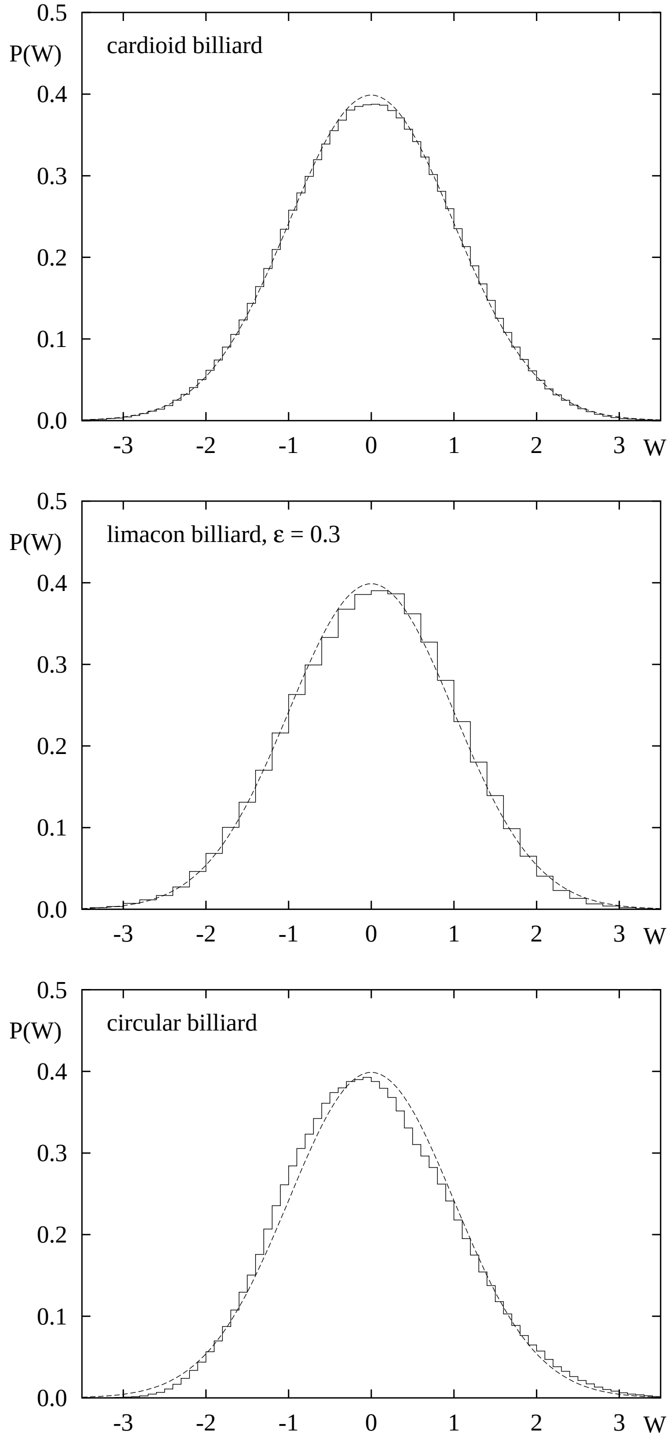

Figure 2.12: The value distribution of $W(\lambda)$, the normalized fluctuations of the spectral counting function (2.93), for three billiards, [Bäc98]. The chaotic cardioid billiard shows rather good agreement with a Gaussian, whereas the integrable circle billiard and the limaçon with mixed phase space show clear deviations.

which corresponds to substituting for ξ the differential operator $\hbar D_x$ instead of D_x. More details on the symbols and properties of such operators will be discussed in the next section.

In a similar way Fourier integral operators depending on $\hbar$ can be introduced. A typical example of such a Fourier integral operator is the time evolution operator

$$\mathcal{U}_\hbar(t) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} t \mathcal{H}_\hbar} ,$$

where $\mathcal{H}_\hbar$ is a Schrödinger operator of the type (2.94). In particular, there is a Poisson relation and a trace formula for Schrödinger operators depending on $\hbar$, in fact the original trace formula of Gutzwiller [Gut71] was developed for such types of operators. In order to formulate a Poisson relation one needs an analog of the wave front set, which takes the dependence on the parameter into account; this is given by the frequency set [GS77].

Definition 2.4.1. *Let $u_\hbar \in \mathcal{S}'(\mathbb{R}^d)$ be a bounded family of distributions depending smoothly on a parameter $\hbar \in (0, \hbar_0)$ for some $\hbar_0 > 0$. Then the **frequency set** of $u_\hbar$, $\mathrm{FS}(u_\hbar) \subset T^*\mathbb{R}^d$, is the complement of all points $(x_0, \xi_0) \in T^*\mathbb{R}^d$ which possess neighborhoods $\mathcal{U} \ni x_0$, $V \ni \xi_0$ such that for every $\varphi \in C_0^\infty(U)$ and $\xi \in V$*

$$\int \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\langle \xi, x\rangle} \varphi(x) u_\hbar(x) \, \mathrm{d}x = O(\hbar^N)$$

for all $N \in \mathbb{N}$ as $\hbar$ tends to 0.

Notice that in case that $u_\hbar = u$ does not depend on $\hbar$ the frequency set coincides with the wave front set, compare (2.35). In contrast to the wave front set the frequency set will in general not be conical. Consider as an example a family of functions of the form $\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\psi(x)}$, with $\psi(x) \in C^\infty(\mathbb{R}^d, \mathbb{C})$ and $\operatorname{Im}\psi(x) \geq 0$, then one computes easily with the method of stationary phase that

$$\mathrm{FS}(\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\psi}) = \{(x, \psi'(x)) \mid \operatorname{Im}\psi(x) = 0\} .$$

In the following we will denote by $\mathcal{H}_\hbar$ an operator on $\mathbb{R}^d$ or some manifold of the form (2.95) with symbol

$$H(\hbar; \xi, x) \sim \sum_{k=0}^{\infty} \hbar^k H_k(\xi, x) , \quad \text{for } \hbar \to 0 ,$$

which is real valued, has positive principal part $H_0(\xi, x) > 0$ (in fact boundedness from below is sufficient), and where the $H_k(\xi, x)$ satisfy suitable symbol estimates (see [Hel97] for more precise statements). A typical example is (2.94) with smooth potential which is bounded from below. Then $\mathcal{H}_\hbar$ can be shown to be essentially selfadjoint for $\hbar$ small enough, and one studies the eigenvalues and eigenfunctions

$$\mathcal{H}_\hbar \psi_n(\hbar) = E_n(\hbar)\psi_n(\hbar) ,$$

which are functions of the parameter $\hbar$. The Poisson relation for an operator of this type was first proven by Chazarain [Cha80]. Let χ be a smooth function with compact support, define

$$f_{\chi,\hbar}(t) := \operatorname{tr}\left[\chi(\mathcal{H}_\hbar)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}t\mathcal{H}_\hbar}\right] = \sum_n \chi(E_n(\hbar))\mathrm{e}^{\frac{\mathrm{i}}{\hbar}tE_n(\hbar)} ,$$

and let Φ^t be the Hamiltonian flow generated by the principal symbol H_0 of $\mathcal{H}_\hbar$, then the Poisson relation states that

$$\mathrm{FS}(f_{\chi,\hbar}) \subset \{(t,E) \,|\, \exists(\xi,x) \,:\, H_0(\xi,x) = E \text{ and } \Phi^t(\xi,x) = (\xi,x)\} .$$

So $\mathrm{FS}(f_{\chi,\hbar})$ is contained in the set of the graph of the periods of the periodic orbits of ϕ^t as a function of the energy E. This set will usually not be homogeneous, in contrast to the wave front set of the wave trace.

A Weyl type theorem, giving the number of eigenvalues in a fixed energy interval as $\hbar$ tends to zero, is also valid. Let $[E_1,E_2]$ be an interval such that E is a regular value of $H_0(\xi,x)$ for each $E\in[E_1,E_2]$, then the number of eigenvalues in this interval is asymptotically

$$N_\hbar([E_1,E_2]) = \frac{1}{(2\pi\hbar)^d}\iint_{E_1\leq H_0(\xi,x)\leq E_2} \mathrm{d}x\mathrm{d}\xi + O(\hbar^{1-d}) ,$$

and under some additional conditions on the classical flow the remainder can be improved to $o(\hbar^{1-d})$, see [PR85] and Chapter 4. Notice the similarity with the classical Weyl theorem if one replaces $\hbar$ by $1/\lambda$. The Poisson relation suggests that there is a trace formula for such operators too. Let E be a fixed energy value, such that E is a regular value of $H_0(\xi,x)$ and the energy-shell

$$\Sigma_E := \{(\xi,x) \,|\, H_0(\xi,x) = E\}$$

is compact. We will state the trace formula only for the simplest case that all periodic orbits of the Hamiltonian flow ϕ^t generated by $H_0(\xi,x)$ on Σ_E are isolated and nondegenerate. Let φ be a smooth function whose Fourier transform has compact support, then

$$\begin{aligned}\sum_n \varphi\left(\frac{E_n(\hbar)-E}{\hbar}\right) =& \frac{\hat\varphi(0)}{2\pi}\frac{\mathrm{vol}(\Sigma_E)}{(2\pi\hbar)^{d-1}} + \frac{\hat\varphi'(0)}{2\pi}\frac{\overline{\operatorname{sub}\mathcal{H}_\hbar}^{\Sigma_E}}{(2\pi\hbar)^{d-2}} + \cdots \\ &+ \sum_\gamma \frac{\hat\varphi(T_\gamma(E))}{2\pi}\frac{T_\gamma^\# \mathrm{e}^{\mathrm{i}\nu_\gamma\pi/2}\mathrm{e}^{\mathrm{i}T_\gamma^\#\overline{\operatorname{sub}\mathcal{H}_\hbar}^\gamma}}{|\det(P_\gamma(E)-I)|^{1/2}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S_\gamma(E)} + O(\hbar) .\end{aligned} \tag{2.96}$$

Here $S_\gamma(E) := \int_{\gamma(E)}\xi\mathrm{d}x$ denotes the action of the periodic orbit γ at energy E, and all other quantities are the same as the one appearing in the trace formula of Duistermaat and Guillemin. The dots in the first line indicate that there can be further terms of the form $a_n\hbar^{d-n}$ for $n\geq 3$ coming from the big singularity at $t=0$. Notice that because of the factor $1/\hbar$ in the argument of φ on the left hand side, the sum is effectively over a range of eigenvalues lying in an interval which shrinks proportional to $\hbar$. This trace formula is the rigorous version of the original trace formula of Gutzwiller [Gut71], rigorous proofs appeared in [PU91, BU91, Mei92] for the case $M = \mathbb{R}^d$ and in [GU89] for the case of compact M.

In a provocative way one could say that the main disadvantage of this formula is the dependence on $\hbar$. In the Duistermaat Guillemin case the physical meaning of the limit taken was clear, here it is generally not, since $\hbar$ is a constant in nature. On the other hand this formula is much more general, it is not only valid for systems on compact manifolds, but on arbitrary manifolds and for a much larger class of operators.

To see the relations more explicit we take as Hamilton operator a first order operator, $\mathcal{H}_\hbar = \hbar\sqrt{-\Delta}$, on a compact Riemannian manifold. The symbol of $\mathcal{H}_\hbar$ is $|\xi|_g$. Let λ_n be the eigenvalues of $\sqrt{-\Delta}$, then the eigenvalues of $\mathcal{H}_\hbar$ are $\hbar\lambda_n$. For a Hamilton function which is homogeneous, like $|\xi|_g$, we will see below that the periods of the periodic orbits and the Poincaré maps are independent of the energy, whereas the actions are proportional to the energy. Hence, if we evaluate (2.96) for this operator at $E = 1$, and if we call $1/\hbar = \lambda$, we arrive at the same expression as the Duistermaat Guillemin trace formula for the operator $\mathcal{H} = \sqrt{-\Delta}$. This example can be generalized: let $\mathcal{H} \in \Psi^1_{\mathrm{phg}}(M)$ be a first order operator, then $\mathcal{H}_\hbar = \hbar\mathcal{H}$ is in $\Psi^1_\hbar(M)$ with symbol

$$H(\hbar;\xi,x) = \hbar H(x, 1/\hbar\,\xi) \sim \sum_{k=0}^{\infty} \hbar^k H_{1-k}(\xi,x) \ .$$

Therefore the principal symbols of the two operators coincide, and the general $\hbar$ dependent trace formula for $\mathcal{H}_\hbar$ reduces to the Duistermaat Guillemin formula for $\mathcal{H}$.

2.5 Semiclassical operators

In the last section we have seen that when performing the limit $\hbar \to 0$ literally, one has to study operators depending explicitly on $\hbar$ and the behavior for $\hbar \to 0$. In particular, the asymptotic expansions for $|\xi| \to \infty$ are replaced by expansions for $\hbar \to 0$. There exists a pseudodifferential operator-calculus for these operators parallel to the the one described in Section 2.2, and we will collect here some results which we will need in the following chapters. Parts of this calculus have already been developed by physicists on a more formal level in order to describe the semiclassical limit, see, e.g. [Wig32, Moy49]. Then Maslov, [Mas72, MF81], was very active in this field. The techniques of microlocal analysis were applied to this field by Voros [Vor76, Vor77], and later on spread out widely. For reviews see [DS99, Hel97, Rob87]. Instead of calling the parameter $\hbar$ we use $1/\lambda$ as parameter and study the case of large λ.

The explicit appearance of a semiclassical parameter λ in this semiclassical calculus of pseudodifferential and Fourier integral operators is an advantage which often facilitates the computations and the performance of the semiclassical limit. The usual theory which we have outlined in the last sections has some limitations. In particular the results we are interested in in quantum chaos are limited to systems on compact manifolds. Many important type of systems, like atoms or molecules do not belong to this class. For these systems the methods of the last section are applicable, but they suffer from the drawback that they are only valid in the limit $\hbar \to 0$, whose physical meaning is not clear a priori, since $\hbar$ is a constant in nature, although a very small one.

Intuitively, the semiclassical limit is the limit of large quantum numbers, meaning small de Broglie wavelength, as far as eigenfunctions are concerned. For the eigenvalues, and the time evolution, one usually needs that the mean spectral density becomes large. This can be seen, e.g., in the trace formulas of the last sections. One can interpret this by recalling that the spectrum of the classical time evolution operator is typically continuous, and in order that the quantum mechanical time evolution should be close to the classical one, one needs at least a high spectral density in order to simulate on short time scales a continuous spectrum.

In the following we will describe a formalism by which these intuitive ideas are implemented in order to give a physical meaningful version of the $\hbar$-dependent calculus. This is by no means the only way to arrive for physical problems at such type of calculi, and we would like to mention for instance adiabatic problems and studies on stability of matter, where similar techniques are used, see e.g. [HST01, FFG97].

We want to discuss now a method by which a rather large class of Hamiltonians can be mapped to λ-dependent operators. We start with scaling systems: let $\mathcal{H}$ be the Weyl quantization of the classical Hamilton function H, then H is called scaling if there are numbers $\alpha, \beta \in \mathbb{R}$ such that

$$H(\lambda^{\alpha}\xi, \lambda^{\beta}x) = \lambda H(\xi, x) \tag{2.97}$$

for all $\lambda > 0$. Typical examples are the Hydrogen atom with

$$H(\xi, x) = \frac{1}{2}\langle \xi, \xi \rangle + \frac{\alpha_0}{|x|}$$

where we have $\alpha = 1/2$, $\beta = -1$, or the harmonic oscillator where $\alpha = \beta = 1/2$. Such an operator can be mapped to a λ-dependent operator by conjugation with a unitary dilatation operator of the form

$$\mathcal{S}_\lambda \psi(x) := \lambda^{\frac{d\gamma}{2}} \psi(\lambda^{\gamma} x)$$

with γ chosen suitably.

Proposition 2.5.1. *Let $\mathcal{H}$ be a pseudodifferential operator with Weyl symbol $H(\xi, x)$, and let*

$$\mathcal{S}_\lambda \psi(x) := \lambda^{\frac{d\beta}{2(\alpha+\beta)}} \psi(\lambda^{\frac{\beta}{\alpha+\beta}} x) \ ,$$

then

$$\mathcal{S}_\lambda \mathcal{H} \mathcal{S}_\lambda^* = \mathcal{H}_\lambda$$

where $\mathcal{H}_\lambda$ denotes the λ-quantization of the λ dependent symbol

$$H(\lambda^{\alpha/(\alpha+\beta)}\xi, \lambda^{\beta/(\alpha+\beta)}x) \ .$$

Proof. We have

$$\begin{aligned}
\mathcal{S}_\lambda\mathcal{H}\mathcal{S}_\lambda^*\psi(x) &= \left(\frac{1}{2\pi}\right)^d \iint \mathrm{e}^{\mathrm{i}\langle\lambda^{\beta/(\alpha+\beta)}x-y,\xi\rangle} H(\xi, (\lambda^{\beta/(\alpha+\beta)}x+y)/2)\psi(\lambda^{-\beta/(\alpha+\beta)}y)\ \mathrm{d}y\mathrm{d}\xi \\
&= \left(\frac{1}{2\pi}\right)^d \iint \mathrm{e}^{\mathrm{i}\lambda^{\beta/(\alpha+\beta)}\langle x-y,\xi\rangle} H(\xi, \lambda^{\beta/(\alpha+\beta)}(x+y)/2)\psi(y)\lambda^{d\beta/(\alpha+\beta)}\ \mathrm{d}y\mathrm{d}\xi \\
&= \left(\frac{1}{2\pi}\right)^d \iint \mathrm{e}^{\mathrm{i}\lambda\langle x-y,\xi\rangle} H(\lambda^{1-\beta/(\alpha+\beta)}\xi, \lambda^{\beta/(\alpha+\beta)}(x+y)/2)\psi(y)\lambda^d\ \mathrm{d}y\mathrm{d}\xi \\
&= \left(\frac{\lambda}{2\pi}\right)^d \iint \mathrm{e}^{\mathrm{i}\lambda\langle x-y,\xi\rangle} H(\lambda^{\alpha/(\alpha+\beta)}\xi, \lambda^{\beta/(\alpha+\beta)}(x+y)/2)\psi(y)\ \mathrm{d}y\mathrm{d}\xi
\end{aligned}$$

where we have used

$$1-\beta/(\alpha+\beta) = \alpha/(\alpha+\beta) \ .$$

□

So it follows that if H is scaling with exponents α and β in the sense (2.97), then the symbol of $\mathcal{H}_\lambda$ becomes

$$\lambda^{1/(\alpha+\beta)}H(\xi, x) \ .$$

Generally, a system need not be scaling, but a fairly large class of Hamiltonians is mapped by conjugation with an dilatation operator $\mathcal{S}_\lambda$ to a λ-dependent operator whose symbol has an asymptotic expansion in λ. Before coming to precise definitions we want to discuss some examples.

Examples 2.5.2:
We discuss the action of the scaling operator $\mathcal{S}_\lambda$ for some standard types of operators.

(i) Assume $\mathcal{H} \in \Psi^m_{\mathrm{phg}}(M)$ with Weyl symbol H, then we can take

$$\alpha = 1/m \ , \quad \beta = 0 \ ,$$

and get that $\mathcal{S}_\lambda\mathcal{H}\mathcal{S}_\lambda^* = \mathcal{H}_\lambda$ is the λ quantization of

$$H(\lambda\xi, x) \sim \lambda^m \sum_{k=0}^{\infty} \lambda^{-k}H_k(\xi, x) \ .$$

(ii) Assume $\mathcal{H} = -\frac{1}{2}\Delta + V(x)$ with $V(x) \sim \sum_{k=0}^{\infty} V_{2-k}(x)$ for $|x| \to \infty$ with $V_{2-k}(x)$ homogeneous of degree $2-k$, that means V is close to an harmonic oscillator potential for large $|x|$. We choose

$$\alpha = 1/2 , \quad \beta = 1/2 ,$$

and get that $\mathcal{S}_\lambda \mathcal{H} \mathcal{S}_\lambda^* = \mathcal{H}_\lambda$ is the λ quantization of

$$H(\lambda^{1/2}\xi, \lambda^{1/2}x) \sim \lambda \sum_{k=0}^{\infty} \lambda^{-k/2} H_k(\xi, x) ,$$

with $H_0(\xi, x) = \frac{1}{2}\langle \xi, \xi \rangle + V_2(x)$ and $H_k(\xi, x) = V_{2-k}(x)$ for $k \geq 1$.

(iii) Assume $\mathcal{H} = -\frac{1}{2}\Delta + V(x)$ where $V(x)$ decays like $1/|x|$ for $|x| \to \infty$, such that, e.g., $V(x) = \alpha_0/|x| + V^{(0)}(x)$ with $V^{(0)}(x)$ of compact support. Then we can choose

$$\alpha = 1/2 , \quad \beta = -1 ,$$

and get that $\mathcal{S}_\lambda \mathcal{H} \mathcal{S}_\lambda^* = \mathcal{H}_\lambda$ is the λ quantization of

$$H(\lambda^{-1}\xi, \lambda^2 x) = \lambda^{-2} \left(\frac{1}{2}\langle \xi, \xi \rangle + \frac{\alpha_0}{|x|} \right) + V^{(0)}(\lambda^2 x) ,$$

We see that the symbols which appear belong to the following type of symbol classes, which we borrow from [DS99].

Definition 2.5.3. *For $a, b \in \mathbb{R}$ we define an order function*

$$m_{a,b}(\xi, x) := (1 + \langle \xi, \xi \rangle)^{a/2} (1 + \langle x, x \rangle)^{b/2} ,$$

then we say that $p(\lambda; \xi, x) \in C^\infty$ belongs to $S^0(m_{a,b})$ if

$$|\partial_\xi^\alpha \partial_x^\beta p(\lambda; \xi, x)| \leq C_{\alpha,\beta} m_{a,b}(\xi, x) ,$$

for all $\alpha, \beta \in \mathbb{Z}_+^d$ and $\lambda > 0$. Furthermore, for $k \in \mathbb{R}$, $p(\lambda; \xi, x) \in C^\infty$ is said to be in $S^k(m_{a,b})$ if $(1 + \lambda^2)^{-k/2} p \in S^0(m_{a,b})$.

These symbol classes have the standard properties which such objects usually possess. They are Fréchet spaces, and they are well behaved under multiplication and inversion of positive elements. If $p \in S^k(m_{a,b})$, $q \in S^{k'}(m_{a',b'})$ then $pq \in S^{k+k'}(m_{a,b} m_{a',b'}) = S^{k+k'}(m_{a+a',b+b'})$ and if $p > 0$ is in $S^k(m_{a,b})$ then $1/p \in S^{-k}(1/m_{a,b}) = S^{-k}(m_{-a,-b})$. We also have asymptotic expansions; if there is a sequence $p_j \in S^{k_j}(m_{a,b})$ with $k_j > k_{j+1}$ and $k_j \to -\infty$ then we say for $p \in S^{k_0}(m_{a,b})$

$$p \sim \sum_{j=0}^{\infty} p_j ,$$

if $p - \sum_{j=0}^{k_n - 1} p_j \in S^{k_n}(m_{a,b})$ for all $j \in \mathbb{N}$. By Borel summation one can find for every such sequence a corresponding p which is unique modulo $S^{-\infty}(m_{a,b}) := \bigcap_{k \in \mathbb{R}} S^k(m_{a,b})$.

We now define the corresponding classes of operators by Weyl quantization.

Definition 2.5.4. *We say that $\mathcal{A} \in \Psi_\lambda^k(m_{a,b})$, if it can be locally represented as*

$$\mathcal{A}\psi(x) = \mathrm{Op}^W[A] := \left(\frac{\lambda}{2\pi}\right)^d \iint \mathrm{e}^{\mathrm{i}\lambda\langle x-y,\xi\rangle} A(\lambda;\xi,(x+y)/2)\psi(y)\, \mathrm{d}y\mathrm{d}\xi\ ,$$

with $A \in S^k(m_{a,b})$.

If the symbol A of $\mathcal{A}$ has an asymptotic expansion

$$A \sim \lambda^{k_0} A_0 + \lambda^{k_1} A_1 + \cdots$$

with A_0 independent of λ, then we will call

$$\sigma(\mathcal{A}) := A_0$$

the principal symbol of $\mathcal{A}$. On calls $\mathcal{A} \in \Psi_\lambda^k(m_{a,b})$ elliptic, if there are constants $\lambda_0 \geq 0$ and $C > 0$ such that

$$|A(\lambda;\xi,x)| \geq C\lambda^k m_{a,b}$$

for $\lambda \geq \lambda_0$ and (ξ,x) outside some compact set. It is easy to see that the same estimate for the principal symbol $\sigma(\mathcal{A})$ is already sufficient. For elliptic operators one can construct parametrices in the same way as in the standard case, once one has established a calculus.

As one expects, the product of two λ-pseudodifferential operators is again a λ-pseudodifferential operator.

Theorem 2.5.5. *Let $P \in \Psi_\lambda^k(m_{a,b})$ and $Q \in \Psi_\lambda^{k'}(m_{a',b'})$, with λ-symbols p and q, respectively, then $PQ \in \Psi_\lambda^{k+k'}(m_{a,b}m_{a',b'}) = \Psi_\lambda^{k+k'}(m_{a+a',b+b'})$ and the symbol of the product is given by*

$$\begin{aligned} p\#q(\lambda;\xi,x) &= \mathrm{e}^{\frac{\mathrm{i}}{2\lambda}[\langle D_y,D_\xi\rangle - \langle D_\eta D_x\rangle]} p(\lambda;\xi,x)q(\lambda;\eta,y)|_{y=x,\eta=\xi} \\ &\sim \sum_{k=0}^{\infty} \frac{1}{k!}\left(\frac{\mathrm{i}}{2\lambda}[\langle D_y,D_\xi\rangle - \langle D_\eta D_x\rangle]\right)^k p(\lambda;\xi,x)q(\lambda;\eta,y)|_{y=x,\eta=\xi} \\ &= p(\lambda;\xi,x)q(\lambda;\xi,x) + \frac{\mathrm{i}}{2\lambda}\{p,q\}(\lambda;\xi,x) + O(\lambda^{k+k'-2})\ , \end{aligned}$$

for $\lambda \to \infty$.

The validity of a product formula implies that the standard results from the classical theory of pseudodifferential operators can be transferred to this case. E.g., the construction of parametrices, a functional calculus and continuity on L^2 if $a, b \leq 0$. We refer to the book of Dimassi and Sjöstrand, [DS99], for a presentation of these results.

One final result in this calculus which we will often need is a criterion for selfadjointness, see [DS99].

Proposition 2.5.6. *Let $\mathcal{H}$ be the λ-quantization of $H \in S^0(m_{a,b})$, assume that H is real valued, and, in case that $m_{a,b}$ is not bounded, that $H + \mathrm{i}$ is elliptic in the sense that there exists a constant $C > 0$ such that $|H + \mathrm{i}| \geq C$. Then there exists a $\lambda_0 \geq 0$ such that $\mathcal{H}$ with domain $\mathcal{S}(\mathbb{R}^d)$ is essentially selfadjoint for $\lambda \geq \lambda_0$.*

From now on we will denote the unique selfadjoint extension of $\mathcal{H}$ as well by $\mathcal{H}$.

In the same manner as for pseudodifferential operators, one can introduce Fourier integral operators which depend on a parameter λ. We will discuss only the local case, so we can assume that our manifold M is $\mathbb{R}^d$.

Definition 2.5.7. *Let $\Phi : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d \times \mathbb{R}^d$ be a canonical transformation which has a generating function $\varphi(\xi, x)$. Then we say $\mathcal{F} \in I^k_\lambda(\Phi, m_{a,b})$, if $\mathcal{F}$ is of the form*

$$\mathcal{F}\psi(x) = \left(\frac{\lambda}{2\pi}\right)^d \iint \mathrm{e}^{\mathrm{i}\lambda(\varphi(\xi,x) - \langle y,\xi\rangle)} A(\lambda; \xi, x)\psi(y) \; \mathrm{d}y\mathrm{d}\xi \; ,$$

with $A \in S^k(m_{a,b})$.

The most important property of these Fourier integral operator is the validity of an Egorov theorem, analogous to Theorem 2.2.20. Only one subtlety appears here, since the canonical transformation Φ need not be homogeneous anymore, it will in general not respect the symbol classes. In order to avoid this problem we will restrict ourselves to operators $\mathcal{F}$ whose amplitudes have compact support.

Theorem 2.5.8. *Let Φ be a canonical transformation with generating function φ and $\chi \in C_0^\infty(\mathbb{R}^d \times \mathbb{R}^d)$, then the operator*

$$\mathcal{U}(\Phi)\psi(x) = \left(\frac{\lambda}{2\pi}\right)^d \iint \mathrm{e}^{\mathrm{i}\lambda(\varphi(\xi,x) - \langle y,\xi\rangle)} |\det \varphi''_{\xi,x}(\xi, x)|^{1/2} \chi(\xi, x)\psi(y) \; \mathrm{d}y\mathrm{d}\xi \; ,$$

satisfies

$$\mathcal{U}(\Phi)\mathcal{U}(\Phi)^* = \mathrm{Op}^W[\chi^*\chi] + O(\lambda^{-1})$$

and for every $\mathcal{H} \in \Psi^k_\lambda(m_{a,b})$ with symbol $H(\xi, x)$, we have $\mathcal{U}(\Phi)\mathcal{H}\mathcal{U}^*(\Phi) \in \Psi^k_\lambda(1)$ with symbol

$$\tilde{H} = \chi^*\chi H \circ \Phi + O(\lambda^{k-1}) \; .$$

The proof follows exactly the same lines as the one sketched after Theorem 2.2.20.

Now that we have collected some definitions and results on the semiclassical calculus, we can return to our original question how to perform the semiclassical limit for a suitable Schrödinger operator. By Proposition 2.5.1 and the examples 2.5.2 following it, we see that many Schrödinger type operators are mapped by conjugation with a suitably chosen dilatation operator to one of the classes $\Psi^k_\lambda(m_{a,b})$.

If we now assume that $\mathcal{H}$ is positive, we can take powers of it and get

$$\mathcal{S}_\lambda \mathcal{H}^{(\alpha+\beta)} \mathcal{S}_\lambda^* = \lambda \tilde{\mathcal{H}}_\lambda \ ,$$

where

$$\tilde{\mathcal{H}}_\lambda = \frac{1}{\lambda} {\mathcal{H}_\lambda}^{\alpha+\beta}$$

and the Schrödinger equation for $\mathcal{H}^{(\alpha+\beta)}$,

$$\mathrm{i} \frac{\partial}{\partial t} \psi = \mathcal{H}^{(\alpha+\beta)} \psi \ ,$$

becomes upon conjugation with $\mathcal{S}_\lambda$

$$\frac{\mathrm{i}}{\lambda} \frac{\partial}{\partial t} \tilde{\psi} = \tilde{\mathcal{H}}_\lambda \tilde{\psi} \ ,$$

with

$$\tilde{\psi} = \mathcal{S}_\lambda \psi \ .$$

Hence for the Hamiltonian $\tilde{\mathcal{H}}_\lambda$ the semiclassical results with $\lambda = 1/\hbar$ are applicable. What do we get if we express the eigenvalues and eigenfunctions of $\tilde{\mathcal{H}}_\lambda$ through the ones of $\mathcal{H}$? Let us denote the quantities belonging to $\tilde{\mathcal{H}}_\lambda$ with a tilde, then we want to compare ψ_n, E_n, defined by

$$\mathcal{H} \psi_n = E_n \psi_n$$

with $\tilde{\psi}_n$, $\tilde{E}_n$, defined by

$$\tilde{\mathcal{H}}_\lambda \tilde{\psi}_n = \tilde{E}_n \tilde{\psi}_n \ .$$

By applying $\mathcal{H}_\lambda$ to $\tilde{\psi}_n$ we get

$$\mathcal{H}_\lambda \tilde{\psi}_n = \lambda^{1/(\alpha+\beta)} \tilde{E}_n^{1/(\alpha+\beta)} \tilde{\psi}_n \ ,$$

and inserting $\mathcal{H}_\lambda = \mathcal{S}_\lambda \mathcal{H} \mathcal{S}_\lambda^*$ gives

$$\mathcal{H} \mathcal{S}_\lambda^* \tilde{\psi}_n = \lambda^{1/(\alpha+\beta)} \tilde{E}_n^{1/(\alpha+\beta)} \mathcal{S}_\lambda^* \tilde{\psi}_n \ ,$$

hence we have

$$\tilde{\psi}_n = \mathcal{S}_\lambda \psi_n \qquad \text{and} \quad \tilde{E}_n = \frac{1}{\lambda} E_n^{(\alpha+\beta)} \ . \tag{2.98}$$

So we see that if we fix the new energy $\tilde{E}$ and perform the semiclassical limit $\lambda \to \infty$, then this is equivalent to $E_n \to \infty$ if $\alpha + \beta > 0$ and $E_n \to 0$ for $\alpha + \beta < 0$.

This determines the quantum mechanical input for the trace formula, and now we want to determine the effect of the scaling property on the classical system.

Proposition 2.5.9. *Assume the Hamilton function $H(\xi, x)$ is scaling with exponents α, β, i.e.*

$$H(\lambda^\alpha \xi, \lambda^\beta x) = \lambda H(\xi, x)$$

for all $\lambda > 0$, and assume $(p(t), q(t))$ is a solution of Hamilton's equations with energy E, then

$$(\tilde{p}(t), \tilde{q}(t)) := (\lambda^\alpha p(\lambda^{1-(\alpha+\beta)} t), \lambda^\beta q(\lambda^{1-(\alpha+\beta)} t))$$

is a solution of Hamilton's equations with energy λE. Furthermore we get for a periodic orbit $\gamma = \{(p(t), q(t)) \; ; t \in [0, T_\gamma(E)]\}$ with energy E, that

$$\lambda \cdot \gamma := \{(\lambda^\alpha p(t), \lambda^\beta q(t)) \; ; (p(t), q(t)) \in \gamma\}$$

is a periodic orbit with

$$S_{\lambda\cdot\gamma}(\lambda E) = \lambda^{(\alpha+\beta)} S_\gamma(E) \; , \qquad T_{\lambda\cdot\gamma}(\lambda E) = \lambda^{(\alpha+\beta)-1} T_\gamma(E) \; .$$

If γ is isolated and nondegenerate, then

$$\det(P_{\lambda\cdot\gamma}(\lambda E) - I) = \det(P_\gamma(E) - I) \; .$$

Proof. By differentiating the homogeneity relation one obtains

$$\begin{aligned}(\partial_\xi H)(\lambda^\alpha \xi, \lambda^\beta x) &= \lambda^{1-\alpha} (\partial_\xi H)(\xi, x) \\ (\partial_x H)(\lambda^\alpha \xi, \lambda^\beta x) &= \lambda^{1-\beta} (\partial_x H)(\xi, x) \; .\end{aligned}$$

Using this with $(\xi(t), x(t)) = (\lambda^\alpha p(\lambda^\delta t), \lambda^\beta q(\lambda^\delta t))$, where $\delta = 1 - (\alpha + \beta)$, in Hamilton's equations gives

$$\begin{aligned}\lambda^{1-\beta} \dot{p}(\lambda^\delta t) &= \partial_x H(\lambda^\alpha p(\lambda^\delta t), \lambda^\beta q(\lambda^\delta t)) = \lambda^{1-\beta} \partial_x H(p(\lambda^\delta t), q(\lambda^\delta t)) \\ \lambda^{1-\alpha} \dot{q}(\lambda^\delta t) &= -\partial_\xi H(\lambda^\alpha p(\lambda^\delta t), \lambda^\beta q(\lambda^\delta t)) = -\lambda^{1-\alpha} \partial_\xi H(p(\lambda^\delta t), q(\lambda^\delta t)) \; ,\end{aligned}$$

which proves that $(\lambda^\alpha p(\lambda^{1-(\alpha+\beta)} t), \lambda^\beta q(\lambda^{1-(\alpha+\beta)} t))$ satisfies Hamilton's equations. The behavior of the period $T_\gamma(E)$ under scaling can be read off immediately, and for the action we get

$$\begin{aligned}S_{\lambda\cdot\gamma}(\lambda E) &= \int_0^{T_{\lambda\gamma}(\lambda E)} \langle \lambda^\alpha p(\lambda^{1-(\alpha+\beta)} t), \lambda^{1-\alpha} \dot{q}(\lambda^{1-(\alpha+\beta)} t) \rangle \, \mathrm{d}t \\ &= \lambda^{(\alpha+\beta)} \int_0^{T_\gamma(E)} \langle p(t), \dot{q}(t) \rangle \, \mathrm{d}t \\ &= \lambda^{(\alpha+\beta)} S_\gamma(E) \; .\end{aligned}$$

To prove the last assertion we use the classical time evolution operator $V_t(E) : L^2(\Sigma_E) \to L^2(\Sigma_E)$ defined by

$$V_t(E)\varphi(\xi, x) = \varphi(\Phi^t(\xi, x)) \ .$$

If γ is nondegenerate with period $T_\gamma(E)$, then there is a neighborhood $\mathcal{U}$ of $T_\gamma(E)$ and a bounded function $a \in C^\infty$ which is one in a neighborhood of $\bigcup_{\lambda\in\mathbb{R}} \lambda \cdot \gamma$ such that for $t \in U$

$$\operatorname{tr} aV_t(E) = \frac{T_\gamma^\#(E)}{|\det(P_\gamma(E) - I)|}\,\delta(t - T_\gamma(E)) \ ,$$

see [Gui77]. Now we introduce an isometry $\mathbf{s}_\lambda(E) : L^2(\Sigma_E) \to L^2(\Sigma_{\lambda E})$ by

$$(\mathbf{s}_\lambda(E)\varphi)(\xi, x) = \lambda^{-d(\alpha+\beta)+1}\varphi(\lambda^{-\alpha}\xi, \lambda^{-\beta}x) \ ,$$

then we have

$$aV_t(E) = \mathbf{s}_\lambda^{-1}(E)aV_{\lambda^{\alpha+\beta-1}t}(\lambda E)\mathbf{s}_\lambda(E)$$

and it follows that for $t \in U$

$$\begin{aligned}
\frac{T_\gamma^\#(E)}{|\det(P_\gamma(E) - I)|}\,\delta(t - T_\gamma(E)) &= \operatorname{tr} aV_t(E) \\
&= \operatorname{tr} S_\lambda^{-1}aV_{\lambda^{\alpha+\beta-1}t}(\lambda E)S_\lambda(E) \\
&= \operatorname{tr} aV_{\lambda^{\alpha+\beta-1}t}(\lambda E) \\
&= \frac{T_{\lambda\cdot\gamma}^\#(\lambda E)}{|\det(P_{\lambda\cdot\gamma}(\lambda E) - I)|}\,\delta(\lambda^{\alpha+\beta-1}t - T_{\lambda\cdot\gamma}(\lambda E)) \ .
\end{aligned}$$

Now with $T_{\lambda\cdot\gamma}(\lambda E) = \lambda^{\alpha+\beta-1}T_\gamma(E)$ the last expression can be rewritten as

$$\begin{aligned}
\frac{T_{\lambda\cdot\gamma}^\#(\lambda E)}{|\det(P_{\lambda\cdot\gamma}(\lambda E) - I)|}\,\delta(\lambda^{\alpha+\beta-1}t - T_{\lambda\cdot\gamma}(\lambda E)) &= \frac{T_\gamma^\#(E)\lambda^{\alpha+\beta-1}}{|\det(P_{\lambda\cdot\gamma}(\lambda E) - I)|}\,\delta(\lambda^{\alpha+\beta-1}(t - T_\gamma(E))) \\
&= \frac{T_\gamma^\#(E)}{|\det(P_{\lambda\cdot\gamma}(\lambda E) - I)|}\,\delta(t - T_\gamma(E))
\end{aligned}$$

and hence we arrive at

$$|\det(P_{\lambda\cdot\gamma}(\lambda E) - I)| = |\det(P_\gamma(E) - I)| \ .$$

□

By the functional calculus we know that the symbol of $\tilde{\mathcal{H}}_\lambda$ is given by

$$H^{\alpha+\beta}(\xi, x) + O(\lambda^{-2}) \ ,$$

hence the principal symbol defining the classical system which determines the classical side of the trace formula for $\tilde{\mathcal{H}}_\lambda$ is $H^{\alpha+\beta}(\xi,x)$. This is scaling in the sense of (2.97) with exponents $\alpha'=\alpha/(\alpha+\beta)$ and $\beta'=\beta/(\alpha+\beta)$ which gives

$$\alpha'+\beta'=1\ .$$

Therefore it follows from Proposition 2.5.9 that

$$\tilde{S}_\gamma(\lambda E)=\lambda\tilde{S}_\gamma(E) \quad \text{and} \quad \tilde{T}_\gamma(\lambda E)=\tilde{T}_\gamma(E)\ ,$$

for all $\lambda>0$. Let us denote by $\tilde{\mathcal{T}}$ the set of periods $\tilde{T}_\gamma(E)$, then the Poisson relation for $\tilde{\mathcal{H}}_\lambda$ reads

$$\mathrm{FS}\left(\sum \mathrm{e}^{\mathrm{i}\lambda t\tilde{E}_n}\right)\subset\tilde{\mathcal{T}}\times\mathbb{R}^+\ .$$

But with (2.98) and the remark after Definition 2.4.1 we see that the Poisson relation reads in terms of the original eigenvalues E_n

$$\mathrm{WF}\left(\sum \mathrm{e}^{\mathrm{i}tE_n^{(\alpha+\beta)}}\right)\subset\tilde{\mathcal{T}}\times\mathbb{R}^+\ .$$

Along the same lines of reasoning we can establish a trace formula (2.96) in terms of E_n, the left-hand side of which is

$$\sum\varphi(\lambda(\tilde{E}_n-E))=\sum\varphi(E_n^{(\alpha+\beta)}-\lambda E)\ .$$

For the classical side we then get from (2.96)

$$\begin{aligned}\sum\varphi(E_n^{(\alpha+\beta)}-\lambda E)=&\frac{\hat{\varphi}(0)}{2\pi}\frac{\lambda^{d-1}|\tilde{\Sigma}_E|}{(2\pi)^{d-1}}\\&+\sum_\gamma\frac{\hat{\varphi}(\tilde{T}_\gamma(E))}{2\pi}\frac{\tilde{T}_\gamma^{\#}(E)\mathrm{e}^{\mathrm{i}\tilde{\mu}_\gamma\pi/2}}{|\det(\tilde{P}_\gamma(E)-I)|^{1/2}}\mathrm{e}^{\mathrm{i}\lambda\tilde{S}_\gamma(E)}+O(\lambda^{-1})\end{aligned}$$

Since the Hamiltonian vectorfield of H, X_H and the one of $H^{\alpha+\beta}$, $X_{H^{\alpha+\beta}}$ are related by

$$X_{H^{\alpha+\beta}}=(\alpha+\beta)H^{(\alpha+\beta)-1}X_H,$$

we get that at $E=E_0$ defined by $(\alpha+\beta)E_0^{(\alpha+\beta)-1}=1$ the two flows coincide and we can express everything in terms of the original Hamiltonian $\mathcal{H}$. Therefore for scaling systems the trace formula (2.96) now reads

$$\begin{aligned}\sum\varphi(E_n^{(\alpha+\beta)}-\lambda E_0)=&\frac{\hat{\varphi}(0)}{2\pi}\frac{\lambda^{d-1}|\Sigma_{E_0}|}{(2\pi)^{d-1}}\\&+\sum_\gamma\frac{\hat{\varphi}(T_\gamma(E_0))}{2\pi}\frac{T_\gamma^{\#}(E_0)\mathrm{e}^{\mathrm{i}\nu_\gamma\pi/2}}{|\det(P_\gamma(E_0)-I)|^{1/2}}\mathrm{e}^{\mathrm{i}\lambda S_\gamma(E_0)}+O(\lambda^{-1})\ .\end{aligned}$$

We will now extend the previous discussion of operators with scaling symbols to more general cases. As an example take the case of an operator

$$\mathcal{H} = -\frac{1}{2}\Delta + V(x) \ ,$$

where for large x the potential $V(x)$ is approximately quadratic, i.e. we assume that $V(\lambda x)$ has an asymptotic expansion

$$V(\lambda x) \sim \sum_{k=0}^{\infty} \lambda^{2-k} V_{2-k}(x)$$

for $\lambda \to \infty$, with $V_{2-k}(x)$ homogeneous of degree $2-k$ in x. From the proof of Proposition 2.5.1 we know that the Weyl symbol of $\mathcal{S}_\lambda^* \mathcal{H} \mathcal{S}_\lambda$ is given by $H(\lambda^{1/2}\xi, \lambda^{1/2}x)$ and so we have

$$H(\lambda^{1/2}\xi, \lambda^{1/2}x) \sim \lambda \sum_{l=0}^{\infty} \lambda^{-l/2} H_l(\xi, x)$$

with $H_0(\xi, x) = \langle \xi, \xi \rangle/2 + V_2(x)$ and $H_l(\xi, x) = V_{2-l}(x)$ for $l \geq 1$. To this kind of semiclassical operators one can now apply the standard techniques. The physical meaning of this construction is a kind of asymptotic perturbation theory, i.e. for large energies the quadratic term of the potential is dominant, and we can treat the lower order terms as a perturbation which is proportional to the inverse square root of the energy.

Definition 2.5.10. *A smooth function $H(\xi, x)$ is called **polyhomogeneous** with exponents $\alpha, \beta \in \mathbb{R}$, if there is a strictly monotonically increasing sequence $\{m_j\}_{j\in\mathbb{N}} \subset \mathbb{R}^+$ with $m_j \to \infty$, such that*

$$H(\lambda^\alpha \xi, \lambda^\beta x) \sim \lambda \sum_{j=0}^{\infty} \lambda^{-m_j} H_j(\xi, x)$$

for $\lambda \to \infty$ where the H_j are homogeneous of degree m_j in the sense that

$$H_j(\lambda^\alpha \xi, \lambda^\beta x) = \lambda^{1-m_j} H_j(\xi, x) \ ,$$

for $\lambda > 0$.

As in the preceeding example, operators with polyhomogeneous symbols can be mapped by conjugation with the scaling operators $\mathcal{S}_\lambda$ of Proposition 2.5.1 to semiclassical operators.

So assume that H is polyhomogeneous with exponents α, β, and with $m_j = 0$. The conjugation of the Weyl quantization $\mathcal{H}$ of H with the corresponding scaling operator $\mathcal{S}_\lambda$ gives according to Proposition 2.5.1

$$\mathcal{S}_\lambda \mathcal{H} \mathcal{S}_\lambda^* = \lambda^{\frac{1}{\alpha+\beta}} \mathcal{H}_\lambda \ ,$$

where $\mathcal{H}_\lambda$ is the λ-quantization of

$$\lambda^{-\frac{1}{\alpha+\beta}} H(\lambda^{\frac{\alpha}{\alpha+\beta}}\xi, \lambda^{\frac{\beta}{\alpha+\beta}}x) \sim \sum_{j=0}^{\infty} \lambda^{-\frac{m_j}{\alpha+\beta}} H_j(\xi, x) = H_0(\xi, x) + \cdots \ .$$

Assume now that $\mathcal{H}_\lambda$ is elliptic in the sense that $H_0 > 0$, then the functional calculus for λ-dependent operators, see [DS99], allows to take the $(\alpha+\beta)$'th power of $\mathcal{S}_\lambda \mathcal{H} \mathcal{S}_\lambda^*$,

$$\left(\mathcal{S}_\lambda \mathcal{H} \mathcal{S}_\lambda^*\right)^{\alpha+\beta} = \lambda \tilde{\mathcal{H}}_\lambda$$

where $\tilde{\mathcal{H}}_\lambda$ is the λ-quantization of the symbol $\tilde{H} \in S^0(m)$ with

$$\tilde{H} \sim H_0 + \cdots \ .$$

So we have now extended the previously constructed mapping of a scaling system to a semiclassical system to the case of a polyhomogeneous system. As the examples show, this covers already a fairly large class of systems. The application of the techniques of semiclassical analysis to the these scaled operators gives now asymptotic results which are valid in the high energy limit.

Note that the results are different from the naive application of the standard semiclassical calculus. Let us illustrate this with the example of a potential system with asymptotic quadratic potential

$$\mathcal{H} = -\frac{\hbar^2}{2m}\Delta + V(x) \ , \tag{2.99}$$

with

$$V(\lambda x) = \lambda^2 V_2(x) + \lambda^1 V_1(x) + \cdots$$

for $\lambda \to \infty$, where V_i is homogeneous of degree i. If we apply the standard semiclassical calculus from Section 2.4 this operator is the $\hbar$ quantization of the symbol

$$H(\xi, x) = \frac{1}{2m}\langle \xi, \xi \rangle + V(x) \ . \tag{2.100}$$

So the properties of the system defined by the Hamiltonian (2.99) are in the limit of $\hbar \to 0$ governed by the classical system generated by (2.100), and furthermore, no subprincipal terms occur. If we compare this with the result of our scaling transformation, the operator is mapped to the λ-quantization of

$$\tilde{H} = \frac{1}{2m}\langle \xi, \xi \rangle + \lambda^{-1} V(\lambda^{1/2} x) \sim \sum_{j=0}^{\infty} \lambda^{-j/2} H_j(\xi, x) \ ,$$

where

$$H_0(\xi, x) = \frac{1}{2m}\langle \xi, \xi \rangle + V_2(x) \ , \quad H_1(\xi, x) = V_1(x) \ .$$

Hence the corresponding classical system differs from (2.100), it contains only the leading part in the high-energy limit. Furthermore, there occur subprincipal terms.

So this second approach can be viewed as a kind of asymptotic perturbation theory. It gives a precise meaning to the semiclassical limit and shows how the usual semiclassical calculus naturally appears in that limit. A further nice property of this construction is that the classical system defined by the principal symbol is always scaling, this facilitates a lot the determination of the classical quantities one needs for instance in the trace formula. But note that in contrast to the standard cases, we obtain typically non-integer powers of the semiclassical parameter, depending on the scaling properties of the principal symbol.

We have sketched in this section how one can implement the intuitive idea of the semiclassical limit as the limit of large quantum numbers, or small de Broglie wavelength, and large semiclassical density, with a scaling transformation which leads to a semiclassical calculus. The parameter is now no longer $\hbar$, but a kind of effective energy. On the level of states, the scaling transformation $\mathcal{S}_\lambda$ implements a parameter λ which governs the de Broglie wavelength. The observables are mapped to semiclassical λ dependent observables. Furthermore, we saw that in general also observables with expansions into non-integer powers of the semiclassical parameter occur.

We have been rather brief, with the principal aim to show how the semiclassical limit can be understood physically, and how it can be formalized in a mathematical language which then leads basically to the known semiclassical calculus, but now with a more physical interpretation of the semiclassical parameter, namely as a parameter which can be controlled experimentally by preparing, e.g., suitable states at $t = 0$. Certainly, this approach needs a refined and a more careful study, in order to incorporate for instance decaying potentials, like the Coulomb potential, which we have ignored in the last part of the section. But we hope we have convinced the reader that it is worth it, and that the semiclassical limit can be implemented in principle in a physically sound way.

In the following chapter we will only use that standard semiclassical calculus, where, motivated by the results of this section, we will call the semiclassical parameter λ instead of $1/\hbar$. But we will ignore the second lesson from this section, namely that one also needs expansions into non-integer powers of the semiclassical parameter. This is just because it is simpler, and in the future one should study the more general case, too.

Chapter 3

Lagrangian states

We have argued in the preceeding chapter that the semiclassical limit is the limit of small de Broglie wavelength, and have shown how this idea is implemented through the theory of microlocal analysis. The basic idea was to study the action of operators on simple states which oscillate as $\mathrm{e}^{\mathrm{i}\lambda\langle x,p\rangle}$, and we have studied how in the limit $\lambda \to \infty$ quantities belonging to classical mechanics appear and govern the behavior of the operators. So the accuracy of the semiclassical approximations is governed by the states.

The aim in this chapter is to describe a class of states with particularly nice semiclassical properties, the Lagrangian states. They will depend on a parameter λ which governs the semiclassical limit. Basic examples are on the one hand coherent states of the form

$$\left(\frac{\lambda}{\pi}\right)^{d/4} (\det \operatorname{Im} B)^{1/4} \mathrm{e}^{\mathrm{i}\lambda[\langle p, x-q\rangle + \langle (x-q), B(x-q)\rangle/2]} ,$$

where $(p, q) \in \mathbb{R}^d \times \mathbb{R}^d$ and B is a symmetric $d \times d$ matrix with strictly positive imaginary part. Such states are concentrated semiclassically, i.e. in the limit $\lambda \to \infty$, at the point (p, q) in phase space, and can therefore be thought of as a quantization of the classical observable $\delta_{(p,q)}$. The other basic class of examples consists of functions of the form

$$\mathrm{e}^{\mathrm{i}\lambda\varphi(x)} ,$$

with $\operatorname{Im} \varphi(x) = 0$, or, more generally, linear superpositions of such functions of the form

$$\left(\frac{\lambda}{2\pi}\right)^{\kappa/2} \int_{\mathbb{R}^\kappa} \mathrm{e}^{\mathrm{i}\lambda\varphi(x,\theta)} a(x,\theta) \mathrm{d}\theta , \tag{3.1}$$

again with $\operatorname{Im} \varphi(x, \theta) = 0$ and some non-degeneracy assumptions on φ. Such functions are semiclassically concentrated on a submanifold of the phase space determined by the phase function,

$$\Lambda_\varphi = \{(x, \varphi_x'(x, \theta))\,;\ \varphi_\theta'(x, \theta) = 0\} ,$$

in fact these manifolds are Lagrangian.

The more general class of functions we will consider is of the same form as (3.1), but now φ is allowed to be complex, with $\operatorname{Im}\varphi > 0$. For such function the set Λ_φ will be complex, so it cannot be considered as a subset of phase space. Instead, the function (3.1) is semiclassically concentrated on,

$$\{(x, \varphi_x'(x,\theta))\,;\ \varphi_\theta'(x,\theta) = 0\,,\ \operatorname{Im}\varphi(x,\theta) = 0\}\ ,$$

which is an isotropic submanifold of phase space. Nevertheless its extension Λ_φ to the complex domain will play an important role in the theory and, because Λ_φ can be thought of as a complex Lagrangian submanifold, the set of states will be called Lagrangian states.

Their possible applications are manifold, but we will use them primarily for two purposes. First they give a framework for studying the semiclassical limit rather generally. We are in particular interested in the time evolution of these states in order to get sharp estimates on the time up to which a semiclassical time evolution is valid. The second purpose is the construction of approximate solutions to the eigenvalue equation, so called quasimodes. It is well known that Lagrangian states can be used to construct quasimodes on invariant tori in integrable or near integrable systems. Furthermore, the Lagrangian states with complex-valued phase functions can be used to construct quasimodes concentrated on elliptic periodic orbits of the classical system.

Our second application of Lagrangian states will be the use of a special class, the so called coherent states, as a basis for the method of Anti-Wick quantization which we will discuss in Chapter 4. To this end we will study the geometry of families of coherent states.

We will start with a short nontechnical review of the main steps leading to a quasimode construction based on real Lagrangian submanifolds, e.g., invariant tori in integrable systems. This serves as a motivation to develop the necessary mathematical tools on a rigorous basis in the next section. Especially for the case of complex valued phase functions we need a rather large technical apparatus, but since we can use it for other purposes as well, we take the time to go into some detail. Not all of this material is needed later on in this work, but it is intended to use it for further applications and therefore we have included it. The last two sections are then devoted to a study of the time evolution.

3.1 Quantization of real Lagrangian manifolds

Let M be a C^∞ manifold of dimension d and $\mathcal{H} \in \Psi^0(m_{a,b})$ a selfadjoint pseudodifferential operator on M, see Definition 2.5.4 and Proposition 2.5.6. We look for approximate solutions of the eigenvalue equation

$$(\mathcal{H} - E)\psi = 0\ , \tag{3.2}$$

that is for a function $\psi(\lambda, x)$ and an $E(\lambda) \in \mathbb{R}$, both depending on a parameter λ, with

$$(\mathcal{H} - E(\lambda))\psi(\lambda, x) = O(\lambda^{-N})\ , \tag{3.3}$$

for some or all $N \in \mathbb{N}$, and a sequence of $\lambda \to \infty$. The classical ansatz in WKB-theory is (see e.g. [Dui74, BW97]) to choose $\psi(\lambda, x)$ to be locally of the form

$$\mathrm{e}^{\mathrm{i}\lambda\varphi(x)} a(\lambda, x) \ , \tag{3.4}$$

where $\varphi(x)$ is a smooth real valued function, and $a(\lambda, x)$ has an asymptotic expansion in powers of $1/\lambda$,

$$a(\lambda, x) \sim \sum_{n=0}^{\infty} \lambda^{-n} a_n(x) \qquad \text{for } \lambda \to \infty \ . \tag{3.5}$$

A slightly more general ansatz is often preferred, given by a superposition of functions of the form (3.4),

$$\psi(\lambda, x) = \left(\frac{\lambda}{2\pi}\right)^{\kappa/2} \int_{\mathbb{R}^\kappa} \mathrm{e}^{\mathrm{i}\lambda\varphi(x,\theta)} a(\lambda, x, \theta) \, \mathrm{d}\theta \ , \tag{3.6}$$

where $a(\lambda, x, \theta)$ has uniformly compact support in θ and has an asymptotic expansion as (3.5), and $\varphi(x, \theta)$ is assumed to be smooth and non-degenerate, i.e. the differentials

$$\mathrm{d}\frac{\partial\varphi}{\partial\theta_1}, \dots, \mathrm{d}\frac{\partial\varphi}{\partial\theta_d}$$

are linearly independent on the set of (x, θ) with $\varphi'_\theta(x, \theta) = 0$. Furthermore, $E(\lambda)$ is assumed to have an asymptotic expansion for $\lambda \to \infty$,

$$E(\lambda) \sim \sum_{k=0}^{\infty} \lambda^{-k} E_k \ .$$

At a point x where $\varphi'_\theta(x, \theta) = 0$ has only one solution $\theta(x)$ in a neighborhood of x, the method of stationary phase, see Appendix D, applied to (3.6) gives

$$\psi(\lambda, x) = \mathrm{e}^{\mathrm{i}\lambda\varphi(x,\theta(x))} \tilde{a}(\lambda, x) \ ,$$

with

$$\tilde{a}(\lambda, x) = \frac{\mathrm{e}^{\mathrm{i}\frac{\pi}{4} \operatorname{sign} \varphi''_{\theta,\theta}(x,\theta(x))}}{|\det \varphi''_{\theta,\theta}(x, \theta(x))|^{1/2}} a_0(x, \theta(x)) + O(\lambda^{-1}) \ , \tag{3.7}$$

if the stationary point of $\varphi(x, \theta)$ is nondegenerate at x. So the function (3.6) is there of the same type as the simpler one (3.4), but at the degenerate points, or if the equation $\varphi'_\theta(x, \theta) = 0$ has a whole manifold of solutions θ, the asymptotic expansion is different. The main point in choosing an ansatz like (3.6) is to treat all stationary points on the same footing, and furthermore to get asymptotics which are uniform in x and possibly further system parameters.

If for a given x there is no θ with $(x,\theta)\in \operatorname{supp} a$ and for which φ is stationary, then the non-stationary phase theorem, Theorem D.1, shows that

$$\psi(\lambda,x)=O(\lambda^{-\infty})\ ,$$

so the function (3.6) is modulo $O(\lambda^{-\infty})$ determined by the germ of a on the set of stationary points

$$\hat{\Lambda}_\varphi:=\{(x,\theta)\,|\,\varphi'_\theta(x,\theta)=0\}\ .$$

When one inserts the ansatz (3.6) in the eigenvalue equation (3.2), one has to determine the action of the operator $\mathcal{H}$ on an oscillating function $\mathrm{e}^{\mathrm{i}\lambda\varphi}a(\lambda)$. We will do this in detail in the next section, see Theorem 3.2.10, and quote here only the well known result, see, e.g., [Dui73],

$$\mathcal{H}(\mathrm{e}^{\mathrm{i}\lambda\varphi}a(\lambda))(x)=\mathrm{e}^{\mathrm{i}\lambda\varphi(x)}b(\lambda,x)\ ,$$

where $b(\lambda,x)$ is given by

$$b(\lambda,x)=\mathrm{e}^{\frac{\mathrm{i}}{\lambda}(\langle\partial_y,\partial_\xi\rangle+\frac{1}{2}\langle\partial_\xi,\varphi''(x)\partial_\xi\rangle)}\mathrm{e}^{\mathrm{i}\lambda R(x,y)}a(\lambda,x+y)H(x+y/2,\lambda(\xi+\varphi'(x)))|_{y=0,\xi=0}\ ,$$

with $R(x,y)=\varphi(y)-\varphi(x)-\varphi'(x)y-\frac{1}{2}y\varphi''(x)y$, which has again an asymptotic expansion in powers of $1/\lambda$ if $\mathcal{H}$ is classical. More precisely, if the Weyl symbol H of $\mathcal{H}$ has the expansion $H\sim H_0+H_1+\cdots$, and $a\sim a_0+\lambda^{-1}a_1+\cdots$ one obtains for b the expansion $b\sim b_0+\lambda^{-1}b_1+\cdots$ with the first two terms given by

$$\begin{aligned}
b_0(x)&=a_0(x)H_0(x,\varphi'_x)\\
b_1(x)&=a_1(x)H_0(x,\varphi'_x)+a_0(x)H_1(x,\varphi'_x)+\mathrm{i}\Big(\partial_x a_0(x)\partial_\xi H_0(x,\varphi'(x))\\
&\qquad+\frac{1}{2}a_0(x)\partial_x\partial_\xi H_0(x,\varphi'(x))+\frac{1}{2}a_0(x)\partial_\xi\varphi''(x)\partial_\xi H_0(x,\varphi'(x))\Big)\ .
\end{aligned}$$

Inserting the ansatz (3.6) into the equation (3.2) leads to

$$(\mathcal{H}-E(\lambda))\psi(\lambda,x)=\left(\frac{\lambda}{2\pi}\right)^{\kappa/2}\int_{\mathbb{R}^\kappa}\mathrm{e}^{\mathrm{i}\lambda\varphi(x,\theta)}[b(\lambda,x,\theta)-E(\lambda)a(\lambda,x,\theta)]\,\mathrm{d}\theta\ ,$$

and the right-hand side is $O(\lambda^{-\infty})$ if $b(\lambda,x,\theta)-E(\lambda)a(\lambda,x,\theta)$ and all its derivatives are $O(\lambda^{-\infty})$ on $\hat{\Lambda}_\varphi$. For the first two terms we hence require

$$a_0(x,\theta)H_0(x,\varphi'_x(x,\theta))-E_0a_0(x,\theta)=0 \tag{3.8}$$

$$a_1H_0+a_0H_1+\mathrm{i}\Big(\partial_x a_0\partial_\xi H_0+\frac{1}{2}a_0\partial_x\partial_\xi H_0+\frac{1}{2}a_0\partial_\xi\varphi''\partial_\xi H_0\Big)-E_0a_1-E_1a_0=0\ , \tag{3.9}$$

where we have supressed the arguments in the second equation. The first one, (3.8), reduces to an equation for φ,

$$H_0(x,\varphi'_x(x,\theta))=E_0 \tag{3.10}$$

for $\varphi'_\theta(x,\theta)=0$. This is a classical Hamilton-Jacobi equation. The set

$$\Lambda_\varphi = \{(x,\varphi'_x(x,\theta)) \mid \varphi'_\theta(x,\theta)=0\} \tag{3.11}$$

is an (immersed) Lagrangian submanifold of T^*X. From (3.10) it follows that the Hamiltonian vector-field X_{H_0} is tangent to Λ_φ, because by (3.10) one has $\mathrm{d}H_0|_{\Lambda_\varphi}=0$, and by the definition of X_{H_0} one has $\mathrm{d}H_0(\cdot)=\omega(\cdot,X_{H_0})$ where ω is the symplectic two-form. Therefore X_{H_0} is skew-orthogonal to every tangent vector of Λ_φ, which implies by the Lagrangianess that X_{H_0} is tangent to Λ_φ. So in order that our ansatz should work, there should at least exist a Lagrangian submanifold of T^*M which is invariant under the Hamiltonian flow generated by the principal symbol of $\mathcal{H}$.

What we have just seen is an expression of a fundamental fact, namely that the basic geometric object associated with an oscillating function like (3.6) is the Lagrangian manifold (3.11). We will interpret the leading term of (3.7) as an object on Λ. The phase function φ defines a density on Λ by $\mathrm{d}_\varphi=\delta(\varphi'_\theta(x,\theta))|\mathrm{d}x||\mathrm{d}\theta|$, for let f be a function on Λ, then the integral of f against d_φ is given by

$$\int f\ \mathrm{d}_\varphi := \iint f(x,\varphi'_x(x,\theta))\,\delta(\varphi'_\theta(x,\theta))\ \mathrm{d}x\mathrm{d}\theta = \int f(x,\varphi'_x(x,\theta(x)))\frac{1}{|\varphi''_{\theta,\theta}(x,\theta(x))|}\ \mathrm{d}x\ .$$

So the factor $\frac{1}{|\varphi''_{\theta,\theta}(x,\theta(x))|^{1/2}}$ in (3.7) suggests that we should interpret the term as a half-density. In fact, if we slightly modify our point of view, and choose the ansatz (3.6) as a half-density, then this interpretation of the term $\frac{a_0(x,\theta(x))}{|\varphi''_{\theta,\theta}(x,\theta(x))|^{1/2}}$ is perfectly natural. Working with half-densities instead of functions on M is well known to be more natural in microlocal analysis. See Appendix A for the definition and an overview of the properties and applications of half-densities.

Until now we have worked only locally, but now we want to see if such a function as $\psi(\lambda,x)$ can be defined globally. In order to decide that one has to study how different local expressions of the form (3.6) can be patched together. From (3.7) it follows that if we have two expressions of the type (3.6) with different phase functions and amplitudes in different coordinate patches, and both admitting an expansion of the form (3.7), then a necessary condition that they coincide is

$$\mathrm{e}^{\mathrm{i}\lambda\varphi(x,\theta(x))}\frac{\mathrm{e}^{\mathrm{i}\frac{\pi}{4}\,\mathrm{sign}\,\varphi''_{\theta,\theta}(x,\theta(x))}}{|\det\varphi''_{\theta,\theta}(x,\theta(x))|^{1/2}}a_0(x,\theta(x)) = \mathrm{e}^{\mathrm{i}\lambda\tilde\varphi(\tilde x,\theta(\tilde x))}\frac{\mathrm{e}^{\mathrm{i}\frac{\pi}{4}\,\mathrm{sign}\,\tilde\varphi''_{\theta,\theta}(\tilde x,\theta(\tilde x))}}{|\det\tilde\varphi''_{\theta,\theta}(\tilde x,\theta(\tilde x))|^{1/2}}\tilde a_0(\tilde x,\theta(\tilde x))\ ,$$

where $x\mapsto\tilde x(x)$ denotes the coordinate-change. So with every change of coordinates, the half-density $\frac{a}{|\det\varphi''_{\theta,\theta}|^{1/2}}|\mathrm{d}x|^{1/2}$ picks up a factor

$$\mathrm{e}^{\mathrm{i}\lambda(\varphi-\tilde\varphi)}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}(\mathrm{sign}\,\varphi''-\mathrm{sign}\,\tilde\varphi'')}\ . \tag{3.12}$$

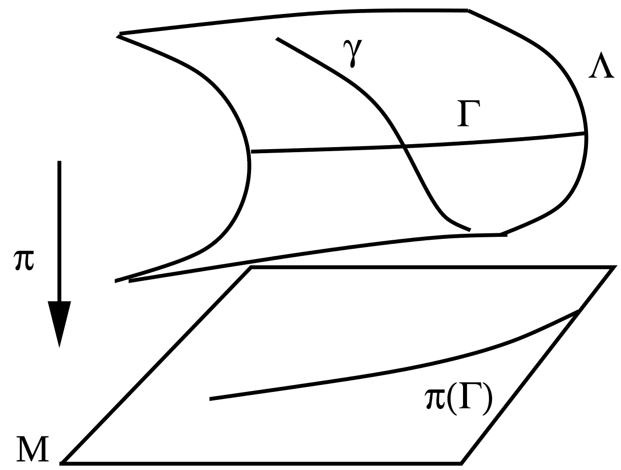

Figure 3.1: On the definition of the Maslov index of a curve γ on the Lagrangian submanifold Λ of T^*M. The Maslov index $\alpha(\gamma)$ is defined as the intersection number of γ with the subset $\Gamma \subset \Lambda$ on which the projection $\pi : \Lambda \to M$ is singular.

Hence the leading term in (3.7) should be considered as section in the half density bundle over Λ tensored with the bundle defined by the transition function (3.12), which is the Liouville bundle tensored with the Maslov bundle of Λ.

We first discuss the Liouville bundle, see e.g. [Dui74, BW97]. By the definition (3.11) of Λ the phase function $\varphi(x, \theta(x))$ satisfies

$$d\varphi(x, \theta(x)) = \left(\frac{\partial \varphi}{\partial x}(x, \theta(x)) + \frac{\partial \varphi}{\partial \theta}(x, \theta(x))\frac{\partial \theta(x)}{\partial x}\right) dx = \xi dx|_{\Lambda} \ ,$$

therefore the difference $\varphi - \tilde{\varphi}$ is locally constant and the line bundle defined by the transition functions $\mathrm{e}^{\mathrm{i}\lambda(\varphi - \tilde{\varphi})}$ is the one associated with the cohomology class of the Liouville one-form ξdx on Λ.

The meaning of the Maslov bundle is well known, too, see, e.g., [GS77, BW97]. The projection of the Lagrangian manifold Λ to the base space M might have singularities. The set of singularities Γ consists of a codimension-one submanifold, and possible further points of codimension three; the codimension-one submanifold furthermore carries a natural orientation. The value of the Maslov cohomology class α, which is the one associated with the Maslov bundle, on a closed loop γ on Λ is now defined as the number of intersections of γ with the codimension-one submanifold of singularities, counted with sign according to the orientation, see figure 3.1. So the Liouville class takes values in $\mathbb{R}$, and the Maslov class in $2\mathbb{Z}$.

The basic condition on the existence of a globally defined oscillating integral associated with Λ is the existence of a global section of the Maslov-Liouville bundle. This means, that if we take a closed loop γ in Λ and a covering of γ with open sets $\Lambda_j \subset \Lambda$ on which we have different local representations ψ_j of the same oscillating function, then after one traversal of the loop the amplitude has picked up a factor

$$\mathrm{e}^{\mathrm{i}(\lambda\sum_j(\varphi_j(x_j)-\varphi_{j-1}(x_j))+\frac{\pi}{4}\sum_j(\operatorname{sign}\varphi_j''(x_j)-\operatorname{sign}\varphi_{j-1}''(x_j)))} .$$

This factor has to be one in order that the function is single valued. The first term is the value of the Liouville class $\Theta = \xi\,\mathrm{d}x$ on γ,

$$\sum_j(\varphi_j(x_j)-\varphi_{j-1}(x_j)) = \int_\gamma \xi\,\mathrm{d}x = \Theta(\gamma) ,$$

which is the classical action of the path γ. The second term is the Maslov class evaluated on γ, $\alpha(\gamma)$. Therefore we get the condition that

$$\lambda\sum_j(\varphi_j(x_j)-\varphi_{j-1}(x_j)) + \frac{\pi}{4}\sum_j(\operatorname{sign}\varphi_j''(x_j)-\operatorname{sign}\varphi_{j-1}''(x_j)) = \lambda\Theta(\gamma)+\frac{\pi}{4}\alpha(\gamma)\in 2\pi\mathbb{Z} ,$$

for all closed loops $\gamma\subset\Lambda$, in order that the local functions ψ_j can be patched together to a single-valued function. This is the famous Maslov quantization condition on Λ. In a more sophisticated way it can be expressed as

$$\frac{1}{2\pi}\Big(\lambda\Theta+\frac{\pi}{4}\alpha\Big)\in H^1(\Lambda,\mathbb{Z}) . \tag{3.13}$$

Therefore we have now found two conditions on a Lagrangian manifold Λ to serve as the support of an oscillating function of the type (3.6) satisfying the approximate eigenvalue equation (3.3). The first one, the Hamilton-Jacobi equation (3.10), is a condition on Λ imposed by the classical system, and it implies that Λ is invariant under the Hamiltonian flow. The second condition, the Maslov quantization condition (3.13), is a topological condition to ensure the existence of a global function of the local form (3.6). This condition will allow only certain values of λ, and therefore leads to a discrete set of approximate eigenvalues $E(\lambda)$.

So the first result is, that if there exists a Lagrangian submanifold Λ of T^*X which satisfies $H_0|_\Lambda = E_0$ and a sequence of λ satisfying (3.13), then there is a sequence of functions $\psi(\lambda,x)$ with

$$(\mathcal{H}-E_0\lambda^m)\psi(\lambda,x) = O(\lambda^{-1}) .$$

Now we come to the second equation, (3.9). If the first one, equation (3.8), is satisfied, (3.9) reduces to

$$a_0(H_1-E_1)+\mathrm{i}\Big(\partial_x a_0\partial_\xi H_0+\frac{1}{2}a_0\partial_x\partial_\xi H_0+\frac{1}{2}a_0\partial_\xi\varphi''\partial_\xi H_0\Big)=0 ,$$

so it is an equation for a_0. The last two terms can be written as $\frac{1}{2}a_0\frac{\partial}{\partial x}\partial_\xi H_0(x,\varphi'(x))$, hence we get

$$\begin{aligned} &a_0(x,\theta)\big(H_1(x,\varphi'(x))-E_1\big)\\ &\qquad+\mathrm{i}\Big(\partial_x a_0(x,\theta)\partial_\xi H_0(x,\varphi'(x))+\frac{1}{2}a_0(x,\theta)\frac{\partial}{\partial x}\partial_\xi H_0(x,\varphi'(x))\Big)=0 . \end{aligned} \tag{3.14}$$

To interpret this equation we recall that we found it more convenient to interpret a as the coefficient of a half-density. Assume that X is a vector field and $b(x)|\mathrm{d}x|^{1/2}$ a half-density, then the Lie-derivative of $b(x)|\mathrm{d}x|^{1/2}$ in the direction X is given by

$$\mathcal{L}_X b(x)|\mathrm{d}x|^{1/2} = \Big(X(b) + \frac{1}{2}(\operatorname{div} X)b\Big)|\mathrm{d}x|^{1/2} \ .$$

The Hamiltonian vector field X_{H_0} restricted to the Lagrangian submanifold Λ in the above coordinates is given by $\partial_\xi H_0(x, \varphi'(x))$, so we see that we can write the transport equation for a_0, (3.14), in the invariant form

$$\frac{1}{\mathrm{i}}\mathcal{L}_{X_{H_0}} a_0 - (H_1 - E_1)a_0 = 0 \tag{3.15}$$

on Λ, if we consider a_0 as a half density on Λ.

By Stokes theorem a necessary condition for the solvability of (3.15) is that

$$E_1 = \int_\Lambda H_1 \ \mathrm{d}\mu_\Lambda \ ,$$

where $\mathrm{d}\mu_\Lambda$ is the invariant measure induced by the Liouville measure on Λ. Therefore the subprincipal symbol determines E_1. But this condition is not sufficient in order that the transport equation (3.15) has always a solution, we will discuss this problem in detail in Chapter 5.3. But if $H_1 = 0$, as is for instance the case if our Hamilton operator is the Laplacian on a Riemannian manifold, then $E_1 = 0$ and the canonical invariant half-density is a solution to (3.15).

To summarize, if, in addition to the previous requirements (3.10) and (3.13), a_0 and E_1 satisfy the transport equation (3.15), then we can construct an approximate solution with

$$(\mathcal{H} - E(\lambda))\psi(\lambda, x) = O(\lambda^{-2}) \ . \tag{3.16}$$

To proceed one has to solve the higher order transport equations. We will discuss the solvability of the transport equation (3.15) in detail in Chapter 5.3 and the consequences for the construction of approximate solutions of the Schrödinger equation up to arbitrary order in λ^{-1} in Chapter 5.4.

The procedure which we have described shows how one can associate with certain invariant Lagrangian submanifolds approximate solutions to the eigenvalue equation. In integrable or slightly perturbed integrable systems such Lagrangian submanifolds are very plenty. But in general other types of invariant sets very often occur, e.g., isolated periodic orbits. So the question arises if one can associate with other invariant submanifolds approximate solutions of the Schrödinger equation too, maybe by modifying the procedure for the Lagrangian manifolds.

For the motivation of the further developments let us discuss an example in $d = 2$ dimensions. Assume there is an elliptic periodic orbit γ of the Hamiltonian flow generated by the principal symbol of $\mathcal{H}$. Let us choose local coordinates around γ of the form $(s, \sigma; p, q)$, where $(s, \sigma; 0, 0)$ gives the orbit cylinder through γ, i.e. σ is transversal to the energy shells $H_0 = \text{const.}$. The normal form of the Hamilton function up to second order in the vicinity of the orbit in these coordinates is given by

$$H(s,\sigma;p,q) = \frac{\omega}{2}(p^2+q^2) + \frac{1}{2}\sigma^2 \ .$$

We are looking for a Lagrangian manifold on which the orbit lies, and which satisfies (3.10). If we consider a generating function $\varphi(s,q)$, then the manifold is locally given by

$$\Lambda_\varphi = \left\{ \left(\frac{\partial\varphi}{\partial s}, s; \frac{\partial\varphi}{\partial q}, q \right) , \ (s,q) \in S^1 \times \mathbb{R}^1 \right\} . \tag{3.17}$$

Since we require $\frac{\partial\varphi}{\partial s} = \sigma = \sqrt{2E} = \text{const.}$, we get for the phase function

$$\varphi(s,q) = \sqrt{2E}\, s + \varphi_1(q) \ .$$

This leads for $\varphi_1(q)$ to the Hamilton-Jacobi equation

$$\left(\frac{\partial\varphi_1(q)}{\partial q} \right)^2 = -q^2$$

which is solved by $\varphi_1(q) = \mathrm{i}q^2/2$. That is we get a phase function of the form

$$\varphi(s,q) = \sqrt{2E}\, s + \mathrm{i}q^2/2$$

which is complex valued, and therefore the corresponding Lagrangian manifold (3.17) is shifted to the complex domain. But how should we interpret this? We have started from a C^∞ manifold M, and there is a priori no notion of complex continuation given. So this construction does not seem to make sense, except we are working in the real analytic category instead. But on the other hand, we note that the imaginary part of the phase function is positive, which means that the class of oscillating function defined by it is well behaved, and furthermore is for large λ concentrated around the real part of Λ_φ. This is exactly the elliptic orbit. So if we were able to deal with the global problems arising because of the complex valuedness of φ, we would expect to generate by these functions approximate solutions of the Schrödinger equation concentrated on elliptic orbits. To develop the necessary theory is the aim of the next sections.

3.2 Oscillating integrals with complex phase functions

Motivated by the last example in the previous section we will develop in this and the following sections a global theory for functions on some manifold M, which are locally given by integrals of the form,

$$\psi(\lambda,x) = \left(\frac{\lambda}{2\pi}\right)^{\kappa/2} \int_{\mathbb{R}^\kappa} \mathrm{e}^{\mathrm{i}\lambda\varphi(x,\theta)} a(\lambda,x,\theta)\ \mathrm{d}\theta \ , \tag{3.18}$$

where $a(\lambda, x, \theta)$ is a smooth function with compact support in θ and an asymptotic expansion

$$a(\lambda, x, \theta) \sim \sum_{l=0}^{\infty} \lambda^{m-l} a_{m-l}(x, \theta) \ .$$

The phase function φ will be assumed to be smooth and complex valued, but with

$$\operatorname{Im} \varphi \geq 0 \ , \tag{3.19}$$

in order that (3.18) is well behaved for large λ. Furthermore, it should be nondegenerate, i.e. the differentials

$$\mathrm{d}\frac{\partial \varphi}{\partial \theta_1}, \dots, \mathrm{d}\frac{\partial \varphi}{\partial \theta_d} \tag{3.20}$$

should be linearly independent on the set of (x, θ) where $\frac{\partial \varphi}{\partial \theta} = 0$ and $\operatorname{Im} \varphi = 0$.

We start by developing some of the aspects of the local theory of functions of the form (3.18) and study their dependence on the phase function and the amplitude.

Recall the definition of the frequency set of a family of distributions u_λ (see 2.4.1).

Definition 3.2.1. *Let $u_\lambda \in \mathcal{D}'(M)$ be a bounded family of distributions depending smoothly on a parameter $\lambda \in (\lambda_0, \infty)$ for some $\lambda_0 > 0$. Then the* ***frequency set*** *of u_λ, $\mathrm{FS}(u_\lambda) \subset T^*M$, is the complement of all points $(x_0, \xi_0) \in T^*M$ which possess neighborhoods $U \ni x_0$, $V \ni \xi_0$, such that for every $\varphi \in C_0^\infty(U)$ and $\xi \in V$*

$$\int \mathrm{e}^{-\mathrm{i}\lambda\langle \xi, x\rangle} \varphi(x) u_\lambda(x) \ \mathrm{d}x = O(\lambda^{-N})$$

for all $N \in \mathbb{N}$, as λ tends to ∞.

This is the same definition as 2.4.1, but with $\hbar$ replaced by $1/\lambda$. The frequency set is an extension of the wave front set for distributions, in case that $u \in \mathcal{D}'(M)$ is independent of λ we have

$$\mathrm{FS}(u) = \mathrm{WF}(u) \ .$$

The properties of the frequency set are therefore very similar to the ones of the wave front set. Pseudodifferential operators remain pseudolocal with respect to the frequency set, i.e. for any $\mathcal{A} \in \Psi^k(m_{a,b})$ one has

$$\mathrm{FS}(\mathcal{A} u_\lambda) \subset \mathrm{FS}(u_\lambda)$$

for every bounded family of distributions $u_\lambda \in \mathcal{D}(M)$. Furthermore, the frequency set can be characterized in terms of the action of pseudodifferential operators, analogously to the wave front set.

Proposition 3.2.2. *For $\mathcal{A} \in \Psi^0(m_{a,b})$ define the characteristic set as the zero set of the principal symbol* $\operatorname{char}(\mathcal{A}) := \{(\xi, x) \,|\sigma(\mathcal{A})(\xi, x) = 0\}$*, then we have*

$$\mathrm{FS}(u_\lambda) = \bigcap \operatorname{char} \mathcal{A}$$

where the intersection runs over all $\mathcal{A} \in \Psi^0(1)$ with $\mathcal{A}u_\lambda = O(\lambda^{-\infty})$.

We omit the proof since it is completely analogous to the one in the homogeneous case, see, e.g., [Hör85a].

Physically speaking, the frequency set consists of the points in phase space on which the semiclassical limit of the family of distributions lives. On all other points in phase space the family of distributions is semiclassically negligible in the sense that for any $(p, q) \notin FS(u_\lambda)$ there exists a neighborhood $U \subset T^*M$ of (p, q) such that

$$\mathcal{A}u_\lambda = O(\lambda^{-\infty}) \ ,$$

for all $\mathcal{A} \in \Psi^0(1)$ whose symbols A have support in U. Now the property that a symbol has support in U is unfortunately not invariant under coordinate transformations, but since the contributions of the transformed symbol from outside U are $O(\lambda^{-\infty})$, the support is almost invariant. A suitable notion of a support modulo $O(\lambda^{-\infty})$ is introduced in the following.

Definition 3.2.3. *Let $\mathcal{A} \in \Psi^k(m_{a,b})$, the **frequency set** $FS(\mathcal{A})$ is defined as the complement of all points $(p, q) \in T^*M$, such that there exists a family $u_\lambda \in \mathcal{D}'$ with $(p, q) \in FS(u_\lambda)$ and*

$$FS(\mathcal{A}u_\lambda) = \emptyset \ .$$

The frequency set is sometimes also called essential support. It can also be characterized by the symbol of the operator.

Proposition 3.2.4. *Let $\mathcal{A} \in \Psi^k(m_{a,b})$ and denote the Weyl symbol in some local coordinates by $A(\xi, x)$, then $(p, q) \notin FS(\mathcal{A})$ if there is a neighborhood U of (p, q) such that*

$$A(\xi, x) = O(\lambda^{-\infty})$$

for all $(\xi, x) \in U$.

The non-stationary phase theorem, Theorem D.1, immediately gives the frequency set of the oscillatory integral (3.18).

Proposition 3.2.5. *Let $\psi(\lambda, x)$ be given by* (3.18)*, where the phase function has positive imaginary part* (3.19) *and is non-degenerate* (3.20)*, then*

$$\mathrm{FS}(u(\lambda)) \subset \{(x, \varphi'_x(x, \theta)) \,|\, \varphi'_\theta(x, \theta) = 0 \ , \operatorname{Im} \varphi(x, \theta) = 0\} \ . \tag{3.21}$$

We now want to study the dependence of $\psi(\lambda, x)$ on a change of the amplitude and phase function. If we we change the amplitude away from the set where the imaginary part of the phase function is zero, we expect that the changes in $u(\lambda, x)$ are small.

Lemma 3.2.6. *Assume* $\operatorname{Im}\varphi(x,\theta)\geq 0$ *and*

$$|a(x,\theta)|\leq C'_N(\operatorname{Im}\varphi(x,\theta))^N\ , \tag{3.22}$$

then we have for $\lambda\geq 1$

$$\left|\mathrm{e}^{\mathrm{i}\lambda\varphi(x,\theta)}a(x,\theta)\right|\leq C_N\lambda^{-N}\ . \tag{3.23}$$

Similarly, we have if $a(\lambda,x,\theta)\sim\sum_{k=0}^{\infty}\lambda^{m-k}a_k(x,\theta)$ *with*

$$|a_k(x,\theta)|\leq C_{N,k}(\operatorname{Im}\varphi(x,\theta))^{N-k}\ ,\quad \textit{for } k\leq N\ , \tag{3.24}$$

that there exists a λ_N *such that for* $\lambda>\lambda_N$

$$\left|\mathrm{e}^{\mathrm{i}\lambda\varphi(x,\theta)}a(\lambda,x,\theta)\right|\leq C_N\lambda^{m-N}\ . \tag{3.25}$$

Proof. We can estimate $\mathrm{e}^{\mathrm{i}\lambda\varphi(x,\theta)}a(x,\theta)$ as

$$\left|\mathrm{e}^{\mathrm{i}\lambda\varphi(x,\theta)}a(x,\theta)\right|\leq \mathrm{e}^{-\lambda\operatorname{Im}\varphi(x,\theta)}|a(x,\theta)|\leq C'_N\mathrm{e}^{-\lambda\operatorname{Im}\varphi(x,\theta)}(\operatorname{Im}\varphi(x,\theta))^N\ ,$$

where we have used the assumption (3.22). Now the first result (3.23) follows from the trivial inequality

$$\mathrm{e}^{-\lambda y}y^N\leq\max_{x\geq 0}\{e^{-x}x^N\}\,\lambda^{-N}\ ,$$

for $y\geq 0$. To show the second estimate (3.25) we write $a(\lambda,x,\theta)=\sum_{k=0}^{N-1}\lambda^{m-k}a_k(x,\theta)+r(\lambda,x,\theta)$ with $|r(\lambda,x,\theta)|\leq C\lambda^{m-N}$, and apply the first result (3.23) to the terms in the sum. □

As an immediate consequence we get an estimate on the difference of oscillating integrals whose amplitudes are equal on the set where the phase function is real.

Proposition 3.2.7. *Assume* $a(\lambda,x,\theta)$ *and* $b(\lambda,x,\theta)$ *have compact support in* θ*, and the difference* $a(\lambda,x,\theta)-b(\lambda,x,\theta)$ *satisfies* (3.24)*, then*

$$\left|\int\mathrm{e}^{\mathrm{i}\lambda\varphi(x,\theta)}(a(\lambda,x,\theta)-b(\lambda,x,\theta))\,\mathrm{d}\theta\right|\leq C\lambda^{m-N}\ .$$

More generally, the same ideas can be used to show that an oscillatory integral ψ is determined modulo $\lambda^{-\infty}$ by the germ of the amplitude a on the critical manifold $C_\varphi=\{(x,\theta)\,;\,\varphi'_\theta(x,\theta)=0\,,\ \operatorname{Im}\varphi(x,\theta)=0\}$.

3.2.1 The action of a pseudodifferential operator on an oscillating integral with complex phase function

Next we want to determine the action of a pseudodifferential operator on an oscillating function with complex phase function. As a first step we will look at functions of the form

$$u_\lambda(x) = \mathrm{e}^{\mathrm{i}\lambda\varphi(x)} ,$$

where $\operatorname{Im}\varphi(x) \geq 0$ and $\varphi(x)$ is smooth. Let $\mathcal{P}$ be a partial differential operator,

$$\mathcal{P} = \sum_{|\alpha|\leq m} p_\alpha(x) D^\alpha ,$$

then we get

$$\mathcal{P}u_\lambda(x) = \lambda^m p_m(x, \varphi'_x)\mathrm{e}^{\mathrm{i}\lambda\varphi(x)} + O(\lambda^{m-1}) ,$$

where $p_m(\xi, x) = \sum_{|\alpha|=m} p_\alpha(x)\xi^\alpha$ is the principal symbol of $\mathcal{P}$. For real valued $\varphi(x)$ we have encountered this formula already several times, and its validity transfers to general pseudodifferential operators. But now we have allowed for a complex valued phase function. This makes no problems for a differential operator $\mathcal{P}$, because then the symbol is a polynomial in ξ and inserting a complex quantity for it causes no harm. But for a general pseudodifferential operator the principal symbol is just assumed to be smooth, and need not be polynomial or analytic, therefore it is not clear how one should evaluate it at a complex ξ.

A way out of this problem is given by the method of almost analytic extensions, which have been introduced by Hörmander and Nirenberg, see e.g. [MS75, Tre80].

Definition 3.2.8. *Let $f \in C^\infty(\mathbb{R}^d)$, then an* ***almost analytic extension*** *of f is a function $\tilde{f}(x, y) \in \mathbb{C}^\infty(\mathbb{R}^d \times \mathbb{R}^d)$ which satisfies*

$$\tilde{f}(x, 0) = f(x)$$

and

$$|\overline{\partial}\tilde{f}(x, y)| \leq C_N|y|^N , \quad \textit{for all } N \in \mathbb{N} , \tag{3.26}$$

where $\overline{\partial} = \partial_x + \mathrm{i}\partial_y$ denotes the Cauchy-Riemann operator.

If we had $|\overline{\partial}\tilde{f}(x, y)| = 0$, $\tilde{f}$ would be analytic, and therefore $\tilde{f}$ would be an analytic continuation of f. But this is only possible if f is already real analytic. The first questions which arise are wether such an almost analytic extension always exists, and if it is unique then. To answer the first question we consider the Taylor series of f around x,

$$\sum_\alpha \frac{f^\alpha(x)}{\alpha!} u^\alpha ,$$

which need not converge if f is not analytic. But by the Borel theorem on the summation of asymptotic series one can find a sequence $\{\varepsilon_\alpha\}$ with $\varepsilon_\alpha \to 0$ for $|\alpha| \to \infty$, and a smooth function $\rho(t)$, $t \in \mathbb{R}$, which is 0 for $t > 2$ and 1 for $t < 1$, such that

$$\sum_\alpha \frac{f^{(\alpha)}(x)}{\alpha!}\rho(|u|/\varepsilon_\alpha)u^\alpha$$

is absolutely convergent and in $C^\infty(\mathbb{R}^d \times \mathbb{R}^d)$. Then we claim that

$$\tilde{f}(x,y) := \sum_\alpha \frac{f^{(\alpha)}(x)\mathrm{i}^{|\alpha|}}{\alpha!}\rho(|y|/\varepsilon_\alpha)y^\alpha$$

defines an almost analytic extension of f. The condition $\tilde{f}(x,0) = f(x)$ follows from the definition, and in order to show the almost analyticity we compute

$$\overline{\partial}\tilde{f}(x,y) = \sum_\alpha \frac{f^{(\alpha)}(x)\mathrm{i}^{|\alpha|}}{\alpha!}\rho'(|y|/\varepsilon_\alpha)\frac{y}{|y|\varepsilon_\alpha}y^\alpha \ ,$$

which obviously satisfies the estimate (3.26), because ρ' has its support in the interval $[1,2]$.

Because the Borel summation is non-unique, it follows that the almost analytic extension of a smooth function is non-unique too. In order to describe the difference between almost analytic continuations of the same function we introduce a further notion from [MS75, Tre80].

Definition 3.2.9. *Let S be a closed subset of $\mathbb{R}^n$. A function g which is defined in some neighborhood of S, and is smooth there, is called **flat** at S if g and all its derivatives are vanishing at S.*

It follows immediately from the definition that g being flat at S is equivalent to

$$|g(x)| \leq C_N(\mathrm{dist}(S,x))^N$$

for all $N \in \mathbb{N}$, and where $\mathrm{dist}(S,x)$ denotes the distance from x to S. Furthermore, it is clear that if g is flat at S, then all derivatives of g are flat at S too. Now the condition that $\tilde{f}$ and $\tilde{g}$ are almost analytic continuations of the same function is equivalent to the fact that $\tilde{f} - \tilde{g}$ is flat at $y = 0$.

After this preparations we can return to our original problem to determine the action of a pseudodifferential operator on an oscillating function with complex valued phase function. We will state the theorem only for operators with symbols in $S^0(m_{a,b})$, since the passage to $S^k(m_{a,b})$ is just a multiplication with λ^k.

Theorem 3.2.10. *Let $\mathcal{H}$ be a pseudodifferential operator with Weyl symbol $H(\lambda,\xi,x) \in S^0(m_{a,b})$, and $a(x)$, $\varphi(x)$ smooth functions with $\operatorname{Im}\varphi(x) \geq 0$; $a(x)$ shall moreover be compactly supported. Then*

$$\mathcal{H}(a\mathrm{e}^{\mathrm{i}\lambda\varphi})(x) = b(\lambda,x)\mathrm{e}^{\mathrm{i}\lambda\varphi(x)} + O(\lambda^{-\infty}) \ ,$$

and the amplitude $b(\lambda, x)$ is given by

$$b(\lambda, x) = \mathrm{e}^{\frac{\mathrm{i}}{\lambda}(\langle D_y, D_\xi\rangle + \frac{1}{2}\langle D_\xi, \varphi''(x) D_\xi\rangle)} \mathrm{e}^{\mathrm{i}\lambda R(x,y)} \tilde{H}(\lambda; \xi + \varphi'(x), x + y/2) a(x+y)|_{y=0,\xi=0} \ , \quad (3.27)$$

where $\tilde{H}(\lambda, \xi, x)$ denotes an almost analytic extension of the Weyl symbol H of $\mathcal{H}$, and $R(x, y)$ is given by

$$R(x, y) = \varphi(x+y) - \varphi(x) - \langle \varphi'(x), y\rangle - \frac{1}{2}\langle y, \varphi''(x) y\rangle \ .$$

In the formula (3.27) the exponential can be expanded in a Taylor series to give the asymptotic expansion

$$\begin{aligned} b(\lambda, x) \sim \sum_{k=0}^{\infty} \frac{\mathrm{i}^k}{k!\lambda^k}(\langle D_y, D_\xi\rangle + \frac{1}{2}\langle D_\xi, \varphi''(x) D_\xi\rangle)^k \mathrm{e}^{\mathrm{i}\lambda R(x,y)} \\ \tilde{H}(\lambda; \xi + \varphi'(x), x + y/2) a(x+y)|_{y=0,\xi=0} \ , \end{aligned} \quad (3.28)$$

for $\lambda \to \infty$, where the k'th term is of order $\lambda^{m+[k/3]-k}$.

In the λ-independent homogeneous theory this result was proven in [MS75], but we will follow mainly the proof in [Tre80]. In the context of Maslov's canonical operator a similar result was proven in [MS73, MSS90].

It can sometimes be useful to choose a different expansion of $b(\lambda, x)$ than the one in (3.28). Note that the operator $\exp\left[\frac{\mathrm{i}}{2\lambda}\langle D_\xi, \varphi''(x) D_\xi\rangle\right]$ acts only on $\tilde{H}(\lambda, \xi + \varphi'(x), x + y/2)$, so with the abbreviation

$$\hat{H}(\lambda; \xi, x, y) := \mathrm{e}^{\frac{\mathrm{i}}{2\lambda}\langle D_\xi, \varphi''(x) D_\xi\rangle} \tilde{H}(\lambda, \xi + \varphi'(x), x + y/2) \ ,$$

we can write for the amplitude b,

$$\begin{aligned} b(\lambda, x) &= \mathrm{e}^{\frac{\mathrm{i}}{\lambda}\langle D_y, D_\xi\rangle} \mathrm{e}^{\mathrm{i}\lambda R(x,y)} \hat{H}(\lambda, \xi, x, y) a(x+y)|_{y=0,\xi=0} \\ &\sim \sum_{k=0}^{\infty} \frac{\mathrm{i}^k}{k!\lambda^k}\langle D_y, D_\xi\rangle^k \mathrm{e}^{\mathrm{i}\lambda R(x,y)} \hat{H}(\lambda, \xi, x, y) a(x+y)|_{y=0,\xi=0} \ . \end{aligned} \quad (3.29)$$

Due to the factor $\mathrm{e}^{\mathrm{i}\lambda R(x,y)}$ the k'th term in the asymptotic sum is not a monomial in $1/\lambda$ of order k times some derivatives of $\hat{H}$, but a polynomial of order $[k/3]$ in $1/\lambda$ times some derivatives of $\hat{H}$. This makes the ordering according to powers of $1/\lambda$ more complicated. In contrast, the asymptotic expansion of $\hat{H}$ is simple, if we furthermore assume that H has an asymptotic expansion $H \sim H_0 + \frac{1}{\lambda} H_1 + \frac{1}{\lambda^2} H_2 + O(\lambda^{-3})$. We then get

$$\begin{aligned}\hat{H}(\lambda\xi, x, y) &\sim \sum_{k=0}^{\infty} \frac{(\mathrm{i})^k}{k!(2\lambda)^k} \langle D_\xi, \varphi''(x) D_\xi\rangle^k \tilde{H}(\lambda; \xi + \varphi'(x), x + y/2) \\ &= \tilde{H}_0(\xi + \varphi'(x), x + y/2,) \\ &\quad + \lambda^{-1}\Big[\tilde{H}_1(\xi + \varphi'(x), x + y/2) - \frac{\mathrm{i}}{2}\langle \partial_\xi, \varphi''(x)\partial_\xi\rangle \tilde{H}_0(\xi + \varphi'(x), x + y/2)\Big] \\ &\quad + \lambda^{-2}\Big[\tilde{H}_2(\xi + \varphi'(x), x + y/2) - \frac{\mathrm{i}}{2}\langle \partial_\xi, \varphi''(x)\partial_\xi\rangle \tilde{H}_1(\xi + \varphi'(x), x + y/2) \\ &\qquad\qquad - \frac{1}{8}\langle \partial_\xi \varphi''(x)\partial_\xi\rangle^2 \tilde{H}_0(\xi + \varphi'(x), x + y/2)\Big] \\ &\quad + O(\lambda^{-3}) ,\end{aligned}$$

and the k'th term in the sum is of order λ^{-k}. Finally we can write down the first few terms in the asymptotic expansion of $b(\lambda, x)$ for $\lambda \to \infty$,

$$\begin{aligned}b(\lambda, x) =& \tilde{H}_0(\varphi'(x), x)a(x) \\ &+ \lambda^{-1}\Big[\tilde{H}_1(\varphi'(x), x)a(x) - \frac{\mathrm{i}}{2}\langle \partial_\xi, \varphi''(x)\partial_\xi\rangle \tilde{H}_0(\varphi'(x), x)a(x) \\ &\qquad - \frac{\mathrm{i}}{2} a(x)\langle \partial_x, \partial_\xi\rangle \tilde{H}_0(\varphi'(x), x) - \mathrm{i}\langle \partial_\xi \tilde{H}_0(\varphi'(x), x), \partial_x a(x)\rangle\Big] \\ &+ O(\lambda^{m-2}) .\end{aligned}$$

Before we come to the proof of Theorem 3.2.10 we state a lemma which allows us to handle the contribution of $\mathrm{e}^{\mathrm{i}\lambda R(x,y)}$ to the asymptotic sums (3.28) and (3.29).

Lemma 3.2.11. *Assume $\varphi \in C^\infty(\mathbb{R}^d)$ satisfies $\partial^\alpha \varphi(0) = 0$ for all $|\alpha| < k$, then*

$$\partial^\alpha \mathrm{e}^{\mathrm{i}\lambda\varphi(x)}|_{x=0} = O(\lambda^{[\frac{|\alpha|}{k}]}) \quad \text{for } \lambda \to \infty ,$$

and for all $\alpha \in \mathbb{Z}_+^d$, where $\left[\frac{|\alpha|}{k}\right]$ denotes the integer part of $\frac{|\alpha|}{k}$.

Proof. We first treat the simplest case that the phase function is a monomial, $\varphi(x) = a_\alpha x^\alpha$, $\alpha \in \mathbb{Z}_+^d$, then

$$\mathrm{e}^{\mathrm{i}\lambda\varphi(x)} = \mathrm{e}^{\mathrm{i}\lambda a_\alpha x^\alpha} = \sum_{l=0}^{\infty} \frac{(\mathrm{i}\lambda a_\alpha)^l}{l!} x^{\alpha l} ,$$

and so one can read off the derivatives as

$$\partial^\beta \mathrm{e}^{\mathrm{i}\lambda a_\alpha x^\alpha}|_{x=0} = \begin{cases} \frac{\beta!}{l!}(\mathrm{i}\lambda a_\alpha)^{\frac{|\beta|}{|\alpha|}} & \text{if } \beta = l\alpha \text{ for some } l \in \mathbb{N} \\ 0 & \text{if } \beta \text{ is not an integer multiple of } \alpha \end{cases} . \tag{3.30}$$

To treat the general case we expand φ into a Taylor series. Since

$$\partial^\beta \mathrm{e}^{\mathrm{i}\lambda\varphi(x)}|_{x=0} = 0$$

if $\partial^\alpha \varphi(x)|_{x=0} = 0$ for all $\alpha \le \beta$, it is sufficient to take the Taylor series up to order $|\beta|$ if one wants to study derivatives up to order $|\beta|$. So we can take

$$\varphi(x) = \sum_{k \le |\alpha| \le |\beta|} a_\alpha x^\alpha ,$$

and then use the factorization

$$\mathrm{e}^{\mathrm{i}\lambda \sum_{k\le|\alpha|\le|\beta|} a_\alpha x^\alpha} = \prod_{k\le|\alpha|\le|\beta|} \mathrm{e}^{\mathrm{i}\lambda a_\alpha x^\alpha} .$$

The derivative of a product $\prod_{j\in J} f_j$, where J is some index set, is given by the Leibnitz rule,

$$\partial^\beta \left(\prod_{j\in J} f_j \right) = \sum_{\substack{\{\gamma_j\}_{j\in J} \\ \sum_{j\in J}\gamma_j = \beta}} \frac{\beta!}{\prod_{j\in J}\gamma_j!} \prod_{j\in J} \partial^{\gamma_j} f_j ,$$

see e.g. [Com74]. The sum is over all partitions of $\beta \in \mathbb{Z}^d_+$ into $|J|$ multiindices $\gamma_j \in \mathbb{Z}^d_+$. In our case the index set consists of all multiindices α with $k \le |\alpha| \le |\beta|$, which we call $J_{k,\beta}$. Then we obtain

$$\partial^\beta \mathrm{e}^{\mathrm{i}\lambda\varphi(x)} = \sum_{\substack{\{\gamma_\alpha\}_{\alpha\in J_{k,\beta}} \\ \sum_{\alpha\in J_{k,\beta}}\gamma_\alpha = \beta}} \frac{\beta!}{\prod_{\alpha\in J_{k,\beta}}\gamma_\alpha!} \prod_{\alpha\in J_{k,\beta}} \partial^{\gamma_\alpha} \mathrm{e}^{\mathrm{i}\lambda a_\alpha x^\alpha} .$$

By equation (3.30) we know that $\partial^{\gamma_\alpha}\mathrm{e}^{\mathrm{i}\lambda a_\alpha x^\alpha}$ is not zero at $x = 0$ if and only if $\gamma_\alpha = l_\alpha \alpha$ for some $l_\alpha \in \mathbb{N}$, therefore we get as a necessary condition that the whole product

$$\prod_{k\le|\alpha|\le|\beta|} \partial^{\gamma_\alpha} \mathrm{e}^{\mathrm{i}\lambda a_\alpha x^\alpha} \tag{3.31}$$

is not zero at $x = 0$, that

$$\beta = \sum_{k\le|\alpha|\le|\beta|} \gamma_\alpha = \sum_{k\le|\alpha|\le|\beta|} l_\alpha \alpha , \tag{3.32}$$

for some $l_\alpha \in \mathbb{N}$. Now according to (3.30) the product (3.31) evaluated at $x = 0$ is of order

$$\lambda^{\sum l_\alpha} ,$$

so we must estimate $\sum l_\alpha$. But by taking the absolute value of (3.32) (in the sense of multi-indices, i.e. $|\beta| = \sum_1^d \beta_j$) we get

$$|\beta| = \left| \sum_{k\le|\alpha|\le|\beta|} l_\alpha \alpha \right| = \sum_{k\le|\alpha|\le|\beta|} l_\alpha |\alpha| \ge k \sum l_\alpha \ ,$$

and since $\sum l_\alpha$ is an integer we obtain the estimate

$$\sum l_\alpha \le \left[\frac{|\beta|}{k} \right] \ ,$$

and the proof is complete. □

Proof of Theorem 3.2.10. The action of $\mathcal{H}$ on the oscillating function $a(x)\mathrm{e}^{\mathrm{i}\lambda\varphi(x)}$ is given by

$$\begin{aligned} \mathcal{H}(a\mathrm{e}^{\mathrm{i}\lambda\varphi})(x) &= \left(\frac{\lambda}{2\pi}\right)^d \iint \mathrm{e}^{\mathrm{i}\lambda\langle x-y,\xi\rangle} H(\lambda;\xi,(x+y)/2)a(y)\mathrm{e}^{\mathrm{i}\lambda\varphi(y)}\ \mathrm{d}y\mathrm{d}\xi \\ &= \left(\frac{\lambda}{2\pi}\right)^d \iint \mathrm{e}^{\mathrm{i}\lambda[\langle x-y,\xi\rangle+\varphi(y)]} H(\lambda;\xi,(x+y)/2)a(y)\ \mathrm{d}y\mathrm{d}\xi \ . \end{aligned}$$

The main contributions to this integral come from the points where the phase function $\langle x-y,\xi\rangle + \varphi(y)$ is real valued and stationary. The stationary points are determined by the equations

$$-\xi + \varphi'(y) = 0 \ , \qquad x - y = 0 \ ,$$

so we get as stationary points

$$y = x \ , \quad \text{and} \quad \xi = \varphi'(x) \ .$$

Now we introduce a smooth cutoff function $\chi(\xi)$, such that $\chi(\xi) = 1$ in a neighborhood of $\xi = \varphi'(x)$ and with support in a larger neighborhood of $\xi = \varphi'(x)$. Then we split the integral into two parts,

$$\mathcal{H}(a\mathrm{e}^{\mathrm{i}\lambda\varphi})(x) = I_1(\lambda,x) + I_2(\lambda,x) \ ,$$

with

$$\begin{aligned} I_1(\lambda,x) &= \left(\frac{\lambda}{2\pi}\right)^d \iint \mathrm{e}^{\mathrm{i}\lambda[\langle x-y,\xi\rangle+\varphi(y)]}\chi(\xi)H(\lambda;\xi,(x+y)/2)a(y)\ \mathrm{d}y\mathrm{d}\xi \ , \\ I_2(\lambda,x) &= \left(\frac{\lambda}{2\pi}\right)^d \iint \mathrm{e}^{\mathrm{i}\lambda[\langle x-y,\xi\rangle+\varphi(y)]}(1-\chi(\xi))H(\lambda;\xi,(x+y)/2)a(y)\ \mathrm{d}y\mathrm{d}\xi \ . \end{aligned}$$

According to the principle of non-stationary phase, Theorem D.1, the second integral can be estimated as [1]

$$|I_2(\lambda,x)| \leq C_N \lambda^{-N}$$

for every $N \in \mathbb{N}$, so we are left with the integral $I_1(\lambda,x)$. Here we introduce the Taylor series of $\varphi(y)$ around the stationary point $y = x$,

$$\varphi(y) = \varphi(x) + \langle \varphi'(x), y-x\rangle + \frac{1}{2}\langle y-x, \varphi''(x)(y-x)\rangle + r(x,y) \ ,$$

which gives, together with a substitution $y \mapsto y + x$,

$$I_1(\lambda,x) = \mathrm{e}^{\mathrm{i}\lambda\varphi(x)} \left(\frac{\lambda}{2\pi}\right)^d \iint \mathrm{e}^{-\mathrm{i}\lambda[\langle y,\xi-\varphi'(x)\rangle - \frac{1}{2}\langle y,\varphi''(x)y\rangle - R(x,y)]} \\ \chi(\xi) H(\lambda;\xi,x+y/2) a(x+y)\ \mathrm{d}y\mathrm{d}\xi \ ,$$

where

$$R(x,y) = r(x,y+x) = \varphi(x+y) - \varphi(x) - \langle \varphi'(x), y\rangle - \frac{1}{2}\langle y, \varphi''(x) y\rangle \ .$$

A further substitution $\xi \mapsto \xi + \varphi'(x)$ would now be desirable, but since $\varphi'(x)$ can be complex valued, we can not simply insert it into $\chi(\xi)H(\lambda;\xi,x+y/2)$. Instead we choose an almost analytic extension $\tilde{\chi}(\xi)\tilde{H}(\lambda;\xi,x+y/2)$. Then Stokes theorem in d-dimensions gives for the ξ-integral

$$\int \mathrm{e}^{-\mathrm{i}\lambda\langle y,\xi-\varphi'(x)\rangle} \chi(\xi) H(\lambda;\xi,x+y/2)\ \mathrm{d}\xi = \\ \int \mathrm{e}^{-\mathrm{i}\lambda\langle y,\xi\rangle} \tilde{\chi}(\xi+\varphi'(x))) \tilde{H}(\lambda;\xi+\varphi'(x),x+y/2,))\ \mathrm{d}\xi \\ - \int_D \mathrm{d}\big(\mathrm{e}^{-\mathrm{i}\lambda\langle y,\xi-\varphi'(x)\rangle} \left[\tilde{\chi}(\xi)\tilde{H}(\lambda;\xi,x+y/2)\right]\ \mathrm{d}\xi\big) \ ,$$

where D is the $d+1$ dimensional (over $\mathbb{R}$) submanifold of $\mathbb{C}^d$ which is bounded by $\mathbb{R}^d$ and $\mathbb{R}^d + \varphi'(x)$, and $\mathrm{d}\xi$ stands for the differential form $\mathrm{d}\xi_1 \wedge \cdots \wedge \mathrm{d}\xi_d$. Now the $(d+1)$-form

[1] Strictly speaking Theorem D.1 is not applicable, because the support of the integrand of I_2 is not compact. But by using a suitable partition of unity, e.g., the one in the proof of [Hör83, Theorem7.8.2], one can extend the case with compact support to the case of non-compact support if the integrand satisfies some symbol estimates, as the one in I_2 does.

in the last integral is

$$\begin{aligned}\mathrm{d}\big(\mathrm{e}^{-\mathrm{i}\lambda\langle y,\xi-\varphi'(x)\rangle}\tilde f(\xi)\,\mathrm{d}\xi_1\wedge\cdots\wedge\mathrm{d}\xi_d\big) &= \sum_{i=1}^{d} -\mathrm{i}\lambda y_i \mathrm{e}^{-\mathrm{i}\lambda\langle y,\xi-\varphi'(x)\rangle}\tilde f(\xi)\,\mathrm{d}\xi_i\wedge\mathrm{d}\xi_1\wedge\cdots\wedge\mathrm{d}\xi_d \\ &\quad + \sum_{i=1}^{d}\mathrm{e}^{-\mathrm{i}\lambda\langle y,\xi-\varphi'(x)\rangle}\frac{\partial\tilde f}{\partial\bar\xi_i}(\xi)\,\mathrm{d}\bar\xi_i\wedge\mathrm{d}\xi_1\wedge\cdots\wedge\mathrm{d}\xi_d \\ &= \mathrm{e}^{-\mathrm{i}\lambda\langle y,\xi-\varphi'(x)\rangle}\sum_{i=1}^{d}\frac{\partial\tilde f}{\partial\bar\xi_i}(\xi)\,\mathrm{d}\bar\xi_i\wedge\mathrm{d}\xi_1\wedge\cdots\wedge\mathrm{d}\xi_d\end{aligned}$$

where we have used the abbreviation $\tilde f(\xi)=\tilde\chi(\xi)\tilde H(\lambda;\xi,x+y/2)$. Hence we get for the integral over D

$$\begin{aligned}&\int_D \mathrm{d}\big(\mathrm{e}^{-\mathrm{i}\lambda\langle y,\xi-\varphi'(x)\rangle}\Big[\tilde\chi(\xi)\tilde H(\lambda;\xi,x+y/2)\Big]\,\mathrm{d}\xi\big) \\ &\quad = \int_D \mathrm{e}^{-\mathrm{i}\lambda\langle y,\xi-\varphi'(x)\rangle}\sum_{i=1}^{d}\partial[\tilde\chi(\xi)\tilde H(\lambda;\xi,x+y/2)]/\partial\bar\xi_i\,\mathrm{d}\bar\xi_i\wedge\mathrm{d}\xi_1\wedge\cdots\wedge\mathrm{d}\xi_d\ ,\end{aligned}$$

and if we insert the asymptotic expansion for the symbol, we obtain a sum of terms of the form

$$K_k := \lambda^{m-k}\int_D \mathrm{e}^{-\mathrm{i}\lambda\langle y,\xi-\varphi'(x)\rangle}\sum_{i=1}^{d}\partial[\tilde\chi(\xi)\tilde H_{m-k}(\lambda;\xi,x+y/2)]/\partial\bar\xi_i\,\mathrm{d}\bar\xi_i\wedge\mathrm{d}\xi_1\wedge\cdots\wedge\mathrm{d}\xi_d$$

and by the almost analyticity condition and the fact that the integral is over a compact domain, we can estimate this integral as

$$|K_k|\le\lambda^{m-k}C_N|\operatorname{Im}\varphi'(x)|^N\ ,$$

for all $N\in\mathbb{N}$. But since $|\operatorname{Im}\varphi'(x)|\le C\operatorname{Im}\varphi(x)^{1/2}$, see [Hör83, Lemma 7.7.2], we have by Lemma 3.2.6

$$|\mathrm{e}^{\mathrm{i}\lambda\varphi}K_k|\le\lambda^{m-k}C_N\lambda^{-N/2}\ ,$$

for all $N\in\mathbb{N}$ and each k. Therefore we have now arrived at

$$\begin{aligned}&\mathcal{H}(a\mathrm{e}^{\mathrm{i}\lambda\varphi})(x) \\ &\quad = \mathrm{e}^{\mathrm{i}\lambda\varphi(x)}\left(\frac{\lambda}{2\pi}\right)^d\iint \mathrm{e}^{-\mathrm{i}\lambda[\langle y,\xi\rangle-\frac12\langle y,\varphi''(x)y\rangle]} \\ &\qquad\qquad \mathrm{e}^{\mathrm{i}\lambda R(x,y)}\tilde\chi(\xi+\varphi'(x))\tilde H(\lambda;\xi+\varphi'(x),x+y/2,)a(x+y)\ \mathrm{d}y\mathrm{d}\xi \\ &\qquad\qquad + O(\lambda^{-\infty})\ .\end{aligned}$$

To proceed we use Lemma B.1, the quadratic form is given by $Q = \lambda\mathrm{i}\left(\begin{smallmatrix} 0 & -I \\ -I & \varphi''(x)\end{smallmatrix}\right)$, so we have $[\det Q/2\pi]^{-1/2} = (2\pi/\lambda)^d$ and $Q^{-1} = \mathrm{i}/\lambda\left(\begin{smallmatrix} \varphi''(x) & I \\ I & 0\end{smallmatrix}\right)$. Hence we can finally write $\mathcal{H}(a\mathrm{e}^{\mathrm{i}\lambda\varphi})(x)$ modulo terms of order $O(\lambda^{-\infty})$ as

$$\begin{aligned} &\mathcal{H}(a\mathrm{e}^{\mathrm{i}\lambda\varphi})(x) \\ &\quad\equiv \mathrm{e}^{\mathrm{i}\lambda\varphi(x)}\mathrm{e}^{\frac{\mathrm{i}}{\lambda}(\langle D_y, D_\xi\rangle + \frac{1}{2}\langle D_\xi, \varphi''(x) D_\xi\rangle)}\mathrm{e}^{\mathrm{i}\lambda R(x,y)}\tilde{H}(\lambda; \xi + \varphi'(x), x + y/2,)a(x+y)|_{y=0,\xi=0} \ , \end{aligned}$$

where we have furthermore used the fact that $\tilde{\chi}(\xi + \varphi'(x))$ is flat as a function of ξ in the neighborhood of $\xi = 0$.

Finally, since $\partial_x^\alpha R(x,y)_{x=y} = 0$ for $|\alpha| \leq 3$, we get from Lemma 3.2.11 that the k'th term in the asymptotic sum (3.28) is of order $\lambda^{m+[k/3]-k}$. □

The result becomes much simpler if the phase function is quadratic, because then $R(x,y) = 0$. This is in particular the case for coherent states of the form

$$u_{p,q}^B(\lambda, x) = \left(\frac{\lambda}{\pi}\right)^{d/4} (\det \operatorname{Im} B)^{1/4} \mathrm{e}^{\mathrm{i}\lambda[\langle p, x-q\rangle + \langle x-q, B(x-q)\rangle/2]} \ , \tag{3.33}$$

where B is a complex $d \times d$ matrix with $\operatorname{Im} B \geq 0$.

Corollary 3.2.12. *Let $\mathcal{H}$ have Weyl symbol $H \in S^0(m_{a,b})$, then modulo $O(\lambda^{-\infty})$*

$$\mathcal{H}u_{p,q}^B(\lambda, x) = \mathrm{e}^{\frac{\mathrm{i}}{2\lambda}[\langle\partial_\eta, B\partial_\eta\rangle + \langle\partial_\eta, \partial_y\rangle]}\tilde{H}(\lambda; \eta + p + B(x-q), y + q + (x-q))|_{\eta=y=0}\, u_{p,q}^B(\lambda, x) \ ,$$

where $\tilde{H}$ denotes an almost analytic extension of H.

What kind of classical states can be quantized as oscillating integrals with complex phase functions? One might think that since every classical state is a superposition of delta-functions, we just have to superimpose coherent-states like (3.33). But this will in general not work, because the relative phase-factors cannot be chosen properly. To explain this, we assume that we have a classical state which is concentrated on some κ-dimensional submanifold Λ of phase space which we assume to be locally parameterized by some subset U of $\mathbb{R}^\kappa$,

$$\Lambda = \{(p(\theta), q(\theta)) \ |\theta \in U \subset \mathbb{R}^\kappa\} \ .$$

Furthermore it should have relative weight $a(\theta) \in C_0^\infty(U)$, i.e. the value of the state on a observable $b(p,q)$ is

$$\int b(p(\theta), q(\theta)) a(\theta) \, \mathrm{d}\theta \ . \tag{3.34}$$

Now a natural ansatz for a corresponding quantum state is

$$\begin{aligned} \psi(\lambda, x) &= \int \mathrm{e}^{\mathrm{i}\lambda S(\theta)} u^{B(\theta)}_{p(\theta),q(\theta)}(\lambda, x) a(\theta) \, \mathrm{d}\theta \\ &= \left(\frac{\lambda}{\pi}\right)^{d/4} \int \mathrm{e}^{\mathrm{i}\lambda S(\theta)} \mathrm{e}^{\mathrm{i}\lambda[\langle p(\theta), x-q(\theta)\rangle + \frac{1}{2}\langle B(\theta)(x-q(\theta)), x-q(\theta)\rangle]} a(\theta) \, \mathrm{d}\theta \ , \end{aligned} \tag{3.35}$$

where we have inserted a not yet specified real valued function $S(\theta)$, which determines the relative phases with which the coherent states are superimposed. A minimal condition that $\psi(\lambda, x)$ is a quantization of (3.34) is that the frequency set of $\psi(\lambda, x)$ should be an open subset of Λ. According to (3.21) the frequency set of $\psi(\lambda, x)$ is contained in the set

$$\{(p(\theta), q(\theta)) \,|\, p(\theta)q'_{\theta_i}(\theta) + S'_{\theta_i}(\theta) = 0 \,, i = 1, \dots, \kappa\} \ .$$

We therefore have to find a function $S(\theta)$ which satisfies the equations

$$p(\theta)q'_{\theta_i}(\theta) + S'_{\theta_i}(\theta) = 0 \ , \quad i = 1, \dots, \kappa \ ,$$

in order that the frequency set has the desired property. But this equation for S can be written in the form

$$\mathrm{d}S_\Lambda = -p\mathrm{d}q|_\Lambda \ ,$$

and a necessary and sufficient condition that this equation has a local solution is

$$\mathrm{d}(-q\mathrm{d}p)|_\Lambda = \mathrm{d}p \wedge \mathrm{d}q|_\Lambda = 0 \ ,$$

i.e. the symplectic form $\omega = \mathrm{d}p \wedge \mathrm{d}q$ should vanish on Λ. A manifold Λ with this property is called an isotropic manifold, and its dimension cannot be larger than d and in case it is equal to d the manifold is called Lagrangian. So we arrive at the conclusion that with superpositions of coherent states in the simple form (3.35) with a relative phase of the type $\mathrm{e}^{\mathrm{i}\lambda S(\theta)}$, we can only quantize classical states which are concentrated on isotropic submanifolds of phase space. We will see that this is as well the case for all oscillatory integrals with complex valued phase functions, the one with real valued phase functions allow the quantization of Lagrangian submanifolds, and the more general ones with complex valued phase functions allow the quantization of isotropic submanifolds.

On the other hand one can of course represent every state as a superposition of coherent states, since, as is well known, the set of coherent states (3.33) forms a complete set of states in $L^2(\mathbb{R}^d)$ when (p, q) runs through $\mathbb{R}^d \times \mathbb{R}^d$. But the dependence of the coefficients of the superposition of coherent states on the parameter λ will generally be not of the simple form $\mathrm{e}^{\mathrm{i}\lambda S}$.

3.3 Coherent states and their geometry

An important special case of Lagrangian states are coherent states which are concentrated in one point, and have quadratic phase functions.

Definition 3.3.1. *Let $(p, q) \in T^*M$ and let B be a $d \times d$ matrix with strictly positive imaginary part,*

$$\operatorname{Im} B > 0 \ ,$$

then we will call a state which in some local coordinates on M around $q \in M$ is given by

$$u_{p,q}^B(\lambda, x) := \left(\frac{\lambda}{\pi}\right)^{1/4} (\det \operatorname{Im} B)^{1/4} \mathrm{e}^{\mathrm{i}\lambda[\langle p, x-q\rangle + \frac{1}{2}\langle x-q, B(x-q)\rangle]} \ , \tag{3.36}$$

*a **coherent state** centered at (p, q).*

Coherent states are well known, they have been introduced already in the beginning of quantum mechanics [Sch26], and have been used in many areas since then, see e.g. [Per86]. In a semiclassical context they have been used for instance by Hagedorn, Combescure and coworkers, and a more general class of coherent states has been used by Paul and Uribe, see [Pau97] for a review. We will here concentrate on geometrical properties of them and emphasise especially the link to complex linear symplectic geometry.

Since the phase function of the state (3.36) is quadratic, we expect the corresponding Lagrangian manifold to be linear. In fact, if the phase function is

$$\langle p, x-q\rangle + \frac{1}{2}\langle x-q, B(x-q)\rangle$$

then the associated Lagrangian manifold is

$$\{(p + B(x-q), x);\ x \in \mathbb{R}^d\} = \{(p + Bx, q + x);\ x \in \mathbb{R}^d\} \ ,$$

which is a d-dimensional subspace of the $2d$-dimensional tangent space $T_{(p,q)}(T^*M)$. If B is complex we have to pass to the complexification of the tangent space, and get a complex Lagrangian plane in it.

The geometrical structures associated with this construction will be discussed in the next subsection.

3.3.1 Complex linear symplectic geometry

We have to recapitulate some linear symplectic geometry with emphasis on the complex case. Most material of this section has been collected from [Hör85a, Chapter 21.6], [Fol89, Chapter 4] and [RZ84].

Let V be a symplectic vector space over $\mathbb{R}$ of dimension $2d$ with symplectic form ω and denote by $V^{\mathbb{C}}$ its complexification. It is well known that one can always choose coordinates $(\xi_1, \dots, \xi_d, x_1, \dots, x_d)$ in which the symplectic form is $\omega = \mathrm{d}\xi \wedge \mathrm{d}x$; such coordinates are called symplectic coordinates. Often the symplectic form is represented by a skew-symmetric matrix, in symplectic coordinates this matrix is

$$\mathcal{J}_0 = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \ ,$$

i.e. one has for all $v, v' \in V$

$$\omega(v, v') = \langle v, \mathcal{J}_0 v' \rangle \ .$$

Recall that a subspace $L \subset V$, or $L \subset V^{\mathbb{C}}$, is called Lagrangian if $\dim L = d$, or $\dim_{\mathbb{C}} L = d$, respectively, and $\omega|_L = 0$, i.e.

$$\omega(l, l') = 0 \ , \quad \text{for all } l, l' \in L \ .$$

Definition 3.3.2. *The set of all Lagrangian planes in V is called the **Lagrangian Grassmannian** $\Lambda(V)$ and similarly $\Lambda(V^{\mathbb{C}})$ denotes the set of all Lagrangian planes in the complexification $V^{\mathbb{C}}$. A Lagrangian plane $L \in \Lambda(V^{\mathbb{C}})$ is called **positive** if*

$$\mathrm{i}\omega(\bar{l}, l) \geq 0$$

*for all $l \in L$, and **totally real** if*

$$\mathrm{i}\omega(\bar{l}, l) = 0$$

for all $l \in L$. The set of all positive Lagrangian planes in $V^{\mathbb{C}}$ will be denoted by $\Lambda^+(V^{\mathbb{C}})$.

Let L_0 be a totally real Lagrangian plane in $V^{\mathbb{C}}$ and consider the space of all positive Lagrangian planes transversal to L_0

$$\Lambda^+_{L_0}(V^{\mathbb{C}}) := \{L \in \Lambda^+(V^{\mathbb{C}})\,;\, L \cap L_0 = \{0\}\,\} \ .$$

We can choose symplectic coordinates (ξ, x) in $V^{\mathbb{C}}$ such that L_0 is defined by $x = 0$. Then every $L \in \Lambda^+_{L_0}(V^{\mathbb{C}})$ can be written as the graph of a linear function on $\mathbb{C}^d$,

$$L = \{(Bx, x)\,;\, x \in \mathbb{C}^d\} \ .$$

That L is Lagrangian means that

$$0 = \omega((Bx, x), (Bx', x')) = \langle Bx', x \rangle - \langle x, Bx' \rangle$$

for all $x, x' \in \mathbb{C}^d$, hence B is symmetric. Then the positivity of L gives

$$\mathrm{i}\omega((\bar{B}\bar{x}, \bar{x}), (Bx, x)) = \mathrm{i}(\langle \bar{B}\bar{x}, x \rangle - \langle \bar{x}, Bx \rangle) = 2\langle \bar{x}, \operatorname{Im} Bx \rangle \geq 0 \ ,$$

for all $x \in \mathbb{C}^d$, so $\operatorname{Im} B$ is positive. Therefore, the space $\Lambda^+_{L_0}(V^{\mathbb{C}})$ is isomorphic to the space of all symmetric $d \times d$ matrices with positive imaginary part. Notice that the scalar product $\langle \cdot, \cdot \rangle$ is bilinear and not sesquilinear, hence B is not hermitian.

Definition 3.3.3. *The set of symmetric $d \times d$ matrices B with complex entries and $\operatorname{Im} B > 0$ is called the **Siegel upper half-space** Σ_d.*

Now one can ask how large the set in $\Lambda^+(V^{\mathbb{C}})$ is which is not covered by $\Lambda^+_{L_0}(V^{\mathbb{C}})$. The answer is provided by the following lemma which can be proven exactly as in [Hör85a, Lemma 21.6.3].

Lemma 3.3.4. *If* $L_0 \in \Lambda^+(V^{\mathbb{C}})$ *then*

$$\{L \in \Lambda^+(V^{\mathbb{C}})\,;\ \dim(L \cap L_0) = k\}$$

is a submanifold of dimension $d(d+1)/2 - k(k+1)/2$.

Collecting the results on $\Lambda^+(V^{\mathbb{C}})$ we have:

Proposition 3.3.5. *The set* $\Lambda^+(V^{\mathbb{C}})$ *is an analytic manifold of (complex) dimension* $d(d+1)/2$, *which can be covered by a finite number of charts mapping the sets* $\Lambda^+_{L_0}(V^{\mathbb{C}})$ *onto the set of all symmetric* $d\times d$ *matrices with positive imaginary part. Since the set of symmetric matrices with positive imaginary part is contractible,* $\Lambda^+(V^{\mathbb{C}})$ *is contractible.*

Recall that the linear symplectic group $\mathrm{Sp}(d,\mathbb{R})$ consists of the $2d\times 2d$ matrices with real entries which leave the symplectic form ω invariant; in symplectic coordinates $\mathcal{S} \in \mathrm{Sp}(d,\mathbb{R})$ if

$$\mathcal{S}^\dagger \mathcal{J}_0 \mathcal{S} = \mathcal{J}_0\ , \quad \text{with } \mathcal{J}_0 = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}\ . \tag{3.37}$$

Some properties of $\mathrm{Sp}(d,\mathbb{R})$ which we will need below are collected in the following theorem.

Theorem 3.3.6. *Let* $\mathcal{S} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \in \mathrm{Sp}(d,\mathbb{R})$, *where* S_{ij} *are* $d \times d$ *matrices, then*

$$S_{11}^\dagger S_{21} = S_{21}^\dagger S_{11},\ \ S_{12}^\dagger S_{22} = S_{22}^\dagger S_{12},\ \ \textit{and}\ S_{11}^\dagger S_{22} - S_{21}^\dagger S_{12} = I\ , \tag{3.38}$$

and

$$\mathcal{S}^{-1} = -\mathcal{J}_0 \mathcal{S}^\dagger \mathcal{J}_0 \in \mathrm{Sp}(d,\mathbb{R})\ .$$

Furthermore, the following sets of matrices

$$\mathtt{N} := \left\{ \begin{pmatrix} I & A \\ 0 & I \end{pmatrix}\ ; A = A^\dagger \right\}\ , \quad \mathtt{D} := \left\{ \begin{pmatrix} A & 0 \\ 0 & A^{\dagger -1} \end{pmatrix}\ ; \det A \neq 0 \right\}\ ,$$

are subgroups of $\mathrm{Sp}(d,\mathbb{R})$, *and* $\mathrm{Sp}(d,\mathbb{R})$ *is generated by* $\mathtt{D} \cup \mathtt{N} \cup \{\mathcal{J}_0\}$.

The first assertion (3.38) is just (3.37) written out in block form and the second assertion follows from (3.37) by multiplication with $\mathcal{S}^{-1}$ from the right and $\mathcal{J}_0$ from the left. For the remaining assertions we refer to [Fol89, Propositions 4.9 and 4.10].

The linear symplectic group $\mathrm{Sp}(d,\mathbb{R})$ acts on the set of all Lagrangian planes. Via the representation of a complex Lagrangian plane by a complex symmetric matrix it induces an action on these matrices which we will now determine. Let $\mathcal{S} = \left(\begin{smallmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{smallmatrix}\right)$ be a symplectic matrix and $B \in \Sigma_d$, then we are looking for a matrix $\mathcal{S}_* B$ with

$$\mathcal{S} L_B = L_{\mathcal{S}_* B} \tag{3.39}$$

where $L_B = \{(Bx, x)\ ,\ x \in \mathbb{C}^d\}$ and similarly $L_{\mathcal{S}_*B} = \{(\mathcal{S}_*Bx, x)\ ,\ x \in \mathbb{C}^d\}$. Equation (3.39) means that for every $x \in \mathbb{C}^d$ there is a $y \in \mathbb{C}^d$ such that

$$(S_{11}B + S_{12})x = \mathcal{S}_*By$$
$$(S_{21}B + S_{22})x = y\ .$$

Inserting the second equation in the first one gives

$$\mathcal{S}_*B = (S_{11}B + S_{12})(S_{21}B + S_{22})^{-1}\ , \tag{3.40}$$

hence $\mathrm{Sp}(d, \mathbb{R})$ acts on Σ_d by "linear fractional" transformations. Notice that since B is invertible, (3.40) is well defined and it follows directly from the defining relation (3.39) that $\mathcal{S}_*(\mathcal{T}_*B) = (\mathcal{S}\mathcal{T})_*B$ for all $\mathcal{S}, \mathcal{T} \in \mathrm{Sp}(d, \mathbb{R})$, so it is indeed a group action.

We quote a theorem from [Fol89, Theorem 4.64] which collects some important properties of the action (3.40) of $\mathrm{Sp}(d, \mathbb{R})$ on Σ_d:

Theorem 3.3.7. *(a) If $B \in \Sigma_d$ and $\mathcal{S} \in \mathrm{Sp}(d, \mathbb{R})$ then $\mathcal{S}_*B \in \Sigma_d$.*
(b) For any $B_1, B_2 \in \Sigma_d$, there exists an $\mathcal{S} \in \mathrm{Sp}(d, \mathbb{R})$ with $\mathcal{S}_*B_1 = B_2$.
(c) $\{\mathcal{S} \in \mathrm{Sp}(d, \mathbb{R})\ ;\ \mathcal{S}_*(\mathrm{i}I) = \mathrm{i}I\} = \mathrm{Sp}(d, \mathbb{R}) \cap O(2d)$.

So by (b) $\mathrm{Sp}(d, \mathbb{R})$ acts transitively on Σ_d and (c) means that Σ_d is the quotient of $\mathrm{Sp}(d, \mathbb{R})$ by its maximal compact subgroup $\mathrm{Sp}(d, \mathbb{R}) \cap O(2d)$.

A strictly positive Lagrangian plane $L \subset V^{\mathbb{C}}$ gives V a complex structure, i.e. an endomorphism $\mathcal{J}$ with $\mathcal{J}^2 = -I$, and a compatible Hermitian form whose imaginary part is the symplectic form, see, e.g., [Hör85a, Proposition 21.5.7]. The real dimensions of L and V are equal, and since for $l \in L$, $l \neq 0$,

$$2\omega(\mathrm{Im}\, l, \mathrm{Re}\, l) = \mathrm{i}\omega(\bar{l}, l) > 0\ ,$$

the map

$$L \to V$$
$$l \mapsto \mathrm{Re}\, l \tag{3.41}$$

defines an isomorphism. The complex structure on V is now defined as the image under this map of the complex structure $l \mapsto \mathrm{i}l$ of L. The Hermitian form on V is then the push-forward to V under the isomorphism (3.41) of the form

$$\frac{\mathrm{i}}{2}\omega(\overline{l'}, l)$$

on L.

Proposition 3.3.8. *Denote by $\mathcal{J}_L$ the complex structure on V induced by L under the map (3.41), and by $\mathbf{h}_L$ the corresponding Hermitian form on V. Then we have for every $\mathcal{S} \in \mathrm{Sp}(d, \mathbb{R})$*

$$\mathcal{J}_{SL} = \mathcal{S}\mathcal{J}_L\mathcal{S}^{-1} \quad \text{and} \quad \mathbf{h}_{SL} = \mathcal{S}^{-1^\dagger}\mathbf{h}_L\mathcal{S}^{-1}\ . \tag{3.42}$$

If one has chosen symplectic coordinates (ζ, z) *in* $V^{\mathbb{C}}$ *such that* L *is represented as* $L = \{(Bz, z)\,,\ z \in \mathbb{C}^d\}$ *with* $\operatorname{Im} B > 0$*, then the complex structure is given by*

$$\mathcal{J}_L = \begin{pmatrix} \operatorname{Re} B[\operatorname{Im} B]^{-1} & -(\operatorname{Im} B + \operatorname{Re} B[\operatorname{Im} B]^{-1} \operatorname{Re} B) \\ [\operatorname{Im} B]^{-1} & -[\operatorname{Im} B]^{-1} \operatorname{Re} B \end{pmatrix}$$

and the real part of the Hermitian form $\mathbf{h}_L$ *is the positive definite real symmetric form given by*

$$\begin{aligned} \mathbf{g}_L &= \begin{pmatrix} [\operatorname{Im} B]^{-1} & -[\operatorname{Im} B]^{-1} \operatorname{Re} B \\ -\operatorname{Re} B[\operatorname{Im} B]^{-1} & \operatorname{Im} B + \operatorname{Re} B[\operatorname{Im} B]^{-1} \operatorname{Re} B \end{pmatrix} \\ &= \begin{pmatrix} I & 0 \\ -\operatorname{Re} B & I \end{pmatrix} \begin{pmatrix} [\operatorname{Im} B]^{-1} & 0 \\ 0 & \operatorname{Im} B \end{pmatrix} \begin{pmatrix} I & -\operatorname{Re} B \\ 0 & I \end{pmatrix} . \end{aligned}$$

Furthermore we have $\mathbf{g}_L \in \operatorname{Sp}(d, \mathbb{R})$ *and in particular* $\det \mathbf{g}_L = 1$.

Proof. The complex structure $\mathcal{J}_L$ is defined by

$$\mathcal{J}_L \operatorname{Re} l = \operatorname{Re} \mathrm{i} l \ , \quad \text{for every } l \in L \ . \tag{3.43}$$

Since for any $l \in L$ and $\mathcal{S} \in \operatorname{Sp}(d, \mathbb{R})$ one has $\operatorname{Re} \mathcal{S} l = \mathcal{S} \operatorname{Re} l$ and $\mathrm{i}\mathcal{S} = \mathcal{S}\mathrm{i}$, we get (with $l' = \mathcal{S} l \in \mathcal{S} L$)

$$\mathcal{J}_{\mathcal{S}L} \operatorname{Re} l' = \operatorname{Re} \mathrm{i} l' = \mathcal{S} \operatorname{Re} \mathrm{i} l = \mathcal{S}\mathcal{J}_L \operatorname{Re} l = \mathcal{S}\mathcal{J}_L\mathcal{S}^{-1} \operatorname{Re} \mathcal{S} l = \mathcal{S}\mathcal{J}_L\mathcal{S}^{-1} \operatorname{Re} l'$$

and hence $\mathcal{J}_{\mathcal{S}L} = \mathcal{S}\mathcal{J}_L\mathcal{S}^{-1}$. It is well known that for a given complex structure $\mathcal{J}_L$ on V the unique Hermitian form $\mathbf{h}_L$ with $\mathbf{h}_L(\mathcal{J}v, \mathcal{J}v') = \mathbf{h}_L(v, v')$ and $\operatorname{Im} \mathbf{h}_L = -\omega$ is given by

$$\mathbf{h}_L(v, v') = \omega(v, \mathcal{J}_L v') - \mathrm{i}\omega(v, v') \ ,$$

see e.g. [LM87, Proposition 10.6]. Therefore we get

$$\begin{aligned} \mathbf{h}_{\mathcal{S}L}(v, v') &= \omega(v, \mathcal{J}_{\mathcal{S}L} v') - \mathrm{i}\omega(v, v') \\ &= \omega(v, \mathcal{S}\mathcal{J}_L\mathcal{S}^{-1} v') - \mathrm{i}\omega(v, v') \\ &= \omega(\mathcal{S}^{-1}v, \mathcal{J}_L\mathcal{S}^{-1}v') - \mathrm{i}\omega(\mathcal{S}^{-1}v, \mathcal{S}^{-1}v') = \mathbf{h}_L(\mathcal{S}^{-1}v, \mathcal{S}^{-1}v') \ , \end{aligned}$$

where we have used that $\omega(\mathcal{S}^{-1}v, \mathcal{S}^{-1}v') = \omega(v, v')$ since $\mathcal{S}^{-1}$ is symplectic, and hence (3.42) is proven.

To prove the remaining part of the proposition we transform L by a symplectic transformation to a simple normal form, for which we can simply read off the complex and Hermitian structures. If L is given as $L = \{(Bz, z)\,,\ z \in \mathbb{C}^d\}$, then we can find an $\mathcal{S} \in \operatorname{Sp}(d, \mathbb{R})$ with $B = \mathcal{S}_* \mathrm{i} I$ because $\operatorname{Sp}(d, \mathbb{R})$ acts transitively on Σ_d. Explicitly we have

$$\mathcal{S} = \begin{pmatrix} I & C \\ 0 & I \end{pmatrix} \begin{pmatrix} A & 0 \\ 0 & A^{\dagger -1} \end{pmatrix} \ , \tag{3.44}$$

with $B = AA^\dagger\mathrm{i} + C$. But for $B = \mathrm{i}I$ one computes

$$\mathrm{Re}\,\mathrm{i}\begin{pmatrix}\mathrm{i}z\\ z\end{pmatrix} = \begin{pmatrix}-\mathrm{Re}\,z\\ -\mathrm{Im}\,z\end{pmatrix} = \begin{pmatrix}0 & -I\\ I & 0\end{pmatrix}\mathrm{Re}\begin{pmatrix}\mathrm{i}z\\ z\end{pmatrix} ,$$

and hence we get $\mathcal{J} = -\mathcal{J}_0$. Now the explicit expressions for $\mathcal{J}_L$ and $\mathbf{h}_L$ follow with (3.42) for $B = S_*\mathrm{i}I$

$$\mathcal{J}_L = -\mathcal{S}\mathcal{S}^\dagger\mathcal{J}_0 , \quad \text{and } h_L = (\mathcal{S}\mathcal{S}^\dagger)^{-1} - \mathrm{i}\mathcal{J}_0 ,$$

and inserting (3.44) gives the final expressions. The fact that $\mathbf{g}_L \in \mathrm{Sp}(d,\mathbb{R})$ follows from $\mathcal{S}, \mathcal{S}^\dagger \in \mathrm{Sp}(d,\mathbb{R})$. □

So every strictly positive Lagrangian plane L defines a positive definite quadratic form $\mathbf{g}_L$, i.e. a metric, on V, which is furthermore symplectic. We will call the space of these metrics G_d,

$$G_d := \{\mathbf{g} \in \mathrm{Sp}(d,\mathbb{R}) \,;\, \mathbf{g}^\dagger = \mathbf{g} \,, \mathbf{g} > 0\} .$$

Then the question arises if every element of G_d defines a Lagrangian plane. Let $\mathbf{g} \in G_d$, then by [Fol89, Proposition 4.22] there exists an $\mathcal{S} \in \mathrm{Sp}(d,\mathbb{R})$ with

$$\mathcal{S}^\dagger\mathbf{g}\mathcal{S} = \begin{pmatrix}D & 0\\ 0 & D\end{pmatrix} ,$$

where D is diagonal. And since $\mathcal{S}^\dagger\mathbf{g}\mathcal{S} \in \mathrm{Sp}(d,\mathbb{R})$ it follows from Theorem 3.3.6 that $D = I$, hence there exists an $\mathcal{S} \in \mathrm{Sp}(d,\mathbb{R})$ with

$$\mathbf{g} = (\mathcal{S}^\dagger\mathcal{S})^{-1} .$$

Now assume we have two such representations, i.e. there are $\mathcal{S}, \tilde{\mathcal{S}} \in \mathrm{Sp}(d,\mathbb{R})$ with

$$\mathbf{g} = (\mathcal{S}^\dagger\mathcal{S})^{-1} = (\tilde{\mathcal{S}}^\dagger\tilde{\mathcal{S}})^{-1} ,$$

then $\tilde{\mathcal{S}} = \mathcal{T}\mathcal{S}$ with $\mathcal{T} = \tilde{\mathcal{S}}\mathcal{S}^{-1} \in \mathrm{Sp}(d,\mathbb{R})$ and

$$\mathcal{T}^\dagger\mathcal{T} = 1 ,$$

hence $\mathcal{T} \in \mathrm{Sp}(d,\mathbb{R}) \cap O(2d)$. So the metric $\mathbf{g}$ determines $\mathcal{S}$ modulo an orthogonal matrix and together with Theorem 3.3.7 and Proposition 3.3.8 we get isomorphism between the sets of positive Lagrangian subspaces, the set of symmetric matrices with strictly positive imaginary part and the set of symplectic metrics on V:

Theorem 3.3.9.

$$\Sigma_d \cong \mathrm{Sp}(d,\mathbb{R})/(\mathrm{Sp}(d,\mathbb{R}) \cap O(2d)) \cong G_d .$$

In connection with the action of $\mathrm{Sp}(d,\mathbb{R})$ on Σ_d we will meet as well the so called multiplier

$$m(\mathcal{S},B) := [\det(S_{21}B+S_{22})]^{-1/2} \ , \tag{3.45}$$

for $B \in \Sigma_d$ and $\mathcal{S} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \in \mathrm{Sp}(d,\mathbb{R})$, see [Fol89]. We will not fix the sign at this place, but later on we will encounter the function $m(\mathcal{S},B)$ for a path of symplectic matrices starting at the identity, and then the sign will be fixed by continuity and the condition that $m(I,B)=1$. As can be checked by a direct calculation, the multiplier satisfies a cocycle identity

$$m(\mathcal{S}\mathcal{T},B) = m(\mathcal{S},\mathcal{T}_*B)m(\mathcal{T},B) \ . \tag{3.46}$$

We will now compute $m(\mathcal{S},B)$ for some simple examples. We introduce the totally real Lagrangian subspace

$$L_0 = \{(\xi,0)\,|\,\xi \in \mathbb{C}^d\} \ .$$

Lemma 3.3.10. *Assume L_0 is invariant under $\mathcal{S} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \in \mathrm{Sp}(d,\mathbb{R})$, i.e.*

$$\mathcal{S}L_0 = L_0 \ ,$$

then we have for any $B \in \Sigma_d$

$$m(\mathcal{S},B) = [\det S_{22}]^{-1/2}$$

Proof. That $\mathcal{S}L_0 = L_0$ means that $\mathcal{S}$ is of the form

$$\mathcal{S} = \begin{pmatrix} S_{11} & S_{12} \\ 0 & S_{22} \end{pmatrix} \ ,$$

and so the result follows from the definition (3.45). □

Next we want to study the case that B is invariant under the action of $\mathcal{S}$, $\mathcal{S}_*B = B$, which means that $\mathcal{S}$ is orthogonal with respect to the Euclidean form $\mathbf{g}$ defined by B on V. In order to simplify the calculations we transform B to the form $\mathrm{i}I$ for which the Euclidean form is the standard one. To this end we define

$$\mathcal{T}^{-1} := \begin{pmatrix} (\operatorname{Im} B)^{1/2} & \operatorname{Re} B(\operatorname{Im} B)^{-1/2} \\ 0 & (\operatorname{Im} B)^{-1/2} \end{pmatrix} \ ,$$

then $\mathcal{T} \in \mathrm{Sp}(d,\mathbb{R})$ and $\mathcal{T}_*^{-1}\mathrm{i}I = B$, $\mathcal{T}_*B = \mathrm{i}I$ and furthermore $\mathcal{T}L_0 = L_0$. Then

$$\begin{aligned} m(\mathcal{T}\mathcal{S}\mathcal{T}^{-1},\mathrm{i}I) &= m(\mathcal{T}\mathcal{S},\mathcal{T}_*^{-1}\mathrm{i}I)m(\mathcal{T}^{-1},\mathrm{i}I) \\ &= m(\mathcal{T},\mathcal{S}_*B)m(\mathcal{S},B)m(\mathcal{T}^{-1},\mathrm{i}I) \\ &= m(\mathcal{T},B)m(\mathcal{S},B)m(\mathcal{T}^{-1},\mathrm{i}I) \ , \end{aligned}$$

but since

$$\begin{aligned} m(\mathcal{T},B)m(\mathcal{T}^{-1},\mathrm{i}I) &= m(\mathcal{T},\mathcal{T}_*^{-1}\mathrm{i}I)m(\mathcal{T}^{-1},\mathrm{i}I) \\ &= m(\mathcal{T}\mathcal{T}^{-1},\mathrm{i}I) = m(1,\mathrm{i}I) = 1 \ , \end{aligned}$$

we get

$$m(\mathcal{T}\mathcal{S}\mathcal{T}^{-1},\mathrm{i}I) = m(\mathcal{S},B) \ .$$

Note that $\mathcal{T}\mathcal{S}\mathcal{T}^{-1} \in \mathrm{Sp}(d,\mathbb{R}) \cap O(2d)$, so we can restrict ourselves to the case that $B = \mathrm{i}I$ and $\mathcal{S} = \mathcal{O} \in \mathrm{Sp}(d,\mathbb{R}) \cap O(2d)$.

The behavior of $\mathcal{O}$ with respect to L_0 plays an important role. Define

$$D_{\mathcal{O}} := L_0 \cap \mathcal{O}L_0 \ ,$$

then $D_{\mathcal{O}}$ is isotropic and invariant under $\mathcal{O}$. Furthermore, its skew-orthogonal complement $D_{\mathcal{O}}^{\omega} := \{v \in V \,|\, \omega(v,w) = 0 \text{ for all } w \in D_{\mathcal{O}}\}$ is invariant under $\mathcal{O}$ too, and therefore $\mathcal{O}$ defines an orthogonal map on the reduced symplectic space

$$\hat{V}_{\mathcal{O}} := D_{\mathcal{O}}^{\omega}/D_{\mathcal{O}} \ ,$$

$$\hat{\mathcal{O}} : \hat{V}_{\mathcal{O}} \to \hat{V}_{\mathcal{O}} \ . \tag{3.47}$$

Lemma 3.3.11. *Let $\mathcal{O} \in \mathrm{Sp}(d,\mathbb{R}) \cap O(2d)$ and let $\hat{\mathcal{O}}$ be the reduced map* (3.47)*, then*

$$m(\mathcal{O},\mathrm{i}I) = m(\hat{\mathcal{O}},\mathrm{i}I) \ .$$

Let furthermore

$$(\mathrm{e}^{\mathrm{i}\varphi_1},\dots,\mathrm{e}^{\mathrm{i}\varphi_n},\mathrm{e}^{-\mathrm{i}\varphi_1},\dots,\mathrm{e}^{-\mathrm{i}\varphi_n})$$

be the eigenvalues of $\hat{\mathcal{O}}$ with $\varphi_i \in [0,\pi)$ for $i = 1,\cdots,n$, where $n = d - \dim(L_0 \cap \mathcal{O}L_0)$. Then we have

$$m(\hat{\mathcal{O}},\mathrm{i}I) = \mathrm{e}^{-\mathrm{i}\frac{1}{2}\sum_{j=1}^{n}\varphi_j} \ .$$

Proof. Since $B = \mathrm{i}I$ defines a Euclidean structure on V we can choose an orthogonal basis $v_1,\dots,v_d$ of L_0, such that $D_{\mathcal{O}}$ is spanned by $v_1,\dots,v_{d-n}$, and complete it to an symplectic and orthogonal basis $v_1,\dots,v_d,w_1,\cdots,w_d$ of V. The subspace $D_{\mathcal{O}}^{\omega}$ is spanned by $v_1,\dots,v_d,w_{d-n+1},\cdots,w_d$ and therefore we can identify $\hat{V}_{\mathcal{O}}$ with the subspace of V spanned by the vectors

$$v_{d-n+1},\dots,v_d,w_{d-n+1},\cdots,w_d \ .$$

If we denote the orthogonal complement of $\hat{V}_{\mathcal{O}}$, spanned by $v_1, \dots, v_{d-n}, w_1, \cdots, w_{d-n}$, by V_0 we have a decomposition of the symplectic vector space V into two symplectic subspaces

$$V = V_0 \oplus \hat{V}_{\mathcal{O}} \ .$$

Now both subspaces are invariant under $\mathcal{O}$, so $\mathcal{O}$ is in this basis block-diagonal

$$\mathcal{O} = \begin{pmatrix} \hat{\mathcal{O}} & 0 \\ 0 & \mathcal{O}_0 \end{pmatrix} \ ,$$

and therefore

$$m(\mathcal{O}, \mathrm{i}I) = m(\hat{\mathcal{O}}, \mathrm{i}I) m(\mathcal{O}_0, \mathrm{i}I) \ .$$

Now we have $V_0 = D_{\mathcal{O}} \oplus D_{\mathcal{O}}^{\perp}$, where $D_{\mathcal{O}}^{\perp}$ denotes the orthogonal complement of $D_{\mathcal{O}}$ in V_0. Since $D_{\mathcal{O}}$ is invariant under $\mathcal{O}_0$, $D_{\mathcal{O}}^{\perp}$ is invariant under $\mathcal{O}_0$ too, and so $\mathcal{O}_0$ is block-diagonal with respect to the splitting $V_0 = D_{\mathcal{O}} \oplus D_{\mathcal{O}}^{\perp}$. Because $D_{\mathcal{O}}$ and $D_{\mathcal{O}}^{\perp}$ are Lagrangian in V_0 we are in the situation of Lemma 3.3.10 with $L_0 = D_{\mathcal{O}}$ and S_{22} orthogonal, therefore we obtain

$$m(\mathcal{O}_0, \mathrm{i}I) = 1 \ .$$

In order to compute the remaining term, we can assume that $L_0 \cap \mathcal{O} L_0 = \{0\}$. We denote by $L_0^{\perp}$ the orthogonal complement of L_0 in V, and it is easy to see that $L_0^{\perp} \cap \mathcal{O} L_0^{\perp} = \{0\}$. Now V splits into two-dimensional $\mathcal{O}$ invariant subspaces V_j on which

$$\mathcal{O}|_{V_j} = \begin{pmatrix} \cos\varphi_j & -\sin\varphi_j \\ \sin\varphi_j & \cos\varphi_j \end{pmatrix} \qquad j = 1, \cdots, d \ ,$$

and since $L_0^{\perp} \cap \mathcal{O} L_0^{\perp} = \{0\}$ and $L_0 \cap \mathcal{O} L_0 = \{0\}$ we have $\dim V_j \cap L_0 = 1$ Then we find

$$m(\mathcal{O}, \mathrm{i}I) = \prod_j m(\mathcal{O}|_{V_j}, \mathrm{i}I) = \prod_j \mathrm{e}^{-\mathrm{i}\frac{1}{2}\varphi_j} = \mathrm{e}^{-\mathrm{i}\frac{1}{2}\sum_j \varphi_j} \ .$$

□

We can now give a general formula for the multiplier.

Proposition 3.3.12. *For any* $B \in \Sigma_d$ *and* $\mathcal{S} \in \mathrm{Sp}(d, \mathbb{R})$, *there are* $\mathcal{T}, \mathcal{P} \in \mathrm{Sp}(d, \mathbb{R})$ *with* $\mathcal{P}_* \mathrm{i}I = \mathcal{S}_* B$, $\mathcal{T}_* B = \mathrm{i}I$ *and* $\mathcal{T} L_0 = L_0$, $\mathcal{P} L_0 = L_0$ *such that*

$$\mathcal{S} = \mathcal{P}\mathcal{O}\mathcal{T}$$

with $\mathcal{O} \in \mathrm{Sp}(d, \mathbb{R}) \cap O(2d)$. *The multiplier is then given by*

$$m(\mathcal{S}, B) = \frac{(\det \mathrm{Im}\, \mathcal{S}_* B)^{1/4}}{(\det \mathrm{Im}\, B)^{1/4}} m(\mathcal{O}, \mathrm{i}I) \ .$$

Proof. Let $\mathcal{T},\mathcal{P}\in \mathrm{Sp}(d,\mathbb{R})$ be defined as

$$\mathcal{P} := \begin{pmatrix} (\operatorname{Im} S_*B)^{1/2} & \operatorname{Re} B(\operatorname{Im} S_*B)^{-1/2} \\ 0 & (\operatorname{Im} S_*B)^{-1/2} \end{pmatrix} \;, \quad \mathcal{T}^{-1} := \begin{pmatrix} (\operatorname{Im} B)^{1/2} & \operatorname{Re} B(\operatorname{Im} B)^{-1/2} \\ 0 & (\operatorname{Im} B)^{-1/2} \end{pmatrix} \;, \tag{3.48}$$

then $\mathcal{P}_*\mathrm{i}I = \mathcal{S}_*B$ and $\mathcal{T}^{-1}{}_*\mathrm{i}I = B$ and therefore there is a unique $\mathcal{O}\in \mathrm{Sp}(d,\mathbb{R})\cap O(2d)$ such that

$$\mathcal{S} = \mathcal{P}\mathcal{O}\mathcal{T} \;.$$

Now with the cocycle property (3.46) we obtain

$$\begin{aligned} m(\mathcal{S},B) &= m(\mathcal{P}\mathcal{O}\mathcal{T},B) \\ &= m(\mathcal{P}\mathcal{O},\mathcal{T}_*B)m(\mathcal{T},B) \\ &= m(\mathcal{P}\mathcal{O},\mathrm{i}I)m(\mathcal{T},B) \\ &= m(\mathcal{P},\mathcal{O}_*\mathrm{i}I)m(\mathcal{O},\mathrm{i}I)m(\mathcal{T},B) \\ &= m(\mathcal{P},\mathrm{i}I)m(\mathcal{O},\mathrm{i}I)m(\mathcal{T},B) \end{aligned}$$

and inserting the expressions (3.48) for $\mathcal{P}$ and $\mathcal{T}$ gives

$$m(\mathcal{P},\mathrm{i}I) = (\det \operatorname{Im} S_*B)^{1/4} \;, \quad \text{and} \quad m(\mathcal{T},B) = (\det \operatorname{Im} B)^{-1/4} \;.$$

□

3.3.2 Creation and annihilation operators

We have seen in the last section that a coherent state is associated with a complex Lagrangian plane L. Let $v\in V^{\mathbb{C}}\cong T^{\mathbb{C}}_{p,q}T^*\mathbb{R}^d$ and consider the linear form $\omega(v,\cdot)$ together with its Weyl quantization

$$\mathcal{P}_v := -\langle a, \frac{\mathrm{i}}{\lambda}\,\partial_x - p\rangle + \langle b, x-q\rangle$$

where $v=(a,b)$. Applying this operator to a coherent state $u^L_{p,q}$ centered at (p,q) gives

$$\begin{aligned} \mathcal{P}_v u^L_{p,q}(\lambda,x) &= [-\langle a, B(x-q)\rangle + \langle b, x-q\rangle] u^L_{p,q}(\lambda,x) \\ &= \omega(v,l_x)u^L_{p,q}(\lambda,x) \;, \end{aligned}$$

with $l_x := (B(x-q),(x-q))$. And since L is Lagrangian and $l_x\in L$ we get that

$$\mathcal{P}_v u^B_{p,q}(\lambda,x) = 0 \tag{3.49}$$

if and only if $v\in L$. As we will see in Section 3.4.3, the validity of condition (3.49) for all $v\in L$ characterizes the state $u^B_{p,q}(\lambda,x)$ uniquely. Because of relation (3.49) the operators $\mathcal{P}_l$

with $l \in L$ are called annihilation operators. The adjoint operators $\mathcal{P}_l^*$ are called creation operators.

From the product formula and the linearity of the symbols it follows immediately that

$$[\mathcal{P}_v, \mathcal{P}_{v'}] = \frac{\mathrm{i}}{\lambda}\, \omega(v, v')$$

and furthermore we have

$$\mathcal{P}_v^* = \mathcal{P}_{\bar{v}} \ .$$

Now, since $\mathrm{i}\omega(l, \bar{l}')$ is a nondegenerate Hermitian form on L, we can choose a basis l_j, $j = 1, \cdots, d$, of L which is orthonormal with respect to this form,

$$\mathrm{i}\omega(l_i, \bar{l}_j) = \delta_{ij} \ .$$

For the corresponding annihilation and creation operators we then obtain the relations

$$[\mathcal{P}_{l_i}, \mathcal{P}_{l_j}] = [\mathcal{P}_{l_i}^*, \mathcal{P}_{l_j}^*] = 0$$
$$[\mathcal{P}_{l_i}, \mathcal{P}_{l_j}^*] = \frac{1}{\lambda}\, \delta_{ij} \ ,$$

which are the classical commutator relations for annihilation and creation operators.

Given a basis l_j, $j = 1, \cdots, d$, of L, and $\alpha \in \mathbb{Z}_+^d$ being a multi-index, we define a higher order coherent state

$$u_{p,q}^L(\alpha) := \Pi_{j=1}^d \mathcal{P}_{l_j}^{*\,\alpha_j}\, u_{p,q}^L \ . \tag{3.50}$$

These states are orthogonal, more precisely, they satisfy

$$\langle u_{p,q}^L(\alpha), u_{p,q}^L(\alpha') \rangle = \frac{1}{\lambda^{|\alpha|}}\, \delta_{\alpha\alpha'} \ ,$$

which follows easily from the commutation relations for the creation and annihilation operators.

We finally want to study the representation of certain operators as polynomials in creation and annihilation operators. Since the set of vectors $l_1, \ldots, l_d, \bar{l}_1, \ldots, \bar{l}_d$ spans $V^{\mathbb{C}}$, we can represent any $v \in V^{\mathbb{C}}$ as a superposition

$$v = \sum_{j=1}^d \nu_j l_j + \mu_j \bar{l}_j \ ,$$

and therefore the corresponding linear differential operator is a linear combination of annihilation and creation operators,

$$\mathcal{P}_v = \sum_{j=1}^d \nu_j \mathcal{P}_{l_j} + \mu_j \mathcal{P}_{l_j}^* \ .$$

By iterating this procedure, it follows that for an operator $\mathcal{A}$ with Weyl symbol

$$a(z) = \sum_{|\alpha|\leq m} a_\alpha (z - z_0)^\alpha$$

one has a representation

$$\mathcal{A} = \sum_{|\alpha|\leq m} \frac{b_\alpha}{\lambda^{|\alpha|}} \mathcal{P}^\alpha \ .$$

Applying this representation to a state $u(\beta)$ yields

$$\mathcal{A}u(\beta) = \sum_{|\alpha|\leq m} \frac{c_\alpha}{\lambda^{|\alpha|}} u(\alpha + \beta) \ .$$

With some more work it is possible to get explicit expressions for the coefficients c_α in terms of the a_α, see, e.g., [Com92]. But for later applications it is sufficient to know that a state $u(\beta)$ is mapped by an operator whose Weyl symbol is a polynomial of degree m to a linear combination of states $u(\alpha + \beta)$ with $0 \leq |\beta| \leq m$.

3.3.3 Families of coherent states

We are now prepared for a closer study of the properties of coherent states. We have learned in Section 3.3.1 that the proper geometrical object associated with a coherent state is the complex Lagrangian plane L associated with the symmetric matrix B by

$$L := \{(p + Bz, q + z) \mid z \in \mathbb{C}^d\} \ .$$

Therefore we will denote the corresponding state by

$$u^L_{p,q}(\lambda, x) = \left(\frac{\lambda}{\pi}\right)^{d/4} (\det \operatorname{Im} B)^{1/4} \mathrm{e}^{\mathrm{i}\lambda[\langle p, x-q\rangle + \frac{1}{2}\langle x-q, B(x-q)\rangle]} \ ,$$

where B is the matrix which generates L.

It is well known that in $\mathbb{R}^d$ the usual set of coherent states form a complete set of states. For sake of completeness we here give a proof of it.

Proposition 3.3.13. *Let B be a complex symmetric $d \times d$ matrix with $\operatorname{Im} B > 0$, then the set of states*

$$u^L_{p,q}(\lambda, x) = \left(\frac{\lambda}{\pi}\right)^{d/4} (\det \operatorname{Im} B)^{1/4} \mathrm{e}^{\mathrm{i}\lambda[\langle p, x-q\rangle + \frac{1}{2}\langle x-q, B(x-q)\rangle]} \tag{3.51}$$

form a complete set of states in $L^2(\mathbb{R}^d)$ in the sense that we have

$$\left(\frac{\lambda}{2\pi}\right)^d \iint \overline{u^L_{p,q}}(\lambda, y) u^L_{p,q}(\lambda, x) \ \mathrm{d}p\mathrm{d}q = \delta(x - y) \ .$$

One can give a straightforward proof by directly calculating the integral, one only has to use Gaussian integrals. Since we will need the Wigner function of the coherent state (3.51) later on as well, we now give a proof via the Wigner function.

Lemma 3.3.14. *Let* $(p,q) \in \mathbb{R}^{2d}$ *and* B *be a complex symmetric matrix with strictly positive imaginary part, then the Wigner function of the coherent state*

$$u^L_{p,q}(\lambda,x) = \left(\frac{\lambda}{\pi}\right)^{d/4} (\det \operatorname{Im} B)^{1/4} \mathrm{e}^{\mathrm{i}\lambda[\langle p, x-q\rangle + \frac{1}{2}\langle x-q, B(x-q)\rangle]}$$

is given by

$$W^L_{p,q}(\xi,x) = \left(\frac{\lambda}{\pi}\right)^{d} \mathrm{e}^{-\lambda\langle(\xi-p,x-q),\mathbf{g}_L(\xi-p,x-q)\rangle} , \tag{3.52}$$

with

$$\begin{aligned}\mathbf{g}_L &= \begin{pmatrix} [\operatorname{Im} B]^{-1} & -[\operatorname{Im} B]^{-1}\operatorname{Re} B \\ -\operatorname{Re} B[\operatorname{Im} B]^{-1} & \operatorname{Im} B + \operatorname{Re} B[\operatorname{Im} B]^{-1}\operatorname{Re} B\end{pmatrix} \\ &= \begin{pmatrix} I & 0 \\ -\operatorname{Re} B & I\end{pmatrix}\begin{pmatrix} [\operatorname{Im} B]^{-1} & 0 \\ 0 & \operatorname{Im} B\end{pmatrix}\begin{pmatrix} I & -\operatorname{Re} B \\ 0 & I\end{pmatrix} ,\end{aligned} \tag{3.53}$$

and $\det \mathbf{g}_L = 1$.

Notice that the quadratic form in the exponential of the Wigner function is defined by the metric canonically associated with L by Proposition 3.3.8.

Proof. If we insert the expression for $u^L_{p,q}(\lambda,x)$ in the definition of the Wigner function

$$W^L_{p,q}(\xi,x) = \left(\frac{\lambda}{2\pi}\right)^{d} \int \mathrm{e}^{-\mathrm{i}\lambda\langle\xi,y\rangle}\overline{u}^B_{p,q}(\lambda,x-y/2)u^B_{p,q}(\lambda,x+y/2)\,\mathrm{d}y ,$$

we get

$$\begin{aligned} W^L_{p,q}(\xi,x) &= \left(\frac{\lambda}{2\pi}\right)^{d}\left(\frac{\lambda}{\pi}\right)^{d/2}(\det \operatorname{Im} B)^{1/2} \\ &\qquad \mathrm{e}^{-\lambda\langle x-q,\operatorname{Im} B(x-q)\rangle}\int \mathrm{e}^{-\lambda\langle y,\operatorname{Im} By\rangle/4}\mathrm{e}^{-\mathrm{i}\lambda\langle y,[\xi-p-\operatorname{Re} B(x-q)]\rangle}\,\mathrm{d}y \\ &= \left(\frac{\lambda}{\pi}\right)^{d}\mathrm{e}^{-\lambda\langle x-q,\operatorname{Im} B(x-q)\rangle}\mathrm{e}^{-\lambda\langle[\operatorname{Im} B]^{-1}(\xi-p-\operatorname{Re} B(x-q)),\xi-p-\operatorname{Re} B(x-q)\rangle}\end{aligned}$$

where we have evaluated the Gaussian integral according to Theorem D.2. Now expanding the product in the exponential leads to the result (3.52). □

Proof of Proposition 3.3.13. Since the Wigner function of a state u is by definition the Weyl symbol of the corresponding projection operator $|u\rangle\langle u|$, the completeness of the coherent states is equivalent to the relation

$$\iint W^L_{p,q}(\xi, x)\ \mathrm{d}p\mathrm{d}q = 1\ ,$$

which follows by inserting the formula (3.52) and then using $\det \mathbf{g}_L = 1$ in the evaluation of the Gaussian integral. □

We will sometimes find it useful to let the Lagrangian plane L vary with the point (p, q) on which the coherent state is concentrated. In other words, the metric tensor $\mathbf{g}$ defined by L is now no longer constant. This does not affect the normalization of $u^L_{p,q}(\lambda, x)$, but the completeness relation is only true asymptotically.

Theorem 3.3.15. *Let $B(p, q)$ be a smooth function with values in the complex symmetric $d \times d$ matrices with strictly positive imaginary part, and assume that for any $\alpha, \beta \in \mathbb{Z}^d_+$ there exists a constant $C_{\alpha,\beta}$ with*

$$||\partial_p^\alpha \partial_q^\beta B(p, q)|| \leq C_{\alpha,\beta}\ .$$

Then the states

$$u^L_{p,q}(\lambda, x) = \left(\frac{\lambda}{\pi}\right)^{d/4} (\det \operatorname{Im} B(p, q))^{1/4} \mathrm{e}^{\mathrm{i}\lambda[\langle p, x-q\rangle + \frac{1}{2}\langle x-q, B(p,q)(x-q)\rangle]}$$

satisfy the relation

$$\left(\frac{\lambda}{2\pi}\right)^d \iint |u^L_{p,q}\rangle\langle u^L_{p,q}|\ \mathrm{d}p\mathrm{d}q = 1 - \frac{1}{12\lambda}\mathbf{s}$$

where $\mathbf{s}$ is a pseudodifferential operator in $\Psi^0(1)$, with principal symbol given by the scalar curvature $s(p, q)$ of the Riemannian metric $\mathbf{g}_L$,

$$\sigma(\mathbf{s}) = s(p, q).$$

Proof. The Weyl symbol of the operator

$$\left(\frac{\lambda}{2\pi}\right)^d \iint |u^L_{p,q}\rangle\langle u^L_{p,q}|\ \mathrm{d}p\mathrm{d}q$$

is given by

$$\iint W^L_{p,q}(\xi, x)\ \mathrm{d}p\mathrm{d}q \tag{3.54}$$

with

$$W^L_{p,q}(\xi,x) = \left(\frac{\lambda}{\pi}\right)^d \mathrm{e}^{-\lambda\langle(p-\xi,q-x),\mathbf{g}(p,q)(p-\xi,q-x)\rangle}$$

being the Wigner function of $u^L_{p,q}(\lambda,x)$, see (3.52). Introducing the abbreviations $z=(\xi,x)$, $z'=(p,q)$ we can write (3.54) as

$$\begin{aligned}\left(\frac{\lambda}{\pi}\right)^d \int \mathrm{e}^{-\lambda\langle z'-z,\mathbf{g}(z')(z'-z)\rangle}\,\mathrm{d}z' &= \left(\frac{\lambda}{\pi}\right)^d \int \mathrm{e}^{-\lambda\langle z',\mathbf{g}(z+z')z'\rangle}\,\mathrm{d}z' \\ &= \left(\frac{\lambda}{\pi}\right)^d \int \mathrm{e}^{-\lambda\langle z',\mathbf{g}(z)z'\rangle}\mathrm{e}^{-\lambda\langle z',[\mathbf{g}(z+z')-\mathbf{g}(z)]z'\rangle}\,\mathrm{d}z'\ .\end{aligned}$$

We could easily evaluate the last integral using Lemma B.1, which gives

$$\mathrm{e}^{-\frac{1}{4\lambda}\langle D_{z'},\mathbf{g}^{-1}(z)D_{z'}\rangle}\mathrm{e}^{-\lambda\langle z',[\mathbf{g}(z+z')-\mathbf{g}(z)]z'\rangle}|_{z'=0}\ ,$$

and shows by the results of Appendix B that it defines a symbol in $S^0(1)$.

But in order to determine the next-to-leading part for $\lambda\to\infty$ it will be more convenient to introduce Riemannian normal coordinates for the metric $\mathbf{g}$ centered at z. Recall that (see, e.g., Theorem 2.17 and Corollary 2.3 in [Cha93]) in such coordinates the entries g_{ij} of the metric $\mathbf{g}$ are of the form

$$g_{ij}(z+z') = \delta_{ij} - \frac{1}{3}\mathrm{R}_{nimj}(z)z'^n z'^m + O(|z'|^3)\ ,$$

and for the determinant one has

$$\det\mathbf{g}(z+z') = 1 - \frac{1}{3}\mathrm{Ric}_{nm}(z)z'^n z'^m + O(|z'|^3)\ .$$

Here $\mathrm{R}_{nimj}(z)$ is the Riemann tensor of $\mathbf{g}$ at z, $\mathrm{Ric}_{nm}(z) := \mathrm{R}^i{}_{nim}(z) := g^{ij}\mathrm{R}_{injm}(z)$ is the Ricci tensor, where the summation convention is used, and g^{ij} are the entries of $\mathbf{g}^{-1}$. Since the change to normal coordinates will typically not be symplectic, the property $\det\mathbf{g}=1$ is lost, and the Riemannian volume element becomes $\sqrt{\det\mathbf{g}(z+z')}\,\mathrm{d}z'$ instead of $\mathrm{d}z'$.

Hence we get by Lemma B.1 for the integral in the new coordinates

$$\left(\frac{\lambda}{\pi}\right)^d \int \mathrm{e}^{-\lambda\langle z',z'\rangle}\mathrm{e}^{-\lambda R(z,z')}\sqrt{\det\mathbf{g}(z+z')}\,\mathrm{d}z' = \mathrm{e}^{\frac{1}{4\lambda}\langle\partial_{z'},\partial_{z'}\rangle}\sqrt{\det\mathbf{g}(z+z')}\mathrm{e}^{-\lambda R(z,z')}|_{z'=0}\ ,$$

with

$$R(z,z') = -\frac{1}{3}\mathrm{R}_{nimj}(z)z'^n z'^m z'^i z'^j + O(|z'|^5)$$

and

$$\sqrt{\det \mathbf{g}(z+z')} = 1 - \frac{1}{6}\mathrm{Ric}_{nm}(z) z'^n z'^m + O(|z'|^3) \ .$$

But since the Riemann tensor is antisymmetric in the first and in the second pair of indices, i.e. $\mathrm{R}_{nimj} = -\mathrm{R}_{inmj}$ and $\mathrm{R}_{nimj} = -\mathrm{R}_{nijm}$, we have $\mathrm{R}_{nimj}(z) z'^n z'^m z'^i z'^j = 0$ and thus

$$R(z,z') = O(|z'|^5) \ .$$

By Lemma 3.2.11 we see that therefore the exponent R gives no contribution of order $1/\lambda$ and so we get

$$\begin{aligned}\left(\frac{\lambda}{\pi}\right)^d \int \mathrm{e}^{-\lambda\langle z'-z, \mathbf{g}(z')(z'-z)\rangle} \, \mathrm{d}z' &= 1 - \frac{1}{24\lambda}\langle \partial_{z'}, \partial_{z'}\rangle \mathrm{Ric}_{nm}(z) z'^n z'^m|_{z'=0} + O(\lambda^{-2}) \\ &= 1 - \frac{1}{12\lambda}\mathrm{Ric}^n{}_n(z) + O(\lambda^{-2})\end{aligned}$$

and since the scalar curvature is defined as $s(z) := \mathrm{Ric}^n{}_n(z)$ the proof is complete. □

If we want to retain the completeness relation, then we have to multiply the coherent states with a parametrix of $(1 - \mathbf{s}/(12\lambda))^{1/2}$,

$$\mathcal{P} = (1 - \mathbf{s}/(12\lambda))^{-1/2} \sim \sum_{k=0}^{\infty} \binom{-1/2}{k} \left(-\frac{\mathrm{s}}{12\lambda}\right)^k \ .$$

More precisely, the states defined by

$$\tilde{u}^L_{p,q}(\lambda, x) := \mathcal{P} u^L_{p,q}(\lambda, x)$$

satisfy

$$\left(\frac{\lambda}{2\pi}\right)^d \iint |\tilde{u}^L_{p,q}\rangle\langle\tilde{u}^L_{p,q}| \, \mathrm{d}p\mathrm{d}q = 1 \ , \qquad (3.55)$$

but they are now no longer normalized. Instead we have

$$\begin{aligned}\langle \tilde{u}^L_{p,q}, \tilde{u}^L_{p,q}\rangle &= \langle u^L_{p,q}, u^L_{p,q}\rangle + \frac{1}{12\lambda}\langle u^L_{p,q}, \mathrm{s}u^L_{p,q}\rangle + O(\lambda^{-2}) \\ &= 1 + \frac{1}{12\lambda} s(p,q) + O(\lambda^{-2}) \ .\end{aligned}$$

Hence the scalar curvature of the metric induced by L is the leading order obstruction for the corresponding set of coherent states to be simultaneously complete and normalized.

Since the completeness relation will be the more important property, we will often use the modified coherent states

$$\tilde{u}^L_{p,q}(\lambda, x) := \mathcal{P} u^L_{p,q}(\lambda, x) \ .$$

Proposition 3.3.16. *The Wigner function of a modified coherent state*

$$\tilde{u}^B_{p,q}(\lambda, x) := \mathcal{P} u^B_{p,q}(\lambda, x)$$

is given by

$$\begin{aligned} W_{z_0}(z) &= A(\lambda, z) \left(\frac{\lambda}{\pi}\right)^d \mathrm{e}^{-\lambda\langle z-z_0, \mathbf{g}_L(z-z_0)\rangle} \\ &= \left(1 + \frac{1}{12\lambda}\left[s(z) + O(z-z_0)\right] + O(\lambda^{-2})\right) \left(\frac{\lambda}{\pi}\right)^d \mathrm{e}^{-\lambda\langle z-z_0, \mathbf{g}_L(z-z_0)\rangle} \end{aligned} \tag{3.56}$$

where $A(\lambda, z) \in S^0(1)$ *and* $z = (\xi, x)$, $z_0 = (p, q)$.

Proof. We start by expressing the Wigner function of $\mathcal{P}u$ through the Wigner function of u, for an arbitrary state u and a pseudodifferential operator $\mathcal{P}$. We have

$$\mathcal{P}u(x) = \left(\frac{\lambda}{2\pi}\right)^d \iint \mathrm{e}^{\mathrm{i}\lambda\langle x-z,\eta\rangle} p(\eta, (x+z)/2) u(z) \, \mathrm{d}z\mathrm{d}\eta \ ,$$

where p is the Weyl symbol of $\mathcal{P}$, and the Wigner function of $\mathcal{P}u$ is

$$\begin{aligned} W(\xi, x) &= \left(\frac{\lambda}{2\pi}\right)^d \int \mathrm{e}^{-\mathrm{i}\lambda\langle y,\xi\rangle} \overline{\mathcal{P}u}(x-y/2) \mathcal{P}u(x+y/2) \, \mathrm{d}y \\ &= \left(\frac{\lambda}{2\pi}\right)^{3d} \iiiint\!\!\int \mathrm{e}^{-\mathrm{i}\lambda[\langle y,\xi\rangle + \langle x-y/2-z,\eta\rangle - \langle x+y/2-z',\eta'\rangle]} \bar{p}(\eta, (x+z)/2 - y/4) \bar{u}(z) \\ &\qquad \bar{p}(\eta, (x+z)/2 - y/4) p(\eta', (x+z')/2 + y/4) u(z') \, \mathrm{d}z\mathrm{d}z'\mathrm{d}\eta\mathrm{d}\eta'\mathrm{d}y \, . \end{aligned}$$

If we substitute now first $z \mapsto z - z'/2$, $z' \mapsto z + z'/2$ and afterwards $y \mapsto y - z'$, we obtain

$$\begin{aligned} W(\xi, x) &= \left(\frac{\lambda}{2\pi}\right)^{3d} \iiiint\!\!\int \mathrm{e}^{-\mathrm{i}\lambda[\langle y,\xi\rangle + \langle x-z-y/2+z'/2,\eta\rangle - \langle x-z+y/2-z'/2,\eta'\rangle]} \\ &\qquad \bar{p}(\eta, (x+z)/2 - y/4 - z'/4) p(\eta', (x+z')/2 + y/4 + z'/4) \\ &\qquad \bar{u}(z - z'/2) u(z + z'/2) \, \mathrm{d}z\mathrm{d}z'\mathrm{d}\eta\mathrm{d}\eta'\mathrm{d}y \\ &= \left(\frac{\lambda}{2\pi}\right)^{3d} \iiiint\!\!\int \mathrm{e}^{-\mathrm{i}\lambda[\langle y-z',\xi\rangle + \langle x-z-y/2+z',\eta\rangle - \langle x-z+y/2-z',\eta'\rangle]} \\ &\qquad \bar{p}(\eta, (x+z)/2 - y/4) p(\eta', (x+z)/2 + y/4) \\ &\qquad \bar{u}(z - z'/2) u(z + z'/2) \, \mathrm{d}z\mathrm{d}z'\mathrm{d}\eta\mathrm{d}\eta'\mathrm{d}y \\ &= \left(\frac{\lambda}{2\pi}\right)^{2d} \iiiint \mathrm{e}^{-\mathrm{i}\lambda[\langle y,\xi-(\eta+\eta')/2\rangle + \langle x-z,\eta-\eta'\rangle]} \bar{p}(\eta, (x+z)/2 - y/4) \\ &\qquad p(\eta', (x+z)/2 + y/4) W_0(\eta + \eta' - \xi, z) \, \mathrm{d}z\mathrm{d}\eta\mathrm{d}\eta'\mathrm{d}y \ , \end{aligned}$$

where $W_0(\xi,x)$ denotes the Wigner function of u. A further substitution $\eta\mapsto\eta-\eta'/2$, $\eta'\mapsto\eta+\eta'/2$ leads to

$$\left(\frac{\lambda}{2\pi}\right)^{2d}\iiiint \mathrm{e}^{-\mathrm{i}\lambda[\langle y,\xi-\eta\rangle-\langle x-z,\eta'\rangle]}\bar{p}(\eta-\eta'/2,(x+z)/2-y/4)$$
$$p(\eta+\eta'/2,(x+z)/2+y/4)W_0(2\eta-\xi,z)\ \mathrm{d}z\mathrm{d}\eta\mathrm{d}\eta'\mathrm{d}y\ ,$$

and then $2\eta-\xi\mapsto\eta$, $y/2\mapsto y$ finally gives

$$W(\xi,x)=\left(\frac{\lambda}{2\pi}\right)^{2d}\iiiint \mathrm{e}^{-\mathrm{i}\lambda[\langle y,\xi-\eta\rangle-\langle x-z,\eta'\rangle]}\bar{p}((\eta+\xi-\eta')/2,(x+z-y)/2)$$
$$p((\eta+\xi+\eta')/2,(x+z+y)/2)W_0(\eta,z)\ \mathrm{d}z\mathrm{d}\eta\mathrm{d}\eta'\mathrm{d}y\ .$$

For the further evaluation of this integral we introduce the abbreviations $z=(\xi,x)$, $z'=(\eta,z)$ and $z''=(\eta',y)$, and with

$$W_0(z')=\left(\frac{\lambda}{\pi}\right)^{d}\mathrm{e}^{-\lambda\langle z'-z_0,\mathbf{g}(z'-z_0)\rangle}$$

we get

$$W(z)=\left(\frac{\lambda}{\pi}\right)^{d}\left(\frac{\lambda}{2\pi}\right)^{2d}\iint \mathrm{e}^{\mathrm{i}\lambda[\mathrm{i}\langle z'-z_0,\mathbf{g}(z'-z_0)\rangle+\langle z'',\mathcal{J}(z'-z)\rangle]}$$
$$\bar{p}((z+z'-z'')/2)p((z+z'+z'')/2)\ \mathrm{d}z'\mathrm{d}z''\ .$$

With the substitution $z'\mapsto z'+z$ this can be rewritten as

$$W(z)=W_0(z)\left(\frac{\lambda}{2\pi}\right)^{2d}\iint \mathrm{e}^{\mathrm{i}\lambda[\mathrm{i}\langle z',\mathbf{g}z'\rangle+\langle z',2\mathrm{i}\mathbf{g}(z-z_0)-\mathcal{J}z''\rangle]}$$
$$\bar{p}(z+(z'-z'')/2)p(z+(z'+z'')/2)\ \mathrm{d}z'\mathrm{d}z''\ ,$$

so this gives (3.56) with

$$A(\lambda,z)=\left(\frac{\lambda}{2\pi}\right)^{2d}\iint \mathrm{e}^{\mathrm{i}\lambda[\mathrm{i}\langle z',\mathbf{g}z'\rangle+\langle z',2\mathrm{i}\mathbf{g}(z-z_0)-\mathcal{J}z''\rangle]}\bar{p}(z+(z'-z'')/2)p(z+(z'+z'')/2)\ \mathrm{d}z'\mathrm{d}z''\ .$$

A substitution $z''\mapsto z''-2\mathrm{i}\mathcal{J}\mathbf{g}(z-z_0)$ followed by $z'\mapsto z'+z''$, $z''\mapsto z'-z''$ gives

$$A(\lambda,z)=\left(\frac{\lambda}{2\pi}\right)^{2d}\iint \mathrm{e}^{-\lambda\langle(z'z''),\mathbf{G}(z',z'')\rangle}\bar{p}(z+z''+\mathrm{i}\mathcal{J}\mathbf{g}(z-z_0))p(z+z'-\mathrm{i}\mathcal{J}\mathbf{g}(z-z_0))\,4^d\mathrm{d}z'\mathrm{d}z''\,,$$

with

$$\mathbf{G} = \begin{pmatrix} \mathbf{g} & \mathbf{g} - \mathrm{i}\mathcal{J} \\ \mathbf{g} - \mathrm{i}\mathcal{J}^\dagger & \mathbf{g} \end{pmatrix} .$$

Now using $\det \mathbf{G} = 1$, we obtain

$$A(\lambda, z) = \mathrm{e}^{-\frac{1}{4\lambda}\langle(\partial_{z'},\partial_{z''}),\mathbf{G}^{-1}(\partial_{z'},\partial_{z''})\rangle}\bar{p}(z + z'' + \mathrm{i}\mathcal{J}\mathbf{g}(z - z_0))p(z + z' - \mathrm{i}\mathcal{J}\mathbf{g}(z - z_0))|_{z'=z''=0}$$

where

$$\mathbf{G}^{-1} = \begin{pmatrix} \mathbf{g}^{-1} & \mathbf{g}^{-1} + \mathrm{i}\mathcal{J} \\ \mathbf{g}^{-1} + \mathrm{i}\mathcal{J}^\dagger & \mathbf{g}^{-1} \end{pmatrix} ,$$

which can be easily seen using the fact that $\mathbf{g}$ is symplectic. By evaluating the leading order terms we get

$$A(\lambda, z)W_0(z) = \left(1 + \frac{1}{12\lambda}s(z)\right) W_0(z) + O(\lambda^{-1})$$

□

Proposition 3.3.16 gives a pointwise result. If one is only interested in weak results, which is in some sense natural for Wigner functions, on can use the following lemma.

Lemma 3.3.17. *Let $u \in L^2(M)$ with Wigner function $W[u]$, and denote by $W[\mathcal{P}u]$ the Wigner function of $\mathcal{P}u$ for $\mathcal{P} \in \Psi^0(1)$. Then we have $W[\mathcal{P}u] = |P|^2 W[u]\big(1 + O(\lambda^{-1})\big)$ weakly, i.e.*

$$\int W[\mathcal{P}u](z)A(z)\,\mathrm{d}z = \int |\mathcal{P}|^2(z)W[u](z)A(z)\,\mathrm{d}z(1 + O(\lambda^{-1}) ,$$

for all $A \in S^0(1)$, where P denotes the Weyl symbol of $\mathcal{P}$. If the symbol of $\mathcal{P}$ is furthermore real valued then the error is in fact $O(\lambda^{-2})$.

Proof. We just write down the equality

$$\langle \mathcal{P}u, \mathcal{A}\mathcal{P}u\rangle = \langle u, \mathcal{P}^*\mathcal{A}\mathcal{P}u\rangle$$

in terms of the symbols, which gives

$$\int W[\mathcal{P}u](z)A(z)\,\mathrm{d}z = \int W[u](z)P^*\#A\#P(z)\,\mathrm{d}z .$$

Since by Theorem 2.5.5

$$P^*\#A\#P(z) = |P(z)|^2A(z) + \frac{1}{2\lambda}\big[P^*\{A, P\} + \{P^*, A\}P + A\{P^*, P\}\big] + O(\lambda^{-2}) ,$$

and the term in brackets vanishes for $P^* = P$, the result follows. □

In the situation in Proposition 3.3.16 we therefore obtain that the Wigner function of a modified coherent state is given by

$$W_{z_0}(z) \equiv \left(1 + \frac{1}{12\lambda}\, s(z) + O(\lambda^{-2})\right) \left(\frac{\lambda}{\pi}\right)^d \mathrm{e}^{-\lambda\langle z - z_0, \mathbf{g}_L(z-z_0)\rangle}$$

in the weak sense.

If one wants to expand a state $\psi \in L^2(\mathbb{R}^d)$ into a basis of coherent states, one has to compute the scalar product $\langle u^L_{p,q}, \psi\rangle$. The square of its absolute value, multiplied by a normalization factor, is called a Husimi function of ψ:

$$H^L_\psi(p,q) := \left(\frac{\lambda}{2\pi}\right)^d |\langle u^L_{p,q}, \psi\rangle|^2 \ . \tag{3.57}$$

Since

$$|\langle u^L_{p,q}, \psi\rangle|^2 = \operatorname{tr}\left[|u^L_{p,q}\rangle\langle u^L_{p,q}|\ |\psi\rangle\langle\psi|\right] = \iint W^L_{p,q}(\xi, x) W_\psi(\xi, x)\ \mathrm{d}x\mathrm{d}\xi \ ,$$

the Husimi function is a Gaussian smoothing of the Wigner function.

The normalization factor ensures that we have

$$\iint H^L_\psi(p,q)\ \mathrm{d}p\mathrm{d}q = \langle \psi, \psi\rangle$$

by the completeness relation for the coherent states.

Of special interest will be the scalar product of two coherent states located at different points, which gives the deviation of the set of coherent states from being orthonormal.

Lemma 3.3.18. *Let* $(p,q), (p',q') \in \mathbb{R}^{2d}$ *and let* $u^L_{p,q}(\lambda, x)$*be the coherent state* (3.51)*, then*

$$\langle u^L_{p,q}, u^L_{p',q'}\rangle = \mathrm{e}^{\mathrm{i}\lambda\langle p+p', q-q'\rangle/2}\mathrm{e}^{-\lambda g_L(p-p', q-q')/4} \ ,$$

and hence the Husimi function is

$$H^L_{u^L}(p,q) := \left(\frac{\lambda}{2\pi}\right)^d |\langle u^L_{p,q}, u^L_{p',q'}\rangle|^2 = \left(\frac{\lambda}{2\pi}\right)^d \mathrm{e}^{-\lambda g_L(p-p', q-q')/2} \ ,$$

where $g_L(p-p', q-q') := \langle (p-p', q-q'), \mathbf{g}_L(p-p', q-q')\rangle$ *denotes the quadratic form defined by the metric* $\mathbf{g}_L$*, see* (3.53)*.*

Proof. The proof consists of a simple evaluation of a Gaussian integral, similar as in the proof of Lemma 3.3.14. Inserting the expressions fur $u^L_{p,q}$, we get

$$\begin{aligned}
\langle u^L_{p,q}, u^L_{p',q'}\rangle &= \left(\frac{\lambda}{\pi}\right)^{d/2} (\det \operatorname{Im} B)^{1/2} \int \mathrm{e}^{\mathrm{i}\lambda[\langle p'-p, x\rangle - \langle p', q'\rangle + \langle p, q\rangle + \frac{1}{2}\langle B(x-q'), x-q'\rangle - \frac{1}{2}\langle \overline{B}(x-q), x-q\rangle]}\ \mathrm{d}x \\
&= \mathrm{e}^{\mathrm{i}\lambda[\frac{1}{2}\langle Bq', q'\rangle - \frac{1}{2}\langle \overline{B}q, q\rangle - \langle p', q'\rangle + \langle p, q\rangle]} \\
&\qquad \left(\frac{\lambda}{\pi}\right)^{d/2} (\det \operatorname{Im} B)^{1/2} \int \mathrm{e}^{-\lambda\langle \operatorname{Im} Bx, x\rangle} \mathrm{e}^{\mathrm{i}\lambda\langle x, p'-p-Bq'+\overline{B}q\rangle}\ \mathrm{d}x \\
&= \mathrm{e}^{\mathrm{i}\lambda[\frac{1}{2}\langle Bq', q'\rangle - \frac{1}{2}\langle \overline{B}q, q\rangle - \langle p', q'\rangle + \langle p, q\rangle]} \mathrm{e}^{-\lambda\langle [\operatorname{Im} B]^{-1}(p'-p-Bq'+\overline{B}q), p'-p-Bq'+\overline{B}q\rangle/4} \ ,
\end{aligned}$$

where we have used Theorem D.2. Now splitting the exponent into its real and imaginary part gives

$$\begin{aligned}\langle u^L_{p,q}, u^L_{p',q'}\rangle &= \mathrm{e}^{\mathrm{i}\lambda[\frac{1}{2}\langle \mathrm{Re}\, Bq',q'\rangle-\frac{1}{2}\langle \mathrm{Re}\, Bq,q\rangle+\frac{1}{2}\langle p'-p,q'+q\rangle+\frac{1}{2}\langle q+q',\mathrm{Re}\, B(q-q')\rangle-\langle p',q'\rangle+\langle p,q\rangle]}\\ &\quad \mathrm{e}^{-\lambda[\langle[\mathrm{Im}\, B]^{-1}(p'-p),(p'-p)\rangle/4-\langle[\mathrm{Im}\, B]^{-1}(p'-p),\mathrm{Re}\, B(q'-q)\rangle/4-\langle[\mathrm{Im}\, B]^{-1}\mathrm{Re}\, B(q'-q),p'-p\rangle/4]}\\ &\quad\quad \mathrm{e}^{-\lambda[\frac{1}{2}\langle \mathrm{Im}\, Bq',q'\rangle+\frac{1}{2}\langle \mathrm{Im}\, Bq,q\rangle-\langle \mathrm{Im}\, B(q'+q),q'+q\rangle/4]}\\ &= \mathrm{e}^{\mathrm{i}\lambda\langle p'+p,q-q'\rangle/2}\\ &\quad \mathrm{e}^{-\lambda[\langle[\mathrm{Im}\, B]^{-1}(p'-p),(p'-p)\rangle/4+\langle[\mathrm{Im}\, B]^{-1}(p'-p),\mathrm{Re}\, B(q'-q)\rangle/4+\langle[\mathrm{Im}\, B]^{-1}\mathrm{Re}\, B(p'-p),q'-q\rangle/4]}\\ &\quad\quad \mathrm{e}^{-\lambda[\langle \mathrm{Im}\, B(q'-q),q'-q\rangle/4]}\\ &= \mathrm{e}^{\mathrm{i}\lambda\langle p'+p,q-q'\rangle/2}\mathrm{e}^{-\lambda g(p'-p,q'-q)/4}\ .\end{aligned}$$

□

In analogy with the definition of the Wigner function of a single function one sometimes defines the Wigner function of a pair of functions $f(x)$, $g(x)$, by

$$W[f,g](\xi,x) = \left(\frac{\lambda}{2\pi}\right)^d \int \mathrm{e}^{-\mathrm{i}\lambda\langle\xi,y\rangle}\overline{f}(x-y/2)g(x+y/2)\ \mathrm{d}y\ , \tag{3.58}$$

see, e.g., [Fol89]. The usefulness of this function lies mainly in the fact that for a pseudo-differential operator $\mathcal{H}$ with Weyl symbol $H(\xi,x)$ one has

$$\langle f,\mathcal{H}g\rangle = \iint W[f,g](\xi,x)H(\xi,x)\ \mathrm{d}\xi\mathrm{d}x\ .$$

We want to determine this Wigner function for two coherent states centered at different points in phase space.

Lemma 3.3.19. *Let $(p,q),(p',q')\in T^*\mathbb{R}^d$, and let $\bar p := (p+p')/2$, $\bar q := (q+q')/2$ and $\delta p := p-p'$, $\delta q := q-q'$, then*

$$W[u^L_{p,q},u^L_{p',q'}](\xi,x) = \left(\frac{\lambda}{\pi}\right)^d \mathrm{e}^{\mathrm{i}\lambda[\langle\bar p,\delta q\rangle-\langle\delta p,x-\bar q\rangle+\langle\delta q,\xi-\bar p\rangle]}\mathrm{e}^{-\lambda\mathbf{g}_L(\xi-\bar p,x-\bar q)}\ .$$

Proof. By inserting the expressions for $u^L_{p,q}$ and $u^L_{p',q'}$ into the definition 3.58 of the Wigner function we get

$$W[u^L_{p,q},u^L_{p',q'}](\xi,x)=\left(\frac{\lambda}{2\pi}\right)^d\int \mathrm{e}^{-\mathrm{i}\lambda\langle\xi,y\rangle}\overline{u}^L_{p,q}(\lambda,x-y/2)u^L_{p',q'}(\lambda,x+y/2)\,\mathrm{d}y$$
$$=\mathrm{e}^{\mathrm{i}\lambda[\langle p',x-q'\rangle-\langle p,x-q\rangle+\langle x-q',B(x-q')\rangle/2-\langle x-q,\bar{B}(x-q)\rangle/2]}$$
$$\left(\frac{\lambda}{2\pi}\right)^d\left(\frac{\lambda}{\pi}\right)^{d/2}[\det\operatorname{Im}B]^{-1/2}\int \mathrm{e}^{-\mathrm{i}\lambda[\langle\xi-(p+p')/2-\bar{B}(x-q')/2-B(x-q)/2,y\rangle}$$
$$\mathrm{e}^{-\lambda\langle y,\operatorname{Im}By\rangle/4}\,\mathrm{d}y$$
$$=\left(\frac{\lambda}{\pi}\right)^d\mathrm{e}^{\mathrm{i}\lambda[\langle p',x-q'\rangle-\langle p,x-q\rangle+\langle x-q',B(x-q')\rangle/2-\langle x-q,\bar{B}(x-q)\rangle/2]}$$
$$\mathrm{e}^{-\lambda\langle\xi-(p+p')/2-\bar{B}(x-q)/2-B(x-q')/2,[\operatorname{Im}B]^{-1}(\xi-(p+p')/2-\bar{B}(x-q)/2-B(x-q')/2)\rangle},$$

where we have used Lemma D.2. Rewriting this expression in terms of $\bar{p},\bar{q}$ and $\delta p,\delta q$ gives

$$W[u^L_{p,q},u^L_{p',q'}](\xi,x)=\left(\frac{\lambda}{\pi}\right)^d\mathrm{e}^{\mathrm{i}\lambda[\langle\bar{p},\delta q\rangle-\langle\delta p,x-\bar{q}\rangle+\mathrm{i}\langle x-\bar{q},\operatorname{Im}B(x-\bar{q})\rangle+\mathrm{i}\langle\delta q,\operatorname{Im}B\delta q\rangle/4+\langle\delta q,\operatorname{Re}B(x-\bar{q})\rangle]}$$
$$\mathrm{e}^{-\lambda\langle\xi-\bar{p}-\operatorname{Re}B(x-\bar{q})-\mathrm{i}\operatorname{Im}B\delta q/2,[\operatorname{Im}B]^{-1}(\xi-\bar{p}-\operatorname{Re}B(x-\bar{q})-\mathrm{i}\operatorname{Im}B\delta q/2)\rangle}$$
$$=\left(\frac{\lambda}{\pi}\right)^d\mathrm{e}^{\mathrm{i}\lambda[\langle\bar{p},\delta q\rangle-\langle\delta p,x-\bar{q}\rangle+\langle\delta q,\xi-\bar{p}\rangle]}$$
$$\mathrm{e}^{-\lambda[\langle\xi-\bar{p}-\operatorname{Re}B(x-\bar{q}),[\operatorname{Im}B]^{-1}(\xi-\bar{p}-\operatorname{Re}B(x-\bar{q}))\rangle+\langle x-\bar{q},\operatorname{Im}B(x-\bar{q})\rangle]}$$
$$=\left(\frac{\lambda}{\pi}\right)^d\mathrm{e}^{\mathrm{i}\lambda[\langle\bar{p},\delta q\rangle-\langle\delta p,x-\bar{q}\rangle+\langle\delta q,\xi-\bar{p}\rangle]}\mathrm{e}^{-\lambda g(\xi-\bar{p},x-\bar{q})}\ .$$

□

This lemma can be used to derive an asymptotic expansion of the matrix elements between coherent states of a pseudodifferential operator.

Proposition 3.3.20. *Let $\mathcal{H}$ be a pseudodifferential operator with Weyl symbol $H\in S^0(m_{a,b})$, then we have*

$$\langle u^L_{p,q},\mathcal{H}u^L_{p',q'}\rangle=\mathrm{e}^{\mathrm{i}\lambda\langle\bar{p},\delta q\rangle}\mathrm{e}^{-\lambda\langle\delta z,\mathbf{g}\delta z\rangle/4}\mathrm{e}^{-\frac{1}{4\lambda}\langle D_{\bar{z}},\mathbf{g}^{-1}D_{\bar{z}}\rangle}\tilde{H}(\bar{z}+\frac{\mathrm{i}}{2}\mathcal{J}_0\mathbf{g}\delta z)+O(\lambda^{-\infty})\ ,$$

where $\tilde{H}$ denotes an almost analytic extension of H, $\bar{z}=(\bar{p},\bar{q})=((p+p')/2,(q+q')/2)$ and $\delta z=(\delta p,\delta q)=(p-p',q-q')$.

Proof. We introduce the abbreviations $z=(p,q)$, $z'=(p',q')$. We need to compute

$$\langle u^L_{p,q},\mathcal{H}u^L_{p',q'}\rangle=\left(\frac{\lambda}{2\pi}\right)^d\iiint \mathrm{e}^{\mathrm{i}\lambda\langle x-y,\xi\rangle}H(\xi,(x+y)/2)\overline{u}_z(x)u_{z'}(y)\,\mathrm{d}x\mathrm{d}y\mathrm{d}\xi$$
$$=\left(\frac{\lambda}{2\pi}\right)^d\iiint \mathrm{e}^{-\mathrm{i}\lambda\langle y,\xi\rangle}H(\xi,x)\overline{u}_z(x-y/2)u_{z'}(x+y/2)\,\mathrm{d}x\mathrm{d}y\mathrm{d}\xi$$
$$=\iint W_{z,z'}(\xi,x)H(\xi,x)\,\mathrm{d}x\mathrm{d}\xi\ ,$$

with

$$W_{z,z'}(z_0) := \left(\frac{\lambda}{2\pi}\right)^d \int \mathrm{e}^{-\mathrm{i}\lambda\langle y,\xi\rangle} \overline{u}_z(x-y/2)u_{z'}(x+y/2)\ \mathrm{d}y$$
$$= \left(\frac{\lambda}{\pi}\right)^d \mathrm{e}^{\mathrm{i}\lambda(\langle\bar p,\delta q\rangle - \langle \delta z, \mathcal{J}_0(z_0-\bar z)\rangle)} \mathrm{e}^{-\lambda g(z_0-\bar z)} \ .$$

Hence we get

$$\langle u^L_{p,q}, \mathcal{H} u^L_{p',q'}\rangle\langle z, \mathcal{H}\, z'\rangle = \mathrm{e}^{\mathrm{i}\lambda\langle\bar p,\delta q\rangle} \left(\frac{\lambda}{\pi}\right)^d \int \mathrm{e}^{\mathrm{i}\lambda(-\langle\delta z,\mathcal{J}_0 z''\rangle + \mathrm{i}\langle z'',\mathbf{g}z''\rangle)} H(\bar z + z'')\ \mathrm{d}z'' \ .$$

The stationary point of the phase of the integral is given by

$$z_0 = \frac{\mathrm{i}}{2}\mathbf{g}^{-1}\mathcal{J}_0\delta z \ ,$$

and the substitution $z'' \mapsto z'' + z_0$ gives

$$\langle u^L_{p,q}, \mathcal{H} u^L_{p',q'}\rangle = \mathrm{e}^{\mathrm{i}\lambda\langle\bar p,\delta q\rangle} \mathrm{e}^{-\lambda\langle\delta z,\mathcal{J}_0^t\mathbf{g}^{-1}\mathcal{J}_0\delta z\rangle/4} \left(\frac{\lambda}{\pi}\right)^d \int \mathrm{e}^{-\lambda\langle z'',\mathbf{g}z''\rangle} \tilde H(\bar z + z_0 + z'')\ \mathrm{d}z''$$
$$= \mathrm{e}^{\mathrm{i}\lambda\langle\bar p,\delta q\rangle} \mathrm{e}^{-\lambda\langle\delta z,\mathbf{g}\delta z\rangle/4} \mathrm{e}^{-\frac{1}{4\lambda}\langle D_z,\mathbf{g}^{-1}D_z\rangle} \tilde H(\bar z + z_0) \ ,$$

where we have used Lemma B.1 and that

$$\mathcal{J}_0^t\mathbf{g}^{-1}\mathcal{J}_0 = \mathbf{g} \ ,$$

which follows from the fact that $\mathbf{g}$ is symplectic.

□

3.4 Global Theory

3.4.1 Lagrangian ideals

In Section 3.1 we have seen that the appropriate invariant object associated with an oscillating integral of the type (3.18) with a real valued phase function is the Lagrangian submanifold in T^*M generated by the phase function. But if we now have a complex valued phase function we face the problem that we do not know how to immerse a complex Lagrangian manifold into T^*M. A way out of this problem can be found by using a more algebraic formulation. Following Hörmander [Hör85b], we consider for a Lagrangian submanifold $\Lambda \subset T^*M$ the corresponding vanishing ideal in $C^\infty(T^*M,\mathbb{R})$, defined by

$$J_\Lambda := \{f \in C^\infty(T^*M,\mathbb{R}) \mid f = 0 \text{ on } \Lambda\} \ . \tag{3.59}$$

The following proposition says that there is a one-to-one correspondence between Lagrangian submanifolds in T^*M and certain ideals in $C^\infty(T^*M,\mathbb{R})$.

Proposition 3.4.1. *The ideal $J_\Lambda = \{f \in C^\infty(T^*M, \mathbb{R}) \mid f = 0 \text{ on } \Lambda\}$ has the following three properties:*

(i) J_Λ is closed under Poisson brackets, i.e. for $f, g \in J_\Lambda$ one has $\{f, g\} \in J_\Lambda$.

(ii) J_Λ is locally generated by d functions, that is for every point in T^*M exists a neighborhood U and d functions $f_1, \dots, f_d \in J_\Lambda$ with $\mathrm{d}f_1, \dots, \mathrm{d}f_d$ linear independent on every point in U, such that every $g \in J_\Lambda$ with support in U can be written as $g = \sum a_j f_j$ for some $a_j \in C^\infty(U, \mathbb{R})$.

(iii) If $af \in J_\Lambda$ for every $a \in C^\infty(T^*M, \mathbb{R})$, then $f \in J_\Lambda$.

Conversely, assume that an ideal $J \subset C^\infty(T^*M, \mathbb{R})$ satisfies the conditions (i) to (iii), then the set of common zeros $\Lambda := \{(\xi, x) \mid f(\xi, x) = 0 \text{ for all } f \in J\}$ is a Lagrangian submanifold in T^*M.

Proof. Assume $f, g \in J_\Lambda$, then they are constant on Λ and therefore their Hamiltonian vector-fields X_f, X_g are tangent to Λ. Thus $\{f, g\}|_\Lambda = \omega(X_f, X_g)|_\Lambda = 0$ because Λ is involutive.

As any d-dimensional submanifold, Λ can locally be represented as the common zeros of d independent functions, $\Lambda \cap U' = \{(\xi, x) \mid f_1(\xi, x) = \cdots f_d(\xi, x) = 0\}$ for some open set $U' \subset T^*M$. In a neighborhood U of $\Lambda \cap U'$ one can choose new coordinates $(y_1, \dots, y_{2d})$ such that $y_i = f_i$ for $i = 1, \dots d$, because of the independence of the f_i. By Taylor's formula we have for any $g \in J_\Lambda$ with support in U,

$$g = \sum_{j=1}^{d} a_j y_j = \sum_{j=1}^{d} a_j f_j$$

with $a_j = \int_0^1 \frac{\partial g}{\partial y_j}(y_1, \dots, t y_j, \dots y_{2d})\, \mathrm{d}t \in C^\infty(T^*M, \mathbb{R})$. This proves (ii), and (iii) is obvious.

Now the converse; assume we have an ideal J which satisfies conditions (i) to (iii), and let Λ be the set of common zeros. Because of (ii) Λ can locally be represented as the set of common zeros of d linearly independent functions f_j, $\Lambda \cap U = \{f_1 = \cdots f_d = 0\}$ for some open set U, and is therefore a d-dimensional submanifold of T^*M. Moreover, the Hamiltonian vector fields X_{f_j} are tangent to Λ and span the tangent space at every point in $\Lambda \cap U$; but because of (i) $0 = \{f_j, f_i\}_\Lambda = \omega(X_{f_j}, X_{f_i})$, therefore Λ is Lagrangian. Finally, condition (iii) ensures that J consists of all functions which vanish on Λ, i.e. $J = J_\Lambda$. ☐

We will call an ideal J with the properties (i) to (iii) of Proposition 3.4.1 a real Lagrangian ideal. It seems now natural to remove the condition that the functions are real valued.

Definition 3.4.2. *An ideal $J \subset C^\infty(T^*M, \mathbb{C})$ which satisfies conditions (i) to (iii) of Proposition 3.4.1, where now the independence in (ii) is meant over $\mathbb{C}$, is called a* ***complex Lagrangian ideal****.*

The set

$$J_{\mathbb{R}} := \{(\xi, x) \mid f(\xi, x) = 0 \text{ for all } f \in J\}$$

is now no longer a Lagrangian manifold. But if it is smooth, the following discussion will show that it is an isotropic submanifold then.

One can define a tangent space $T_z^{\mathbb{C}} J$ for every $z \in J_{\mathbb{R}}$ as the subspace in the complexified tangent space to T^*M at $z \in T^*M$ which is annihilated by all $\mathrm{d}f_j$,

$$T_z^{\mathbb{C}} J := \{X \in T_z^{\mathbb{C}} T^*M \ ; \langle \mathrm{d}f_j(z), X\rangle = 0 \ , \ j = 1, \dots, d\} \ .$$

Algebraically the complexified tangent space to T^*M at $z \in T^*M$, $T_z^{\mathbb{C}} T^*M$, is given as the dual to I_z/I_z^2, where

$$I_z := \{f \in C^\infty(T^*M, \mathbb{C}) \ , \ f(z) = 0\}$$

is the vanishing ideal of $z \in T^*M$. To see this, note that the elements of I_z/I_z^2 are equivalence classes of functions whose differentials $\mathrm{d}f$ coincide at z, therefore

$$I_z/I_z^2 \cong T_z^{*\mathbb{C}} T^*M \ ,$$

and the dual space is the tangent space

$$T_z^{\mathbb{C}} T^*M \cong (I_z/I_z^2)^* \ .$$

Hence the tangent space to J at $z \in J_{\mathbb{R}}$ can be identified with the dual of $J/I_z^2 \subset I_z/I_z^2$,

$$T_z^{\mathbb{C}} J \cong [J/I_z^2]^* \ .$$

The Poisson bracket gives a natural identification of $T_z^{\mathbb{C}} T^*M$ with I_z/I_z^2, every $f \in I_z$ defines via

$$I_z/I_z^2 \ni g \mapsto \{f, g\}(z) \in \mathbb{C}$$

a linear form on I_z/I_z^2, which depends only on the equivalence class of g in I_z/I_z^2, and gives therefore an identification of these two spaces. Furthermore, the Poisson bracket defines a symplectic structure on I_z/I_z^2 by

$$(f, g) \mapsto \{f, g\}(z) \ ,$$

and since $\{f, g\} \in J$ for $f, g \in J$ we have $\{f, g\}(z) = 0$ for $z \in J_{\mathbb{R}}$ and $\{f, g\}$, hence J/I_z^2 is Lagrangian in I_z/I_z^2. Since the Poisson structure is dual to the symplectic structure on $T_z^{\mathbb{C}} T^*M$ this implies that the complex tangent space $T_z^{\mathbb{C}} J$ to J at $z \in J_{\mathbb{R}}$ is Lagrangian in $T_z^{\mathbb{C}} T^*M$.

So there is a complex Lagrangian tangent space to J at every $z \in J_{\mathbb{R}}$ and since the tangent space to $J_{\mathbb{R}}$ at z is a subspace thereof,

$$T_z J_{\mathbb{R}} \subset T_z^{\mathbb{C}} J \ ,$$

it follows that $J_{\mathbb{R}}$ is isotropic.

Lagrangian manifolds can always locally be represented by generating functions, and therefore the natural question arises, if complex Lagrangian ideals admit such a simple local representation, too.

Example 3.4.3. Take for example a function $\varphi(x)$ on M, which is complex valued. If it were real valued, $\Lambda = \{(x, \varphi'(x))\}$ would define a Lagrangian submanifold. So let us take the ideal generated by the functions $\xi_j - \partial\varphi/\partial x_j(x)$ instead, that is the one locally given by

$$J(\varphi) = \Big\{ \sum_j a_j(\xi, x)\Big(\xi_j - \frac{\partial\varphi}{\partial x_j}(x)\Big) \;\mid a_j \in C^\infty(T^*M, \mathbb{C}) \Big\} \;.$$

In order that condition (ii) is fulfilled the $\xi_j - \partial\varphi/\partial x_j(x)$ have to be linearly independent, which is equivalent to

$$\det \varphi''(x) \neq 0 \;. \tag{3.60}$$

Then condition (i) and (iii) are easy to check, so $J(\varphi)$ is a complex Lagrangian ideal if the non-degeneracy condition (3.60) is fulfilled. The zero set is determined by the critical values of the imaginary part of $\varphi(x)$,

$$J_{\mathbb{R}}(\varphi) = \{(x, \varphi'(x)) \mid \operatorname{Im} \varphi'(x) = 0\} \;.$$

If we take, e.g., $\varphi(\xi, x) = \langle x, p\rangle + \mathrm{i}(x-q)^2/2$, then the zero set

$$J_{\mathbb{R}}(\varphi) = \{(p, q)\}$$

consists of one point.

The following theorem gives the existence of a generating function for arbitrary complex Lagrangian ideals J close to their real parts $J_{\mathbb{R}}$. It is the non-homogeneous version of [Hör85b, Proposition 25.4.2].

Theorem 3.4.4. *Let M be a C^∞ manifold and let J be a complex Lagrangian ideal in $C^\infty(T^*M)$. For every $z_0 \in J_{\mathbb{R}}$ the local coordinates x at the projection $x_0 \in M$ of z_0 can be chosen, with the corresponding coordinates (ξ, x) in T^*M, so that the Lagrangian plane defined by $\mathrm{d}\xi = 0$ in $T^{\mathbb{C}}_{z_0}T^*M$ is transversal to $T_{z_0}J$. If $z_0 = (x_0, \xi_0)$, one can find a C^∞ function $F(\xi)$ defined in a neighborhood of ξ_0, such that J is generated by $x_j - \partial F(\xi)/\partial\xi_j$ in a neighborhood of z_0. Conversely, such functions always generate a complex Lagrangian ideal, and if $\tilde{F}(\xi)$ is another function with the same properties, then in a neighborhood of ξ_0 we have for every $N \in \mathbb{N}$*

$$|F'(\xi) - \tilde{F}'(\xi)| \leq C_N |\operatorname{Im} F'(\xi)|^N \;.$$

Proof. If L is a complex Lagrangian plane in $T^*\mathbb{C}^d$, then by [Hör85a, Corollary 21.2.11], see also Lemma 3.3.4, it follows that one can find a real Lagrangian plane L_1 which is transversal to L and to the Lagrangian plane L_0 defined by $\mathrm{d}x_j = 0$, $j = 1, \dots, d$. Hence we can find, as in the proof of [Hör85a, Theorem 21.2.16], local coordinates x such that $x_0 = 0$ and L_1 is the tangent plane to the zero-section of T^*M at z.

With such coordinates let $u_j(\xi, x)$, $j = 1, \cdots, d$, be local generators of J at z_0. Since $T_{z_0}J$ is defined by $\mathrm{d}u_j = 0$, $j = 1, \ldots, d$, the transversality of $T_{z_0}J$ and the plane L_0 defined by $\mathrm{d}\xi_j$, $j = 1, \ldots, d$, means that the equations $\mathrm{d}u_j = 0$, $\mathrm{d}\xi_j = 0$, $j = 1, \ldots, d$, imply that $\mathrm{d}x_j = 0$, $j = 1, \ldots, d$, hence $\det \partial u_j/\partial x_i \neq 0$. Therefore, by Theorem C.3, one can find in a neighborhood of z_0 new generators of J of the form $x_j - h_j(\xi)$, $j = 1, \ldots, d$.

Since J is Lagrangian, we have

$$g_{i,j}(\xi) := \{x_i - h_i(\xi), x_j - h_j(\xi)\} = \frac{\partial h_j(\xi)}{\partial \xi_i} - \frac{\partial h_i(\xi)}{\partial \xi_j} \in J \ , \tag{3.61}$$

and we are looking for a $F(\xi) \in C^\infty(\mathbb{R}^d, \mathbb{C})$ with $\partial F(\xi)/\partial \xi_j - h_j(\xi) \in J$, $j = 1, \ldots, d$, so that we can take $x_j - \partial F(\xi)/\partial \xi_j$, $j = 1, \ldots, d$, instead of $x_j - h_j(\xi)$ as generators of J.

Set

$$F(\xi) = \int_0^1 \sum_{i=1}^d h_i(t\xi)\xi_i \,\mathrm{d}t \ ,$$

then we get with (3.61) and partial integration

$$\begin{aligned}
\frac{\partial F(\xi)}{\partial \xi_j} &= \int_0^1 \sum_{i=1}^d \frac{\partial h_i}{\partial \xi_j}(t\xi)t\xi_i \,\mathrm{d}t + \int_0^1 h_j(t\xi)\,\mathrm{d}t \\
&= \int_0^1 \sum_{i=1}^d \frac{\partial h_j}{\partial \xi_i}(t\xi)t\xi_i \,\mathrm{d}t - \int_0^1 \sum_{i=1}^d g_{i,j}(t\xi)t\xi_i \,\mathrm{d}t + \int_0^1 h_j(t\xi)\,\mathrm{d}t \\
&= \int_0^1 t\frac{\mathrm{d}}{\mathrm{d}t} h_j(t,\xi)\,\mathrm{d}t - \int_0^1 \sum_{i=1}^d g_{i,j}(t\xi)t\xi_i \,\mathrm{d}t + \int_0^1 h_j(t\xi)\,\mathrm{d}t \\
&= h_j(\xi) - \int_0^1 \sum_{i=1}^d g_{i,j}(t\xi)t\xi_i \,\mathrm{d}t \ .
\end{aligned}$$

But according to Theorem C.4 the fact that $g_{i,j}(\xi) \in J$ is equivalent to

$$|g_{i,j}(\xi)| \leq C_N |\operatorname{Im} h(\xi)|^N$$

for every N, where $h(\xi)$ denotes the vector with components $h_j(\xi)$. So we get

$$\left|\frac{\partial F(\xi)}{\partial \xi_j} - h_j(\xi)\right| = \left|\int_0^1 \sum_{i=1}^d g_{i,j}(t\xi)t\xi_i \,\mathrm{d}t\right| \leq \sup_{t\in[0,1]} \sum_{i=1}^d |g_{i,j}(t\xi)\xi_i| \leq \tilde{C}_N |\operatorname{Im} h(\xi)|^N \ ,$$

in a neighborhood of ξ_0, since $\operatorname{Im} h(\xi) = 0$ for $\xi = \xi_0$. Therefore, Theorem C.4 gives $\frac{\partial F(\xi)}{\partial \xi_j} - h_j(\xi) \in J$, and we can choose $x_j - \frac{\partial F(\xi)}{\partial \xi_j}$, $j = 1, \ldots, d$, as generators for J. Assume now that we have another function $\tilde{F}(\xi)$ with this property, then the components of $F'(\xi) - \tilde{F}'(\xi)$ are in J, and hence the remaining part follows again from Theorem C.4. □

This theorem gives the existence of a special type of generating functions. In practice, as we have already seen in the last sections, the phase functions which occur in oscillating integrals are of the following form.

Definition 3.4.5. *Let M be a C^∞ manifold, $x_0 \in M$, and let $\varphi(x,\theta)$ be a C^∞ function in a neighborhood $U \subset \mathbb{R}^d \times \mathbb{R}^\kappa$ of (x_0,θ_0) with $\operatorname{Im}\varphi(x_0,\theta_0) = 0$. Then $\varphi(x,\theta)$ will be called a* ***non-degenerate phase function*** *of* ***positive type*** *at (x_0,θ_0), if*

(i) $\varphi'_\theta(x_0,\theta_0) = 0$;

(ii) the differentials $\mathrm{d}(\partial\varphi/\partial\theta_1), \dots, \mathrm{d}(\partial\varphi/\partial\theta_\kappa)$ *are linearly independent over the complex numbers at (x_0,θ_0);*

(iii) $\operatorname{Im}\varphi(x,\theta) \geq 0$ *in U.*

Such a phase function of positive type always generates a complex Lagrangian ideal, and we can ask how two phase functions which generate the same Lagrangian ideal differ.

Proposition 3.4.6. *If $\varphi(x,\theta)$ is a non-degenerate phase function of positive type at (x_0,θ_0), then $\xi_0 := \varphi'_x(x_0,\theta_0) \in T^*_{x_0}M$. Let $\hat{J}$ be the ideal generated by*

$$\frac{\partial\varphi}{\partial\theta_i}(x,\theta)\ , \quad i = 1,\dots,\kappa\,; \qquad \frac{\partial\varphi}{\partial\theta_j}(x,\theta) - \xi_j\ , \quad j = 1,\dots,d\ ,$$

then the ideal J formed by the functions in $\hat{J}$ which are independent of θ is a complex Lagrangian ideal in $C^\infty(T^*M)$. Furthermore, T_zJ is a positive Lagrangian plane. If the local coordinates and $F(\xi)$ are chosen as in Theorem 3.4.4, then $\operatorname{Im}F(\xi) \leq 0$ *and*

$$\varphi(x,\theta) - (\langle\xi,x\rangle - F(\xi)) \in \hat{J}^2\ .$$

Proof. The proof is identical to the proof of the analogous homogeneous result [Hör85b, Proposition 25.4.4], and therefore we will only give a sketch. From $\operatorname{Im}\varphi(x_0,\theta_0) = 0$ and $\operatorname{Im}\varphi \geq 0$ it follows that $\operatorname{Im}\mathrm{d}\varphi(x_0,\theta_0) = 0$, and therefore $\varphi'_\theta(x_0,\theta_0) = 0$ implies that $\operatorname{Im}\varphi'_x(x_0,\theta_0) = 0$ and hence $\varphi'_x(x_0,\theta_0) \in T^*_{x_0}M$.

As in the the proof of Theorem 3.4.4 one can show that one can choose local coordinates x such that

$$\det\begin{pmatrix} \varphi''_{xx} & \varphi''_{x\theta} \\ \varphi''_{\theta x} & \varphi''_{\theta\theta} \end{pmatrix} \neq 0$$

at (x_0,θ_0), and then it follows from Theorem C.3 that there are generators of $\hat{J}$ of the form

$$x_j - X_j(\xi)\,, \qquad \theta_j - \Theta_j(\xi)\ .$$

By (C.8) there is a function $F(\xi)$ with

$$\varphi(x,\theta) - (\langle\xi,x\rangle - F(\xi)) \in \hat{J}^2\ , \tag{3.62}$$

in the notation of (C.8) $F(\xi)$ is $-[\varphi(x,\theta)-\langle\xi,x\rangle]^0$, and by Lemma C.5 there is a constant $C>0$ such that near 0

$$-\operatorname{Im} F(\xi) \geq C(|\operatorname{Im} X(\xi)|^2 + |\operatorname{Im}\Theta(\xi)|^2) \geq 0\ . \tag{3.63}$$

Hence one can replace the generators $x_j - X_j(\xi)$ by $x_j + \partial F(\xi)/\partial\xi_j$. Now according to the Malgrange preparation theorem, every smooth function $g(\xi,x)$ can be written in a neighborhood of (x_0,ξ_0) as

$$g(\xi,x) = \sum_j q_j(\xi,x)(x_j - \partial F(\xi)/\partial\xi_j) + r(\xi)\ ,$$

and if $g \in J$ then $r(\xi)$ is in $\hat{J}$ and by Theorem C.4 follows

$$|r(\xi)| \leq C_N(|\operatorname{Im} X(\xi)| + |\operatorname{Im}\Theta(\xi)|)^N\ ,$$

for every $N \in \mathbb{N}$. But from (3.63) together with $|\operatorname{Im} F(\xi)| \leq C|\operatorname{Im} F'(\xi)|^{1/2}$ we then get

$$|r(\xi)| \leq C'_N|\operatorname{Im} F'(\xi)|^N\ ,$$

for all $N \in \mathbb{N}$, hence by Theorem C.4 $r(\xi)$ is in the ideal generated by $x_j - \partial F(\xi)/\partial\xi_j$. Therefore J is generated by

$$x_j - \partial F(\xi)/\partial\xi_j\ .$$

The positivity of the tangent plane is now straightforward by the fact that $\operatorname{Im} F'' \leq 0$. □

The theorem implies that the property that a complex Lagrangian ideal is generated by a phase function of positive type is invariant under a change of the generating function. Hence this property can be used to define the positivity of a complex Lagrangian ideal.

Definition 3.4.7. *A complex Lagrangian ideal will be called* ***positive****, if every $z \in J_{\mathbb{R}}$ possesses a neighborhood in which J can be parameterized by a phase function of positive type.*

Recall that a Lagrangian plane L in a complex symplectic space V is called positive, if $\mathrm{i}\omega(\bar{l},l) \geq 0$ for all $l \in L$, see Definition 3.3.2. It follows from Theorem 3.4.6 that the positivity of J implies that the tangent space $T_z^{\mathbb{C}}J$ is positive for each $z \in J_{\mathbb{R}}$. It is tempting to think that the converse holds as well, i.e., that the positivity of each tangent plane is already sufficient to imply the positivity of J. But this is generally not the case, only in certain situations one of which is covered in the next proposition.

Proposition 3.4.8. *Assume that the complex Lagrangian ideal J is* ***non-degenerate*** *in the sense that it satisfies*

$$T_z J_{\mathbb{R}} = T_z^{\mathbb{C}} J \cap T_z^{\mathbb{R}}(T^*M) \tag{3.64}$$

for all $z \in J_{\mathbb{R}}$, then positivity of all $T_z^{\mathbb{C}}J$ implies positivity of J.

Proof. One always has

$$T_z J_{\mathbb{R}} \subset T_z^{\mathbb{C}} J \cap T_z^{\mathbb{R}}(T^*M) ,$$

so we have to study the consequences if there is equality. By Theorem 3.4.4 we can assume that locally there exists a generating function of J of the form $\langle \xi, x\rangle - F(\xi)$ and then the tangent space to J at $z_0 = (x_0, \xi_0) \in J_{\mathbb{R}}$ is given by

$$T_{z_0}^{\mathbb{C}} J = \{(F''(\xi_0)p, p)\,;\, p \in \mathbb{C}^d\} ,$$

hence we get

$$\begin{aligned} T_z^{\mathbb{C}} J \cap T_z^{\mathbb{R}}(T^*M) &= \{(F''(\xi_0)p, p)\,;\, p \in \mathbb{R}^d ,\ \operatorname{Im} F''(\xi_0)p = 0\} \\ &= \{(\operatorname{Re} F''(\xi_0)p, p)\,;\, p \in \mathbb{R}^d \cap \ker \operatorname{Im} F''(\xi_0)\} . \end{aligned} \tag{3.65}$$

The positivity of $T_{z_0}^{\mathbb{C}} J$ implies that $\operatorname{Im} F''(\xi_0) \leq 0$. Let us choose a splitting of the coordinates $\xi = (\xi', \xi'')$ such that $J_{\mathbb{R}}$ is parameterized by $(\xi', 0)$, then we get $\operatorname{Im} F((\xi', 0)) = 0$ and by (3.64) and (3.65) we have $\langle p'', \operatorname{Im} F'' p''\rangle < 0$ for $p'' \neq 0$, hence $\operatorname{Im} F(\xi) \leq 0$ in a neighborhood of ξ_0. Therefore J is positive then. □

In general it could for instance happen that $F''(\xi_0) = 0$. Then the tangent space to J is totally real, but unless we have no information on the higher order terms of F in the Taylor series around ξ_0, we cannot conclude anything on the positivity of J.

3.4.2 Invariant definition of Lagrangian states

Since by Theorem 3.4.4 we can always find a simple generating function of the form $\langle \xi, x\rangle - F(\xi)$ in suitable local coordinates, it is important to study the corresponding representation of Lagrangian states using such a function.

Theorem 3.4.9. *Let φ, J, $\hat{J}$ and F be as in Proposition 3.4.6 and let $a(\lambda, x, \theta) \in C_0^\infty(\mathbb{R}^d \times \mathbb{R}^\kappa)$ have support in a small neighborhood of (x_0, θ_0) and be of order λ^m, and consider the function*

$$u(\lambda, x) = \left(\frac{\lambda}{2\pi}\right)^{\kappa/2} \int \mathrm{e}^{\mathrm{i}\lambda\varphi(x,\theta)} a(\lambda, x, \theta)\ \mathrm{d}\theta .$$

Then one can find a $v(\lambda, \xi) \in C_0^\infty(\mathbb{R}^d)$ with support in a neighborhood of ξ_0 such that

$$u(\lambda, x) = \left(\frac{\lambda}{2\pi}\right)^{d/2} \int \mathrm{e}^{\mathrm{i}\lambda(\langle \xi, x\rangle - F(\xi))} v(\lambda, \xi)\ \mathrm{d}\xi + O(\lambda^{-\infty}) \tag{3.66}$$

and

$$\frac{1}{\lambda^m}\big(v(\lambda, \xi) - a(\lambda, x, \theta)(\det \Phi/\mathrm{i})^{-1/2}\big) \in \hat{J} ,$$

in a neighborhood of (x_0, θ_0, ξ_0). Here Φ is the matrix given by

$$\Phi(x, \theta) = \begin{pmatrix} \varphi''_{x,x}(x,\theta) & \varphi''_{x,\theta}(x,\theta) \\ \varphi''_{\theta,x}(x,\theta) & \varphi''_{\theta,\theta}(x,\theta) \end{pmatrix} .$$

Proof. We start by computing the λ-Fourier transformation of u defined as

$$\hat{u}^\lambda(\lambda,\xi) := \left(\frac{\lambda}{2\pi}\right)^{d/2} \int \mathrm{e}^{-\mathrm{i}\lambda\langle\xi,x\rangle} u(\lambda,x)\ \mathrm{d}x\ . \tag{3.67}$$

Inserting the integral representation for u gives

$$\hat{u}^\lambda(\lambda,\xi) = \left(\frac{\lambda}{2\pi}\right)^{(d+\kappa)/2} \iint \mathrm{e}^{\mathrm{i}\lambda[\varphi(x,\theta)-\langle\xi,x\rangle]} a(\lambda,x,\theta)\ \mathrm{d}x\mathrm{d}\theta\ ,$$

and we will use the stationary phase formula, Theorem D.4, to determine $\hat{u}^\lambda(\lambda,\xi)$ up to order $O(\lambda^{-\infty})$. The stationary points as functions of ξ are determined by the equations

$$\varphi'_x(x,\theta) - \xi = 0\ , \quad \varphi'_\theta(x,\theta) = 0\ ,$$

and by the assumptions of the theorem the matrix of second derivatives

$$\Phi = \begin{pmatrix} \varphi''_{x,x}(x,\theta) & \varphi''_{x,\theta}(x,\theta) \\ \varphi''_{\theta,x}(x,\theta) & \varphi''_{\theta,\theta}(x,\theta) \end{pmatrix}$$

is non-degenerate. By Theorem C.2 there is a smooth function $F(\xi)$ with $F(\xi)+\varphi(x,\theta)-\langle\xi,x\rangle \in \hat{J}$ and $\operatorname{Im} F(\xi) \leq 0$. Thus Theorem D.4 gives

$$\hat{u}^\lambda(\lambda,\xi) = \mathrm{e}^{-\mathrm{i}\lambda F(\xi)} v(\lambda,\xi) + O(\lambda^{-\infty}) \tag{3.68}$$

with

$$v(\lambda,\xi) \sim \frac{1}{[\det \Phi/\mathrm{i}]^{1/2}} \sum_{k=0}^{\infty} \lambda^{m-k} v_k(\xi)$$

where the functions $v_k(\xi)$ are smooth and compactly supported. If we now take the inverse λ-Fourier transformation we get for u the desired representation

$$u(\lambda,x) = \left(\frac{\lambda}{2\pi}\right)^{d/2} \int \mathrm{e}^{\mathrm{i}\lambda(\langle\xi,x\rangle - F(\xi))} v(\lambda,\xi)\ \mathrm{d}\xi + O(\lambda^{-\infty})\ .$$

□

This simple representation of an oscillating function associated with a complex Lagrangian ideal J can now be used to derive further properties of the set of all such functions. First we want to determine the action of an operator $\mathcal{A}_j \in \Psi^0(m_{a,b})$ with principal symbol in J on such a function. Since J is locally generated by

$$x_j - \partial F(\xi)/\partial\xi_j\ ,\ \ j = 1,\ldots,d\ ,$$

we will assume that $\mathcal{A}_j$ has symbol $x_j - \partial F(\xi)/\partial \xi_j$. Then we get with (3.68)

$$\begin{aligned}\widehat{\mathcal{A}_j u}^{\lambda}(\lambda,\xi) &= \Big(-\frac{\mathrm{i}}{\lambda}\frac{\partial}{\partial \xi_j} - \frac{\partial F}{\partial \xi_j}(\xi)\Big)\hat{u}^{\lambda}(\lambda,\xi) \\ &= -\Big(\frac{\mathrm{i}}{\lambda}\frac{\partial}{\partial \xi_j} + \frac{\partial F}{\partial \xi_j}(\xi)\Big)\mathrm{e}^{-\mathrm{i}\lambda F(\xi)} v(\lambda,\xi) + O(\lambda^{-\infty}) \\ &= -\frac{\mathrm{i}}{\lambda}\frac{\partial v(\lambda,\xi)}{\partial \xi_j}\,\mathrm{e}^{-\mathrm{i}\lambda F(\xi)} + O(\lambda^{-\infty}) \ .\end{aligned}$$

Hence, $\mathcal{A}_j u(\lambda, x)$ is given by

$$\mathcal{A}_j u(\lambda,x) = -\frac{\mathrm{i}}{\lambda}\left(\frac{\lambda}{2\pi}\right)^{d/2}\int \mathrm{e}^{\mathrm{i}\lambda(\langle \xi,x\rangle - F(\xi))}\partial v(\lambda,\xi)/\partial\xi_j \,\mathrm{d}\xi + O(\lambda^{-\infty})$$

and has therefore lost one order in λ compared to (3.66).

We will now give an invariant definition of the space of oscillating functions associated with a given positive complex Lagrangian ideal, analogous to the definition of real Lagrangian distributions in [Hör85b]. Based on the preceeding example we will define them as the set of functions which loose one order in λ under application of a pseudodifferential operator with principal symbol in the complex Lagrangian ideal J.

First we need to define the notion of order for λ-dependent functions and half-densities.

Definition 3.4.10. *Let M be a C^∞ manifold. We will denote by $H^m_\lambda(M)$ the space of functions (half-densities) $u(\lambda)$ on M which depend on a parameter $\lambda \in \mathbb{R}^+$ and satisfy*

$$||u(\lambda)|| \leq C\lambda^m$$

for all λ, where $||\cdot||$ denotes the L^2 norm on M. By $H^m_{\lambda,\mathrm{phg}}(M)$ we will denote the subspace of $H^m_\lambda(M)$, where

$$||u(\lambda)|| \sim \sum_{k=0}^{\infty} \lambda^{m-k}\alpha_k(u) \ ,$$

and the $\alpha_k(u)$ depend smoothly on u.

According to Theorem 3.2.10 the application of a pseudodifferential operator on an oscillatory function leads to the multiplication of the leading term of the amplitude with the principal symbol evaluated on the corresponding Lagrangian manifold. If the principal symbol vanishes on this Lagrangian manifold, then the order of the oscillating function is reduced by one. But the fact that the principal symbol vanishes on the Lagrangian manifold means that it belongs to the corresponding Lagrangian ideal. We will now use this property to give an invariant definition of the set of oscillating functions associated with a given positive Lagrangian ideal.

Definition 3.4.11. *Let M be a C^∞ manifold and J be a positive complex Lagrangian ideal in $C^\infty(T^*M,\mathbb{C})$. We will denote by $I_\lambda^m(M,J)$ the set of smooth functions $u(\lambda)$ on M which depend smoothly on the parameter $\lambda\in\mathbb{R}^+$ and satisfy for all $N\in\mathbb{N}$ and $\mathcal{A}_j\in\Psi_\lambda^0(m_{a,b})$, $j=1,\dots,N$,*

$$\mathcal{A}_1\cdots\mathcal{A}_N u(\lambda)\in H_\lambda^{m-N}(M)\ ,\quad \text{if } \sigma(\mathcal{A}_j)\in J \text{ for } j=1,\dots,N\ . \tag{3.69}$$

Analogously we say that $u(\lambda)$ belongs to $I_{\lambda,\mathrm{phg}}^m(M,J)$ if (3.69) is valid with $H_\lambda^{m-N}(M)$ replaced by $H_{\lambda,\mathrm{phg}}^{m-N}(M)$. The elements of $I_\lambda^m(M,J)$ are called the ***Lagrangian functions*** *associated with J.*

The conceptual advantage of this rather abstract definition of the spaces $I_\lambda^m(M,J)$ and $I_{\lambda,\mathrm{phg}}^m(M,J)$ is that it characterizes them in terms of observables, i.e., in terms of physically meaningful quantities. The set of pseudodifferential operators $\mathcal{A}$ with the property $\sigma(\mathcal{A})\in J$ form an ideal in Ψ, which can be thought of as the quantization of J, and the set of functions in H_λ^0 which is mapped by this ideal to H_λ^{-1}, a set of function which are semiclassically vanishing, can be thought of as the analog of $J_\mathbb{R}$. So in this sense the Definition 3.4.11 resembles on the classical side the definition of the complex Lagrangian ideal. It has furthermore some technical advantages, because it allows to transfer easily properties of pseudodifferential operators to Lagrangian functions. E.g., the theorem of Egorov gives immediately the behavior of $I_\lambda^m(M,J)$ under the action of Fourier integral operators.

Theorem 3.4.12. *Let M be a C^∞ manifold, $\chi: T^*M\to T^*M$ a canonical transformation, and J a positive complex Lagrangian ideal on M. Then $J\circ\chi$ is a positive complex Lagrangian ideal and for every $U(\chi)\in I^k(M,\chi)$ we have*

$$U(\chi): I_\lambda^m(M,J)\to I_\lambda^{m+k}(M,J\circ\chi)\ ,$$

and similarly operators in $I_{\mathrm{phg}}^k(M,\chi)$ map $I_{\lambda,\mathrm{phg}}^m(M,J)$ to $I_{\lambda,\mathrm{phg}}^{m+k}(M,J\circ\chi)$.

Proof. It is obvious from the definition that $J\circ\chi$ is a Lagrangian ideal; what remains to be shown is that it is positive. By Theorem 3.4.4 we can assume that J has the generating function $\langle\xi,x\rangle-F(\xi)$; let $\psi(x,\eta)$ be a generating function for χ in the sense of (2.67), then one can check that

$$\varphi(y;x,\eta,\xi)=\langle\xi,x\rangle-F(\xi)-\psi(x,\eta)+\langle y,\eta\rangle$$

is a generating function for $J\circ\chi$, where (x,η,ξ) are now considered as auxiliary parameters. It is obvious that it has positive imaginary part, and therefore $J\circ\chi$ is positive[2].

The remaining part then follows simply from the fact that by the Theorem of Egorov

$$\sigma(U^*\mathcal{A}U)\in J\circ\chi$$

if $\sigma(\mathcal{A})\in J$. □

[2] We have been cheating a little bit, because the function $\varphi(y;x,\eta,\xi)$ is not non-degenerate in the sense of Definition 3.4.5, but it is clean, see [Hör85a, Definition 21.5.15], and it can be shown as in [Hör85a, chapter 21.2] that clean phase functions as well generate Lagrangian ideals.

Our next aim is to show that the elements of $I_\lambda^m(M,J)$ and $I_{\lambda,\mathrm{phg}}^m(M,J)$ can locally be represented as oscillating integrals. Since the generating phase functions given, e.g., by Theorem 3.4.4, are defined only locally, we have to localize the study of $I_\lambda^m(M,J)$.

Lemma 3.4.13. *Let $u(\lambda) \in I_\lambda^m(M,J)$, then $\mathrm{FS}(u(\lambda)) \subset J_\mathbb{R}$ and $\mathcal{A}u(\lambda) \in I_\lambda^m(M,J)$ for every $\mathcal{A} \in \Psi^0_{\lambda,\mathrm{phg}}(1)$ and every $\mathcal{A} \in \Psi^0(1)$. Conversely, $u(\lambda) \in I_\lambda^m(M,J)$ if for every $(x_0,\xi_0) \in T^*M$ one can find an $\mathcal{A} \in \Psi^0_{\lambda,\mathrm{phg}}(1)$ with $\sigma(\mathcal{A})(x_0,\xi_0) \neq 0$ such that $\mathcal{A}u(\lambda) \in I_\lambda^m(M,J)$.*

We omit the proof, since it is almost identical to the one of [Hör85b, Lemma 25.1.2]. This lemma reduces the study of $I_\lambda^m(M,J)$ to the case that $\mathrm{FS}(u(\lambda))$ is contained in a small neighborhood of some point $z_0 \in J_\mathbb{R}$. In view of Theorem 3.4.4 we may therefore assume that the local coordinates are chosen in a such way that in a neighborhood of z_0 J is generated by $x_j - \partial F(\xi)/\partial\xi_j$, $j = 1,\dots,d$, with some smooth function $F(\xi)$ which satisfies $\operatorname{Im} F(\xi) \leq 0$. We will furthermore restrict ourselves to the case that J satisfies the non-degeneracy condition (3.64). This is not essential, but it will facilitate the proof at some points and make the determination of the order of the functions simpler.

Theorem 3.4.14. *Let M be a C^∞ manifold, and J a positive complex Lagrangian ideal satisfying (3.64). If $u(\lambda) \in I_\lambda^m(M,J)$ has support in some small neighborhood of $z_0 \in J_\mathbb{R}$, then*

$$u(\lambda,x) = \left(\frac{\lambda}{2\pi}\right)^{d/2} \int \mathrm{e}^{\mathrm{i}\lambda(\langle\xi,x\rangle - F(\xi))} a(\lambda,\xi)\, \mathrm{d}\xi$$

with $a(\lambda,\xi)$ satisfying $|\partial_\xi^\beta a(\lambda,\xi)| \leq C_\beta \lambda^m$ for all $\beta \in \mathbb{Z}_+^d$. If $u(\lambda) \in I_{\lambda,\mathrm{phg}}^m(M,J)$ then $a(\lambda,\xi) \sim \sum_{k=0}^\infty \lambda^{m-k} a_k(\xi)$ with $a_k \in C^\infty(\mathbb{R}^d)$.

Proof. Since the ideal J is locally generated by $x_j - \partial F(\xi)/\partial\xi_j$, $j = 1,\dots,d$ we choose $\mathcal{A}_j \in \Psi^0(1)$ with symbols $x_j - \partial F(\xi)/\partial\xi_j$ in a neighborhood of z_0. Then we have

$$\widehat{\mathcal{A}_j u}^\lambda(\lambda,\xi) = \left(\frac{\mathrm{i}}{\lambda}\partial_{\xi_j} - \partial F(\xi)/\partial\xi_j\right) \widehat{u}^\lambda(\lambda,\xi) \; ,$$

where $\widehat{u}^\lambda(\lambda,\xi)$ denotes the λ-Fourier transformation defined in (3.67). Since $||\widehat{u}^\lambda(\lambda,\xi)|| = ||u(\lambda)||$ we get, if we define $a(\lambda,\xi)$ by $\widehat{u}^\lambda(\lambda,\xi) = \mathrm{e}^{-\mathrm{i}\lambda F(\xi)} a(\lambda,\xi)$, that

$$\left(\frac{\mathrm{i}}{\lambda}\partial_{\xi_j} - \partial F(\xi)/\partial\xi_j\right) \widehat{u}^\lambda(\lambda,\xi) = \mathrm{e}^{-\mathrm{i}\lambda F(\xi)} \frac{\mathrm{i}}{\lambda}\partial_{\xi_j} a(\lambda,\xi) \in F_\lambda^{m-1}(\mathbb{R}^d) \; .$$

Iterating this procedure we obtain for every $\beta \in \mathbb{N}$

$$\left(\frac{\mathrm{i}}{\lambda}\right)^{|\beta|} \mathrm{e}^{-\mathrm{i}\lambda F(\xi)} \partial_\xi^\beta a(\lambda,\xi) \in F_\lambda^{m-|\beta|}(\mathbb{R}^d) \; ,$$

and therefore

$$||e^{\lambda \operatorname{Im} F}\partial_\xi^\beta a(\lambda)|| \leq C_\beta \lambda^m \ .$$

In the same way we get for $u(\lambda) \in I^m_{\lambda,\mathrm{phg}}(M,J)$ that for all $\beta \in \mathbb{Z}^d_+$

$$||e^{\lambda \operatorname{Im} F}\partial_\xi^\beta a(\lambda)|| \sim \sum_{k=0}^{\infty} \lambda^{m-k}\alpha_{\beta,k} \ .$$

Let us assume first that J is real, then $\operatorname{Im} F = 0$ and we have in the case that $u \in I^m_\lambda(M,J)$

$$||\partial_\xi^\beta a(\lambda)|| \leq C_\beta \lambda^m$$

for every $\beta \in \mathbb{Z}^d_+$. By the Sobolev inequalities we can pass from the L^2 norms to sup-norms and get

$$|\partial_\xi^\beta a(\lambda,\xi)| \leq C'_\beta \lambda^m$$

for every $\beta \in \mathbb{Z}^d_+$. In the case $u(\lambda) \in I^m_{\lambda,\mathrm{phg}}(M,J)$, we start by studying the sequence $a(\lambda,\xi)/\lambda^m$ for which we get for every $\alpha \in \mathbb{Z}^d_+$ and every fixed $\delta > 0$

$$\begin{aligned}|\partial_\xi^\alpha(a(\lambda,\xi)/\lambda^m - &a(\lambda+\delta,\xi)/(\lambda+\delta)^m)| \\ &\leq C_\alpha ||\partial_\xi^\beta(a(\lambda)/\lambda^m - a(\lambda+\delta)/(\lambda+\delta)^m)|| \to 0\end{aligned}$$

in the limit $\lambda \to \infty$, where $|\beta| \geq |\alpha| + d/2$. Hence $a(\lambda,\xi)/\lambda^m$ is a Cauchy-sequence in $C^\infty(\mathbb{R}^d)$ and there exists a smooth $a_m(\xi)$ with

$$\lim_{\lambda\to\infty} a(\lambda,\xi)/\lambda^m = a_m(\xi) \ .$$

By applying the same procedure to $a(\lambda,\xi) - \lambda^m a_m(\xi)$ and iterating this we get a sequence of smooth $a_k(\xi)$ giving an asymptotic expansion of the amplitude.

Now we come to the case that $\operatorname{Im} F$ is not zero, but that J satisfies the non-degeneracy condition (3.64). This means that there exist a splitting $\xi = (\xi', \xi'')$ such that $J_\mathbb{R}$ is parameterized by $(\xi', 0)$ and $\operatorname{Im} F''$ is non-degenerate when restricted to the complementary space. Then we can evaluate the L^2 norm $||e^{\lambda \operatorname{Im} F}\partial_\xi^\beta a(\lambda)||$ in the limit $\lambda \to \infty$, giving

$$||e^{\lambda \operatorname{Im} F}\partial_\xi^\beta a(\lambda)||^2 \sim \left(\frac{2\pi}{\lambda}\right)^{(d-\dim J_\mathbb{R})/2} \int [\det(\operatorname{Im} F)^\#]^{-1/2} |\partial_\xi^\beta a(\lambda,(\xi',0))|^2 \, d\xi'$$

for $\lambda \to \infty$. The integral is nothing but the L^2 norm of the restriction of the amplitude to $J_\mathbb{R}$. Now, in the same way as for the real case we can use the Sobolev inequalities to see that a defines a unique C^∞ germ on $J_\mathbb{R}$, and similarly in the second case there is a unique germ of an asymptotic expansion. Hence choosing a representative gives the desired conclusion. □

Let us discuss as an example the coherent states in the light of this invariant characterization. The quantizations $\mathcal{A}_j$ of the generators of J in this case satisfy

$$\mathcal{A}_j u^L_{p,q}(\lambda, x) = 0 \ ,$$

hence they are the annihilation operators. The adjoints are then the creation operators.

The existence of creation operators is characteristic for complex ideals. Since in the real case the algebra generated by quantizations of J is self-adjoint, in leading order no such phenomenon occurs there.

We will now consider the problem of defining a principal symbol of a Lagrangian function. The principal symbol will determine the leading asymptotic behavior of the oscillating function, and will furthermore play an important role in the quantization conditions which we will encounter in the study of approximate eigenstates. As a preparation to the general case we will first study the linear case, i.e. $M = \mathbb{R}^d$, and where the complex Lagrangian ideal is generated by linear generators, so J can be identified with a positive complex Lagrangian plane in $T^*\mathbb{C}^d$.

3.4.3 The linear case and the Maslov bundle

We will now discuss the special case of Lagrangian function defined on some Lagrangian subspace of a symplectic vector space.

In case that the symplectic space is the tangent space to a cotangent bundle at some point, $V = T_{(\xi,x)}T^*M$, there is a distinguished real Lagrangian plane given, the kernel of the projection

$$\mathrm{d}\pi : T_{(\xi,x)}T^*M \to T_xM \ .$$

Therefore, we will in the following assume that there is a distinguished real element $L_0 \in \Lambda(V^{\mathbb{C}})$ given.

Let us now choose a real Lagrangian plane $L_1 \in \Lambda_{L_0}(V^{\mathbb{C}})$, that is $L_1 \cap L_0 = \{0\}$. Then the symplectic form defines a non-degenerate bilinear map

$$L_0 \times L_1 \ni (l, l') \mapsto \omega(l, l') \tag{3.70}$$

which gives an isomorphism of L_1 with the dual space of L_0, $L_1 \to L_0'$, and hence can be used to identify half-densities in L_1 and L_0'. We will call symplectic coordinates (ξ, x) ***adapted*** to L_1, if $x = 0$ in L_0 and $\xi = 0$ in L_1, hence L_1 is identified with the base of $T^*\mathbb{R}^d$ and L_0 with the fiber of the projection. Given a linear form P on V and let, in symplectic coordinates adapted to L_1, $P(D_\lambda, x)$ be the operator $\sum_{j=1}^d a_j x_j + \sum_{j=1}^d b_j \frac{1}{\mathrm{i}\lambda}\partial_{x_j}$, when $P = \sum_{j=1}^d a_j x_j + \sum_{j=1}^d b_j \xi_j$.

Definition 3.4.15. *With the previous notations, let $L \in \Lambda^+(V^{\mathbb{C}})$ and define*

$$I(L, L_1) := \{u(\lambda) \in \mathcal{S}'(L_0', \Omega_{1/2})\, ;\, P(D_\lambda, x)u(\lambda) = 0 \quad \textit{for all linear forms } P \textit{ vanishing on } L\ \} \ .$$

This is the linear analog of Definition 3.4.11 where we have allowed the oscillatory integrals to take values in the space of distributions, in order that we can allow the amplitudes to be constant.

In this definition the auxiliary space L_1 appeared, and we want to study the dependence of $I(L, L_1)$ on L_1. So let L_2 be any other real element in $\Lambda_{L_0}(V^{\mathbb{C}})$. In the coordinates (ξ, x) adapted to L_1 it can be written as

$$L_2 = \{(Ax, x)\} ,$$

where A is a real symmetric matrix. Hence the new coordinates (η, y) given by $y = x$ and $\eta = \xi - Ax$ are symplectic and adapted to L_2. Now, if $P(\xi, x) = 0$ on L then $P(\eta + Ay, y) = 0$ on L in the new coordinates, but if $P(D_\lambda, x)u_1(\lambda) = 0$, then $P(D_\lambda + Ay, y)u_2(\lambda) = 0$ if

$$u_2(\lambda, y) = u_1(\lambda, y)\mathrm{e}^{-\mathrm{i}\lambda\langle Ay,y\rangle/2} . \tag{3.71}$$

Hence the map

$$I(L, L_1) \ni u_1(\lambda) \mapsto u_2(\lambda) = u_1(\lambda)\mathrm{e}^{-\mathrm{i}\lambda\langle A\cdot,\cdot\rangle/2} \in I(L, L_2)$$

is an isomorphism which allows to identify the two spaces.

There is clearly a description of the space $I(L, L_1)$ analogous to Theorem 3.4.14.

Lemma 3.4.16. *If $L_1 \cap L = \{0\}$ and (ξ, x) are coordinates adapted to L_1, then every $u(\lambda) \in I(L, L_1)$ is an oscillatory integral*

$$u(\lambda, x) = c\left(\frac{\lambda}{2\pi}\right)^d \int \mathrm{e}^{\mathrm{i}\lambda(\langle\xi,x\rangle - \langle B\xi,\xi\rangle/2)}\, \mathrm{d}\xi\, |\mathrm{d}x|^{1/2} ,$$

where B is a symmetric matrix with negative imaginary part defining L by

$$L = \{(\xi, B\xi)\} ,$$

and c is a constant depending only on λ.

Notice that $\mathrm{i}\omega((\bar{B}\bar{\xi}, \bar{\xi}), (B\xi, \xi)) = \mathrm{i}(\langle\bar{\xi}, B\xi\rangle - \langle\bar{B}\bar{\xi}, \xi\rangle) = -2\langle\bar{\xi}, (\operatorname{Im} B)\xi\rangle \geq 0$, so L is indeed positive. The pre-factor in front of the integral is just a matter of convention; it will turn out to be convenient later on. We omit the proof, since it can be found in [Hör85a, Lemma 21.6.4] and is analogous to the proof of Theorem 3.4.14, but simpler.

The distribution $u(\lambda)$ is uniquely determined by the factor c, so the question arises how it changes if we change L_1, i.e. the coordinates on the base. First we note that with

$$c\left(\frac{\lambda}{2\pi}\right)^d \int \mathrm{e}^{\mathrm{i}\lambda(\langle\xi,x\rangle - \langle B\xi,\xi\rangle/2)}\, \mathrm{d}\xi\, |\mathrm{d}x|^{1/2} = \frac{c}{|\mathrm{d}x|^{1/2}}\left(\frac{\lambda}{2\pi}\right)^d \int \mathrm{e}^{\mathrm{i}\lambda(\langle\xi,x\rangle - \langle B\xi,\xi\rangle/2)}\, \mathrm{d}\xi\, |\mathrm{d}x|$$

we get

$$c\,|\mathrm{d}x|^{-1/2} = \int u(\lambda)\, |\mathrm{d}x|^{1/2} , \tag{3.72}$$

so c can be naturally identified with a $-\frac{1}{2}$ density on L_1. By the duality (3.70) this $-\frac{1}{2}$ density on L_1 is mapped to the $\frac{1}{2}$ density $c|\mathrm{d}\xi|^{1/2}$ on L_0, and since L_1 is transversal to L, the projection

$$\pi_{L_1} : L \to L_0$$

of L to L_0 along L_1 is bijective. Hence, the half-density on L_0 can be pulled back to a half-density on L,

$$u(\lambda)^{\#}_{L_1} := \pi^*_{L_1} c|\mathrm{d}\xi|^{1/2} \ . \tag{3.73}$$

This is an object on L which characterizes uniquely the distribution in $I(L)$, it only depends on L_1. Now let $L_2 \in \Lambda_{L_0}(V^{\mathbb{C}})$ be totally real. According to (3.71) the element $u(\lambda) \in I(L)$ is in coordinates (y, η), which are adapted to L_2, given by

$$u_2(\lambda, y) = c \left(\frac{\lambda}{2\pi}\right)^d \mathrm{e}^{-\mathrm{i}\lambda\langle Ay,y\rangle/2} \int \mathrm{e}^{\mathrm{i}\lambda(\langle y,\xi\rangle - \langle B\xi,\xi\rangle/2)} \,\mathrm{d}\xi \,|\mathrm{d}y|^{1/2} \ .$$

Now the same reasoning which lead to (3.73) leads to a half-density

$$u(\lambda)^{\#}_{L_2} := \pi^*_{L_2} c_2 |\mathrm{d}\eta|^{1/2}$$

on L, where according to (3.72) c_2 is given by

$$\begin{aligned} c_2\,|\mathrm{d}y|^{-1/2} = \int u_2(\lambda, y)\,|\mathrm{d}y|^{1/2} &= c\left(\frac{\lambda}{2\pi}\right)^d \iint \mathrm{e}^{\mathrm{i}\lambda(\langle y,\xi\rangle - \langle B\xi,\xi\rangle/2 - \langle Ay,y\rangle/2)} \,\mathrm{d}\xi\mathrm{d}y \\ &= c\left[\det \frac{1}{\mathrm{i}} \begin{pmatrix} -B & I \\ I & -A \end{pmatrix}\right]^{-1/2} \ . \end{aligned}$$

In order to complete the determination of the transformation property of $u(\lambda)^{\#}_{L_1}$ to $u(\lambda)^{\#}_{L_2}$ we have to compare the densities $\pi^*_{L_1}|\mathrm{d}\xi|$ and $\pi^*_{L_2}|\mathrm{d}\eta|$ on L. In the (ξ, x) coordinates ξ parameterizes L via $(\xi, B\xi) \in L$. In the (η, y) coordinates the same point is parameterized by $\eta = \xi - Ay = \xi - AB\xi$, since $y = x = B\xi$ on L, so

$$\pi_{L_2}\pi^{-1}_{L_1}\xi = (I - AB)\xi \ .$$

But since $\det(I - AB) = \det \frac{1}{\mathrm{i}} \begin{pmatrix} -B & I \\ I & -A \end{pmatrix}$, we get

$$u(\lambda)^{\#}_{L_2} = \mathrm{e}^{\mathrm{i}\pi s(L_0, L; L_1, L_2)/4} u(\lambda)^{\#}_{L_1} \tag{3.74}$$

with

$$\begin{aligned} s(L_0, L; L_1, L_2) &:= -\frac{1}{\pi} \arg\det \frac{1}{\mathrm{i}} \begin{pmatrix} -B & I \\ I & -A \end{pmatrix} \\ &= -\frac{1}{\pi} \arg\det(I - AB) = -\frac{1}{\pi} \arg\det \pi_{L_2}\pi^{-1}_{L_1} \ . \end{aligned} \tag{3.75}$$

This number $s(L_0, L; L_1, L_2)$ is defined modulo $2\pi\mathbb{Z}$ for each four Lagrangian planes L_0, L, L_1, L_2 such that the two former ones are transversal to the two others, and L is positive while all others are totally real. The definition can be extended to the case that $\operatorname{Im} A \leq 0$, i.e. L_1 is negative, and since the space of complex matrices with negative imaginary part is simply connected, there is a unique choice of $\arg\det \pi_{L_2}\pi_{L_1}^{-1}$ such that

$$s(L_0, L; L_1, L_1) = 0 \ .$$

This number is the generalization of the Hörmander index [Hör71, GS77] to the case of a complex Lagrangian manifold L and it has been studied in [Mei94, RZ84]. It follows immediately from the representation as $s(L_0, L; L_1, L_2) = -\frac{1}{\pi}\arg\det \pi_{L_2}\pi_{L_1}^{-1}$ that it satisfies the following cocycle conditions

$$\begin{aligned} s(L_0, L; L_1, L_2) + s(L_0, L; L_2, L_1) &= 0 \\ s(L_0, L; L_1, L_2) + s(L_0, L; L_2, L_3) + s(L_0, L; L_3, L_1) &= 0 \ . \end{aligned} \tag{3.76}$$

These cocycle conditions imply that the transition functions $\mathrm{e}^{\mathrm{i}\pi s(L_0,L;L_1,L_2)/4}$ define a complex $U(1)$ bundle on Λ^+.

Definition 3.4.17. *The complex $U(1)$ line bundle on Λ^+ defined by a covering with the open sets $\Lambda^+_{L_1}(V^{\mathbb{C}})$, $L_1 \in \Lambda^+_{L_0}(V^{\mathbb{C}})$, and the transition functions*

$$g_{L_1,L_2} = \mathrm{e}^{\mathrm{i}\pi s(L_0,L;L_1,L_2)/4} \ , \quad L \in \Lambda^+_{L_1}(V^{\mathbb{C}}) \cap \Lambda^+_{L_2}(V^{\mathbb{C}}) \ ,$$

with $s(L_0, L; L_1, L_2)$ defined in (3.75), *is called the* ***Maslov bundle*** *$M(\Lambda^+)$ of Λ^+.*

The Maslov bundle additionally depends on L_0, but in the applications there will be a canonical choice for it, so we have not mentioned it explicitly in the definition.

Therefore (3.74) means that $u(\lambda)^{\#}$ gives rise to a section of the Maslov bundle $M(\Lambda^+)$ over Λ^+. We will view the quantity $u(\lambda)^{\#}$ as the principal symbol of $u(\lambda)$: it is a section of the Maslov bundle tensored with the half-density bundle on L,

$$\Omega_{1/2}(L) \otimes M(\Lambda^+) \ .$$

The representation $s(L_0, L; L_1, L_2) = -\frac{1}{\pi}\arg\det \pi_{L_2}\pi_{L_1}^{-1}$ suggests that we might represent $s(L_0, L; L_1, L_2)$ as well as $s(L_0, L; L_1, L_2) = -\frac{1}{\pi}\arg\det \pi_{L_2} - (-\frac{1}{\pi}\arg\det \pi_{L_1})$ if we could make sense of the expression $\arg\det \pi_{L_2}$. This is done in the following definition taken from [RZ84].

Definition 3.4.18. *Let $L_0, L_1 \in \Lambda(V^{\mathbb{C}})$ be real, $L \in \Lambda^+(V^{\mathbb{C}})$ with $L \cap L_1 = \{0\}$ and let $\pi_{L_1} : L \to L_0$ be the projection along L_1, then*

$$L \ni l \mapsto \omega(l, \pi_{L_1} l)$$

defines a quadratic form on L with positive imaginary part. Let Q be the matrix representing this quadratic form in some basis, then we define

$$s(L_0, L, L_1) := \frac{1}{\pi}\operatorname{sign}_+ Q \ ,$$

where $\operatorname{sign}_+ Q$ *is defined in Appendix D, eq.* (D.2).

That $\omega(l, \pi_{L_1} l)$ has positive imaginary part will be shown in the proof of the next proposition, which gives the desired decomposition of the Hörmander index.

Proposition 3.4.19. *Let $L_0, L_1, L_2 \in \Lambda(V^{\mathbb{C}})$ be real and $L \in \Lambda^+(V^{\mathbb{C}})$ with $L_0 \cap L_1 = L_0 \cap L_2 = \{0\}$ and $L \cap L_1 = L \cap L_2 = \{0\}$ then*

$$s(L_0, L; L_1, L_2) = s(L_0, L, L_1) - s(L_0, L, L_2) \ .$$

Since the right-hand side is defined without any restrictions on $L \in \Lambda^+(V^{\mathbb{C}})$, it defines an extension of the function $s(L_0, L; L_1, L_2)$ to the case that $L \cap L_1 \neq \{0\}$, $L \cap L_2 \neq \{0\}$.

Proof. Let (ξ, x) be symplectic coordinates in $V^{\mathbb{C}}$ adapted to L_1, i.e. $L_1 = \{(0, x);\ x \in \mathbb{C}^d\}$ and $L_0 = \{(\xi, 0);\ \xi \in \mathbb{C}^d\}$ in these coordinates, then there is a complex symmetric matrix B with $\operatorname{Im} B < 0$ such that L is given as $L = \{(\xi, B\xi);\ \xi \in \mathbb{C}^d\}$. Since $L_0 \cap L_1 = \{0\}$ they span $V^{\mathbb{C}}$ and each element $l \in L$ can be uniquely decomposed into $l = l_0 + l_1$ with $l_0 \in L_0$ and $l_1 \in L_1$, then $\pi_{L_1} l = l_0$ in the coordinates (ξ, x). This means that

$$(\xi, B\xi) = (\xi, 0) + (0, x)$$

with $x = B\xi$, hence $\pi_{L_1}(\xi, B\xi) = (\xi, 0)$ and

$$\langle \xi, Q\xi \rangle = \omega((\xi, B\xi), \pi_{L_1}(\xi, B\xi)) = \omega((\xi, B\xi), (\xi, 0)) = -\langle \xi, B\xi \rangle \ .$$

Therefore we have found that the quadratic form $\omega(l, \pi_{L_1} l)$ has positive imaginary part and that

$$s(L_0, L, L_1) = \frac{1}{\pi} \operatorname{sign}_+(-B) \ . \tag{3.77}$$

In the same coordinates L_2 is given by (Ax, x) for some real symmetric matrix A and to determine the corresponding decomposition of an element of L into a sum of elements from L_0 and L_2, and to find π_{L_2}, we have to solve the equation

$$(\xi, B\xi) = (\xi', 0) + (Ax, x)$$

for ξ'. From the second component we get $B\xi = x$ and inserting this into the first component gives $\xi' = \xi - Ax = (I - AB)\xi$, hence $\pi_{L_2}(\xi, B\xi) = ((I - AB)\xi, 0)$. This leads to $\omega((\xi, B\xi), \pi_{L_2}(\xi, B\xi)) = -\langle \xi, B(I - AB)\xi \rangle$, and therefore

$$s(L_0, L, L_2) = \frac{1}{\pi} \operatorname{sign}_+(-B(I - AB)) \ .$$

By taking the difference of $s(L_0, L, L_1)$ and $s(L_0, L, L_2)$ we get

$$\begin{aligned} s(L_0, L, L_1) - s(L_0, L, L_2) &= \frac{1}{\pi} \operatorname{sign}_+(-B) - \frac{1}{\pi} \operatorname{sign}_+(-B(I - AB)) \\ &= -\frac{1}{\pi} \operatorname{sign}_+[(-B(I - AB))(-B)^{-1}] \\ &= -\frac{1}{\pi} \operatorname{sign}_+(I - AB) \\ &= s(L_0, L; L_1, L_2) \end{aligned}$$

by (3.75). □

The meaning of this result is that the functions $e^{i\pi s(L_0,L,L_1)}$ define local trivialisations of the Maslov bundle.

For a real Lagrangian space L, the indices $s(L_0,L;L_1,L_2)$ and $s(L_0,L,L_1)$ and their properties have been studied intensively in the literature, see, e.g., [Hör85a, GS77, Dui76] and [CLM94] for a review. We will now show that if $L\in\Lambda^+(V^{\mathbb{C}})$ contains a real subspace D, i.e. $D\cap\overline{D}=\{0\}$, then we can represent the index $s(L_0,L,L_1)$ as a sum of two indices $s(L_0',L',L_1')+s(L_0'',L'',L_1'')$ on different spaces, with L'' real, so we can use the known results for part of $s(L_0,L,L_1)$.

If $D\subset L$ and $D\cap\overline{D}=\{0\}$, then D is isotropic in V and we can study the reduced space

$$V':=D^{\omega}/D\ .$$

It is a symplectic vector space, and there is a map of Lagrangian subspaces

$$\begin{aligned}\Lambda^+(V^{\mathbb{C}})&\to\Lambda^+(V'^{\mathbb{C}})\\ L&\mapsto L':=(L\cap D^{\omega})/(L\cap D)\ ,\end{aligned}\tag{3.78}$$

see, e.g. [Hör85a]. On the other hand, if we choose a subspace $E\subset V$ which is complementary to D^{ω}, $E\cap D^{\omega}=\{0\}$ there is a projection along E, $\pi_E:V\to D^{\omega}$, and the space V_E'' defined by

$$0\to V_E''\to V\xrightarrow{\pi_E}D^{\omega}\to V'\to 0\ ,$$

is symplectic. The exact sequence furthermore induces a map of Lagrangian subspaces

$$\Lambda(V)\ni L\to L_E''=L\cap V_E''\in\Lambda(V_E'')\ ,$$

where L_E'' is the pre-image of L'.

Proposition 3.4.20. *Let $L\in\Lambda^+(V^{\mathbb{C}})$, $L_0,L_1\in\Lambda_{\mathbb{R}}(V^{\mathbb{C}})$ with $L_0\cap L_1=L\cap L_1=\{0\}$ and $D\subset L$ be real, then in the notation just defined*

$$s(L_0,L,L_1)=s(L_0',L',L_1')+s(L_0'',L'',L_1'')\ ,$$

where $s(L_0',L',L_1')$ is the index on V' and $s(L_0'',L'',L_1'')=s(L_0{}_E'',L_E'',L_1{}_E'')$ is the index on V_E'' and is independent of E. For the Hörmander index then follows

$$s(L_0,L;L_1,L_2)=s(L_0',L';L_1',L_2')+s(L_0'',L'';L_1'',L_2'')$$

if $L_2\in\Lambda_{\mathbb{R}}(V^{\mathbb{C}})$ with $L_0\cap L_2=L\cap L_2=\{0\}$.

Proof. Let (ξ,x) be coordinates in $V^{\mathbb{C}}$ adapted to L_0 and L_1, i.e. $L_0=\{(\xi,0)\ \xi\in\mathbb{C}^d\}$ and $L_1=\{(0,x)\,;\ x\in\mathbb{C}^d\}$, then L can be represented as

$$L=\{(\xi,B\xi)\,;\ \xi\in\mathbb{C}^d\}\ .$$

Assume furthermore that the coordinates are chosen such that there is a splitting $\xi = (\xi', \xi'')$ with

$$D = \{((0,\xi''), B(0,\xi''))\,;\ \xi'' \in \mathbb{C}^k\}\ ,$$

and write B in block-diagonal form corresponding to the splitting (ξ', ξ''),

$$B = \begin{pmatrix} B_1 & 0 \\ 0 & B_2 \end{pmatrix}\ ,$$

which can be achieved with a change of coordinates respecting the splitting (ξ', ξ'') corresponding to D. That D is real is equivalent to B_2 being real. By (3.77) we therefore have

$$s(L_0, L, L_1) = \frac{1}{\pi}\,\mathrm{sign}_+(-B) = \frac{1}{\pi}\,\mathrm{sign}_+(-B_1) + \frac{1}{\pi}\,\mathrm{sign}_+(-B_2)\ . \tag{3.79}$$

Now we come to the computation of $s(L'_0, L', L'_1)$. In the preceeding coordinates we have

$$\begin{aligned} D &= \{((0,\xi''), (0, B_2\xi''))\,;\ \xi'' \in \mathbb{C}^k\}\ ,\\ D^\omega &= \{((\xi',\xi''), (x', B_2\xi''))\,;\ x' \in \mathbb{C}^{d-k}\ (\xi',\xi'') \in \mathbb{C}^{d-k} \oplus \mathbb{C}^k\}\ , \end{aligned}$$

so $V' = D^\omega/D$ can be identified with the subspace

$$\{((\xi',0),(x',0))\,;\ x' \in \mathbb{C}^{d-k}\, \xi' \in \mathbb{C}^{d-k}\} \cong \{(\xi',x')\,;\ (\xi',x') \in \mathbb{C}^{d-k} \oplus \mathbb{C}^{d-k}\} \cong S'$$

of V. Furthermore, we get in the coordinates (x', ξ') of V'

$$L'_0 = \{(\xi',0)\,;\ \xi' \in \mathbb{C}^{d-k}\}\ ,\quad L'_1 = \{(0,x')\,;\ x' \in \mathbb{C}^{d-k}\}\ ,\quad L' = \{(\xi', B_1\xi')\,;\ \xi' \in \mathbb{C}^{d-k}\}\ ,$$

and therefore by (3.77)

$$s(L'_0, L', L'_1) = \frac{1}{\pi}\,\mathrm{sign}_+(-B_1)\ . \tag{3.80}$$

The second index $s(L''_0, L'', L''_1)$ can be computed similarly. The space

$$E = \{((0,0),(0,x''))\,;\ x'' \in \mathbb{C}^k\}\ ,$$

in the same coordinates (ξ, x) as above, is complementary to D^ω and V''_E can identified with a subspace of V,

$$S''_E \cong \{((0,\xi''),(0,x''))\,;\ x'' \in \mathbb{C}^k\, \xi'' \in \mathbb{C}^k\}\ .$$

The Lagrangian subspaces L_0, L, L_1, are mapped to

$$L_0{}''_E = \{(\xi'',0)\,;\ \xi'' \in \mathbb{C}^k\}\ ,\quad L_1{}''_E = \{(0,x'')\,;\ x'' \in \mathbb{C}^k\}\ ,\quad L''_E = \{(\xi'', B_2\xi'')\,;\ \xi'' \in \mathbb{C}^k\}\ ,$$

in the coordinates (ξ'', x'') of V''_E, and hence we get by (3.77)

$$s({L_0}''_E, L''_E, {L_1}_E'') = \frac{1}{\pi}\,\mathrm{sign}_+(-B_1)\ . \tag{3.81}$$

Therefore, by (3.79), (3.80) and (3.81) we have arrived at

$$s(L_0, L, L_1) = s(L'_0, L', L'_1) + s({L_0}''_E, L''_E, {L_1}''_E)\ ,$$

and since $s(L_0, L, L_1)$ and $s(L'_0, L', L'_1)$ are independent of E, $s({L_0}''_E, L''_E, {L_1}''_E)$ is independent of E too. □

Of special interest will be the case $D = L \cap \overline{L}$. This is the largest possible D, then L' is strictly positive.

We will now study representations of elements of $I(L)$ with arbitrary quadratic phase functions. Let $Q(x, \theta)$, $(x, \theta) \in \mathbb{R}^d \times \mathbb{R}^\kappa$, be nondegenerate and positive, in the sense that the differentials

$$\mathrm{d}\frac{\partial Q}{\partial \theta_1}, \dots, \mathrm{d}\frac{\partial Q}{\partial \theta_\kappa}$$

are linear independent on the set $\partial Q/\partial\theta = 0$, and that $\operatorname{Im} Q \geq 0$. Then one can show as in [Hör85a, Chapter 21.6] that the integral

$$u(x) = a\left(\frac{\lambda}{2\pi}\right)^{(d+\kappa)/2} \int \mathrm{e}^{\mathrm{i}\lambda Q(x,\theta)}\ \mathrm{d}\theta\ |\mathrm{d}x|^{1/2} \tag{3.82}$$

is well defined as an oscillatory integral. We have for any linear form P

$$P(D_\lambda, x)u(x) = a\left(\frac{\lambda}{2\pi}\right)^{(d+\kappa)/2} \int P(\partial Q/\partial x, x)\mathrm{e}^{\mathrm{i}\lambda Q(x,\theta)}\ \mathrm{d}\theta\ |\mathrm{d}x|^{1/2}\ ,$$

and so if $P(\partial Q/\partial x, x) = \sum t_i \partial Q/\partial\theta_i$ we obtain by partial integration

$$P(D_\lambda, x)u(x) = 0.$$

Hence we get for such P, that $P(\xi, x) = 0$ for

$$(\xi, x) \in L := \{(\partial Q/\partial x, x)\,;\ \partial Q/\partial\theta = 0\}$$

so $u \in I(L, L_1)$, where $L_1 = \{(0, x)\}$. If $L \cap L_1 = \{0\}$ we have for u a representation as in Lemma 3.4.16, with c given according to (3.72) by

$$c = a\left(\frac{\lambda}{2\pi}\right)^{(d+\kappa)/2} \iint \mathrm{e}^{\mathrm{i}\lambda Q(x,\theta)}\ \mathrm{d}\theta\mathrm{d}x = a\frac{1}{\sqrt{\det Q''/\mathrm{i}}} = a\frac{\mathrm{e}^{\mathrm{i}\pi\,\mathrm{sign}_+ Q''/4}}{\sqrt{|\det Q''|}}\ ,$$

where we have used Theorem D.2 and eq. (D.3). We are now going to interpret the term $1/\sqrt{|\det Q''|}$. The exact sequence

$$0 \longrightarrow C_Q \longrightarrow \mathbb{R}^d \times \mathbb{R}^\kappa \xrightarrow{Q'_\theta} \mathbb{R}^\kappa \longrightarrow 0$$

together with the Lebesgue densities in $\mathbb{R}^d \times \mathbb{R}^\kappa$ and $\mathbb{R}^\kappa$ induces a density σ_Q on

$$C_Q := \{(x,\theta)\ ;\ \partial Q/\partial\theta = 0\,\}$$

defined by

$$\sigma_Q\,|\mathrm{d}\partial Q/\partial\theta_1 \wedge \ldots \wedge \mathrm{d}\partial Q/\partial\theta_\kappa| = |\mathrm{d}x_1 \wedge \ldots \wedge \mathrm{d}x_d \wedge \mathrm{d}\theta_1 \wedge \ldots \wedge \mathrm{d}\theta_\kappa|\ .$$

Since Q is nondegenerate, the map

$$C_Q \ni (x,\theta) \mapsto (\partial Q/\partial x, x) \in L$$

is an isomorphism, hence defines a bijection between the densities on these two vector-spaces. If $L \cap L_1 = \{0\}$, we can identify the densities on L with the densities on L_0 via the projection along L_1 and a density ρ on L can be written as $\rho = b|\mathrm{d}\xi|$. In order that it coincides with the push-forward of the density σ_Q to L, its pullback to C_Q, $b|\mathrm{d}\partial Q/\partial x_1 \wedge \ldots \wedge \mathrm{d}\partial Q/\partial x_d|$, has to coincide with σ_Q, hence we get the condition

$$\begin{aligned} b\,|\mathrm{d}\partial Q/\partial x_1 \wedge \ldots \wedge \mathrm{d}\partial Q/\partial x_d|\,|\mathrm{d}\partial Q/\partial\theta_1 \wedge \ldots \wedge \mathrm{d}\partial Q/\partial\theta_\kappa| \\ = |\mathrm{d}x_1 \wedge \ldots \wedge \mathrm{d}x_d \wedge \mathrm{d}\theta_1 \wedge \ldots \wedge \mathrm{d}\theta_\kappa|\ , \end{aligned}$$

and therefore $b = 1/|\det Q''|$. If we recall that $u^\#_{L_1} = c|\mathrm{d}\xi|^{1/2}$, we can summarize that we have found

$$u^\#_{L_1} = a\sigma_Q^{1/2}\mathrm{e}^{\mathrm{i}\pi\,\mathrm{sign}_+ Q''/4}\ . \tag{3.83}$$

If we have another representation

$$\tilde{u}(\lambda, x) = \tilde{a}\left(\frac{\lambda}{2\pi}\right)^{(d+\tilde{\kappa})/2} \int \mathrm{e}^{\mathrm{i}\lambda\tilde{Q}(x,\tilde{\theta})}\ \mathrm{d}\tilde{\theta}\ |\mathrm{d}x|^{1/2}$$

of the same element as in (3.82), then $\tilde{Q}$ must parameterize the same Lagrangian plane L then Q, and it follows from (3.83) that we have

$$a\sigma_Q^{1/2}\mathrm{e}^{\mathrm{i}\pi[\mathrm{sign}_+ Q'' - \mathrm{sign}_+ \tilde{Q}'']/4} = \tilde{a}\sigma_{\tilde{Q}}^{1/2}\ .$$

This gives another description of the Maslov bundle $M(\Lambda^+)$ on Λ^+. For a fixed L_1 choose an open cover of Λ^+ with sets Λ such that L is defined by a non-degenerate quadratic form Q_L depending continuously on $L \in \Lambda$. Then for another $\tilde{Q}_L$, with $L \in \tilde{\Lambda}$ we get the transition functions

$$\mathrm{e}^{\mathrm{i}\pi[\mathrm{sign}_+ Q''_L - \mathrm{sign}_+ \tilde{Q}''_L]/4}\ , \quad L \in \tilde{\Lambda} \cap \Lambda\ , \tag{3.84}$$

which define the Maslov bundle.

We will now extend the definition of the Maslov bundle to the global case, i.e. to symplectic vector bundles. A symplectic vector bundle is a vector bundle with a symplectic vector space as a fiber, such that the symplectic form varies smoothly, see, e.g., [MS98] for details. The basic examples which we will encounter is the tangent bundle $T(T^*M)$ of the cotangent bundle of a smooth manifold M, and the restrictions of this bundle to submanifolds $\Lambda \subset T^*M$, $T(T^*M)|_\Lambda$, where the fiber at each point in Λ is given by the tangent space of T^*M at this point.

In $T(T^*M)$ there is a distinguished Lagrangian subbundle L_0 defined as

$$L_0(p,q) := \ker \mathrm{d}\pi(p,q) \ ,$$

where $\pi : T^*M \to M$ is the canonical projection of T^*M. The set of positive Lagrangian planes $\mathcal{L}^+(T^{\mathbb{C}}_{(p,q)}(T^*M))$ in the complexification $T^{\mathbb{C}}_{(p,q)}(T^*M)$ of the tangent space to T^*M at $(p,q) \in T^*M$ for each $(p,q) \in T^*M$ defines another fiber bundle $\mathcal{L}^+(T^{\mathbb{C}}(T^*M))$ over T^*M with fiber Λ^+. The Lagrangian subbundle L_0 defines a section in this bundle, which in turn defines on every fiber $\mathcal{L}^+(T^{\mathbb{C}}_{(p,q)}(T^*M))$ a Maslov bundle $M(\mathcal{L}^+(T^{\mathbb{C}}_{(p,q)}(T^*M)))$. The resulting bundle

$$M(T(T^*M)) \to \mathcal{L}^+(T^{\mathbb{C}}(T^*M))$$

is called the Maslov bundle of T^*M.

Now let J be a positive complex Lagrangian ideal on T^*M, and denote by $L(p,q) = T_{(p,q)}J$ the positive Lagrangian plane in $T^{\mathbb{C}}_{(p,q)}T^*M$ at $(p,q) \in J_{\mathbb{R}}$. Furthermore, let $M \to U_1$ be a local chart of M near q and (ξ, x) the local coordinates then $L_1(p,q) = \{(0,x)\,;\, x \in \mathbb{C}^d\}$ is a real Lagrangian plane in $T^{\mathbb{C}}_{(p,q)}T^*M$ which is transversal to L_0. Let $M \to U_2$ and L_2 be another such pair. Then a complex $U(1)$ line bundle on $J_{\mathbb{R}}$ is defined by a covering of a neighborhood of $J_{\mathbb{R}}$ by open sets Λ_j with $\pi(\Lambda_j) = U_j$ and the transition functions

$$g_{i,j}(p,q) = \mathrm{e}^{\mathrm{i}\pi s(L_0(p,q), L(p,q); L_i, L_j)/4} \ , \quad (p,q) \in \Lambda_i \cap \Lambda_j \ .$$

This is called the Maslov bundle of J.

One can give as well a description of the Maslov bundel in terms of generating functions, analogous to (3.84). Cover a neighborhood of $J_{\mathbb{R}}$ in T^*M with open sets Λ_j such that on each Λ_j, J is can parameterized by a nondegenerate phase function φ_j. Then the Maslov bundle on J is defined by the transition functions

$$\mathrm{e}^{\mathrm{i}\pi[\mathrm{sign}_+ \varphi_i'' - \mathrm{sign}_+ \varphi_j'']/4} \qquad \text{on } \Lambda_i \cap \Lambda_j \cap J_{\mathbb{R}} \ . \tag{3.85}$$

3.4.4 The principal symbol

Now we will turn back to general Lagrangian states and use the facts we have learned on the linear case to define a principal symbol in the general case. Let M be a smooth manifold, $J \subset C^\infty(T^*M, \mathbb{C})$ be a positive complex Lagrangian ideal on M, $u \in I^m_\lambda(M, J)$

and $(p,q) \in J_{\mathbb{R}}$, then by Theorem 3.4.14 and Theorem 3.4.9 in a neighborhood of q u can modulo $\lambda^{-\infty}$ be represented as

$$u(\lambda,x) = \left(\frac{\lambda}{2\pi}\right)^{\kappa/2} \int \mathrm{e}^{\mathrm{i}\lambda\varphi(x,\theta)} a(\lambda,x,\theta)\, \mathrm{d}\theta \;,$$

with $\varphi(x,\theta)$ a non-degenerate generating function for J and $a \in S^m_\lambda(\mathbb{R}^d \times \mathbb{R}^\kappa)$. Since $(p,q) \in J_{\mathbb{R}}$, there is a $\theta_0 \in \mathbb{R}^\kappa$ with

$$p = \varphi'_x(q,\theta_0) \qquad \text{and} \quad \varphi'_\theta(q,\theta_0) = 0 \;.$$

Let us now consider the Taylor-expansion of $\varphi(x,\theta)$ around (q,θ_0) up to second order,

$$\begin{aligned}\varphi(x,\theta) &= \varphi(q,\theta_0) + \varphi'_x(q,\theta_0)(x-q) + \varphi'_\theta(q,\theta_0)(\theta-\theta_0) + Q(x-q,\theta-\theta_0) + \cdots \\ &= \varphi(q,\theta_0) + p(x-q) + Q(x-q,\theta-\theta_0) + \cdots \;,\end{aligned}$$

with

$$Q(x,\theta) = \frac{1}{2}(x,\theta) \begin{pmatrix} \varphi''_{x,x}(q,\theta_0) & \varphi''_{x,\theta}(q,\theta_0) \\ \varphi''_{\theta,x}(q,\theta_0) & \varphi''_{\theta,\theta}(q,\theta_0)\end{pmatrix} \begin{pmatrix} x \\ \theta \end{pmatrix} \;,$$

and the corresponding "linearized" state around (p,q),

$$u_{(p,q)}(\lambda, q+x) = \left(\frac{\lambda}{2\pi}\right)^{\kappa/2} a(\lambda,q,\theta_0)\mathrm{e}^{\mathrm{i}\lambda(\varphi(q,\theta_0)+pq)} \int \mathrm{e}^{\mathrm{i}\lambda Q(x,\theta)}\, \mathrm{d}\theta \;. \tag{3.86}$$

This state is in $I(L)$ with $L = T_{(p,q)}J \subset T^{\mathbb{C}}_{(p,q)}T^*M$, and we want to compare it at (p,q) with the full state u.

Proposition 3.4.21. *Let M be a smooth manifold, $J \subset C^\infty(T^*M,\mathbb{C})$ be a positive complex Lagrangian ideal on M, $u \in I^m_\lambda(M,J)$, $(p,q) \in J_{\mathbb{R}}$ and $u_{(p,q)} \in I(T_{(p,q)}J)$ be the corresponding linearization* (3.86) *of u at (p,q), then*

$$\langle u_{(p,q)}, u^L_{(p,q)}\rangle = O(\lambda^{m-d/4}) \;, \quad \text{and } \langle u - u_{(p,q)}, u^L_{(p,q)}\rangle = O(\lambda^{m-d/4-1}) \;,$$

for all L with $\overline{L} \cap T_{(p,q)}J = \{0\}$ and $u^L_{(p,q)}$ given by (3.33). *Hence $u_{(p,q)}$ determines the leading order behavior of u at $(p,q) \in T^*M$ for $\lambda \to \infty$.*

Proof. The proof is a straightforward application of the stationary phase theorem. We start by computing $\langle u_{(p,q)}, u^L_{(p,q)}\rangle$. With (3.86) and (3.33) we get

$$\begin{aligned}\langle u_{(p,q)}, u^L_{(p,q)}\rangle &= \left(\frac{\lambda}{2\pi}\right)^{\kappa/2} \left(\frac{\lambda}{\pi}\right)^{d/4} \bar{a}(\lambda,q,\theta_0)\mathrm{e}^{-\mathrm{i}\lambda(\bar{\varphi}(q,\theta_0)+pq)}(\det \operatorname{Im} B)^{1/4} \\ &\qquad \iint \mathrm{e}^{-\mathrm{i}\lambda\bar{Q}(x-q,\theta)} \mathrm{e}^{\mathrm{i}\lambda[\langle x,p\rangle + \frac{1}{2}\langle B(x-q),x-q\rangle]}\, \mathrm{d}\theta\mathrm{d}x \\ &= \left(\frac{\lambda}{2\pi}\right)^{\kappa/2} \left(\frac{\lambda}{\pi}\right)^{d/4} \bar{a}(\lambda,q,\theta_0)\mathrm{e}^{-\mathrm{i}\lambda\bar{\varphi}(q,\theta_0)}(\det \operatorname{Im} B)^{1/4} \\ &\qquad \iint \mathrm{e}^{\mathrm{i}\lambda\langle(\theta,x),\mathcal{Q}(\theta,x)\rangle/2} \mathrm{e}^{\mathrm{i}\lambda\langle x,p\rangle}\, \mathrm{d}\theta\mathrm{d}x \;,\end{aligned}$$

where we have introduced the matrix

$$\mathcal{Q} = \begin{pmatrix} -\bar{\varphi}''_{\theta\theta}(q,\theta_0) & -\bar{\varphi}''_{\theta x}(q,\theta_0) \\ -\bar{\varphi}''_{x\theta}(q,\theta_0) & -\bar{\varphi}''_{xx}(q,\theta_0)+B \end{pmatrix} .$$

Recall that

$$\begin{aligned} L &= \{(Bx,x)\, ;\ x\in\mathbb{C}^d\} \\ \overline{T_{(p,q)}J} &= \{(\overline{\varphi}''_{xx}x+\overline{\varphi}''_{x\theta}\theta,x)\, ;\ \overline{\varphi}''_{\theta\theta}\theta+\overline{\varphi}''_{\theta x}x=0\,\} , \end{aligned}$$

hence if there is a (θ,x) with $\mathcal{Q}\binom{\theta}{x}=0$, i.e.

$$\begin{aligned} -\overline{\varphi}''_{\theta\theta}\theta-\overline{\varphi}''_{\theta x}x &= 0 \\ -\overline{\varphi}''_{xx}x-\overline{\varphi}''_{x\theta}\theta+Bx &= 0 , \end{aligned}$$

then the vector $(\overline{\varphi}''_{xx}x+\overline{\varphi}''_{x\theta}\theta,x)$ is in $L\cap\overline{T_{(p,q)}J}$. Therefore $\overline{L}\cap T_{(p,q)}J=\{0\}$ implies that the matrix $\mathcal{Q}$ is non-degenerate.

So we can apply Theorem D.2 and (D.3) and get

$$\langle u_{(p,q)},u^L_{(p,q)}\rangle = \left(\frac{4\pi}{\lambda}\right)^{d/4} \bar{a}(\lambda,q,\theta_0)\mathrm{e}^{-\mathrm{i}\lambda\bar{\varphi}(q,\theta_0)}\frac{(\det\operatorname{Im}B)^{1/4}}{|\det\mathcal{Q}|^{1/2}}\mathrm{e}^{-\mathrm{i}\lambda\langle(0,p),\mathcal{Q}^{-1}(0,p)\rangle} .$$

On the other hand the evaluation of the stationary phase formula (D.8) gives

$$\langle u,u^L_{(p,q)}\rangle = \langle u_{(p,q)},u^L_{(p,q)}\rangle + O(\lambda^{m-d/4-1}) .$$

□

By this proposition we can transfer the notion of a principal symbol from the linear case to the general case, and it will characterize the Lagrangian state in leading order. In contrast to the linear case an additional phase factor appears, due to the so-called Liouville class.

In order to determine the nature of the leading part of u at (p,q) we have to study its behavior under a change of the representation of u. So let $\tilde{\varphi}(x,\tilde{\theta})\in C^\infty(\mathbb{R}^d\times\mathbb{R}^{\tilde{\kappa}})$ be another phase function parameterizing J in a neighborhood of (p,q) and $\tilde{a}(\lambda,x,\tilde{\theta})$ be a corresponding amplitude, such that the same u is given by

$$u(\lambda,x) = \left(\frac{\lambda}{2\pi}\right)^{\tilde{\kappa}/2}\int \mathrm{e}^{\mathrm{i}\lambda\tilde{\varphi}(x,\tilde{\theta})}a(\lambda,x,\tilde{\theta})\,\mathrm{d}\tilde{\theta}$$

in a neighborhood of $x=q$. Then we get for the linearized u at (p,q) the expression

$$u_{(p,q)}(\lambda,q+x) = \left(\frac{\lambda}{2\pi}\right)^{\tilde{\kappa}/2}\tilde{a}(\lambda,q,\tilde{\theta}_0)\mathrm{e}^{\mathrm{i}\lambda(\tilde{\varphi}(q,\tilde{\theta}_0)+pq)}\int \mathrm{e}^{\mathrm{i}\lambda\tilde{Q}(x,\tilde{\theta})}\,\mathrm{d}\tilde{\theta} ,$$

and comparison with the linear case and (3.84) shows that in order that it coincides with (3.86), $\tilde{a}$ and a have to satisfy

$$\tilde{a}(q,\tilde{\theta}_0)\sigma_{\tilde{Q}}^{1/2} = \mathrm{e}^{\mathrm{i}\lambda[\varphi(q,\theta_0)-\tilde{\varphi}(q,\tilde{\theta}_0)]}\mathrm{e}^{\mathrm{i}\pi[\mathrm{sign}_+ Q''-\mathrm{sign}_+ \tilde{Q}'']/4}a(q,\theta_0)\sigma_Q^{1/2} \; .$$

The new term which appears here in contrast to (3.84) is

$$\mathrm{e}^{\mathrm{i}\lambda[\varphi(q,\theta_0)-\tilde{\varphi}(q,\tilde{\theta}_0)]} \; , \tag{3.87}$$

and we will now interpret it. For comparison see Section 3.1, where we have discussed it already briefly for real Lagrangian manifolds. Recall the map

$$\begin{aligned} \iota_\varphi : C_\varphi &\to J_{\mathbb{R}} \\ (x,\theta) &\mapsto (x,\varphi_x'(x,\theta)) \; , \end{aligned}$$

where $C_\varphi \subset \mathbb{R}^d \times \mathbb{R}^\kappa$ is defined as

$$C_\varphi := \{(x,\theta)\, ;\; \varphi_\theta'(x,\theta) = 0\, ,\; \mathrm{Im}\,\varphi(x,\theta) = 0\,\} \; .$$

The phase function $\varphi(q,\theta_0(p,q))$ on $J_{\mathbb{R}}$ is the push-forward $\iota_{\varphi *}\varphi$ of the function $\varphi(x,\theta)$ on C_φ. Now we have

$$\mathrm{d}\varphi|_{C_\varphi} = (\varphi_x' + \varphi_\theta')|_{C_\varphi}\mathrm{d}x = \iota_\varphi^*(\xi \mathrm{d}x) \; , \tag{3.88}$$

so $\mathrm{d}\varphi|_{C_\varphi}$ is the pullback of the Liouville one form $\xi\mathrm{d}x$ on $J_{\mathbb{R}}$ to C_φ, and we get

$$\mathrm{d}[\iota_{\varphi *}\varphi - \iota_{\tilde{\varphi} *}\tilde{\varphi}] = 0 \; .$$

Therefore the phase factor (3.87) is constant. The $U(1)$ line bundle on $J_{\mathbb{R}}$ which is defined by choosing these functions as transition function will be called the Liouville bundle $\mathcal{L}_\lambda(J_{\mathbb{R}})$; note that it depends on the parameter λ.

We can interpret the preceeding constructions now as providing a map

$$\sigma : I_\lambda^m(M,J) \to C^\infty(J_{\mathbb{R}}, \Omega_{1/2}(J) \otimes M_J \otimes \mathcal{L}_\lambda(J_{\mathbb{R}})) \; , \tag{3.89}$$

which in local coordinates $x \in \mathbb{R}^d$ and with a generating function $\varphi(x,\theta) \in C^\infty(\mathbb{R}^d \times \mathbb{R}^\kappa)$ for J is given by

$$u(x) = \left(\frac{\lambda}{2\pi}\right)^{\kappa/2} \int \mathrm{e}^{\mathrm{i}\lambda\varphi(x,\theta)}a(\lambda,x,\theta)\; \mathrm{d}\theta \mapsto \sigma(u) = \frac{\mathrm{e}^{\mathrm{i}\lambda(\varphi(q,\theta_0)+pq)}}{(\det\varphi''(q,\theta_0)/\mathrm{i})^{1/2}}a_0(q,\theta_0) \; . \tag{3.90}$$

Definition 3.4.22. *Let M be a C^∞ manifold and $J \subset C^\infty(T^*M,\mathbb{C})$ be a positive complex Lagrangian ideal, then the map* (3.89) *is called the* ***principal symbol map****, and $\sigma(u)$ defined in local coordinates by* (3.90) *is called the* ***principal symbol*** *of u.*

By (3.90) every generating function φ defines a local trivialization of the bundle

$$C^\infty(J_{\mathbb{R}}, \Omega_{1/2}(J) \otimes M_J \otimes \mathcal{L}_\lambda(J_{\mathbb{R}})) \ ,$$

because

$$\frac{\mathrm{e}^{\mathrm{i}\lambda(\varphi(q,\theta_0)+pq)}}{(\det \varphi''(q,\theta_0)/\mathrm{i})^{1/2}} \tag{3.91}$$

is a local section of this bundle. Using these local trivializations one can show that the principal symbol characterizes a Lagrangian state up to leading order.

Proposition 3.4.23. *Let M be a C^∞ manifold and $J \subset C^\infty(T^*M, \mathbb{C})$ be a positive complex Lagrangian ideal, then the principal symbol map provides an isomorphism*

$$I_\lambda^m(M,J)/I_\lambda^{m-1}(M,J) \cong C^\infty(J_{\mathbb{R}}, \Omega_{1/2}(J) \otimes M_J \otimes \mathcal{L}_\lambda(J_{\mathbb{R}}))$$

Proof. What remains to do, is to construct an inverse of the principal symbol map, i.e. to an arbitrary element of $C^\infty(J_{\mathbb{R}}, \Omega_{1/2}(J) \otimes M_J \otimes \mathcal{L}_\lambda(J_{\mathbb{R}}))$ we have to associate an element of $I_\lambda^m(M,J)/I_\lambda^{m-1}(M,J)$.

So let there be given an element $\sigma \in C^\infty(J_{\mathbb{R}}, \Omega_{1/2}(J) \otimes M_J \otimes \mathcal{L}_\lambda(J_{\mathbb{R}}))$, and choose a cover $\{\Lambda_j\}$ of a neighborhood of $J_{\mathbb{R}}$ in T^*M such that near each $J_{\mathbb{R}j} := J_{\mathbb{R}} \cap \Lambda_j$, J is generated by a non-degenerate phase function φ_j. Each phase function φ_j defines a local trivialization by which σ is mapped to an element of $C^\infty(J_{\mathbb{R}})$ which we will call a_j. Now pulling this back to C_{φ_j} by ι_{φ_j} and choosing a smooth extension to $\mathbb{R}^d \times \mathbb{R}^{\kappa_j}$ gives an element of $C^\infty(\mathbb{R}^d \times \mathbb{R}^{\kappa_j})$ which we will call $a_j(x,\theta_j)$; it defines an element of S^m/S^{m-1}. If we choose for each j one representative $a_j(\lambda,x,\theta_j)$ of this equivalence class and define

$$u_j(x) = \left(\frac{\lambda}{2\pi}\right)^{\kappa_j/2} \int \mathrm{e}^{\mathrm{i}\lambda\varphi_j(x,\theta_j)} a_j(\lambda,x,\theta_j)\; \mathrm{d}\theta_j \ ,$$

then these functions are unique modulo $I_\lambda^{m-1}(M,J)$ and coincide on the intersections of the covering $\{\Lambda_j\}$ modulo $I_\lambda^{m-1}(M,J)$, hence they define the unique element of

$$I_\lambda^m(M,J)/I_\lambda^{m-1}(M,J) \ ,$$

which we were looking for. □

The inverse of the principal symbol map which we constructed in the proof is called the canonical operator, or Maslov's canonical operator. It was first introduced by Maslov for the case of real Lagrangian manifolds [Mas72], see as well [MF81], and later extended to the case of complex Lagrangian manifolds also, see [MSS90] for an exposition of the theory. In our exposition we have followed more closely the theory of Fourier Integral Operators and the way Duistermaat presented the theory of oscillatory integrals with real phase functions along these lines [Dui74].

3.5 Time evolution

In this section we will study the time evolution of Lagrangian states in the semiclassical limit. Special emphasis will be put on the time dependence of the remainder terms, since this is the place where the stability of the classical system manifests itself. For systems with positive Lyapunov exponent typically the remainder term will grow exponentially with time, whereas for regular systems it will only grow polynomially. We will concentrate on coherent states, since on the one hand they are sufficiently simple to treat, and on the other hand by their completeness we can use them to get information on arbitrary states. We will follow mainly the work of Combescure and Robert [CR97], with some minor changes. The time evolution of coherent states was also extensively discussed from a more physical point of view in [Lit86].

3.5.1 Time evolution of coherent states

We will now study the time evolution of coherent states. As we have learned in Section 3.3, a coherent state is characterized by a point (p, q) in phase space and a strictly positive Lagrangian subspace L of the complexified tangent space at (p, q). Given these data the state is

$$u_{p,q}^{L}(\lambda, x) = \left(\frac{\lambda}{\pi}\right)^{d/4} (\det \operatorname{Im} B)^{1/4} \mathrm{e}^{\mathrm{i}\lambda(\langle p, x-q\rangle + \frac{1}{2}\langle B(x-q),(x-q)\rangle)} ,$$

where the matrix B is determined by L through

$$L = \{(Bx, x) \; ; x \in \mathbb{C}^d\} .$$

Let $\mathcal{H}$ be a selfadjoint pseudodifferential operator of λ-order zero on M with Weyl symbol

$$H(\lambda, \xi, x) \sim \sum_{k \geq 0} \lambda^{-k} H_k(\xi, x) ,$$

principal symbol $\sigma(\mathcal{H}) = H_0$ and subprincipal symbol $\operatorname{sub}(\mathcal{H}) = H_1$. Let $(p(t), q(t))$ be the solution of Hamilton's equations

$$\dot{q} = \frac{\partial H_0(p, q)}{\partial p} , \qquad \dot{p} = -\frac{\partial H_0(p, q)}{\partial q} , \tag{3.92}$$

with initial conditions $(p(0), q(0)) = (p, q)$. We know from the propagation of frequency sets that a state centered initially at (p, q) will after time t be centered at $(p(t), q(t))$.

In order to determine the semiclassical time evolution we have to solve the Schrödinger equation

$$\left(\frac{\mathrm{i}}{\lambda}\frac{\partial}{\partial t} - \mathcal{H}\right) \psi(t, x) = 0 ,$$

with initial condition $\psi(0,x)=u^L_{p,q}(x)$ in the limit $\lambda\to\infty$. Since we expect that $\psi(t,x)$ will microlocally be concentrated around $(p(t),q(t))$ we will approximate the operator $\mathcal{H}$ microlocally around $(p(t),q(t))$ with a simpler operator $\mathcal{H}^{(2)}(t)$ such that

$$(\mathcal{H}-\mathcal{H}^{(2)}(t))u^{L'}_{p(t),q(t)}=O(\lambda^{-3/2}) \ ,$$

for every L'. The time evolution generated by $\mathcal{H}^{(2)}(t)$ can be computed directly, and the error we make with this approximation will then be estimated using Duhamel's principle.

The approximate Hamiltonian $\mathcal{H}^{(2)}(t)$ is obtained by taking as its Weyl symbol all terms in the Taylor expansion of $H(\lambda,\xi,x)$ around $(p(t),q(t))$ which contribute to $\mathcal{H}u^{L'}_{p(t),q(t)}$ up to order λ^{-1}. So we need the Taylor series of H_0 up to order 2 and of H_1 only the zeroth-order term. Hence we will start by discussing the time evolution of a state with quadratic phase function generated by a quadratic time dependent Hamiltonian.

Let us denote in the following the points in phase space T^*M by $z=(\xi,x)$. The Weyl symbol of $\mathcal{H}^{(2)}_{z_0(t)}(t)$ then is

$$\begin{aligned}H^{(2)}(t,z)=&H_0(t,z_0(t))+\langle H_0'(t,z_0(t)),z-z_0(t)\rangle+\frac{1}{2}\langle z-z_0(t),H_0''(t,z_0(t))(z-z_0(t))\rangle\\&+\frac{1}{\lambda}H_1(t,z_0(t)) \ ,\end{aligned} \tag{3.93}$$

where $z_0(t)=(p(t),q(t))$ denotes a solution to Hamilton's equations (3.92) with initial conditions $z_0(0)=(p,q)$, and $H_0'(t,z_0(t))$ and $H_0''(t,z_0(t))$ denote the gradient and the matrix of second derivatives of H_0 at $z_0(t)$, respectively.

By $\mathcal{S}_{z_0}(t)$ we denote the linearized flow along the trajectory $z_0(t)$, i.e.

$$\mathcal{S}_{z_0}(t):T_{z_0}T^*M\to T_{z_0(t)}T^*M$$

is the solution of the differential equation

$$\frac{\partial\mathcal{S}_{z_0}(t)}{\partial t}=\mathcal{J}_0H_0''(t,z_0(t))\mathcal{S}_{z_0}(t) \ , \quad \text{with } \mathcal{S}_{z_0}(0)=I \ , \tag{3.94}$$

where $\mathcal{J}_0=\left(\begin{smallmatrix}0&I\\-I&0\end{smallmatrix}\right)$. $\mathcal{S}_{z_0}(t)$ is a one parameter group of symplectic matrices, and the map

$$T^*M\times T_{z_0}T^*M\ni(z_0,v)\mapsto(z_0(t),\mathcal{S}_{z_0}(t)v)\in T^*M\times T_{z_0(t)}T^*M$$

is the standard skew-product defined by the linearized flow, see, e.g., [BDD+00].

By the action on the Siegel upper half plane, see (3.40), the family of symplectic transformations $\mathcal{S}(t)$ defines a family of matrices

$$B(t):=\mathcal{S}(t)_*B_0=(S_{11}B_0+S_{12})(S_{21}B_0+S_{22})^{-1} \ . \tag{3.95}$$

Recall that by Proposition 3.3.12 there exist unique symplectic matrices $\mathcal{P}(t)$ and $\mathcal{T}(t)$ with $\mathcal{P}(t)_*\mathrm{i}I=B(t)$, $\mathcal{T}(t)_*B_0=\mathrm{i}I$, and wich leave the vertical space $L_0=\{(\xi,0)\}$ invariant. So there is a unique symplectic orthogonal matrix $\mathcal{O}(t)$ defined by

$$\mathcal{S}(t)=\mathcal{P}(t)\mathcal{O}(t)\mathcal{T}(t) \ . \tag{3.96}$$

By the correspondence principle one expects that the coherent state centered at $z_0 = (p,q)$ with Lagrangian L is mapped under the time evolution in leading order to a coherent state centered at $z_0(t) = (p(t), q(t))$ with Lagrangian $\mathcal{S}(t)L$. Modulo a phase factor this is indeed the case.

Theorem 3.5.1. *Let $\mathcal{H}^{(2)}_{z_0(t)}$ denote the Weyl-quantization of the symbol* (3.93)*, then the unique solution of the differential equation*

$$\frac{\mathrm{i}}{\lambda}\frac{\partial\psi(t,x)}{\partial t} = \mathcal{H}^{(2)}_{z_0(t)}\psi(t,x) \tag{3.97}$$

with initial condition

$$\psi(0,x) = u^L_{p,q}(\lambda,x) = \left(\frac{\lambda}{\pi}\right)^{d/4}(\det \operatorname{Im} B)^{1/4}\mathrm{e}^{\mathrm{i}\lambda(\langle p,x-q\rangle+\frac{1}{2}\langle B(x-q),x-q\rangle)} \tag{3.98}$$

is given by

$$\begin{aligned}\psi(t,x) &= \left(\frac{\lambda}{\pi}\right)^{d/4}(\det \operatorname{Im} B(t))^{1/4}\mathrm{e}^{-\mathrm{i}(\lambda\Theta(t)-\sigma(t))}\mathrm{e}^{\mathrm{i}\lambda[\langle p(t),x-q(t)\rangle+\frac{1}{2}\langle B(t)(x-q(t)),x-q(t)\rangle]}\\ &= \mathrm{e}^{\mathrm{i}(\lambda\Theta(t)+\sigma(t))}u^{\mathcal{S}(t)L}_{p(t),q(t)}(\lambda,x)\ .\end{aligned} \tag{3.99}$$

Here $(p(t),q(t))$ are the solutions of Hamilton's equations with initial condition $(p(0),q(0)) = (p,q)$, $B(t)$ is the image of B under the action of $\mathcal{S}(t)$, $B(t) = \mathcal{S}(t)_*B_0$, $\Theta(t)$ is the classical action along the path $(p(t),q(t))$,

$$\Theta(t) = \int_0^t \left[H_0(p(t'),q(t'),t') - \langle p(t),\dot q(t)\rangle\right]\,\mathrm{d}t'\ ,$$

and

$$\sigma(t) = \int_0^t H_1(t',p(t'),q(t'))\,\mathrm{d}t' + \frac{\pi}{2}\sigma'(t)\ ,$$

where the Maslov phase $\sigma'(t)$ is defined by the multiplier, see (3.45)*,*

$$m(\mathcal{O}(t),\mathrm{i}I) = \mathrm{e}^{\mathrm{i}\frac{\pi}{2}\sigma'(t)}$$

with $\mathcal{O}(t)$ given by (3.96).

Proof. We only have to check that the function (3.99) satisfies the equation (3.97). This will be a tedious but straightforward computation. If we make an ansatz

$$\psi(t,x) = \left(\frac{\lambda}{\pi}\right)^{d/4}\alpha(t)\mathrm{e}^{-\mathrm{i}\lambda\Theta(t)}\mathrm{e}^{\mathrm{i}\lambda[\langle p(t),x-q(t)\rangle+\frac{1}{2}\langle B(t)(x-q(t)),(x-q(t))\rangle]}$$

we get for the left hand side of (3.97),

$$\frac{\mathrm{i}}{\lambda}\frac{\partial\psi(t,x)}{\partial t} = \bigg[\frac{\mathrm{i}}{\lambda}\dot{\alpha}/\alpha + \dot{\Theta} + \langle p,\dot{q}\rangle - \langle\dot{p},x-q\rangle + \langle B\dot{q},(x-q)\rangle - \frac{1}{2}\langle\dot{B}(x-q),(x-q)\rangle\bigg]\psi(t,x) \ ,$$

where the dot denotes a derivative with respect to time. For the right-hand side of (3.97) we get

$$\begin{aligned}\mathcal{H}^{(2)}\psi(t,x) = \bigg[&H_0 + \left\langle\frac{\partial H_0}{\partial x}, x-q\right\rangle + \left\langle\frac{\partial H_0}{\partial\xi}, B(x-q)\right\rangle \\ &+ \frac{1}{2}\langle x-q, H_0{}''_{x,x}(x-q)\rangle + \frac{1}{2}\langle x-q, H_0{}''_{\xi,x}B(x-q)\rangle \\ &+ \frac{1}{2}\langle x-q, BH_0{}''_{\xi,x}(x-q)\rangle + \frac{1}{2\mathrm{i}\lambda}\operatorname{tr} H_0{}''_{\xi,x} + \frac{1}{2}\langle x-q, BH_0{}''_{\xi,\xi}B(x-q)\rangle \\ &+ \frac{1}{2\mathrm{i}\lambda}\operatorname{tr} H_0{}''_{\xi,\xi}B + \frac{1}{\lambda}H_1\bigg]\psi(t,x) \ ,\end{aligned}$$

where we have used the relation

$$\langle\partial_x, Qx\rangle\psi(x) = \operatorname{tr} Q\,\psi(x) + \langle\partial_x\psi(x), Qx\rangle$$

for a matrix Q. By equating equal powers of λ and of $(x-q)$ we get the following set of equations

$$\dot{\alpha}/\alpha = -\frac{1}{2}[\operatorname{tr} H''_{\xi,x} + \operatorname{tr} H''_{\xi,\xi}B] - \mathrm{i}H_1 \tag{3.100}$$

$$\dot{\Theta} = -\langle\dot{q},p\rangle + H_0 \tag{3.101}$$

$$-\dot{p} + B\dot{q} = \frac{\partial H_0}{\partial x} + B\frac{\partial H_0}{\partial\xi} \tag{3.102}$$

$$-\dot{B} = H_0{}''_{x,x} + H_0{}''_{\xi,x}B + BH_0{}''_{\xi,x} + BH_0{}''_{\xi,\xi}B \ . \tag{3.103}$$

The second equation (3.101) is just solved by integration and the third one, (3.102), follows from Hamilton's equations (3.92), so we are left with the first and the fourth one. In order to determine the derivative of B it is useful to write out the differential equation (3.94) for $\mathcal{S}$ more explicitly. A short computation gives

$$\begin{pmatrix}\dot{S}_{11} & \dot{S}_{12}\\ \dot{S}_{21} & \dot{S}_{22}\end{pmatrix} = \begin{pmatrix}-H_0{}''_{\xi,x}S_{11} - H_0{}''_{x,x}S_{21} & -H_0{}''_{\xi,x}S_{12} - H_0{}''_{x,x}S_{22}\\ H_0{}''_{\xi,\xi}S_{11} + H_0{}''_{\xi,x}S_{21} & H_0{}''_{\xi,\xi}S_{12} + H_0{}''_{\xi,x}S_{22}\end{pmatrix} \ . \tag{3.104}$$

Now differentiating (3.95) with respect to t gives

$$\begin{aligned}\dot{B} &= (\dot{S}_{11}B + \dot{S}_{12})(S_{21}B + S_{22})^{-1} \\ &\quad - (S_{11}B + S_{12})(S_{21}B + S_{22})^{-1}(\dot{S}_{21}B + \dot{S}_{22})(S_{21}B + S_{22})^{-1} \\ &= (\dot{S}_{11}B + \dot{S}_{12})(S_{21}B + S_{22})^{-1} - B(\dot{S}_{21}B + \dot{S}_{22})(S_{21}B + S_{22})^{-1} \ .\end{aligned}$$

But with (3.104) we get

$$\begin{aligned}\dot{S}_{11}B + \dot{S}_{12} &= (-H_0{}''_{\xi,x}S_{11} - H_0{}''_{x,x}S_{21})B - H_0{}''_{\xi,x}S_{12} - H_0{}''_{x,x}S_{22} \\ &= -H_0{}''_{\xi,x}(S_{11}B + S_{12}) - H_0{}''_{x,x}(S_{21}B + S_{22})\end{aligned}$$

and

$$\begin{aligned}\dot{S}_{21}B + \dot{S}_{22} &= (H_0{}''_{\xi,\xi}S_{11} + H_0{}''_{\xi,x}S_{21})B + H_0{}''_{\xi,\xi}S_{12} + H_0{}''_{\xi,x}S_{22} \\ &= H_0{}''_{\xi,\xi}(S_{11}B + S_{12}) + H_0{}''_{\xi,x}(S_{21}B + S_{22}) \ ,\end{aligned} \tag{3.105}$$

which together lead to the desired result (3.103),

$$\dot{B} = -H_0{}''_{\xi,x}B - H_0{}''_{x,x} - BH_0{}''_{\xi,\xi}B - BH_0{}''_{\xi,x} \ .$$

In the first equation (3.100) we make an ansatz

$$\alpha(t) = \mathrm{e}^{-\mathrm{i}\int_0^t H_1 \mathrm{d}t'} a(t)$$

which leads together with (3.105) to

$$\begin{aligned}\frac{\partial}{\partial t}\ln a &= -\frac{1}{2}\,\mathrm{tr}[H_0{}''_{\xi,x} + H_0{}''_{\xi,\xi}B] \\ &= -\frac{1}{2}\,\mathrm{tr}[(\dot{S}_{21}B + \dot{S}_{22})(S_{21}B + S_{22})^{-1}] \\ &= -\frac{1}{2}\frac{\partial}{\partial t}\,\mathrm{tr}\ln(S_{21}B + S_{22}) \ ,\end{aligned}$$

hence we get with the initial condition $a(0) = (\det \operatorname{Im} B_0)^{1/4}$ and the definition (3.45) of $m(\mathcal{S}, B_0)$

$$\begin{aligned}a(t) &= (\det \operatorname{Im} B_0)^{1/4}\mathrm{e}^{-\frac{1}{2}\mathrm{tr}\ln(S_{21}B_0 + S_{22})} \\ &= (\det \operatorname{Im} B_0)^{1/4}[\det(S_{21}B_0 + S_{22})]^{-1/2} \\ &= (\det \operatorname{Im} B_0)^{1/4} m(\mathcal{S}, B_0) \ .\end{aligned}$$

But $m(\mathcal{S}, B_0)$ was determined in Proposition 3.3.12 to be

$$m(\mathcal{S}, B_0) = \frac{(\det \operatorname{Im} \mathcal{S}_* B_0)^{1/4}}{(\det \operatorname{Im} B_0)^{1/4}}\, m(\mathcal{O}, \mathrm{i}I) \ ,$$

and so we get

$$a(t) = (\det \operatorname{Im} B)^{1/4} m(\mathcal{O}, \mathrm{i}I) \ .$$

□

In the following we will denote the time evolution operator generated by $\mathcal{H}^{(2)}_{z_0(t)}(t)$ by $\mathcal{U}^{(2)}(t,t_0)$. It is the solution of the Schrödinger equation

$$\frac{\mathrm{i}}{\lambda}\frac{\mathrm{d}\mathcal{U}^{(2)}(t,t_0)}{\mathrm{d}t} = \mathcal{H}^{(2)}_{z_0(t)}(t)\mathcal{U}^{(2)}(t,t_0) \ ,$$

with initial condition

$$\mathcal{U}^{(2)}(t_0,t_0) = 1 \ .$$

Corollary 3.5.2. *Let $W^L_{z_0}(z)$ be the Wigner function of the coherent state $u^L_{z_0}$, see Lemma 3.3.14, then the Wigner function of $\mathcal{U}^{(2)}(t,0)u^L_{z_0}$ is given by*

$$W^{\mathcal{S}(t)L}_{z_0(t)}(z) = \left(\frac{\lambda}{\pi}\right)^d \mathrm{e}^{-\lambda\langle z-z_0(t),\mathbf{g}(t)(z-z_0(t))\rangle} \ ,$$

with

$$\mathbf{g}(t) = \mathcal{S}^{-1\dagger}(t)\mathbf{g}_L\mathcal{S}^{-1}(t)$$

and $\mathbf{g}_L$ was given by, see (3.53),

$$\mathbf{g}_L = \begin{pmatrix} \operatorname{Im} B + \operatorname{Re} B[\operatorname{Im} B]^{-1}\operatorname{Re} B & -[\operatorname{Im} B]^{-1}\operatorname{Re} B \\ -\operatorname{Re} B[\operatorname{Im} B]^{-1} & [\operatorname{Im} B]^{-1} \end{pmatrix} \ .$$

Proof. Since the phase factor $\mathrm{e}^{-\mathrm{i}(\lambda\Theta(t)-\sigma(t))}$ in (3.99) drops out in the definition of the Wigner function, we get by Lemma 3.3.14

$$W^{\mathcal{S}(t)L}_{z_0(t)}(z) = \left(\frac{\lambda}{\pi}\right)^d \mathrm{e}^{-\lambda\langle z-z_0(t),\mathbf{g}_{\mathcal{S}(t)L}(z-z_0(t))\rangle} \ .$$

So the result follows from the fact that the symplectic group action on $\mathbf{g}_L$ takes the simple form,

$$\mathbf{g}_{\mathcal{S}L} = \mathcal{S}^{-1\dagger}\mathbf{g}_L\mathcal{S}^{-1}$$

for every symplectic matrix $\mathcal{S}$, which we have shown in Proposition 3.3.8.

□

This result shows that the Wigner function is localized at $z = z(t)$ as long as $\lambda||\mathbf{g}(t)||$ is sufficiently large, so the condition

$$\lambda||\mathbf{g}(t)|| \geq C$$

introduces a time scale $T_E(\lambda)$, sometimes called the Ehrenfest time, up to which a localized state stays localized under time evolution. We want to discuss this time scale more closely for different examples. First of all, it mainly depends on the linearized flow $\mathcal{S}(t)$ along the trajectory $z(t)$. For later use it is more convenient to state an estimate in the norm of $\mathbf{g}^{-1}(t)$.

Lemma 3.5.3. *We have*

$$||\mathbf{g}^{-1}(t)|| \leq \frac{\operatorname{tr} \mathcal{S}(t)\mathcal{S}^{\dagger}(t)}{|\operatorname{tr} \mathbf{g}(0)|} \ .$$

Proof. By Corollary 3.5.2 we have

$$\mathbf{g}(0) = \mathcal{S}^{\dagger}(t)\mathbf{g}(t)\mathcal{S}(t) \ .$$

Taking the trace on both sides gives

$$|\operatorname{tr} \mathbf{g}(0)| = |\operatorname{tr} \mathcal{S}^{\dagger}(t)\mathbf{g}(t)\mathcal{S}(t)| = |\operatorname{tr} \mathbf{g}(t)\mathcal{S}(t)\mathcal{S}^{\dagger}(t)| \leq ||\mathbf{g}(t)|| \operatorname{tr} \mathcal{S}(t)\mathcal{S}^{\dagger}(t) \ ,$$

and therefore

$$||\mathbf{g}^{-1}(t)|| = ||\mathbf{g}(t)||^{-1} \leq \frac{\operatorname{tr} \mathcal{S}(t)\mathcal{S}^{\dagger}(t)}{|\operatorname{tr} \mathbf{g}(0)|} \ .$$

□

For Hamiltonian systems the tangent space splits into two subspaces at every point, $T_z(T^*M) = V_z^{(0)} \oplus V_z^{(1)}$, where $V_z^{(0)}$ is spanned by be the Hamiltonian vectorfield and a vector transversal to the energy shell, hence $\dim V_z^{(0)} = 2$, and $V_z^{(1)}$ is a complementary subspace. Furthermore the splitting can be chosen such that it is invariant under the linearized flow $\mathcal{S}_z(t)$, i.e. $\mathcal{S}_z(t)V_z^{(0)} = V_{z(t)}^{(0)}$ and $\mathcal{S}_z(t)V_z^{(1)} = V_{z(t)}^{(1)}$, so $\mathcal{S}_z(t)$ is block-diagonal with blocks $\mathcal{S}_z^{(1)}(t)$ and $\mathcal{S}_z^{(2)}(t)$. The part $\mathcal{S}_z^{(1)}(t)$ has always two eigenvalues one, and can be brought to the normal form

$$\mathcal{S}_z^{(1)}(t) = \begin{pmatrix} 1 & tT'(E) \\ 0 & 1 \end{pmatrix} \ ,$$

whereas the behavior of $\mathcal{S}_z^{(2)}(t)$ reflects the stability properties of the orbit $z(t)$. We will discuss the different cases that can occur and the corresponding time scales.

(i) The unstable case: The orbit is unstable if $\mathcal{S}^{(2)}(1)$ has an eigenvalue of absolute value larger than 1. The Lyapunov exponent $\gamma(z)$ of the trajectory through z, defined as

$$\gamma(z) := \lim_{t\to\infty} \frac{\ln \left[\operatorname{tr} \mathcal{S}^{(2)\dagger}(t)\mathcal{S}^{(2)}(t)\right]^{1/2}}{t} \ ,$$

is then positive. So we get an Ehrenfest time

$$T_E(\lambda) \sim \frac{\ln \lambda}{2\gamma(z)}$$

up to which a coherent state stays localized in phase space.

(ii) The stable case: If all eigenvalues of $\mathcal{S}^{(2)}(t)$ lie on the unit circle and are $\neq 1$ for some t, then $\operatorname{tr} \mathcal{S}^{(2)\dagger}(t)\mathcal{S}^{(2)}(t) \leq C$ and so by $\operatorname{tr} \mathcal{S}^{(1)\dagger}(t)\mathcal{S}^{(1)}(t) \leq 2 + t^2$ we get as Ehrenfest time

$$T_E(\lambda) \sim \lambda^{1/2} .$$

So the state stays a much longer time localized around $z(t)$ as in the unstable case. Furthermore, note that the state remains localized in the transversa direction for all times. The delocalization takes only place along the orbit, where the system behaves like a one-dimensional free system.

(ii) The marginally stable case: If at least two eigenvalues of $\mathcal{S}^{(2)}(t)$ are one, we expect the same behavior as for $\mathcal{S}^{(1)}(t)$ and get the same result as for the stable case, since there dominated alreadythe $\mathcal{S}^{(1)}(t)$ part,

$$T_E(\lambda) \sim \lambda^{1/2} .$$

The approximate time evolution $\mathcal{U}_{z_0}^{(2)}(t)$ can also be determined exactly on observables. The result is already suggested by Corollary 3.5.2.

Proposition 3.5.4. *Let $\mathcal{P}$ be pseudodifferential operator with Weyl symbol $P(z) \in S^0(m_{a,b})$, then $\mathcal{U}_{z_0}^{(2)}(t)^\dagger \mathcal{P}\mathcal{U}_{z_0}^{(2)}(t)$ is a pseudodifferential operator with symbol*

$$P(t,z) = P(z_0 + \mathcal{S}_{z_0}^{-1}(t)(z - z_0(t))) \in S^0(m_{a,b})$$

for finite t.

Proof. Since $\mathcal{H}^{(2)}(t)$ has a Weyl symbol which is a quadratic polynomial in z the asymptotic series for the symbol of the commutator $[\mathcal{H}^{(2)}, \mathcal{P}]$, which follows from 2.5.5, terminates after the first term. So the quantum mechanical differential equation $\frac{\mathrm{i}}{\lambda}\frac{\mathrm{d}\mathcal{P}}{\mathrm{d}t} = [\mathcal{H}^{(2)}, \mathcal{P}]$ reads in terms of the Weyl symbols

$$\frac{\mathrm{d}P}{\mathrm{d}t} = \{H^{(2)}, P\} . \tag{3.106}$$

The ansatz $P(t,z) = P(z_0 + \mathcal{S}_{z_0}^{-1}(t)(z - z_0(t)))$ satisfies of course the initial condition $P(0,z) = P(z)$, and for the left-hand side of (3.106) we get

$$\frac{\mathrm{d}P(t,z)}{\mathrm{d}t} = -\langle P'(t,z), \mathcal{S}_{z_0}^{-1}(t)\dot{\mathcal{S}}_{z_0}(t)\mathcal{S}_{z_0}^{-1}(t)(z - z_0(t)) + \mathcal{S}_{z_0}^{-1}(t)\mathcal{J}H'(z_0(t))\rangle$$

where $P' := \nabla_z P$ and $H' = \nabla_z H$, and we have used $\mathrm{d}\mathcal{S}_{z_0}^{-1}(t)/\mathrm{d}t = -\mathcal{S}_{z_0}^{-1}(t)\dot{\mathcal{S}}_{z_0}(t)\mathcal{S}_{z_0}^{-1}(t)$ and $\dot{z}_0(t) = \mathcal{J}H'(z_0(t))$. For the right-hand side of (3.106) we obtain

$$\{H^{(2)}, P\} = \langle H'(z_0(t)) + H''(z_0(t))(z - z_0(t)), \mathcal{J}\mathcal{S}_{z_0}^{-1}(t)^\dagger P'(t,z)\rangle ,$$

where we have used the relation $\nabla_z f(\mathcal{A}z) = \mathcal{A}^\dagger f'(\mathcal{A}z)$ valid for an arbitrary matrix $\mathcal{A}$. By comparing the two expressions and using $\mathcal{J}^\dagger = -\mathcal{J}$ (3.106) reduces to

$$\mathcal{S}_{z_0}^{-1}(t)\dot{\mathcal{S}}_{z_0}(t)\mathcal{S}_{z_0}^{-1}(t) = \mathcal{S}_{z_0}^{-1}(t)\mathcal{J}H''(z_0(t)) \ .$$

Multiplication by $\mathcal{S}_{z_0}(t)$ from the left and right then gives (3.94), and so the proof is complete. □

Since $\mathcal{U}_{z_0}^{(2)}(t)$ is unitary, the norm of $\mathcal{P}(t)$ is preserved for all t, but the pseudodifferential operator class to which it belongs depends on the derivative of the symbol, and here the matrix $\mathcal{S}(t)$ forces them to diverge for $t \to \infty$.

As a corollary we get the evolution of creation and annihilation operators, and the higher order coherent states defined in Section 3.3.2.

Corollary 3.5.5. *Let $v \in \mathbb{C}^{2d}$ and let $\mathcal{P}_v(s)$ be the Weyl quantization of the linear form $\omega(v, z - z(s))$, then we have*

$$\mathcal{U}^{(2)}(t,s)\mathcal{P}_v(s)\mathcal{U}^{(2)}(s,t) = \mathcal{P}_{v(t)}(t)$$

where $v(t) = \mathcal{S}(t)v$. Hence, if $u(\alpha) = \mathcal{P}^{\alpha}_{B,z(s)}u^{B}_{z(s)}(\lambda, x)$ is a higher order coherent state, see (3.50)*, then*

$$\mathcal{U}^{(2)}(t,s)u(\alpha) = \mathrm{e}^{\mathrm{i}(\lambda\Theta(t)+\sigma(t))}\mathcal{P}^{\alpha}_{\mathcal{S}(t)_*B,z(t)}u^{\mathcal{S}(t)_*B}_{z(s)}(\lambda, x) \ .$$

In order to estimate the time evolution generated by a more general Hamiltonian $\mathcal{H}(t)$ we will compare it with its quadratic approximation $\mathcal{H}^{(2)}(t)$, the following lemma is then essential;

Lemma 3.5.6. *Let $\mathcal{H}^{(1)}(t)$, $\mathcal{H}^{(2)}(t)$ be two time dependent self adjoint operators and $\mathcal{U}^{(1)}(t,s)$, $\mathcal{U}^{(2)}(t,s)$ the unitary operators generated by them, i.e.*

$$\frac{\mathrm{i}}{\lambda}\frac{\partial}{\partial t}\mathcal{U}^{(k)}(t,s) = \mathcal{H}^{(k)}(t)\mathcal{U}_k(t,s) \ , \quad \mathcal{U}_k(s,s) = I \ ,$$

for $k = 1, 2$. Then for ψ in the intersection of the domains of $\mathcal{H}^{(1)}(t)$ and $\mathcal{H}^{(2)}(t)$ we have

$$||\mathcal{U}^{(1)}(t,s)\psi - \mathcal{U}^{(2)}(t,s)\psi|| \leq \lambda(t-s) \sup_{r\in[s,t]} ||[\mathcal{H}^{(1)}(r) - \mathcal{H}^{(2)}(r)]\mathcal{U}^{(2)}(r,s)\psi|| \ .$$

Proof. The estimate is an immediate consequence of Duhamel's principle (see e.g. [Tay96]), which can be stated as follows

$$\mathcal{U}^{(1)}(t,s) - \mathcal{U}^{(2)}(t,s) = \frac{\lambda}{\mathrm{i}}\int_s^t \mathcal{U}^{(1)}(t,r)[\mathcal{H}^{(1)}(r) - \mathcal{H}^{(2)}(r)]\mathcal{U}^{(2)}(r,s)\ \mathrm{d}r \ .$$

By using that $\mathcal{U}^{(1)}(t,r)$ is unitary, and hence $||\mathcal{U}^{(1)}(t,r)|| = 1$, we get the result. □

Now we can come to our main result, the time evolution of a coherent state generated by a general Hamiltonian.

Theorem 3.5.7. *Let $\mathcal{H}(t)$ be a selfadjoint pseudodifferential operator on M which satisfies the conditions in Proposition 2.5.6 and let $\mathcal{U}(t,s)$ be the corresponding time evolution operator. Let ψ_s be the state (3.98) centered at $z_0 = (q,p)$ and let $\mathcal{H}^{(2)}(t)$ be the Taylor expansion up to second order of $\mathcal{H}$ around $z_0(t) = (q(t), p(t))$, i.e. the operator with Weyl symbol (3.93), and $\psi(t,x)$ be the state (3.99), then*

$$||\mathcal{U}(t,s)\psi_s - \psi(t)|| \leq \lambda(t-s) \sup_{r\in[t,s]} C(r) \sum_{j=0}^{3} \frac{1}{\lambda^j} \left(\frac{||\mathbf{g}^{-1}(t)||}{\lambda}\right)^{(3-j)/2} ,$$

with $\mathbf{g}$ given by (3.53) and

$$C(t) = \left(\sup_z \frac{[(H-H_2)\#(H-H_2)](z)}{|z|^6}\right)^{1/2} .$$

The proof of this and the next theorem will be based on the estimate obtained in the following Lemma.

Lemma 3.5.8. *Let $\mathcal{P}(t)$ be a pseudodifferential operator with $||\mathcal{P}(t)|| \leq C$ for all t, with symbol $P(t,\lambda,z) \in S^0(m_{a,b})$ for finite t, and*

$$P(t,\lambda,z) = \sum_{j=0}^{N} \frac{1}{\lambda^j} P_j(t,z) + R_{N+1}(t,\lambda,z)$$

where $P_j(t,z)$ has a zero of order $N-j$ at $z = z(t)$ and $R_{N+1}(t,\lambda,z) \in S^{-(N+1)}(m_{a,b})$. Then we have

$$||\mathcal{P}(t)\mathcal{U}^{(2)}(t,t_0)u_z^L|| \leq C \sum_{j=0}^{N} \frac{1}{\lambda^j} \left(\frac{||\mathbf{g}^{-1}(t)||}{\lambda}\right)^{(N-j)/2} .$$

Proof. We first show that we can restrict our attention to a neighborhood of $z(t)$. Choose a symbol $A \in S^0(1)$ which has compact support in a neighborhood of z and $A = 1$ in a further neighborhood of z, and denote by $\mathcal{A}$ its Weyl quantization. Then we have

$$||(1-\mathcal{A})u_z^L|| \leq C_N \lambda^{-N}$$

for all $N \in \mathbb{N}$, and hence

$$\begin{aligned} ||\mathcal{P}(t)\mathcal{U}^{(2)}(t,t_0)u_z^L|| &= ||\mathcal{P}(t)\mathcal{U}^{(2)}(t,t_0)[\mathcal{A} + (1-\mathcal{A})]u_z^L|| \\ &\leq ||\mathcal{P}(t)\mathcal{U}^{(2)}(t,t_0)\mathcal{A}u_z^L|| + ||\mathcal{P}(t)\mathcal{U}^{(2)}(t,t_0)(1-\mathcal{A})u_z^L|| \\ &\leq ||\mathcal{P}(t)\mathcal{U}^{(2)}(t,t_0)\mathcal{A}u_z^L|| + ||\mathcal{P}(t)\mathcal{U}^{(2)}(t,t_0)||||(1-\mathcal{A})u_z^L|| \\ &\leq ||\mathcal{P}(t)\mathcal{U}^{(2)}(t,t_0)\mathcal{A}u_z^L|| + CC_N\lambda^{-N} \end{aligned}$$

for all $N \in \mathbb{N}$. If we now define $\mathcal{P}'(t) := \mathcal{P}(t)\mathcal{U}^{(2)}(t,t_0)\mathcal{A}\mathcal{U}^{(2)}(t_0,t)$, then by Proposition 3.5.4 the symbol of $\mathcal{P}'(t)$ will have compact support in a neighborhood of $z(t)$, and satisfies the same conditions as P concerning its zeros. So we can assume from now on that the symbol of $\mathcal{P}(t)$ has compact support in a neighborhood of $z(t)$.

We use the representation

$$\begin{aligned} ||\mathcal{P}(t)\mathcal{U}^{(2)}(t,t_0)u_z^L||^2 &= \langle \mathcal{P}(t)\mathcal{U}^{(2)}(t,t_0)u_z^L, \mathcal{P}(t)\mathcal{U}^{(2)}(t,t_0)u_z^L\rangle \\ &= \langle \mathcal{U}^{(2)}(t,t_0)u_z^L, \mathcal{P}(t)^\dagger\mathcal{P}(t)\mathcal{U}^{(2)}(t,t_0)u_z^L\rangle \\ &= \int \overline{P}\#P(t,\lambda,z)W_{z(t)}^{L(t)}(z)\,\mathrm{d}z\ , \end{aligned}$$

where $W_{z(t)}^{L(t)}(z)$ is the Wigner function of the state $\mathcal{U}^{(2)}(t,t_0)u_z^L$. With Corollary 3.5.2 we then obtain

$$||\mathcal{P}(t)\mathcal{U}^{(2)}(t,t_0)u_z^L||^2 = \left(\frac{\lambda}{\pi}\right)^d \int \overline{P}\#P(t,\lambda,z)\mathrm{e}^{-\lambda\langle z-z(t),\mathbf{g}_{L(t)}(z-z(t))\rangle}\,\mathrm{d}z\ . \tag{3.107}$$

By the assumptions on $P(t,\lambda,z)$ we have

$$\overline{P}\#P(t,\lambda,z) = \sum_{j=0}^{2N}\frac{1}{\lambda^j}p_j(t,z) + r_{2N+1}(t,\lambda,z) \tag{3.108}$$

with $r_{2N+1}(t,\lambda,z) \in S^{-(2N+1)}(m_{a,b})$ and where $p_j(t,z)$ is positive and has a zero of order $2N-j$ at $z-z(t)$, which means that

$$p_j(t,z-z(t)) \le C_j(t)(\langle z-z(t),z-z(t)\rangle)^{N-j/2}\ . \tag{3.109}$$

Furthermore, all functions have compact support. Inserting (3.108) and using (3.109) gives

$$\begin{aligned} &\left(\frac{\lambda}{\pi}\right)^d \int \overline{P}\#P(t,\lambda,z)\mathrm{e}^{-\lambda\langle z-z(t),\mathbf{g}_{L(t)}(z-z(t))\rangle}\,\mathrm{d}z \\ &\quad\le \sum_{j=0}^{2N}\frac{C_j(t)}{\lambda^j}\left(\frac{\lambda}{\pi}\right)^d \int (\langle z-z(t),z-z(t)\rangle)^{N-j/2}\mathrm{e}^{-\lambda\langle z-z(t),\mathbf{g}_{L(t)}(z-z(t))\rangle}\,\mathrm{d}z \\ &\qquad + \left(\frac{\lambda}{\pi}\right)^d \int r_{2N+1}(t,\lambda,z)\mathrm{e}^{-\lambda\langle z-z(t),\mathbf{g}_{L(t)}(z-z(t))\rangle}\,\mathrm{d}z\ . \end{aligned}$$

Using $|r_{2N+1}(t,\lambda,z)| \le C\lambda^{-(2N+1)}$ and that it is compactly supported we can estimate the remainder term as

$$\left(\frac{\lambda}{\pi}\right)^d \int \rho_1(d_t(z-z(t)))r_{2N+1}(t,\lambda,z)\mathrm{e}^{-\lambda\langle z-z(t),\mathbf{g}_{L(t)}(z-z(t))\rangle}\,\mathrm{d}z \le C\lambda^{-(2N+1)}\ .$$

For the terms in the sum we substitute variables in the integral and use $\det \mathbf{g}_B = 1$ to get

$$
\begin{aligned}
&\left(\frac{\lambda}{\pi}\right)^d \int (\langle z - z(t), z - z(t)\rangle)^{N-j/2} \mathrm{e}^{-\lambda\langle z-z(t), \mathbf{g}_{L(t)}(z-z(t))\rangle} \, \mathrm{d}z \\
&\quad = \left(\frac{\lambda}{\pi}\right)^d \int (\langle z, z\rangle)^{N-j/2} \mathrm{e}^{-\lambda\langle z, \mathbf{g}_{L(t)} z\rangle} \, \mathrm{d}z \\
&\quad = \left(\frac{1}{\pi}\right)^d \int \left(\frac{\langle z, \mathbf{g}_{L(t)}^{-1} z\rangle}{\lambda}\right)^{N-j/2} \mathrm{e}^{-\langle z, z\rangle} \, \mathrm{d}z \\
&\quad \leq \left(\frac{||\mathbf{g}_{L(t)}^{-1}||}{\lambda}\right)^{2N-j} \left(\frac{1}{\pi}\right)^d \int (\langle z, z\rangle)^{N-j/2} \mathrm{e}^{-\langle z, z\rangle} \, \mathrm{d}z \\
&\quad = \left(\frac{||\mathbf{g}_{L(t)}^{-1}||}{\lambda}\right)^{2N-j} C_j \; ,
\end{aligned}
$$

and so the proof is complete.

□

Proof of Theorem 3.5.7. According to Lemma 3.5.6 we have to estimate

$$
||[\mathcal{H}(t) - \mathcal{H}^{(2)}(t)]\psi(t)|| \; .
$$

To this end we note that $\mathcal{H} - \mathcal{H}^{(2)}(t)$ satisfies the assumptions on $\mathcal{P}(t)$ in Lemma 3.5.8 with $N = 3$ and so the remainder estimate in Theorem 3.5.7 follows from Lemma 3.5.8. □

One often needs also information on higher order approximations for the time evolution. These can be obtained by iterating Duhamel's principle,

$$
\begin{aligned}
\mathcal{U}^{(1)}(t, t_0) &= \mathcal{U}^{(2)}(t, t_0) + \frac{\lambda}{\mathrm{i}} \int_{t_0}^{t} \mathcal{U}^{(1)}(t, t_1) \Delta\mathcal{H}(t_1) \mathcal{U}^{(2)}(t_1, t_0) \, \mathrm{d}t_1 \\
&= \mathcal{U}^{(2)}(t, t_0) + \frac{\lambda}{\mathrm{i}} \int_{t_0}^{t} \mathcal{U}^{(2)}(t, t_1) \Delta\mathcal{H}(t_1) \mathcal{U}^{(2)}(t_1, t_0) \, \mathrm{d}t_1 \\
&\quad + \left(\frac{\lambda}{\mathrm{i}}\right)^2 \int_{t_0}^{t} \int_{t_2}^{t} \mathcal{U}^{(1)}(t, t_2) \Delta\mathcal{H}(t_2) \mathcal{U}^{(2)}(t_2, t_1) \Delta\mathcal{H}(t_1) \mathcal{U}^{(2)}(t_1, t_0) \, \mathrm{d}t_2 \mathrm{d}t_1 \\
&\quad \vdots
\end{aligned}
$$

with $\Delta\mathcal{H}(t) := \mathcal{H}^{(1)}(t) - \mathcal{H}^{(2)}(t)$. By further iteration we obtain the so called Dyson series

$$\begin{aligned}\mathcal{U}^{(1)}(t,t_0) &= \mathcal{U}^{(2)}(t,t_0)\\ &\quad+\sum_{j=1}^{p}\left(\frac{\lambda}{\mathrm{i}}\right)^j\int_{t_0}^{t}\int_{t_1}^{t}\cdots\int_{t_{j-1}}^{t}\mathcal{U}^{(2)}(t,t_j)\Delta\mathcal{H}(t_j)\mathcal{U}^{(2)}(t_j,t_{j-1})\\ &\quad\times\Delta\mathcal{H}(t_{j-1})\mathcal{U}^{(2)}(t_{j-1},t_{j-2})\cdots\Delta\mathcal{H}(t_1)\mathcal{U}^{(2)}(t_1,t_0)\ \mathrm{d}t_j\cdots\mathrm{d}t_2\mathrm{d}t_1\\ &\quad+\left(\frac{\lambda}{\mathrm{i}}\right)^{p+1}\int_{t_0}^{t}\int_{t_1}^{t}\cdots\int_{t_p}^{t}\mathcal{U}^{(1)}(t,t_{p+1})\Delta\mathcal{H}(t_{p+1})\mathcal{U}^{(2)}(t_{p+1},t_p)\\ &\quad\times\Delta\mathcal{H}(t_p)\mathcal{U}^{(2)}(t_p,t_{p-1})\cdots\Delta\mathcal{H}(t_1)\mathcal{U}^{(2)}(t_1,t_0)\ \mathrm{d}t_{p+1}\cdots\mathrm{d}t_2\mathrm{d}t_1\end{aligned}$$

for every $p \in \mathbb{N}$. Notice that the terms in the sum contain only the approximate time evolution $\mathcal{U}^{(2)}$ and only in the remainder term there appears a contribution of $\mathcal{U}^{(1)}$. If we introduce the shorthand

$$\hat{\mathcal{H}}(t_j) := \mathcal{U}^{(2)}(t_0,t_j)\Delta\mathcal{H}(t_j)\mathcal{U}^{(2)}(t_j,t_0)$$

we can rewrite the Dyson series as

$$\mathcal{U}^{(1)}(t,t_0) = \sum_{j=0}^{p}\mathcal{P}_j(t,t_0)\,\mathcal{U}^{(2)}(t,t_0) + \mathcal{R}_{p+1}(t,t_0)\,\mathcal{U}^{(2)}(t,t_0)$$

with $\mathcal{P}_0(t,t_0) = 1$,

$$\mathcal{P}_j(t,t_0) := \left(\frac{\lambda}{\mathrm{i}}\right)^j\int_{t_0}^{t}\int_{t_1}^{t}\cdots\int_{t_{j-1}}^{t}\hat{\mathcal{H}}(t_j)\hat{\mathcal{H}}(t_{j-1})\cdots\hat{\mathcal{H}}(t_1)\ \mathrm{d}t_j\cdots\mathrm{d}t_2\mathrm{d}t_1\ ,$$

and

$$\begin{aligned}\mathcal{R}_{p+1}(t,t_0) := \left(\frac{\lambda}{\mathrm{i}}\right)^{p+1}\int_{t_0}^{t}\int_{t_1}^{t}\cdots\int_{t_p}^{t}&\mathcal{U}^{(1)}(t,t_{p+1})\mathcal{U}^{(2)}(t_{p+1},t)\hat{\mathcal{H}}(t_{p+1})\\ &\hat{\mathcal{H}}(t_p)\cdots\hat{\mathcal{H}}(t_1)\ \mathrm{d}t_{p+1}\cdots\mathrm{d}t_2\mathrm{d}t_1\ .\end{aligned}$$

Therefore, we get for the time evolution of a coherent state

$$\mathcal{U}^{(1)}(t,t_0)u_z^L = \sum_{j=0}^{p}\mathcal{P}_j(t,t_0)\,\mathcal{U}^{(2)}(t,t_0)u_z^L + \mathcal{R}_{p+1}(t,t_0)\,\mathcal{U}^{(2)}(t,t_0)u_z^L\ .$$

Theorem 3.5.9. *Under the same conditions as in Theorem 3.5.7 we have*

$$\mathcal{U}(t,t_0)u_z^L = \sum_{j=0}^{p}\mathcal{P}_j(t,t_0)\ \mathcal{U}^{(2)}(t,t_0)u_z^L + \mathcal{R}_{p+1}(t,t_0)\,\mathcal{U}^{(2)}(t,t_0)u_z^L\ ,$$

where $\mathcal{P}_j(t,t_0) \in \Psi^0(m_{a,b})$ *is given by*

$$\mathcal{P}_j(t,t_0) := \left(\frac{\lambda}{\mathrm{i}}\right)^j \int_{t_0}^t \int_{t_1}^t \cdots \int_{t_{j-1}}^t \hat{\mathcal{H}}(t_j)\hat{\mathcal{H}}(t_{j-1})\cdots\hat{\mathcal{H}}(t_1)\, \mathrm{d}t_j \cdots \mathrm{d}t_2 \mathrm{d}t_1 \ , \tag{3.110}$$

for $j > 0$ *and* $\mathcal{P}_0(t,t_0) = 1$, *and*

$$\hat{\mathcal{H}}(t_k) := \mathcal{U}^{(2)}(t_0,t_k)[\mathcal{H}(t_k) - \mathcal{H}(t_k)^{(2)}]\mathcal{U}^{(2)}(t_k,t_0) \ .$$

Furthermore, the terms in the sum and the remainder satisfy the estimates

$$||\mathcal{P}_j(t,t_0)\,\mathcal{U}^{(2)}(t,t_0)u_z^L|| \leq C\lambda^j(t-t_0)^j \sum_{k=0}^{3j} \frac{1}{\lambda^k}\left(\frac{||\mathbf{g}^{-1}(t)||}{\lambda}\right)^{(3j-k)/2} \ ,$$

and

$$||\mathcal{R}_{p+1}(t,t_0)\,\mathcal{U}^{(2)}(t,t_0)u_z^L|| \leq C\lambda^{p+1}(t-t_0)^{p+1} \sum_{k=0}^{3(p+1)} \frac{1}{\lambda^k}\left(\frac{||\mathbf{g}^{-1}(t)||}{\lambda}\right)^{(3(p+1)-k)/2} \ .$$

Proof. The proof follows again from Lemma 3.5.8, the operators $\lambda^{-j}\mathcal{P}_j(t,t_0)$ satisfy the assumptions of that Lemma with $N = 3j$, and the remainder $\lambda^{-p-1}\mathcal{R}_{p+1}(t,t_0)$ with $N = 3(p+1)$. □

Notice that for t in a finite interval we obtain

$$||\mathcal{P}_j(t,t_0)\,\mathcal{U}^{(2)}(t,t_0)u_z^L|| \leq C\lambda^{-j/2}$$

and

$$||\mathcal{R}_{p+1}(t,t_0)\,\mathcal{U}^{(2)}(t,t_0)u_z^L|| \leq C\lambda^{-\frac{p+1}{2}} \ ,$$

so we have indeed an asymptotic expansion in powers of λ.

Let us discuss the time scales up to which the remainder terms stay small for the different types of behaviors of the trajectory, in analogy to the discussion after Lemma 3.5.3. The leading term in the upper estimate is always given by the $j = 0$ term.

(i) If the trajectory is unstable with an Liapunov exponent $\gamma(z)$, then for

$$t << \frac{\ln \lambda}{6\gamma(z)}$$

the error term remains small.

(ii) In the stable and marginally stable case, we obtain that for

$$t << \lambda^{1/6}$$

the error term remains small.

The observation that the time up to which the quantum dynamics follows the classical dynamics, i.e. the Ehrenfest time, depends on the dynamical properties of the system is not new, see e.g. [Zas81]. The main new thing in the work of Combescure and Robert is a rigorous proof for the Ehrenfest time.

Since the main ingredient in the proof of the remainder estimates was the localization of the Wigner function of a coherent state, it is quite likely that the above time scales are specific for the time evolution of coherent states. The first time that in a chaotic system a larger time scale was explored rigorously, is in the recent paper [BDB00]. There it is shown that for the discrete time evolution of a quantized cat map, the semiclassical time evolution of a coherent state is valid up to $t = \ln \lambda/\gamma$. Up to $t = \ln \lambda/2\gamma$ it stays localized as discussed after Lemma 3.5.3, and for $\ln \lambda/2\gamma < t < \ln \lambda/\gamma$ it becomes ergodically distributed on phase space, as predicted by the classical dynamics. Probably this continues to be the case for all times up to some multiple of the Heisenberg time.

With Proposition 3.5.4 and Theorem 3.5.1 we can in principle determine all the contributions to the time evolution. The results on time evolution we presented here have been recently improved and generalized. In [HJ99, BGP99] exponentially good estimates for the remainder terms in the time evolution of coherent states and observables have been derived in the caseof analytic Hamiltonians.

The time evolution for more general states than coherent states can now be obtained by expanding them into coherent states. As a special case we mention without proof that for Lagrangian states we obtain

Theorem 3.5.10. *Let $\mathcal{H}$ be a selfadjoint pseudodifferential operator satisfying the same conditions as in Theorem 3.5.7 and denote by $\mathcal{U}(t) = \mathrm{e}^{-\mathrm{i}\lambda t\mathcal{H}}$ the corresponding time evolution. Assume $u \in I^0(M, J)$ has compact support and principal symbol $\sigma(u)$, then $\mathcal{U}(t)u$ is in $I^0(M, \Phi^t J)$ and has principal symbol*

$$\sigma(\mathcal{U}(t)u)(z) = \mathrm{e}^{\mathrm{i}[\lambda\Theta(t,z)+\int^t H_1\,\mathrm{d}t' + \frac{\pi}{2}\sigma'(t,z)]}\sigma(u)\circ\Phi^{-t}(z) \ ,$$

with the same phase factors as in Theorem 3.5.1. Furthermore, if $u^0(t)$ denotes an element in $I^0(M, \Phi^t J)$ with principal symbol $\sigma(u)\circ\Phi^t$, then

$$||\mathcal{U}(t)u - u^0(t)|| \leq \sup_{z\in \operatorname{supp}\sigma(u)} C\lambda \left(\frac{||\mathbf{g}_z^{-1}(t)||}{\lambda}\right)^{3/2} \ .$$

3.6 Time evolution: Remarks on the non-semiclassical case

In the last section we have discussed the time evolution of Lagrangian states for semiclassical Hamiltonians, i.e. for Hamilton operators which depend on the semiclassical parameter λ. We have discussed at the end of Chapter 2, in Section 2.5, the physical interpretation of this limit. We want to complement the considerations there by a concrete example of a non-semiclassical case, the time evolution of coherent states where we set $\lambda = 1$. States can be experimentally prepared in various ways, and one expects that when one studies, e.g., the time evolution of an initial state with small de Broglie wavelength, that it is approximately governed by a classical Hamiltonian flow. In this section we will study the time evolution from this different perspective.

In order to simplify the exposition we will only study a simple type of system. Let

$$\mathcal{H} = -\frac{1}{2}\Delta + V(x)$$

be a Hamiltonian on $\mathbb{R}^d$ with smooth potential $V(x)$. We want to study the time evolution generated by this Hamiltonian for the initial state

$$\psi_0(x) = (\det \operatorname{Im} B_0)^{1/4} \mathrm{e}^{\mathrm{i}[\langle p_0, x-q_0\rangle + \langle B_0(x-q_0), x-q_0\rangle/2]} ,$$

that is we have to solve the differential equation

$$\mathrm{i}\frac{\partial \psi}{\partial t}(t,x) = \mathcal{H}\psi(t,x) , \quad \text{with } \psi(0,x) = \psi_0(x) .$$

If we insert the ansatz

$$\psi(t,x) = \alpha(t)\mathrm{e}^{\mathrm{i}\Theta(t)}\mathrm{e}^{\mathrm{i}[\langle p(t), x-q(t)\rangle + \langle B(t)(x-q(t)), x-q(t)\rangle/2]}$$

into the equation we get

$$\begin{aligned}\big(\mathrm{i}\dot\alpha/\alpha - \dot\Theta - \langle \dot p, x\rangle + \langle B\dot q, (x-q)\rangle - \langle \dot B(x-q), (x-q)\rangle/2\big)\psi \\ = \big(-\mathrm{i}\operatorname{tr} B/2 + (p + B(x-q))^2/2 + V(x)\big)\psi .\end{aligned}$$

Since the state is concentrated at $x = q$ we will order this equation by powers of $(x-q)$ and treat each power separately. Up to second order we then get the following set of equations

$$\mathrm{i}\dot\alpha/\alpha - \dot\Theta - \langle \dot p, q\rangle = -\mathrm{i}\operatorname{tr} B/2 + \langle p,p\rangle/2 + V(q) \tag{3.111}$$

$$-\dot p + B\dot q = Bp + V'_x(q) \tag{3.112}$$

$$-\dot B = B^2 + V''_{x,x}(q) . \tag{3.113}$$

If we compare this with the classical system defined by the Hamilton function

$$H(p,q) = \langle p,p\rangle/2 + V(q)$$

leading to the set of Hamilton equations

$$\dot q = p , \qquad \dot p = -V'_q(q) , \tag{3.114}$$

we see that the second equation (3.112) is fulfilled if we choose $q(t)$ and $p(t)$ to be the solutions of (3.114) with initial conditions (q_0, p_0). If $\mathcal{S}(t)$ is the solution of the linearized Hamilton-equations

$$\dot{\mathcal{S}} = \mathcal{J}_0 H''\mathcal{S} = \begin{pmatrix} 0 & -V''(q(t)) \\ I & 0 \end{pmatrix}\mathcal{S} , \quad \text{with } \mathcal{S}(0) = I$$

then it follows as in the proof of Theorem 3.5.1 that

$$B(t) := \mathcal{S}(t)_* B_0$$

is a solution of (3.113) with initial condition $B(0) = B_0$. Finally the choices

$$\Theta(t) = -\int_0^t \langle \dot{p}(s), q(s) \rangle + H(q(s), p(s)) \, \mathrm{d}s$$

and

$$\alpha(t) = (\det \operatorname{Im} B_0)^{1/4} \mathrm{e}^{-\frac{\mathrm{i}}{2}\int_0^t \operatorname{tr}[\mathcal{S}(s)_* B_0] \, \mathrm{d}s}$$

give the solution to (3.111).

Summarizing, what we have found is that our ansatz $\psi(t,x)$ with the above choices of $(p(t), q(t))$, $B(t)$, $\Theta(t)$ and $\alpha(t)$ inserted in the Schrödinger equation gives

$$\big(\mathrm{i}\partial/\partial t - \hat{H}\big)\psi(t,x) = R\psi(t,x)$$

with

$$R = V(x) - \sum_{|\alpha| \leq 2} V^\alpha(q(t))(x - q(t))^\alpha/\alpha! = O((x - q(t))^3) \ .$$

In view of Lemma 3.2.6 this implies that

$$|R\psi(t,x)| \leq C |\operatorname{Im} B(t)|^{-3/2}$$

where the constant only depends on V but not on $\psi(t,x)$. So we have found an approximate solution to the Schrödinger equation and the error is controlled by the norm of the matrix $\operatorname{Im} B$ which describes the sharpness of the localization of the state $\psi(t,x)$ and acts therefore as a semiclassical parameter.

This result illustrates the general philosophy that the semiclassical limit is performed by preparing the system in suitable states, for which then the system behaves almost classically, and not by changing some parameters of the system like $\hbar$. A semiclassical parameter can then be introduced a posteriori, as we have sketched in Section 2.5.

Chapter 4

Operators localized in phase space

The theory of pseudodifferential operators gives a correspondence between a certain class of quantum mechanical observables, and smooth functions on phase space. It provides a flexible mathematical framework in which many intuitive physical arguments can be made rigorous, and has led to beautiful results in semiclassics and quantum chaos as we have discussed in Chapter 2.

But occasionally one would like to quantize non-smooth classical objects, which do not fit into the framework of classical pseudodifferential operators. The example which was our motivation for the development of the formalism in this chapter is the case of the characteristic function of some open subset D of phase space. One of our aims is to study the influence of invariant domains of the classical system on a corresponding quantum system, for instance, if eigenfunctions are concentrated on them. Given such a domain D, one would like to associate a kind of projection operator with it, whose image is then the part of Hilbert space associated with D. A natural candidate for such an operator would be a quantization of the characteristic function of D. The characteristic function of an invariant open subset of phase space defines an invariant measure on phase space and one is then as well interested in studying more general measures on phase space associated with the classical system.

A way of quantizing non-smooth objects on phase space is provided by Anti-Wick quantization. Anti-Wick quantization uses a complete set of coherent states u_z; the properties of such states have been studied in chapter 3.3. Let $|z\rangle\langle z|$ be the projection operator onto the state u_z, then the Anti-Wick quantization of $a \in C^\infty(T^*M)$ is defined as

$$\mathrm{Op}^{AW}[a] := \left(\frac{\lambda}{2\pi}\right)^d \int a(z)|z\rangle\langle z| \;\mathrm{d}z \ ,$$

and this prescription can be extended to arbitrary distributions. So Anti-Wick quantization allows to quantize very general objects, but the price one has to pay for this is that the algebraic properties are less pleasant than for usual pseudodifferential operators.

In Section 4.1 we give a review of some of the basic properties of Anti-Wick operators. We then restrict ourselves to the quantization of measures, and study estimates for the Anti-Wick quantizations of measures in the following Section 4.1.1. A general version of Cotlar's

Lemma allows to derive very precise estimates on the norm of Anti-Wick quantizations of measures in terms of fractal dimensions of these measures. Since many measures appearing in dynamical systems have fractal properties this might have some interesting applications. We then proceed to study the multiplication of Anti-Wick operators with pseudodifferential operators, and commutators with them.

The Egorov theorem on time evolution of operators and the Szegö limit theorem on the semiclassical limit of expectation values are extended in Section 4.2 to the case of Anti-Wick quantizations of measures. The Egorov theorem is a simple consequence of the time evolution of coherent states, Theorems 3.5.7 and 3.5.9. For the Szegö limit theorem we can use a simplified version of the standard proof in the literature for the case of pseudodifferential operators with smooth symbols.

We then turn to our main application of the formalism developed so far, the construction of approximate projection operators associated with open invariant domains of phase space. They are of the form

$$\boldsymbol{\pi}_D = \left(\frac{\lambda}{2\pi}\right)^d \int_D |z\rangle\langle z| \, \mathrm{d}z \ ,$$

and we first discuss to what extent they can be viewed as approximate projection operators. Our main aim then is to show that one can construct such operators in a way that they commute with the Hamilton operator up to a semiclassically small error. For an arbitrary open domain with piecewise smooth boundary the error is of order $\lambda^{-3/2}$, but with the additional assumption that the domain is stably invariant we can improve the result and obtain an error of order λ^{-N} for every $N \in \mathbb{N}$. The condition of stable invariance will play an important role in the next chapter, too. It means that any sufficiently small perturbation of the classical system possesses an invariant domain close to D. This result will then be applied in the last section, Section 4.4, and in the next chapter, Chapter 5.

The two applications in Section 4.4 are a discussion of almost invariant subspaces of the Hilbert space and a local quantum ergodicity theorem. If the classical system has an invariant open subset D, we have a decomposition into two systems, D and the complement of D, which are invariant under time evolution and do not interact. The corresponding approximate projection operators induce a similar approximate decomposition of the quantum mechanical system. The image of $\boldsymbol{\pi}_D$ is approximately invariant, and we give an estimate of the time a state remains in this subspace. If the flow on D is ergodic, then we furthermore can prove a local quantum ergodicity theorem, which states that in the semiclassical limit the eigenfunctions microlocally become constant on D.

4.1 Anti-Wick quantization

The Anti-Wick quantization provides an alternative way of describing the quantum-to-classical correspondence. Instead of classifying operators by their action on plane waves, one chooses coherent states for the classification. This quantization was introduced in the early seventies by Berezin, [Ber71], and then used in semiclassics by Voros [Vor76, Vor77] and later for the proof of quantum ergodicity by Helffer, Martinez and Robert [HMR87]. Some aspects are also treated in [BBR96], and the procedure is related to Friedrichs symmetrization [Tay81].

We start by recalling some results for the case $M = \mathbb{R}^d$, see, e.g., [Hel97, Pau97]. Let $\mathcal{A}$ be a pseudodifferential operator of order m and $u^L_{p,q}$ a coherent state, see (3.33), then by Theorem 3.2.10, or Corollary 3.2.12, we have approximatly

$$\mathcal{A}u^L_{p,q} \approx \sigma(\mathcal{A})(p,q)u^L_{p,q} ,$$

where $\sigma(\mathcal{A})(p,q)$ is the principal symbol of $\mathcal{A}$, up to a remainder of order $O(\lambda^{m-1/2})$. Using this and the completeness relation, Proposition 3.3.13, we get an approximate decomposition of $\mathcal{A}$ in projection operators onto coherent states,

$$\mathcal{A} = \mathcal{A}\left(\frac{\lambda}{2\pi}\right)^d \iint |u^L_{p,q}\rangle\langle u^L_{p,q}| \; \mathrm{d}p\mathrm{d}q = \left(\frac{\lambda}{2\pi}\right)^d \iint \sigma(\mathcal{A})(p,q)|u^L_{p,q}\rangle\langle u^L_{p,q}| \; \mathrm{d}p\mathrm{d}q + O(\lambda^{m-1/2}) \; .$$

This formula motivates one now to turn it into a prescription of how to associate with a large class of distributions a an operator:

Definition 4.1.1. *Let L be a distribution of positive complex Lagrangian planes on T^*M and $u^L_{p,q}$ be a corresponding set of coherent states, which satisfies the completeness relation* (3.55)*. Then for $a \in \mathcal{D}'(T^*M)$, we call the operator*

$$\mathrm{Op}^{AW}_L[a] := \left(\frac{\lambda}{2\pi}\right)^d \iint a(p,q)|u^L_{p,q}\rangle\langle u^L_{p,q}| \; \mathrm{d}p\mathrm{d}q \; ,$$

the ***Anti-Wick quantization*** *of a. Conversely, a distribution a is called the* ***Anti-Wick symbol*** *of the operator $\mathcal{A}$ if $\mathcal{A} = \mathrm{Op}^{AW}_L[a]$.*

Since we will in the following only need some special classes of distributions, especially measures, as Anti-Wick symbols, we will not discuss the general mapping properties of Anti-Wick operators. We only remark that for instance in the case $M = \mathbb{R}^d$ an Anti-Wick operator with symbol in $\mathcal{S}'(T^*\mathbb{R}^d)$ maps $\mathcal{S}(\mathbb{R}^d)$ to $\mathcal{S}'(\mathbb{R}^d)$.

The Anti-Wick quantization has some nice properties. It reflects very well the properties of the symbol a, e.g., a positive symbol a leads to a positive operator $\mathrm{Op}^{AW}_L[a]$. Explicitly we have the lower bound

$$\mathrm{Op}^{AW}_L[a] \geq \inf a \; ,$$

which follows from the fact that for $\psi \in L^2(\mathbb{R}^d)$

$$\langle \psi, \mathrm{Op}^{AW}_L[a]\psi\rangle = \left(\frac{\lambda}{2\pi}\right)^d \iint a(p,q)|\langle u^L_{p,q}, \psi\rangle|^2 \; \mathrm{d}p\mathrm{d}q = \iint a(p,q)H_\psi(p,q) \; \mathrm{d}p\mathrm{d}q$$

where $H_\psi(p,q)$ is the Husimi function of ψ, see (3.57).

In the other direction it follows directly that

$$|| \operatorname{Op}_L^{AW}[a]|| \leq \sup |a| \ .$$

From the knowledge of the Weyl symbol of the projection operator $|u_{p,q}^L\rangle\langle u_{p,q}^L|$, see Lemma 3.3.14, we can infer the Weyl symbol of an Anti-Wick operator. If $\operatorname{Op}_L^{AW}[a]$ is the Anti-Wick quantization of a, then the Weyl symbol a^W of $\operatorname{Op}_L^{AW}[a]$ is given by

$$\begin{aligned} a^W(\xi,x) &= \iint W_{p,q}^L(\xi,x)a(p,q)\ \mathrm{d}p\mathrm{d}q \\ &= \left(\frac{\lambda}{\pi}\right)^d \iint \mathrm{e}^{-\lambda\langle \mathbf{g}_L(\xi-p,x-q),(\xi-p,x-q)\rangle} a(p,q)\ \mathrm{d}p\mathrm{d}q \ , \end{aligned} \tag{4.1}$$

hence the Weyl symbol is a Gaussian smoothing of the Anti-Wick symbol. The stationary phase formula gives for a smooth Anti-Wick symbol

$$a^W(\xi,x) = a(\xi,x) + O(\lambda^{-1}) \ ,$$

hence the principal symbol of the Anti-Wick operator $\operatorname{Op}_L^{AW}[a]$ is given by the leading part of a.

Similarly as in the case of Weyl quantization one can express the trace of an Anti-Wick operator in terms of the Anti-Wick symbol,

$$\operatorname{tr} \operatorname{Op}^{AW}[a] = \left(\frac{\lambda}{2\pi}\right)^d \int a(z)\ \mathrm{d}z \ ,$$

where we have used the abbreviation $z = (p,q)$.

Since by (4.1) the Weyl symbol is given by a convolution of the Anti-Wick symbol with a Gaussian, we can immediately transfer the product formula from the Weyl calculus, and obtain for a product of a Weyl operator $\mathcal{H}$ with Weyl-symbol H with the Anti-Wick operator $\operatorname{Op}_L^{AW}[a]$,

$$\mathcal{H} \operatorname{Op}_L^{AW}[a] = \operatorname{Op}_L^{AW}[H\#a] \ ,$$

if L is constant.

In order to treat the case that L is not constant it will be useful to introduce the abbreviations $z = (\xi,x)$ and $z' = (p,q)$. Then we can write (4.1) as

$$\tilde{a}(z) = \int a(z')W_{z'}(z)\ \mathrm{d}z' \ ,$$

with

$$W_{z'}(z) = \left(\frac{\lambda}{\pi}\right)^d \mathrm{e}^{-\lambda\langle z-z',\mathbf{g}(z')(z-z')\rangle} \ ,$$

and we get for any pseudodifferential operator $\mathcal{H}$ with Weyl symbol $H(z)$

$$H\#\tilde{a}(z) = \int a(z')H\#W_{z'}(z)\ \mathrm{d}z'$$

and

$$\tilde{a}\#H(z) = \int a(z')W_{z'}\#H(z)\ \mathrm{d}z'\ .$$

Proposition 4.1.2. *Let $H(z)$ be a symbol in $S^k(m_{a,b})$ and $W_{z'}(z) = \left(\frac{\lambda}{\pi}\right)^d \mathrm{e}^{-\lambda\langle z-z',\mathbf{g}(z')(z-z')\rangle}$ the Wigner function of a coherent state, then we have*

$$H\#W_{z'}(z) = \mathrm{e}^{\frac{1}{4\lambda}\langle\partial_{z''},\mathbf{g}(z')^{-1}\partial_{z''}\rangle}\tilde{H}(z''+z-\mathrm{i}\mathcal{J}_0\mathbf{g}(z-z'))|_{z''=0}W_{z'}(z)+O(\lambda^{-\infty})$$

and

$$W_{z'}\#H(z) = \mathrm{e}^{\frac{1}{4\lambda}\langle\partial_{z''},\mathbf{g}(z')^{-1}\partial_{z''}\rangle}\tilde{H}(z''+z+\mathrm{i}\mathcal{J}_0\mathbf{g}(z-z'))|_{z''=0}W_{z'}(z)+O(\lambda^{-\infty})\ ,$$

where $\tilde{H}$ denotes an almost analytic extension of H.

Proof. By the product formula of the Weyl calculus in its integral form, see, e.g., [Hör85a, DS99], we have

$$\begin{aligned}
H\#W_{z'}(z) &= \left(\frac{\lambda}{\pi}\right)^{2d}\iint H(z+z'')W_{z'}(z+z''')\mathrm{e}^{2\mathrm{i}\lambda\langle z''',\mathcal{J}_0z''\rangle}\ \mathrm{d}z''\mathrm{d}z''' \\
&= \left(\frac{\lambda}{\pi}\right)^{3d}\iint H(z+z'')\mathrm{e}^{-\lambda\langle z-z'+z''',\mathbf{g}(z')(z-z'+z''')\rangle}\mathrm{e}^{2\mathrm{i}\lambda\langle z''',\mathcal{J}_0z''\rangle}\ \mathrm{d}z''\mathrm{d}z''' \\
&= \left(\frac{\lambda}{\pi}\right)^{3d}\iint H(z+z'')\mathrm{e}^{-\lambda\langle z''',\mathbf{g}(z')z'''\rangle}\mathrm{e}^{2\mathrm{i}\lambda\langle z''',\mathcal{J}_0z''\rangle}\mathrm{e}^{-2\mathrm{i}\lambda\langle z-z',\mathcal{J}_0z''\rangle}\ \mathrm{d}z''\mathrm{d}z'''\ .
\end{aligned}$$

The z''' integral can be evaluated, giving

$$\left(\frac{\lambda}{\pi}\right)^{d}\int \mathrm{e}^{-\lambda\langle z''',\mathbf{g}(z')z'''\rangle}\mathrm{e}^{2\mathrm{i}\lambda\langle z''',\mathcal{J}_0z''\rangle}\ \mathrm{d}z''' = \mathrm{e}^{-\lambda\langle\mathcal{J}_0z'',\mathbf{g}(z')^{-1}\mathcal{J}_0z''\rangle}\ .$$

Since $\mathbf{g}$ is symplectic, we have $\mathcal{J}_0^t\mathbf{g}(z')^{-1}\mathcal{J}_0 = \mathbf{g}(z')$ and hence we arrive at

$$H\#W_{z'}(z) = \left(\frac{\lambda}{\pi}\right)^{2d}\int H(z+z'')\mathrm{e}^{-\lambda\langle z'',\mathbf{g}(z')z''\rangle}\mathrm{e}^{2\mathrm{i}\lambda\langle\mathcal{J}_0(z-z'),z''\rangle}\ \mathrm{d}z''\ .$$

Now the stationary point of the phase $2\langle\mathcal{J}_0(z-z'),z''\rangle+\mathrm{i}\langle z'',\mathbf{g}(z')z''\rangle$ is given by

$$z_0 = -\mathrm{i}\mathbf{g}(z')^{-1}\mathcal{J}_0(z-z') = -\mathrm{i}\mathcal{J}_0\mathbf{g}(z')(z-z')\ ,$$

and substituting $z'' \mapsto z'' + z_0$ gives together with Lemma B.1

$$\begin{aligned} H\#W_{z'}(z) &= \left(\frac{\lambda}{\pi}\right)^d \mathrm{e}^{-\lambda\langle z-z',\mathbf{g}(z')(z-z')\rangle} \left(\frac{\lambda}{\pi}\right)^d \int \tilde{H}(z+z''+z_0)\mathrm{e}^{-\lambda\langle z'',\mathbf{g}(z')z''\rangle}\,\mathrm{d}z'' + O(\lambda^{-\infty}) \\ &= W_{z'}(z)\mathrm{e}^{\frac{1}{4\lambda}\langle\partial_{z''},\mathbf{g}(z')^{-1}\partial_{z''}\rangle}\tilde{H}(z+z''+z_0)|_{z''=0} + O(\lambda^{-\infty}) \ . \end{aligned}$$

The almost analytic extension has entered because z_0 is imaginary. The price we have to pay for this is that, as in the proof of Theorem 3.2.10 , the result is only determined modulo $O(\lambda^{-\infty})$.

The case $W_{z'}\#H(z)$ is completely analogous with $\mathcal{J}_0$ replaced by $\mathcal{J}_0^t = -\mathcal{J}_0$, which then gives $z_0 = \mathrm{i}\mathcal{J}_0\mathbf{g}(z')(z-z')$. □

4.1.1 Estimates of Anti-Wick operators and fractal dimensions

The most important classical objects which we want to quantize using the Anti-Wick prescription are measures on phase space. As the example of a delta function δ_z concentrated at z shows

$$\mathrm{Op}_L^{AW}[\delta_z] = \left(\frac{\lambda}{2\pi}\right)^d |z\rangle\langle z| \ ,$$

the quantization of a measure will not necessarily yield an operator which for $\lambda \to \infty$ is bounded.

To be precise we will consider complex Radon measures. A complex Radon measure is a distribution of order zero, i.e. a linear map on the set of continuous functions

$$\begin{aligned} \mu : C^0(T^*M) &\to \mathbb{C} \\ \rho &\mapsto \mu(f) \end{aligned}$$

which is continuous in the sense that for every compact set $K \subset T^*M$ there is a constant C_K such that

$$|\mu(\rho)| \leq C_K \sup |\rho(z)|$$

for all $\rho \in C^0(T^*M)$ with $\operatorname{supp}\rho \subset K$. We will usually write

$$\mu(\rho) = \int \rho(z)\, \mu(z)\, \mathrm{d}z \ ,$$

following the conventions in the theory of distributions, and not in measure theory.

Any complex Radon measure can be decomposed into its real and imaginary parts

$$\mu = \operatorname{Re}\mu + \mathrm{i}\operatorname{Im}\mu \ ,$$

which are signed Radon measures. Any signed Radon measure in turn has a unique decomposition into the difference of two Radon, i.e. positive, measures,

$$\mu = \mu_+ - \mu_- \ ,$$

$\mu_+ \geq 0$, $\mu_- \geq 0$, and its absolute value is defined as

$$|\mu| := \mu_+ + \mu_- \ .$$

Furthermore, any Radon measure μ defines a unique Borel measure on T^*M which we denote by μ, too. By the decomposition $\mu = \mu_+ - \mu_-$ we get that any signed Radon measure defines as well a signed Borel measure. For more details see, e.g., [Mal95].

In the following we will always assume that the measures which occur are real signed Radon measures. The case of complex measures can always be reduced to this situation by the decomposition into real and imaginary parts.

The main tool for estimating the norm of an Anti-Wick operator is Cotlar's Lemma, which we state here essentially in the form given in [Fol89].

Lemma 4.1.3 (Cotlar's Lemma). *Let μ be a measure on T^*M and $\mathcal{A}(z)$, $z \in T^*M$, be a family of bounded operators on $L^2(M)$, such that the function $z \mapsto \langle u, \mathcal{A}(z)v\rangle$ is measurable for all $u, v \in L^2(M)$ and*

$$||\mathcal{A}(z)|| \leq M$$

for μ-almost all $z \in T^*M$. Suppose there exists a measurable function $h : T^*M \times T^*M \to [0, \infty)$ such that

$$||\mathcal{A}(z)\mathcal{A}(z')^*||^{1/2} \leq h(z, z') \ , \quad ||\mathcal{A}(z)^*\mathcal{A}(z')||^{1/2} \leq h(z, z') \ ,$$

for $\mu \times \mu$-almost all $(z, z') \in T^*M \times T^*M$, and

$$\int_{T^*M} h(z, z') \ |\mu(z')| \mathrm{d}z' = C < \infty$$

for μ-almost all $z \in T^*M$. Let $\{K_i\}_{i\in\mathbb{N}}$ be a sequence of compact subsets of T^*M with $K_i \subset K_{i+1}$ for all i and $\bigcup_i K_i = T^*M$, then

$$\mathcal{A}(K_i) := \int_{K_i} \mathcal{A}(z) \ \mu(z) \mathrm{d}z$$

is well defined, and the sequence $\mathcal{A}(K_i)$ converges to an operator $\mathcal{A}$ with

$$||\mathcal{A}|| \leq C \ .$$

Since this Lemma is the main tool for estimating norms of Anti-Wick operators we give a proof. We follow [Fol89] almost verbatim, with the only extension that we put more emphasis on the fact that we need all estimates only μ-almost everywhere.

Proof. For any bounded operator $\mathcal{B}$ on $L^2(M)$ one has

$$||\mathcal{B}||^2 = ||\mathcal{B}^*\mathcal{B}|| = ||(\mathcal{B}^*\mathcal{B})^n||^{1/n} , \tag{4.2}$$

and for a set of bounded operators $\mathcal{B}_1, \dots \mathcal{B}_{2n}$

$$\begin{aligned} ||\mathcal{B}_1\mathcal{B}_2\cdots\mathcal{B}_{2n}|| &\leq ||\mathcal{B}_1\mathcal{B}_2||\,||\mathcal{B}_3\mathcal{B}_4||\cdots||\mathcal{B}_{2n-1}\mathcal{B}_{2n}|| , \\ ||\mathcal{B}_1\mathcal{B}_2\cdots\mathcal{B}_{2n}|| &\leq ||\mathcal{B}_1||\,||\mathcal{B}_2\mathcal{B}_3||\cdots||\mathcal{B}_{2n-2}\mathcal{B}_{2n-1}||\,||\mathcal{B}_{2n}|| . \end{aligned}$$

Taking the geometric mean of these inequalities yields

$$||\mathcal{B}_1\mathcal{B}_2\cdots\mathcal{B}_{2n}|| \leq \left[||\mathcal{B}_1||\,||\mathcal{B}_1\mathcal{B}_2||\,||\mathcal{B}_2\mathcal{B}_3||\cdots||\mathcal{B}_{2n-1}\mathcal{B}_{2n}||\,||\mathcal{B}_{2n}||\right]^{1/2} . \tag{4.3}$$

Now consider

$$\begin{aligned} (\mathcal{A}(K_i)^*\mathcal{A}(K_i))^n = \int_{K_i}\cdots\int_{K_i} & \mathcal{A}(z_1)^*\mathcal{A}(z_2)\mathcal{A}(z_3)^*\cdots\mathcal{A}(z_{2n-1})^*\mathcal{A}(z_{2n}) \\ & \mu(z_{2n})\mu(z_{2n-1})^*\cdots\mu(z_1)^*\,\mathrm{d}z_{2n}\cdots\mathrm{d}z_1 . \end{aligned}$$

By (4.3) and the hypothesis on $\mathcal{A}(z)$, $||(\mathcal{A}(K_i)^*\mathcal{A}(K_i))^n||$ is bounded by

$$\int_{K_i}\cdots\int_{K_i} M^{1/2}h(z_1,z_2)\cdots h(z_{2n-1},z_{2n})M^{1/2}\,|\mu(z_{2n})||\mu(z_{2n-1})|\cdots|\mu(z_1)|\,\mathrm{d}z_{2n}\cdots\mathrm{d}z_1 ,$$

and by the hypotheses on h this can be estimated by $M|\mu|(K_i)C^{2n-1}$. Thus we obtain together with (4.2)

$$||\mathcal{A}(K_i)|| = ||(\mathcal{A}(K_i)^*\mathcal{A}(K_i))^n||^{1/2n} \leq (M|\mu|(K_i))^{1/2n}C^{(2n-1)/2n} ,$$

and taking the limit $n \to \infty$ then gives

$$||\mathcal{A}(K_i)|| \leq C .$$

The proof of the convergence of $\mathcal{A}(K_i)$ will be only given for the special case that $\mu(z)$ and $\mathcal{A}(z)$ are positive, for the general case we refer to [Fol89]. Under these conditions the sequence $\mathcal{A}(K_i)$ is non-decreasing,

$$\mathcal{A}(K_{i+1}) \geq \mathcal{A}(K_i) ,$$

and since it is bounded, it converges to a bounded operator $\mathcal{A}$. □

In the case at hand, the family of operators is given by

$$\mathcal{A}(z) = \left(\frac{\lambda}{2\pi}\right)^d |z\rangle\langle z| ,$$

and therefore we have to estimate

$$||\mathcal{A}(z)\mathcal{A}(z')^*||^{1/2} = ||\mathcal{A}(z)^*\mathcal{A}(z')||^{1/2} = \left(\frac{\lambda}{2\pi}\right)^d |\langle z,z'\rangle|^{1/2}||\,|z\rangle\langle z'|\,||^{1/2} = \left(\frac{\lambda}{2\pi}\right)^d |\langle z,z'\rangle|^{1/2} .$$

Lemma 4.1.4. *Assume that the distribution L is constant, then we have*

$$||\mathcal{A}(z)\mathcal{A}(z')^*||^{1/2} = ||\mathcal{A}(z)^*\mathcal{A}(z')||^{1/2} = \left(\frac{\lambda}{2\pi}\right)^d \mathrm{e}^{-\lambda\langle z-z',\mathbf{g}(z-z')\rangle/8} ,$$

where $\mathbf{g}$ *denotes the metric defined by L, see* (3.53). *If the distribution L is not constant, then there exists a constant $C > 0$ such that*

$$||\mathcal{A}(z)\mathcal{A}(z')^*||^{1/2} = ||\mathcal{A}(z)^*\mathcal{A}(z')||^{1/2} \leq C\left(\frac{\lambda}{2\pi}\right)^d \mathrm{e}^{-\lambda\langle z-z',\mathbf{g}(z-z')\,(z-z')\rangle/8} .$$

Proof. In the first case the result follows directly from Lemma 3.3.18. In the second case one has to use an asymptotic version of Lemma 3.3.18 which follows from the method of stationary phase. The details are left to the reader. □

So the function h can be chosen as

$$h(z,z') = C\left(\frac{\lambda}{2\pi}\right)^d \mathrm{e}^{-\lambda\langle z-z',\mathbf{g}(z-z')\,(z-z')\rangle/8} .$$

where C is the constant from Lemma 4.1.4.

To determine the bound on the norm of $\mathrm{Op}_L^{AW}[\mu]$ we therefore have to estimate

$$\rho_\lambda * |\mu|(z) := \int \left(\frac{\lambda}{2\pi}\right)^d \mathrm{e}^{-\lambda\langle z-z',\mathbf{g}(z-z')\,(z-z')\rangle/8}\,|\mu(z')|\mathrm{d}z' \tag{4.4}$$

for large λ, where $\rho_\lambda(z) := \left(\frac{\lambda}{2\pi}\right)^d \mathrm{e}^{-\lambda\langle z,\mathbf{g}(z)\,z\rangle/8}$. For the case that μ belongs to an L^p space, a bound on the norm follows immediately from Young's inequality.

Proposition 4.1.5. *Let μ be in $L^p(T^*M)$, $1 \leq p \leq \infty$, then there is constant $C_{p,L}$, independent on μ, such that*

$$||\,\mathrm{Op}_L^{AW}[\mu]|| \leq C_{p,L}\left(\frac{\lambda}{2\pi}\right)^{d/p} ||\mu||_{L^p} .$$

So the quantization of a bounded function has a bounded norm, and the quantization of an integrable function has a norm which grows not faster than λ^d.

Proof. Young's inequality, see, e.g., [RS80], yields

$$||\rho_\lambda * |\mu|||_{L^\infty} \leq ||\rho_\lambda||_{L^q}||\mu||_{L^p} ,$$

with $1/p + 1/q = 1$, so we only have to determine $||\rho_\lambda||_{L^q}$. But this gives

$$\begin{aligned}
||\rho_\lambda||_{L^q}^q &= C^q \int \left(\frac{\lambda}{2\pi}\right)^{dq} \mathrm{e}^{-\lambda q\langle z,\mathbf{g}(z)\,z\rangle/8}\,\mathrm{d}z \\
&= C^q \left(\frac{\lambda}{2\pi}\right)^{dq} (\lambda q/4)^{-d} \int \mathrm{e}^{-\langle z,\mathbf{g}(0)z\rangle/2}\,\mathrm{d}z\big(1+O(1/\lambda)\big) \\
&= C^q \left(\frac{\lambda}{2\pi}\right)^{dq} (\lambda q/4)^{-d}(2\pi)^d\big(1+O(1/\lambda)\big) ,
\end{aligned}$$

where we have used the stationary phase formula and the fact that $\det \mathbf{g} = 1$. Taking the q'th root leads to

$$||\rho_\lambda||_{L^q} \leq C_{p,L} \left(\frac{\lambda}{2\pi}\right)^{d/p} .$$

□

For more general measures μ a more refined analysis is necessary in order to get good estimates on the norm. As a preparation we will now discuss some fractal dimensions associated with general measures, see [Fal90, Fal97] or the contribution of Pesin in [BDD+00] for an introduction and more details.

Definition 4.1.6. *Let μ be a (Borel-) measure on T^*M, fix some metric on T^*M and denote by $B(z,r) := \{z' \in T^*M \ , \mathrm{dist}(z,z') \leq r\}$ the ball of radius r around z. Then the* ***local lower dimension*** *and the* ***local upper dimension*** *of μ at $z \in \operatorname{supp}\mu$ are defined as*

$$\begin{aligned} \underline{\dim}(\mu, z) &:= \liminf_{r\to 0} \frac{\ln \mu(B(z,r))}{\ln r} , \\ \overline{\dim}(\mu, z) &:= \limsup_{r\to 0} \frac{\ln \mu(B(z,r))}{\ln r} . \end{aligned}$$

If they are equal the common limit is called the ***local dimension*** $\dim(\mu,z)$ *of μ at z. Furthermore,*

$$\dim_H(\mu) := \sup\{s \ , \underline{\dim}(\mu,z) \geq s \text{ for } \mu\text{−almost all } z \in \operatorname{supp}\mu\} \tag{4.5}$$

is called the ***Hausdorff dimension*** *of μ.*

The local dimensions describe the power law behavior of the μ-volume of the ball $B(z,r)$ for $r \to 0$ and thus describe, roughly speaking, how concentrated the mass of μ is at z. The smaller the local dimension is, the higher is the concentration of the measure at z, as the following examples show.

Examples 4.1.7:

1. Let $\mu(x)\mathrm{d}x = a(x)\mathrm{d}x$, where $\mathrm{d}x$ denotes Lebesgue measure on $\mathbb{R}^d$ and $a \in L^\infty(\mathbb{R}^d)$. Then

$$\mu(B(z,r)) \leq ||a||_\infty \int_{B(z,r)} \mathrm{d}x = ||a||_\infty c_d\, r^d ,$$

so we have for $x \in \operatorname{supp} a$ $\underline{\dim}(\mu,z) = \overline{\dim}(\mu,z) = d$ and $\dim_H(\mu) = d$.

2. Let μ_S be concentrated on a submanifold $S \subset \mathbb{R}^n$ of dimension k, in the sense that $\mu_S(x)\mathrm{d}x = a(x)\delta(f_1(x)) \cdots \delta(f_{n-k}(x))\mathrm{d}x$ where the $f_i(x)$ are smooth functions which locally define S through $S = \{x\,;\, f_1(x) = \cdots f_{n-k}(x) = 0\}$; $a \in \mathbb{C}^\infty(\mathbb{R}^d)$ and $\mathrm{d}x$ denotes Lebesgue measure on $\mathbb{R}^d$. Then one obtains for $z \in S \cap \operatorname{supp} a$
$$\mu_S(B(z,r)) \sim r^{\dim S} \quad ,$$
and so $\underline{\dim}(\mu, z) = \overline{\dim}(\mu, z) = \dim S$. The Hausdorff dimension of μ_S then equals the dimension of S, $\dim_H(\mu_S) = \dim S$.

3. To get an impression of what other types of measures can occur, we give an example where we expect a non-integer dimension $\underline{d}_\mu$. Let $f(x)$ be a continuous, but nowhere differentiable function, for instance the Weierstrass function
$$f_s(x) := \sum_{k=1}^{\infty} 2^{(2-s)k} \sin 2^k x \ ,$$
with $1 \leq s < 2$, then the graph of $f_s(x)$ has fractal box dimension equal to s and one expects that its Hausdorff dimension also equals s, see [Fal90, Chapter 11]. Therefore, we expect by (4.6) that the measure μ_f on $\mathbb{R}^2$, defined by $\int \rho(x,y)\ \mathrm{d}\mu_f(x,y) := \int \rho(x, f(x))\ \mathrm{d}x$, has Hausdorff dimension $\dim_H \mu_f = s$, too.

We want to compare the Hausdorff dimension of a measure with the Hausdorff dimension of the sets of positive μ-measure. For completeness we recall the definition of the Hausdorff dimension of sets. Let E be a subset of some metric space X; a countable open cover $\{U_i\}$ of E is called a δ-cover if $|U_i| := \sup\{d(x,y)\,,\, x,y \in U_i\} \leq \delta$. Then for a given $s \geq 0$ and all $\delta > 0$ one defines
$$\mathcal{H}^s_\delta(E) = \inf\left\{ \sum_i |U_i|^s \ ,\ \{U_i\} \text{ is a } \delta\text{-cover of } E \right\} \ ,$$
and then the s-dimensional Hausdorff measure of E is defined as
$$\mathcal{H}^s(E) = \lim_{\delta \to 0} \mathcal{H}^s_\delta(E) \ .$$
The Hausdorff dimension of E is now defined as the smallest s such that $\mathcal{H}^s(E)$ is finite, which is equivalent to
$$\dim_H E := \inf\{s\ :\ \mathcal{H}^s(E) = 0\} = \sup\{s\ :\ \mathcal{H}^s(E) = \infty\} \ .$$
Now the relation between the Hausdorff dimension of a measure and the Hausdorff dimension of sets is given in [Fal97, Proposition 10.2]. For a finite Borel measure μ one has
$$\dim_H \mu = \inf\{\dim_H E\ :\ E \text{ is a Borel set with } \mu(E) > 0\,\} \ . \tag{4.6}$$

We now want to relate the asymptotic behavior of (4.4), which determines the norm of the Anti-Wick quantization of μ, to the Hausdorff dimension.

Lemma 4.1.8. *Let μ be a positive measure on T^*M, and*

$$\rho_\lambda(z) := \left(\frac{\lambda}{\pi}\right)^d \mathrm{e}^{-\lambda\langle z,\mathbf{g}z\rangle}$$

be a Gaussian, where $\mathbf{g}$ *is a positive definite symmetric matrix and* $d = \dim M$. *Denote by* $\rho_\lambda * \mu$ *the convolution of* ρ_λ *and* μ, *then*

$$\liminf_{\lambda\to\infty} \frac{\ln \rho_\lambda * \mu(z)}{\ln\lambda} = d - \frac{1}{2}\underline{\dim}(\mu, z) \tag{4.7}$$

$$\limsup_{\lambda\to\infty} \frac{\ln \rho_\lambda * \mu(z)}{\ln\lambda} = d - \frac{1}{2}\overline{\dim}(\mu, z) \ , \tag{4.8}$$

and

$$\limsup_{\lambda\to\infty} \frac{\ln \rho_\lambda * \mu(z)}{\ln\lambda} \leq d - \frac{1}{2}\dim_H \mu \ , \tag{4.9}$$

for μ *almost every* z.

Proof. Let us denote by $\chi_{[z,r]}(z')$ the characteristic function of the ball $B(z,r)$ and introduce

$$\tilde\rho_\lambda := \mathrm{e}^{-\lambda\langle z,\mathbf{g}z\rangle} \ .$$

We have for $\epsilon > 0$

$$\begin{aligned}\frac{1}{2}\tilde\rho_\lambda(z-z') &= \frac{1}{2}\chi_{[z,1/\lambda^{1/2-\epsilon}]}(z')\tilde\rho_\lambda(z-z') + \frac{1}{2}(1-\chi_{[z,1/\lambda^{1/2-\epsilon}]}(z'))\tilde\rho_\lambda(z-z')\\ &< \chi_{[z,1/\lambda^{1/2-\epsilon}]}(z') + C\mathrm{e}^{-c\lambda^\epsilon}\end{aligned}$$

with some constants $C, c > 0$. On the other hand, there is a λ_0 such that for $\lambda > \lambda_0$

$$2\tilde\rho_\lambda(z-z') > \chi_{[z,1/\lambda^{1/2+\epsilon}]}(z') \ .$$

Now, by taking the convolution of the two inequalities with μ and noting that $\mu(B(z,r)) = \chi_{[z,r]} * \mu(0)$ we get for λ sufficiently large that

$$\frac{\ln\mu(B(z,1/\lambda^{1/2+\epsilon}))}{\ln\lambda} < \frac{\ln\tilde\rho_\lambda * \mu(z)}{\ln\lambda} < \frac{\ln\mu(B(z,1/\lambda^{1/2-\epsilon}))}{\ln\lambda} \ .$$

Therefore we get

$$\begin{aligned}-\frac{1}{2}\underline{\dim}(\mu,z) - 2\epsilon &\leq \liminf_{\lambda\to\infty}\frac{\ln\tilde\rho_\lambda * \mu(z)}{\ln\lambda} \leq -\frac{1}{2}\underline{\dim}(\mu,z) + 2\epsilon\\ -\frac{1}{2}\overline{\dim}(\mu,z) - 2\epsilon &\leq \limsup_{\lambda\to\infty}\frac{\ln\tilde\rho_\lambda * \mu(z)}{\ln\lambda} \leq -\frac{1}{2}\overline{\dim}(\mu,z) + 2\epsilon \ ,\end{aligned}$$

for any $\epsilon > 0$, and hence

$$\liminf_{\lambda\to\infty} \frac{\ln \tilde\rho_\lambda * \mu(z)}{\ln\lambda} = -\frac{1}{2}\underline{\dim}(\mu, z)$$
$$\limsup_{\lambda\to\infty} \frac{\ln \tilde\rho_\lambda * \mu(z)}{\ln\lambda} = -\frac{1}{2}\overline{\dim}(\mu, z) \ .$$

By substituting ρ_λ for $\tilde\rho_\lambda$, this proves the first of the relations (4.7) and (4.8). The second one, (4.9), is then a direct consequence of the definition of $\dim_H \mu$, (4.5). □

By a small variation of the proof we can obtain the following result, which will be useful later.

Lemma 4.1.9. *Let μ be a measure, and*

$$\rho_\lambda^{(n)}(z) := |z|^n e^{-\lambda\langle z, \mathbf{g}z\rangle} \ ,$$

where $\mathbf{g}$ is a positive definite symmetric matrix. Then we have

$$|\mu * \rho_\lambda^{(n)}| \le C\lambda^{-n/2}\, |\mu| * \rho_\lambda^{(0)} \ .$$

Proof. In the proof of Lemma 4.1.8 we have seen that we can replace the Gaussian by the characteristic function of a ball of radius $\lambda^{-1/2}$ without changing the order in λ of the convolution. But on a ball of radius $\lambda^{-1/2}$ around 0, the function $|z|^n$ can be estimated by $\lambda^{-n/2}$. □

We can now put all the pieces together to obtain a description of the behavior of the Anti-Wick quantization of a measure on phase space. Cotlar's Lemma 4.1.3, together with Definition 4.1.6, and Lemma 4.1.8 gives the following theorem.

Theorem 4.1.10. *Let μ be a measure on phase space T^*M such that for μ-almost every z*

$$\left(\frac{\lambda}{2\pi}\right)^d \int_{T^*M} e^{-\lambda\langle z-z', \mathbf{g}(z-z')(z-z')\rangle/8}\, |\mu(z')|\, dz' \le C < \infty \ ,$$

then $\mathrm{Op}_L^{AW}[\mu]$ is well defined and

$$||\,\mathrm{Op}_L^{AW}[\mu]|| \le C \ .$$

Furthermore, we get for large λ that

$$\limsup_{\lambda\to\infty} \frac{\ln ||\,\mathrm{Op}_L^{AW}[\mu]||}{\ln\lambda} \le d - \frac{1}{2}\dim_H \mu \ , \tag{4.10}$$

where $\dim_H \mu$ denotes the Hausdorff dimension of μ, defined in (4.5).

Roughly speaking, (4.10) means that

$$|| \operatorname{Op}_L^{AW}[\mu]|| \leq C\lambda^{d-\frac{1}{2}\dim_H \mu} , \tag{4.11}$$

but one has to be careful: If we multiply for instance powers of $\ln \lambda$ on the right-hand side of (4.11), (4.10) remains true. So (4.11) is generally only true modulo logarithmic terms, and (4.10) is the more precise statement. Alternatively we could reformulate (4.10) in the following form; for every $\varepsilon > 0$ exists a constant $C_\varepsilon > 0$ such that

$$|| \operatorname{Op}_L^{AW}[\mu]|| \leq C_\varepsilon \lambda^{d-\frac{1}{2}\dim_H \mu+\varepsilon} .$$

For the first two examples in 4.1.7 we obtain for their Anti-Wick quantizations:
Examples:

- If $\mathrm{d}\mu(z)$ is of the form $a(z)\mathrm{d}z$, with a bounded function $a(z)$, then we get of course

$$|| \operatorname{Op}_L^{AW}[a]|| \leq \sup_z |a(z)| .$$

- Let $S \subset T^*M$ be a submanifold of codimension κ, and let $\mathrm{d}\mu = a(z)\mathrm{d}\mu_S(z)$, where $\mu_S(z)$ is the measure on S induced by the symplectic measure $\mathrm{d}z$, then

$$|| \operatorname{Op}_L^{AW}[\mu]|| \leq \left(\frac{\lambda}{2\pi}\right)^{\kappa/2} \sup_{z\in S} |a(z)| .$$

4.1.2 Algebraic properties of Anti-Wick operators

The general algebraic properties of Anti-Wick operators are less pleasant than the ones of pseudodifferential operators. For instance, they do not even form an algebra. But for certain special cases products can be studied without too much work. Proposition 4.1.2 allows to draw some conclusions on the semiclassical behavior of Anti-Wick operators under multiplication with ordinary pseudodifferential operators.

Theorem 4.1.11. *Let μ be a measure on T^*M with compact support, then we have for all $\mathcal{A} \in \Psi_\lambda^0(m_{a,b})$*

$$\begin{aligned} ||\mathcal{A} \operatorname{Op}_L^{AW}[\mu] - \operatorname{Op}_L^{AW}[\sigma(\mathcal{A})\mu]|| &\leq C|| \operatorname{Op}_L^{AW}[\mu]||\, \lambda^{-1/2} \\ || \operatorname{Op}_L^{AW}[\mu]\mathcal{A} - \operatorname{Op}_L^{AW}[\sigma(\mathcal{A})\mu]|| &\leq C|| \operatorname{Op}_L^{AW}[\mu]||\, \lambda^{-1/2} , \end{aligned}$$

where the constants depend on $\mathcal{A}$ and μ.

Proof. We have

$$\mathcal{A} \operatorname{Op}_L^{AW}[\mu] = \left(\frac{\lambda}{2\pi}\right)^d \int \mu(z)\, \mathcal{A}|z\rangle\langle z|\, \mathrm{d}z$$

and according to Corollary 3.2.12 $\mathcal{A}|z\rangle$ is given by

$$\mathcal{A}u_{p,q}(\lambda,x) = \sigma(\mathcal{A})(z)u_{p,q}(\lambda,x) + r(\lambda;z,x)$$

with

$$r(\lambda;z,x)) = O((x-q))u_{p,q}(\lambda,x) + O(\lambda^{-1})f(\lambda,z,x)u_{p,q}(\lambda,x) \ , \tag{4.12}$$

where $f(\lambda,z,x) = O(\lambda^0)$ uniformly in z and x. So we get

$$\mathcal{A}\,\mathrm{Op}_L^{AW}[\mu] - \mathrm{Op}_L^{AW}[\sigma(\mathcal{A})\mu] = \left(\frac{\lambda}{2\pi}\right)^d \int \mu(z)\,|r(z)\rangle\langle z|\ \mathrm{d}z \ ,$$

and we will estimate the left-hand side with Cotlar's Lemma. The family of operators is in this case given by

$$\mathcal{B}(z) = \left(\frac{\lambda}{2\pi}\right)^d |r(z)\rangle\langle z| \ ,$$

and we get with (4.12) and Lemma 4.1.9

$$||\mathcal{B}(z)\mathcal{B}(z')^*||^{1/2} \leq \frac{C}{\lambda^{1/2}}\,\mathrm{e}^{-\lambda\langle z-z',\mathbf{g}(z-z')\rangle/8} \qquad ||\mathcal{B}(z')\mathcal{B}(z)^*||^{1/2} \leq \frac{C}{\lambda^{1/2}}\,\mathrm{e}^{-\lambda\langle z-z',\mathbf{g}(z-z')\rangle/8} \ ,$$

which then yields the first estimate. The proof of the second relation is identical.

□

The next quantity we want to discuss is the commutator of an Anti-Wick operator $\mathrm{Op}_L^{AW}[\mu]$ and a pseudodifferential operator $\mathcal{A}$. If $\mathrm{d}\mu$ is of the form $b(z)\mathrm{d}z$ with $b \in S(1)$, then by (4.1) the Weyl symbol $b^W(z)$ of $\mathrm{Op}_L^{AW}[\mu]$ is in $S(1)$, too, and has an asymptotic expansion of the form

$$b^W(z) \sim b(z) + \frac{1}{\lambda}b_1(z) + \cdots \ .$$

So the commutator $[\mathcal{A}, \mathrm{Op}_L^{AW}[\mu]]$ has the Weyl symbol $\frac{1}{\mathrm{i}\lambda}\{\sigma(\mathcal{A}), b\} + O(1/\lambda^2)$, and hence we get for $A \in S(1)$ that

$$||[\mathcal{A}, \mathrm{Op}_L^{AW}[\mu]] - \frac{1}{\mathrm{i}\lambda}\mathrm{Op}_L^{AW}[\{\sigma(\mathcal{A}), b\}]|| \leq C\lambda^{-2} \ .$$

But for more general measures, which are not smooth relative to Liouville measure, additional terms can enter the expression for the commutator. The reason is the presence of the metric $\mathbf{g}$ whose derivative along the Hamiltonian vector field generated by $\sigma(\mathcal{A})$ we have to take into account. It will enter through a kind of covariant derivative,

$$\mathbf{D}_{\sigma(\mathcal{A})}\mathbf{g} := [X_{\sigma(\mathcal{A})}\mathbf{g}] + (\mathcal{J}\sigma(\mathcal{A})'')^\dagger\mathbf{g} + \mathbf{g}\mathcal{J}\sigma(\mathcal{A})'' \ , \tag{4.13}$$

where $[X_{\sigma(\mathcal{A})}\mathbf{g}] := \langle X_{\sigma(\mathcal{A})}, \partial_z\rangle\mathbf{g}$ denotes the application of $X_{\sigma(\mathcal{A})}$ to $\mathbf{g}$.

Theorem 4.1.12. *Let μ be a measure on T^*M and $\mathcal{A}$ be a pseudodifferential operator with symbol in $S(m_{a,b})$, then*

$$[\mathrm{Op}_L^{AW}[\mu], \mathcal{A}] = \frac{1}{\mathrm{i}\lambda} \mathrm{Op}_L^{AW}[\{\mu, \sigma(A)\}] + \mathrm{i}\ \mathrm{Op}_{L,\mathbf{D}}^{AW}[\mu] + \mathcal{R}$$

with

$$||\mathcal{R}|| \leq C|| \mathrm{Op}_L^{AW}[\mu]||\, \lambda^{-3/2} \ ,$$

and where $\mathrm{Op}_{L,\mathbf{D}}^{AW}[\mu]$ denotes the operator with Weyl symbol

$$\int \langle z' - z, \mathbf{D}_{\sigma(\mathcal{A})}\mathbf{g}(z)(z' - z)\rangle \left(\frac{\lambda}{\pi}\right)^d \mathrm{e}^{-\lambda\langle z'-z, \mathbf{g}(z)(z'-z)\rangle}\, \mu(z)\ \mathrm{d}z \ , \tag{4.14}$$

with $\mathbf{D}_{\sigma(\mathcal{A})}\mathbf{g}(z)$ defined in (4.13).

Here the Poisson bracket $\{\mu, \sigma(A)\}$ is defined in the sense of distributions. Of course $\{\mu, \sigma(A)\}$ is then generally no longer a measure, but Anti-Wick quantization is well defined for general distributions.

Proof. We will make a Taylor expansion of the Weyl symbol of $\mathcal{A}$ around z, writing

$$\mathcal{A}u_z = \mathcal{A}_z^{(2)}u_z + [\mathcal{A} - \mathcal{A}_z^{(2)}]u_z$$

where $\mathcal{A}_z^{(2)}$ has Weyl symbol

$$A_2^{(2)}(z') = A_0(z) + \langle A_0'(z), z' - z\rangle + \frac{1}{2}\langle z' - z, A_0''(z)z' - z\rangle + \frac{1}{\lambda}A_1(z) \ ,$$

where A_0 denotes the principal symbol of $\mathcal{A}$ and A_1 the subprincipal symbol. By Corollary 3.2.12 we have

$$[\mathcal{A} - \mathcal{A}_z^{(2)}]u_z(\lambda, x) = [O((x - q)^3) + O(x - q)/\lambda + O(\lambda^{-2})]u_z(\lambda, x) \ ,$$

and so the same argument as in the proof of Theorem 4.1.11 gives

$$||[\mathcal{A}, \mathrm{Op}_L^{AW}[\mu]] - [\mathcal{A}^{(2)}, \mathrm{Op}_L^{AW}[\mu]]|| \leq C\, || \mathrm{Op}_L^{AW}[\mu]||\, \lambda^{-3/2} \ ,$$

where $[\mathcal{A}^{(2)}, \mathrm{Op}_L^{AW}[\mu]]$ is a shorthand for

$$\left(\frac{\lambda}{2\pi}\right)^d \int [\mathcal{A}_z^{(2)}, |z\rangle\langle z|]\, \mu(z)\ \mathrm{d}z \ .$$

Hence we are left with the determination of $[\mathcal{A}^{(2)}, \mathrm{Op}_L^{AW}[\mu]]$.

The Weyl symbol of $\mathcal{A}_z^{(2)}|z\rangle\langle z| - |z\rangle\langle z|\mathcal{A}_z^{(2)}$ can be computed with Proposition 4.1.2 to be

$$\begin{aligned} b_z(z') &= \left(\frac{\lambda}{\pi}\right)^d \big[2\mathrm{i}\langle A_0'(z), \mathcal{J}_0\mathbf{g}(z)(z'-z)\rangle \\ &\qquad\qquad + 2\mathrm{i}\langle z'-z, [A_0''(z)\mathcal{J}_0\mathbf{g}(z)]_+(z'-z)\rangle\big]\mathrm{e}^{-\lambda\langle z'-z,\mathbf{g}(z)(z'-z)\rangle} \\ &= \left(\frac{\lambda}{\pi}\right)^d \big[-2\mathrm{i}\langle X_{A_0}(z), \mathbf{g}(z)(z'-z)\rangle \\ &\qquad\qquad + 2\mathrm{i}\langle z'-z, [A_0''(z)\mathcal{J}_0\mathbf{g}(z)]_+(z'-z)\rangle\big]\mathrm{e}^{-\lambda\langle z'-z,\mathbf{g}(z)(z'-z)\rangle} , \end{aligned}$$

where $X_{A_0}(z) = \mathcal{J}_0 A_0'(z)$ denotes the Hamilton vector field of A_0, and $[A_0''(z)\mathcal{J}_0\mathbf{g}(z)]_+ := [A_0''(z)\mathcal{J}_0\mathbf{g}(z) - \mathbf{g}(z)\mathcal{J}_0A_0''(z)]/2$ denotes the symmetric part of $A_0''(z)\mathcal{J}_0\mathbf{g}(z)$. With

$$\begin{aligned} -\frac{1}{2\lambda}\langle X_{A_0}, \partial_z\rangle \mathrm{e}^{-\lambda\langle z'-z,\mathbf{g}(z)(z'-z)\rangle} = \Big[&\langle X_{A_0}, \mathbf{g}(z)(z'-z)\rangle \\ &+ \frac{1}{2}\langle z'-z, [X_{A_0}\mathbf{g}](z)(z'-z)\rangle\Big]\mathrm{e}^{-\lambda\langle z'-z,\mathbf{g}(z)(z'-z)\rangle} , \end{aligned}$$

where $[X_{A_0}\mathbf{g}](z) := \langle X_{A_0}, \partial_z\rangle\mathbf{g}(z)$ denotes the application of X_{A_0} to $\mathbf{g}$, we can rewrite this as

$$\begin{aligned} b_z(z') &= \left(\frac{\lambda}{\pi}\right)^d \frac{\mathrm{i}}{\lambda}\langle X_{A_0}, \partial_z\rangle \mathrm{e}^{-\lambda\langle z'-z,\mathbf{g}(z)(z'-z)\rangle} \\ &\quad + \left(\frac{\lambda}{\pi}\right)^d \Big[\mathrm{i}\langle z'-z, [X_{A_0}\mathbf{g}](z)(z'-z)\rangle \\ &\qquad\qquad + 2\mathrm{i}\langle z'-z, [A_0''(z)\mathcal{J}_0\mathbf{g}(z)]_+(z'-z)\rangle\Big]\mathrm{e}^{-\lambda\langle z'-z,\mathbf{g}(z)(z'-z)\rangle} \\ &= \mathrm{i}\left(\frac{\lambda}{\pi}\right)^d \left[\frac{1}{\lambda}\langle X_{A_0}, \partial_z\rangle + \langle z'-z, \mathbf{D}_{A_0}\mathbf{g}(z)(z'-z)\rangle\right]\mathrm{e}^{-\lambda\langle z'-z,\mathbf{g}(z)(z'-z)\rangle} . \end{aligned}$$

Now the Weyl symbol of $\mathrm{Op}_L^{AW}[\{\sigma(\mathcal{A}), \mu\}]$ is given by

$$\begin{aligned} &\left(\frac{\lambda}{2\pi}\right)^d \int \langle X_{A_0}(z), \partial_z\rangle\mu(z) \, \left(\frac{\lambda}{\pi}\right)^d \mathrm{e}^{-\lambda\langle z'-z,\mathbf{g}(z),z'-z\rangle}\,\mathrm{d}z \\ &= -\left(\frac{\lambda}{2\pi}\right)^d \int \mu(z)\,\langle X_{A_0}(z), \partial_z\rangle \left(\frac{\lambda}{\pi}\right)^d \mathrm{e}^{-\lambda\langle z'-z,\mathbf{g}(z),z'-z\rangle}\,\mathrm{d}z \end{aligned}$$

where we have used partial integration. Hence we get that the difference

$$[\mathcal{A}^{(2)}, \mathrm{Op}_L^{AW}[\mu]] - \frac{1}{\mathrm{i}\lambda}\,\mathrm{Op}_L^{AW}[\{\sigma(\mathcal{A}), \mu\}]$$

has Weyl symbol

$$h(z') := \int \mu(z) \left(\frac{\lambda}{\pi}\right)^d \mathrm{i}\langle z'-z, \mathbf{D}_{A_0}\mathbf{g}(z)(z)(z'-z)\rangle \mathrm{e}^{-\lambda\langle z'-z,\mathbf{g}(z)(z'-z)\rangle}\, \mathrm{d}z \ .$$

□

The first term in the expression for the commutator, $\mathrm{Op}_L^{AW}[\{\mu, \sigma(A)\}]$, is the one expected from the corresponding results on classical pseudodifferential operators. The second term, (4.14), is related to the smoothness of the measure μ as the following corollary shows.

Corollary 4.1.13. *Assume that the measure μ on T^*M satisfies*

$$\partial_{z_i}\mu \in L^\infty(T^*M) \ , \tag{4.15}$$

for $i = 1, \cdots, 2d$, then we have for $\mathcal{A} \in \Psi(m_{a,b})$

$$||[\mathcal{A}, \mathrm{Op}^{AW}[\mu]] - \frac{1}{\mathrm{i}\lambda}\mathrm{Op}^{AW}[\{\sigma(\mathcal{A}), \mu\}]|| \leq C\lambda^{-3/2} \ .$$

Proof. We have to estimate the second term, (4.14), in the expression for the commutator in Theorem 4.1.12. With a Taylor expansion, $\mathbf{D}_{\sigma(\mathcal{A})}\mathbf{g}(z) = \mathbf{D}_{\sigma(\mathcal{A})}\mathbf{g}(z') + O(z-z')$, and $\mathbf{g}(z) = \mathbf{g}(z') + O(z-z')$, we get

$$h(z') = \int \mu(z) \left(\frac{\lambda}{\pi}\right)^d \mathrm{i}\langle z'-z, (\mathbf{D}_{\sigma(\mathcal{A})}\mathbf{g})(z')(z'-z)\rangle \mathrm{e}^{-\lambda\langle z'-z,\mathbf{g}(z')(z'-z)\rangle}\, \mathrm{d}z\, (1 + O(1/\sqrt{\lambda})) \ .$$

Using $-\frac{1}{2\lambda}\mathbf{g}^{-1}\partial_z \mathrm{e}^{-\lambda\langle z'-z,\mathbf{g}(z')(z'-z)\rangle} = (z-z')\mathrm{e}^{-\lambda\langle z'-z,\mathbf{g}(z')(z'-z)\rangle}$ together with partial integration gives

$$\begin{aligned}
h(z') = &- \int \mu(z)\, \mathrm{i}\langle z'-z, \frac{1}{2\lambda}(\mathbf{D}_{\sigma(\mathcal{A})}\mathbf{g})(z')\mathbf{g}^{-1}(z')\partial_z\rangle \\
&\qquad\qquad \left(\frac{\lambda}{\pi}\right)^d \mathrm{e}^{-\lambda\langle z'-z,\mathbf{g}(z')(z'-z)\rangle}\, \mathrm{d}z\, (1 + O(1/\sqrt{\lambda})) \\
= &\frac{\mathrm{i}}{2\lambda}\int \mu(z)\, \mathrm{tr}((\mathbf{D}_{\sigma(\mathcal{A})}\mathbf{g})(z')\mathbf{g}^{-1}(z')) \left(\frac{\lambda}{\pi}\right)^d \mathrm{e}^{-\lambda\langle z'-z,\mathbf{g}(z')(z'-z)\rangle}\, \mathrm{d}z\, (1 + O(1/\sqrt{\lambda})) \\
&+ \frac{\mathrm{i}}{2\lambda}\int \left[\langle z'-z, (\mathbf{D}_{\sigma(\mathcal{A})}\mathbf{g})(z')\mathbf{g}^{-1}\partial_z\rangle \mu(z)\right] \\
&\qquad\qquad \left(\frac{\lambda}{\pi}\right)^d \mathrm{e}^{-\lambda\langle z'-z,\mathbf{g}(z')(z'-z)\rangle}\, \mathrm{d}z\, (1 + O(1/\sqrt{\lambda})) \ .
\end{aligned}$$

Since

$$\operatorname{tr}[X_{A_0}\mathbf{g}]\mathbf{g}^{-1} = [X_{A_0}\operatorname{tr}\ln\mathbf{g}] = [X_{A_0}\ln\det\mathbf{g}] = 0\ ,$$

because $\det\mathbf{g} = 1$, and

$$\operatorname{tr}[A_0''(z)\mathcal{J}_0\mathbf{g}(z)]_+\mathbf{g}^{-1} = \frac{1}{2}[\operatorname{tr}A_0''(z)\mathcal{J}_0 - \operatorname{tr}\mathcal{J}_0A_0''(z)] = 0\ ,$$

we have $\operatorname{tr}(\mathbf{D}_{\sigma(\mathcal{A})}\mathbf{g})(z')\mathbf{g}^{-1}(z') = 0$ and hence

$$h(z') = \frac{\mathrm{i}}{2\lambda}\int\left[\langle z'-z,(\mathbf{D}_{\sigma(\mathcal{A})}\mathbf{g})(z')\mathbf{g}^{-1}(z')\partial_z\rangle\mu(z)\right]\left(\frac{\lambda}{\pi}\right)^d \mathrm{e}^{-\lambda\langle z'-z,\mathbf{g}(z')(z'-z)\rangle}\,\mathrm{d}z \times(1+O(1/\sqrt{\lambda}))\ .$$

Now the result follows from Lemma 4.1.9 and Cotlars Lemma 4.1.3. □

If the measure does not fulfill the requirement (4.15), then the second term, (4.14), in the expression for the commutator will in general not be smaller than first term containing the Poissonbracket. One application we have in mind is the case that $\mathcal{A} = \mathcal{H}$ is an selfadjoint operator, and μ is an invariant measure, i.e. $\{\sigma(\mathcal{H}),\mu)\} = 0$. Then the naive expectation that the commutator of the operators should be semiclassically small, is spoiled by the term (4.14), which measures the change in the metric $\mathbf{g}$ when transported along the flow. But one might hope that one can adapt the metric $\mathbf{g}$ to the Hamiltonian $\sigma(\mathcal{H})$ and the measure μ, such that for this special choice of $\mathbf{g}$ the term (4.14) indeed becomes small. In Section 4.3.1 we will show that this can be done for the case that μ is the characteristic function of an open smooth and invariant domain in phase space. It would be extremely interesting if one could extend these procedures to more general invariant measures.

One can also consider situations where the measure is only almost invariant, i.e. where the Poissonbracket $\{\sigma(\mathcal{H}),\mu\}$ is small in the sense that it is of smaller fractal dimension than μ. A situation we have in mind, where such a behavior could appear, is the case of a domain in phases space which is bounded by a cantorus. A cantorus is a torus in phase space where only a cantorsubset is invariant under the flow, so if we take in this case for μ the measure $\chi_D\mathrm{d}z$ where χ_D is the characteristic function of a domain D which is bounded by the cantorus, then $\{\sigma(\mathcal{H}),\mu\}$ will be a measure which is concentrated on the cantorus, and hence its quantization will decay with a rate governed by the fractal dimension of the cantorus. If one could adapt the metric again to this situation, such that the term (4.14) is smaller than the quantisation of the Poissonbracket, then we could made for instance estimates on the time evolution through such a partial barrier, similar to the estimates in Section 4.4.

4.2 Time evolution and semiclassical limit of Anti-Wick operators

The results on the time evolution of coherent states, Theorem 3.5.7, allow to derive an Egorov type Theorem for Anti-Wick operators.

Theorem 4.2.1. *Let μ be a Radon measure on T^*M and let $\mathcal{U}(t) = \exp(-\mathrm{i}\lambda t\mathcal{H})$ be the time evolution generated by a selfadjoint pseudodifferential operator $\mathcal{H}$ which satisfies the conditions in Theorem 3.5.7. Denote furthermore by Φ^t the Hamiltonian flow generated by the principal symbol of $\mathcal{H}$, and by Φ^t_*L the distribution of complex positive Lagrangian planes whose element at $z \in T^*M$ is given by $\mathcal{S}_z^{-1}(t)L(\Phi^t(z))$ where $\mathcal{S}_z(t) : T_zT^*M \to T_{\Phi^t(z)}T^*M$ denotes the linearized flow. Then*

$$\mathcal{U}^*(t)\,\mathrm{Op}_L^{AW}[\mu]\mathcal{U}(t) = \mathrm{Op}^{AW}_{\Phi^t_*L}[\mu\circ\Phi^t] + \mathcal{R}(t)\ ,$$

and the remainder $\mathcal{R}$ satisfies

$$||\mathcal{R}(t)|| \le C||\,\mathrm{Op}_L^{AW}[\mu]||\lambda^{-1/2}\ .$$

Proof. The result is a consequence of the time evolution of coherent states, Theorem 3.5.9. With

$$\mathrm{Op}_L^{AW}[\mu] = \left(\frac{\lambda}{2\pi}\right)^d \int \mu(z)|u_z^L\rangle\langle u_z^L|\ \mathrm{d}z$$

and

$$\mathcal{U}^*(t)u_z^L(\lambda,x) = \mathcal{P}^{(N)}(-t)\mathcal{U}^{(2)}(-t)u_z^L(\lambda,x) + \mathcal{R}_{N+1}(-t)\mathcal{U}^{(2)}(-t)u_z^L(\lambda,x)\ ,$$

where

$$\mathcal{P}^{(N)}(-t) = 1 + \sum_{n=1}^N \mathcal{P}_j(-t)\ ,$$

see (3.110) for the definition of the $\mathcal{P}_j$, we get

$$\begin{aligned}
\mathcal{U}^*(t)\,\mathrm{Op}_L^{AW}[\mu]\mathcal{U}(t) &= \left(\frac{\lambda}{2\pi}\right)^d \int \mu(z)\mathcal{U}^{(2)}(-t)|u_z^L\rangle\langle u_z^L|\mathcal{U}^{(2)}(t)\ \mathrm{d}z + \mathcal{R}(t)\\
&= \left(\frac{\lambda}{2\pi}\right)^d \int \mu(z)|u^{\mathcal{S}^{-1}L}_{\Phi^{-t}(z)}\rangle\langle u^{\mathcal{S}^{-1}L}_{\Phi^{-t}(z)}|\ \mathrm{d}z + \mathcal{R}(t)\\
&= \left(\frac{\lambda}{2\pi}\right)^d \int \mu(\Phi^t(z))|u_z^{\mathcal{S}^{-1}L}\rangle\langle u_z^{\mathcal{S}^{-1}L}|\ \mathrm{d}z + \mathcal{R}(t)\\
&= \mathrm{Op}^{AW}_{\Phi^t_*L}[\mu\circ\Phi^t] + \mathcal{R}(t)
\end{aligned}$$

with

$$\mathcal{R}(t) = \left(\frac{\lambda}{2\pi}\right)^d \int \mu(z)\Big(\mathcal{U}^{(2)}(-t)|u_z^L\rangle\langle u_z^L|\Big[\sum_{n=1}^N \mathcal{P}_j(t) + \mathcal{R}_{N+1}\Big]\mathcal{U}^{(2)}(t) + \mathrm{c.c.}\Big)\ \mathrm{d}z\ .$$

By Theorem 3.5.9 the term containing $\mathcal{R}_{N+1}$ is of order

$$\lambda^{d-N-1}\ ,$$

so by choosing $N \geq d$ it becomes semiclassically small. The terms containing the operators $\mathcal{P}_j(t)$ can be estimated with Cotlar's Lemma. From the fact that they have a zero of order $3j$ at $z = z(t)$ we can deduce that we can choose

$$h_j(z, z') = \left(\frac{\lambda}{\pi}\right)^d \lambda^j |z - z'|^{3j} \mathrm{e}^{-\lambda\langle z-z', \mathbf{g}(t)(z-z')\rangle} ,$$

and for $j = 1$ this gives with Lemma 4.1.9 the loss of $\lambda^{-1/2}$ in the order of the norm. □

A Szegö limit theorem for Anti-Wick quantizations of measures is as well valid. Let $\mathcal{H} \in \Psi^0(m_{a,b})$ be selfadjoint, and assume that the spectrum is discrete in the interval $[\alpha, \beta]$, $\beta > \alpha$, then we are interested in the asymptotic behavior of

$$\sum_{\alpha \leq E_n \leq \beta} \langle \psi_n, \mathrm{Op}^{AW}[\mu]\psi_n\rangle \tag{4.16}$$

for $\lambda \to \infty$, where E_n and ψ_n denote the eigenvalues and eigenfunctions of $\mathcal{H}$, and μ is a general measure. In case that $\mathrm{Op}^{AW}[\mu]$ is a bounded pseudodifferential operator, the behavior of this sum is well known, see, e.g., [DS99], and we want to extend the known results to the case of an Anti-Wick quantization of a measure.

We will first derive an a priori estimate for a smoothed form of (4.16). Choose $f \in C_0^\infty(\mathbb{R})$, supported in a neighborhood V of $[\alpha, \beta]$, which satisfies $f \equiv 1$ on $[\alpha, \beta]$. Furthermore, assume that $\mathcal{H}$ has discrete spectrum in V. A sufficient condition for this is that $H_0^{-1}(V)$ is compact. Since by the functional calculus, see [DS99], $f(\mathcal{H}) \in \Psi^0(1)$ with principal symbol $f(H_0)$, we obtain

$$\sum_n f(E_n)\langle \psi_n, \mathrm{Op}^{AW}[\mu]\psi_n\rangle = \mathrm{tr}\left(f(\mathcal{H})\,\mathrm{Op}^{AW}[\mu]\right) = \left(\frac{\lambda}{2\pi}\right)^d \int f(H_0)\ \mu\,\mathrm{d}z + O(\lambda^{d-1}) . \tag{4.17}$$

So by multiplication with $f(\mathcal{H})$ we can make traces finite. We follow the usual approach to estimate (4.16), and study a localized Fouriertransformation of the wave trace, $\mathrm{tr}\left(\mathrm{Op}_L^{AW}[a]f(\mathcal{H})U(t)\right)$, where $\mathcal{U}(t) = \mathrm{e}^{-\mathrm{i}\lambda t\mathcal{H}}$ denotes the time evolution operator. Since

$$\begin{aligned}
\mathrm{tr}\left(\mathrm{Op}_L^{AW}[a]f(\mathcal{H})\mathcal{U}(t)\right) &= \left(\frac{\lambda}{2\pi}\right)^d \int \langle u_{z'}^L, \mathrm{Op}_L^{AW}[a]f(\mathcal{H})\mathcal{U}(t)u_{z'}^L\rangle\ \mathrm{d}z' \\
&= \left(\frac{\lambda}{2\pi}\right)^{2d} \iint \langle u_{z'}^L, u_z^L\rangle a(z)\langle u_z^L, f(\mathcal{H})\mathcal{U}(t)u_{z'}^L\rangle\ \mathrm{d}z'\mathrm{d}z \\
&= \left(\frac{\lambda}{2\pi}\right)^d \int a(z)\langle u_z^L, f(\mathcal{H})\mathcal{U}(t)u_z^L\rangle\ \mathrm{d}z ,
\end{aligned}$$

where we have used the completeness relation, we will first study $\left(\frac{\lambda}{2\pi}\right)^d \langle u_z^L, f(\mathcal{H})\mathcal{U}(t)u_z^L\rangle$. This quantity can be expressed in terms of the Husimi functions

$$H_n^L(z) := \left(\frac{\lambda}{2\pi}\right)^d |\langle u_z^L, \psi_n\rangle|^2$$

of the eigenfunctions as

$$\left(\frac{\lambda}{2\pi}\right)^d \langle u_z^L, f(\mathcal{H})\mathcal{U}(t)u_z^L\rangle = \sum_n f(E_n)H_n^L(z)\mathrm{e}^{-\mathrm{i}\lambda t E_n} \ .$$

We will study a smoothed inverse Fouriertransformation of this quantity. Let $\rho \in C_0^\infty(\mathbb{R})$ then

$$\int \rho(t) \left(\frac{\lambda}{2\pi}\right)^d \langle u_z^L, f(\mathcal{H})\mathcal{U}(t)u_z^L\rangle \mathrm{e}^{\mathrm{i}\lambda t E} \, \mathrm{d}t = \sum_n f(E_n)H_n^L(z)\hat{\rho}(\lambda(E_n - E)) \ .$$

Proposition 4.2.2. *Let $\mathcal{H}$ be a selfadjoint pseudodifferential operator in $\Psi^0(m_{a,b})$. Assume that the Hamiltonian vector field X_{H_0} of $H_0 := \sigma(\mathcal{H})$ is nondegenerate at $z \in T^*M$, that $\Phi^t(z) \neq z$ for all $t \neq 0$ in the interval $(-T(z), T(z))$, and that $f \in C_0^\infty(\mathbb{R})$ with $f \equiv 1$ in a neighborhood of E, and $f(H_0)$ has compact support. Then there are smooth function $a_n(z)$ with*

$$\begin{aligned} &\sum_n f(E_n)H_n^L(z)\hat{\rho}(\lambda(E_n - E)) \\ &\qquad = \rho(0)\left(\frac{\lambda}{2\pi}\right)^{d-1} \delta_{H_0,\lambda}(z,E)\left(1 + \sum_{n=1}^{N-1}\lambda^{-n}a_n(z)\right) + O(\lambda^{-N+1/2+d}) \end{aligned} \tag{4.18}$$

for all $\rho \in C_0^\infty((-T(z), T(z)))$, where

$$\delta_{H_0,\lambda}(z,E) := \left(\frac{\lambda}{\pi}\right)^{1/2} \frac{1}{|X_{H_0}|_g(z)} \, \mathrm{e}^{-\lambda \frac{\left(H_0(z)-E\right)^2}{|X_{H_0}|_g^2(z)}}$$

is concentrated on the energy shell Σ_E, and approaches the Liouville density on Σ_E in the limit $\lambda \to \infty$. Moreover,

$$|X_{H_0}|_g(z) := \sqrt{\langle X_{H_0}(z), \mathbf{g}(z)X_{H_0}(z)\rangle}$$

denotes the length of the vector $X_{H_0}(z)$ measured in the metric $\mathbf{g}(z)$.

Proof. For $t \neq 0$ and $t \in (-T(z), T(z))$ we have $\mathrm{FS}(u_z^L) \cap \mathrm{FS}(\mathcal{U}(t)u_z^L) = \emptyset$, and therefore

$$\left(\frac{\lambda}{2\pi}\right)^d \langle u_z^L, \mathcal{U}(t)u_z^L\rangle = O(\lambda^{-\infty}) \ ,$$

so we only have to care about a neighborhood of $t = 0$. Now we get

$$\langle u_z^L, \mathcal{U}(t)u_z^L\rangle = \mathrm{e}^{\mathrm{i}\lambda[\langle p+p(t), q-q(t)\rangle/2 + \int_0^t H_0(z(t')) - \langle p(t), \dot{q}(t)\rangle \, \mathrm{d}t} \mathrm{e}^{-\lambda\langle z-z(t), \mathbf{g}(z)\,(z-z(t))\rangle/4} \ ,$$

and up to order t^2 in the exponent this is

$$\langle u_z^L, \mathcal{U}(t)u_z^L\rangle = \mathrm{e}^{\mathrm{i}\lambda[H_0(z)t + O(t^3)]}\mathrm{e}^{-\lambda[\langle X_{H_0}(z), \mathbf{g}(z)X_{H_0}(z)\rangle t^2/4 + O(t^3)]} \ .$$

Therefore we obtain by the stationary phase theorem, Theorem D.4,

$$\int \rho(t)\langle u_z^L, \mathcal{U}(t)u_z^L\rangle \mathrm{e}^{-\mathrm{i}\lambda tE}\,\mathrm{d}t = \left(\frac{4\pi}{\lambda}\right)^{1/2} \frac{\rho(0)\mathrm{e}^{-\lambda\langle X_{H_0}(z),\mathbf{g}(z)X_{H_0}(z)\rangle^{-1}(H_0(z)-E)^2}}{\sqrt{\langle X_{H_0}(z),\mathbf{g}(z)X_{H_0}(z)\rangle}} \times \left(1+\sum_{n=1}^{N-1}\frac{1}{\lambda^n}a_n(z)\right) + O(\lambda^{-N-1/2})\ .$$

□

By integration of (4.18) we will now get an estimate of the sum (4.16).

Theorem 4.2.3. *Assume $\mathcal{H} \in \Psi^0(m_{a,b})$ satisfies the same conditions as in Proposition 4.2.2, then*

$$\sum_{\alpha\leq E_n(\lambda)\leq\beta} H_n^L(z) = \left(\frac{\lambda}{2\pi}\right)^d \int_\alpha^\beta \delta_{H_0,\lambda}(z,E)\,\mathrm{d}E + O(\lambda^{d-1})\ , \tag{4.19}$$

and if the set of periodic points with period $\neq 0$ has μ-measure 0, then

$$\sum_{\alpha\leq E_n(\lambda)\leq\beta} \langle\psi_n, \mathrm{Op}^{AW}[\mu]\psi_n\rangle = \left(\frac{\lambda}{2\pi}\right)^d \left[\int_\alpha^\beta \mu\big(\delta_{H_0,\lambda}(\cdot,E)\big)\,\mathrm{d}E + \lambda^{-1}\int_\alpha^\beta \mu\big(a_1\delta_{H_0,\lambda}(\cdot,E)\big)\,\mathrm{d}E\right] + o(\lambda^{d-1})\ . \tag{4.20}$$

The proof will be based on the following simple Lemma, whose proof is left to the reader.

Lemma 4.2.4. *Let $\chi_{[\alpha,\beta]}$ be the characteristic function of the interval $[\alpha,\beta]$, and let $\rho \in C_0^\infty((-1,1))$ with $\rho(0)=1$, such that the Fouriertransform satisfies $\hat\rho \geq 0$. We then define $\rho_T(t) := \rho(t/T)$ and note that $\rho_T \in C_0^\infty((-T,T))$ and $\hat\rho_T(E) = T\hat\rho(TE)$. Then there are constants $c, C > 0$ such that*

$$\int_{\alpha-\varepsilon}^{\beta+\varepsilon} \frac{\lambda}{2\pi}\hat\rho_T(\lambda(E'-E))\,\mathrm{d}E + \frac{c}{2}\varepsilon \geq \chi_{[\alpha,\beta]}(E') \geq \int_{\alpha+\varepsilon}^{\beta-\varepsilon} \frac{\lambda}{2\pi}\hat\rho_T(\lambda(E'-E))\,\mathrm{d}E - \frac{c}{2}\varepsilon\ , \tag{4.21}$$

for $\varepsilon > 0$ and all λ with

$$\lambda \geq \frac{C}{T}\frac{1}{\varepsilon}\ . \tag{4.22}$$

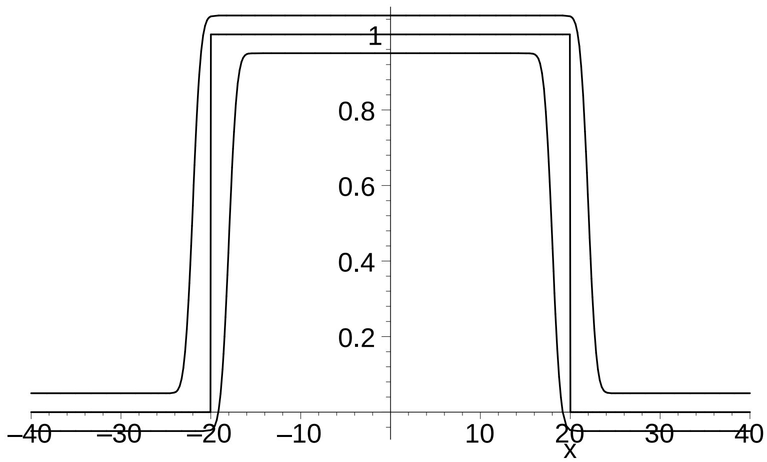

Figure 4.1: Sketch of the three functions in the inequality (4.21)

Proof of Theorem 4.2.3. In Lemma 4.2.4 we choose T smaller or equal to the smallest nonzero period $T(z)$ of z, then we choose in (4.21) $E' = E_n$, multiply (4.21) with $f(E_n)H_n^L(z)$, where f is chosen as in (4.17), and sum over n. This gives that

$$\sum_{\alpha \leq E_n \leq \beta} H_n^L(z)$$

can be estimated from above by

$$\int_{\alpha-\varepsilon}^{\beta+\varepsilon} \sum_n f(E_n) \frac{\lambda}{2\pi} H_n^L(z) \hat{\rho}_T(\lambda(E_n - E)) \, \mathrm{d}E + \frac{c}{2}\varepsilon \sum_n f(E_n) H_n^L(z)$$

and from below by

$$\int_{\alpha+\varepsilon}^{\beta-\varepsilon} \sum_n f(E_n) \frac{\lambda}{2\pi} H_n^L(z) \hat{\rho}_T(\lambda(E_n - E)) \, \mathrm{d}E - \frac{c}{2}\varepsilon \sum_n f(E_n) H_n^L(z) \ .$$

By using (4.17) with $\mu = \delta_z$ we obtain

$$\varepsilon \sum_n f(E_n) H_n^L(z) = \varepsilon O(\lambda^d) \ ,$$

and integrating (4.18) yields

$$\begin{aligned}
&\int_{\alpha\mp\varepsilon}^{\beta\pm\varepsilon} \sum_n f(E_n) \frac{\lambda}{2\pi} H_n^L(z) \hat{\rho}_T(\lambda(E_n - E)) \, \mathrm{d}E \\
&\qquad = \left(\frac{\lambda}{2\pi}\right)^d \int_{\alpha\mp\varepsilon}^{\beta\pm\varepsilon} \delta_{H,\lambda}(z,E)(1 + \lambda^{-1} a_1(z)) \, \mathrm{d}E + O(\lambda^{-2}) \\
&\qquad = \left(\frac{\lambda}{2\pi}\right)^d \int_{\alpha}^{\beta} \delta_{H,\lambda}(z,E)(1 + \lambda^{-1} a_1(z)) \, \mathrm{d}E (1 + O(\varepsilon)) + O(\lambda^{-2})
\end{aligned}$$

So by choosing the smallest possible ε according to (4.22), $\varepsilon = \frac{C}{T}\lambda^{-1}$, we get

$$\limsup_{\lambda\to\infty} \frac{1}{\lambda^{d-1}} \left| \sum_{\alpha \le E_n \le \beta} H_n^L(z) - \left(\frac{\lambda}{2\pi}\right)^d \int_\alpha^\beta \delta_{H,\lambda}(z,E)(1+\lambda^{-1}a_1(z))\, \mathrm{d}E \right| \le C' \frac{1}{T} ,$$

which implies (4.19). Now, if there is no periodic orbit through z we can choose T as large as we wish, and obtain

$$\sum_{\alpha \le E_n \le \beta} H_n^L(z) = \left(\frac{\lambda}{2\pi}\right)^d \int_\alpha^\beta \delta_{H,\lambda}(z,E)(1+\lambda^{-1}a_1(z))\, \mathrm{d}E + o(\lambda^{d-1}) ,$$

which is (4.20) for the case $\mu = \delta_z$. Define now for $\delta > 0$

$$T_\delta^*(z) := \begin{cases} T(z) & \text{if } z \text{ is periodic with minimal period } 0 < T(z) \le \frac{1}{\delta} \\ \frac{1}{\delta} & \text{else} \end{cases} ,$$

then $T_\delta^*(z)$ is lower semicontinuous and we have, since the set of periodic points has μ-measure 0, that

$$\int f(H_0) \frac{1}{T_\delta^*(z)}\, \mu(z)\mathrm{d}z \le C\delta .$$

Therefore, if μ is positive we obtain

$$\limsup_{\lambda\to\infty} \frac{1}{\lambda^{d-1}} \Bigg| \sum_{\alpha \le E_n \le \beta} \langle \psi_n, \mathrm{Op}^{AW}[\mu]\psi_n\rangle - \left(\frac{\lambda}{2\pi}\right)^d \int_\alpha^\beta \mu(\delta_{H,\lambda}(z,E)(1+\lambda^{-1}a_1(z)))\, \mathrm{d}E \Bigg| \le C'\delta ,$$

and since we can choose δ as small as we wish, we obtain (4.20). The general case of non-positive μ is reduced to this one by decomposing it into a difference of positive ones and using that (4.20) is linear. □

By taking $\mu = 1$ we get the standard two-term asymptotics for the counting function of the energy, see [Ivr98, DS99],

$$\begin{aligned} N_{\alpha,\beta}(\lambda) :=& \#\{n\,;\alpha \le E_n \le \beta\} \\ =& \left(\frac{\lambda}{2\pi}\right)^d \left[\int_{\alpha \le H_0(z) \le \beta} \mathrm{d}z + \frac{1}{\lambda} \int_{\alpha \le H_0(z) \le \beta} H_1(z)\, \mathrm{d}z \right] + o(\lambda^{d-1}) \end{aligned}$$

if the set of periodic points with period $\neq 0$ has measure zero. Here we have used the additional fact that $a_1 = H_1$ in Theorem 4.2.3, which we have not proven since we do not need it later on.

Corollary 4.2.5. *Assume that the energy shell $\Sigma_E := \{z\,;\, H(z) = E\}$ is compact, that the Hamiltonian vector field is nondegenerate on Σ_E, and that the set of periodic points on Σ_E with period $\neq 0$ has μ-measure zero, then*

$$\sum_{E-\frac{\alpha}{2\lambda}\leq E_n(\lambda)\leq E+\frac{\alpha}{2\lambda}} \langle \psi_n, \mathrm{Op}^{AW}[\mu]\psi_n\rangle = \left(\frac{\lambda}{2\pi}\right)^{d-1} \frac{\alpha}{2\pi}\mu(\Sigma_E)(1+o(1)) \ ,$$

for all $\alpha > 0$.

The form in which the formula in the corollary is often presented is

$$\lim_{\lambda\to\infty} \frac{1}{N_{E-\frac{\alpha}{2\lambda},E+\frac{\alpha}{2\lambda}}(\lambda)} \sum_{E-\frac{\alpha}{2\lambda}\leq E_n(\lambda)\leq E+\frac{\alpha}{2\lambda}} \langle \psi_n, \mathrm{Op}^{AW}[\mu]\psi_n\rangle = \frac{1}{\mathrm{vol}(\Sigma_E)}\,\mu(\Sigma_E) \ ,$$

where $\mathrm{vol}(\Sigma_E)$ denotes the Liouville measure of Σ_E.

The condition that the set of periodic orbits should have μ measure zero is necessary. For instance, for the case of a two-dimensional isotropic harmonic oscillator and μ the Liouville measure, the result in Corollary 4.2.5 is not true. The same holds true for an arbitrary system, if we choose μ to be a delta function of a periodic orbit, see [PU98a, PU98b].

4.3 Approximate projection operators

In this section we will use the Anti-Wick quantization to construct approximate projection operators associated with subsets in phase space. Similar ideas have been developed by Omnès, see [Omn94, Omn97]. Closer to the applications we have in mind is a construction of approximate projection operators for a perturbed torus by Shnirelman [Shn], but he does not use coherent states.

Let D be a domain in phase space $T^*\mathbb{R}^d$, then we can associate the selfadjoint operator

$$\boldsymbol{\pi}_D^L := \left(\frac{\lambda}{2\pi}\right)^d \int_D |u_z^L\rangle\langle u_z^L| \,\mathrm{d}z$$

with it. This is the Anti-Wick quantization of the characteristic function of D. By the symbol calculus one expects that it behaves like a projection operator onto the set D. In order to make this idea more precise we test this operator on coherent states. Fix a point $z = (p,q) \in \mathbb{R}^d \times \mathbb{R}^d$ and consider the action of $\boldsymbol{\pi}_D^L$ on u_z^L,

$$\boldsymbol{\pi}_D^L u_z^L = \left(\frac{\lambda}{2\pi}\right)^d \int_\Omega \langle u_{z'}^L, u_z^L\rangle\, u_{z'}^L \,\mathrm{d}z' \ .$$

One expects that approximately

$$\boldsymbol{\pi}_D^L u_z^L \approx \chi_D(z) u_z^L \ ,$$

where $\chi_D(z)$ denotes the characteristic function of D. The next proposition says that this is true away from the boundary ∂D.

We will in the following assume for simplicity that $M = \mathbb{R}^d$ and L is constant, so the metric $\mathbf{g}$ defined by L on $T^*\mathbb{R}^d$ is constant. This will facilitate the proofs but it is not necessary, the result in Proposition 4.3.1, Proposition 4.3.2 and Theorem 4.3.3 remain true in the general case. In Section 4.3.1 we will need to introduce non-constant metrizes explicitly.

Proposition 4.3.1. *Let $D \subset T^*\mathbb{R}^d$ be an open domain in phase space and let $\boldsymbol{\pi}_D^L$ be the Anti-Wick quantization of the characteristic function χ_D of D,*

$$\boldsymbol{\pi}_D^L := \left(\frac{\lambda}{2\pi}\right)^d \int_D |u_z^L\rangle\langle u_z^L| \, \mathrm{d}z \ .$$

Then for $z \notin \partial D$ one has

$$||\boldsymbol{\pi}_D^L u_z^L - \chi_D(z) u_z^L|| \leq C \mathrm{e}^{-\lambda[d_{\partial D}^L(z)]^2/4} \ ,$$

where $d_{\partial D}^L(z)$ denotes the distance of z to ∂D measured in the metric $\mathbf{g}$ defined by L, i.e.

$$[d_{\partial D}^L(z)]^2 = \min_{z' \in \partial D} \langle z - z', \mathbf{g}(z - z')\rangle \ . \tag{4.23}$$

Proof. We first treat the case that $z \notin D$, and estimate

$$||\boldsymbol{\pi}_D^L u_z^L||^2 = \left(\frac{\lambda}{2\pi}\right)^{2d} \int_D \int_D \langle u_{z'}^L, u_z^L\rangle \, \langle u_{z''}^L, u_{z'}^L\rangle \, \langle u_z^L, u_{z''}^L\rangle \, \mathrm{d}z' \, \mathrm{d}z'' \ .$$

We have by Lemma 3.3.18

$$\langle u_{z'}^L, u_z^L\rangle = \mathrm{e}^{\mathrm{i}\lambda\langle p+p', q'-q\rangle/2} \mathrm{e}^{-\lambda g_L(p-p', q-q')/4} \ ,$$

hence $|\langle u_{z'}^L, u_z^L\rangle| \leq \mathrm{e}^{-\lambda g_L(z-z')/4}$, so we get

$$\begin{aligned}
||\boldsymbol{\pi}_D^L u_z^L||^2 &\leq \left(\frac{\lambda}{2\pi}\right)^{2d} \int_D \int_D \mathrm{e}^{-\lambda[g_L(z-z')+g_L(z-z'')]/4} \mathrm{e}^{-\lambda g_L(z''-z')/4} \, \mathrm{d}z' \, \mathrm{d}z'' \\
&\leq \mathrm{e}^{-\lambda[d_{\partial D}^L(z)]^2/2} \times \\
&\quad \left(\frac{\lambda}{2\pi}\right)^{2d} \int_D \int_D \mathrm{e}^{-\lambda[g_L(z-z')-[d_{\partial D}^L(z)]^2+g_L(z-z'')-[d_{\partial D}^L(z)]^2]/4} \mathrm{e}^{-\lambda g_L(z''-z')/4} \, \mathrm{d}z' \, \mathrm{d}z'' \ ,
\end{aligned}$$

where $d_{\partial D}^L(z)$ denotes the distance of ∂D to z measured in the metric defined by g, as defined in (4.23).

Since $(\lambda/\pi)^d \mathrm{e}^{-\lambda g_L(z''-z')/4}$ tends to $\delta(z''-z')$ as $\lambda \to \infty$, we get

$$||\boldsymbol{\pi}_D^L u_z^L|| \leq C \mathrm{e}^{-\lambda[d_{\partial D}^L(z)]^2/4}$$

with some constant C depending on D.

The case that $z \in D$ can be reduced to the previous one by using that $\pi_D^L = 1 - \pi_{D'}^L$ with $D' = T^*M \backslash D$,

$$||(\boldsymbol{\pi}_D^L - 1)u_z^L|| = ||\boldsymbol{\pi}_{D'}^L u_z^L|| \leq C' \mathrm{e}^{-\lambda[d_{\partial D}^L(z)]^2/4} .$$

□

What remains to be determined is the behavior of $\boldsymbol{\pi}_D^L u_z^L$ for z in a neighborhood of ∂D.

Proposition 4.3.2. *For z close to ∂D one has*

$$\langle u_z^L, \boldsymbol{\pi}_D^L u_z^L \rangle = \frac{1}{2}\left[1 + \mathrm{erf}\big((\lambda/2)^{1/2}\delta_{\partial D}(z)\big)\right](1 + O(1/\lambda)) ,$$

where $\delta_{\partial D}(z)$ is the signed distance from z to ∂D,

$$\delta_{\partial D}(z) = \begin{cases} d_{\partial D}(z) & \text{for } z \in D \\ -d_{\partial D}(z) & \text{for } z \notin D \end{cases} .$$

Proof. We have

$$\langle u_z^L, \boldsymbol{\pi}_D^L u_z^L \rangle = \left(\frac{\lambda}{2\pi}\right)^d \int_D |\langle z, z' \rangle|^2 \, \mathrm{d}z' = \left(\frac{\lambda}{2\pi}\right)^d \int_D \mathrm{e}^{-\lambda g(z'-z)/2} \, \mathrm{d}z' .$$

Now we introduce a boundary defining function $f(z)$ for ∂D, i. e. ,

$$f(z) = 0 \quad \text{for } z \in \partial D \ , f(z) > 0 \quad \text{for } z \in D \ , \text{and } f(z) < 0 \quad \text{for } z \notin D \ ,$$

and $f'(z) \neq 0$. Then we can write

$$\chi_D(z) = \theta(f(z)) = \int_0^\infty \delta(s - f(z)) \, \mathrm{d}s = \int_0^\infty \frac{\lambda}{2\pi} \int \mathrm{e}^{\mathrm{i}\lambda\eta(s - f(z))} \, \mathrm{d}\eta \, \mathrm{d}s$$

and hence

$$\left(\frac{\lambda}{2\pi}\right)^d \int_D \mathrm{e}^{-\lambda g(z'-z)/2} \, \mathrm{d}z' = \int_0^\infty \left(\frac{\lambda}{2\pi}\right)^{d+1} \iint \mathrm{e}^{\mathrm{i}\lambda[\eta(s - f(z')) + \mathrm{i}g(z'-z)/2]} \, \mathrm{d}\eta \mathrm{d}z' \, \mathrm{d}s .$$

The inner integrals can be evaluated by the method of stationary phase. Since the phase function has positive imaginary part for $z' \neq z$, we will consider only stationary points in a neighborhood of z. The condition for a stationary point then reads

$$\begin{aligned} -\eta(f'(z) + f''(z)(z' - z)) + \mathrm{i}\mathbf{g}(z' - z) + O((z' - z)^2) = 0 \ , \\ s - f(z) - f'(z)(z' - z) + O((z' - z)^2) = 0 \ , \end{aligned}$$

where $\mathbf{g}$ is defined by $g(z) = \langle z, \mathbf{g}z\rangle$. So only for $s = f(z)$ the integral is not exponentially decreasing, and we want to determine the behavior of it in a neighborhood of $s = f(z)$. The stationary points can be computed to be

$$z' - z = \frac{(s - f(z))}{\langle f'(z), \mathbf{g}^{-1} f'(z)\rangle} \mathbf{g}^{-1} f'(z) + O((s - f(z))^2)$$
$$\eta = \mathrm{i}\frac{(s - f(z))}{\langle f'(z), \mathbf{g}^{-1} f'(z)\rangle} + O((s - f(z))^2) \ ,$$

and we then get for the integral

$$\left(\frac{\lambda}{2\pi}\right)^{d+1} \iint \mathrm{e}^{\mathrm{i}\lambda[\eta(s-f(z'))+\mathrm{i}g(z'-z)/2]} \,\mathrm{d}\eta \mathrm{d}z'$$
$$= \left(\frac{\lambda}{2\pi}\right)^{1/2} [\det \Phi(s)/\mathrm{i}]^{-1/2} \mathrm{e}^{-\lambda[\frac{(s-f(z))^2}{\langle f'(z), \mathbf{g}^{-1} f'(z)\rangle}/2 + O((s-f(z))^3)]}(1 + O(\lambda^{-1}))$$

with some nondegenerate matrix $\Phi(s)$. Inserting this in the final integral over s then gives

$$\langle u_z^L, \boldsymbol{\pi}_D^L u_z^L\rangle = \left(\frac{\langle f'(z), \mathbf{g}^{-1} f'(z)\rangle}{\det[\Phi(f(z))/\mathrm{i}]}\right)^{1/2}$$
$$\frac{1}{2}\left[1 + \operatorname{erf}\left(\left(\frac{\lambda}{2}\right)^{1/2} \frac{f(z)}{\langle f'(z), \mathbf{g}^{-1} f'(z)\rangle^{1/2}}\right)\right] (1 + O(\lambda^{-1})) \ .$$

It remains to determine the prefactor and the argument of the error function.

The distance is defined as $[d_{\partial D}(z)]^2 = \min_{z' \in \partial D}\langle z - z', \mathbf{g}(z - z')\rangle$, and in order to find the $z' \in \partial D$ for which the distance is minimal we look for the extremum of

$$\langle z - z', \mathbf{g}(z - z')\rangle + l f(z') \ ,$$

where the Lagrange parameter l is determined by the condition $f(z') = 0$. We find

$$z - z' = -\frac{l}{2}\mathbf{g}^{-1} f'(z') = -\frac{l}{2}\mathbf{g}^{-1} f'(z) + O(\lambda(z - z'))$$

and then the condition $f(z') = 0$ gives

$$-\frac{l}{2} = \frac{f(z)}{\langle f'(z), \mathbf{g}^{-1} f'(z)\rangle} + O(z - z') \ .$$

Putting the pieces together leads to

$$[d_{\partial D}(z)]^2 = \frac{f(z)^2}{\langle f'(z), \mathbf{g}^{-1} f'(z)\rangle} + O((z - z')^2) \ ,$$

which gives the argument of the error function. To determine the prefactor we observe that we have for $z \in D\backslash\partial D$ $\boldsymbol{\pi}_D^L u_z^L = u_z^L + O(\mathrm{e}^{-\lambda[d_{\partial D}(z)]^2/4})$, so in this case by the normalization of u_z^L we have

$$\langle u_z^L, \boldsymbol{\pi}_D^L u_z^L\rangle = 1 + O(\mathrm{e}^{-\lambda[d_{\partial D}(z)]^2/4}) \ ,$$

hence we must have

$$\left(\frac{\langle f'(z), \mathbf{g}^{-1} f'(z)\rangle}{\det[\Phi(f(z))/\mathrm{i}]}\right)^{1/2} = 1 \ .$$

□

We can now determine to what extent $\boldsymbol{\pi}_D^L$ is a projection operator.

Theorem 4.3.3. *Let $\boldsymbol{\pi}_D^L$ be the Anti-Wick quantization of the characteristic function of a smooth open domain $D \subset T^*M$. Then we have for $z \notin \partial D$*

$$||[(\boldsymbol{\pi}_D^L)^2 - \boldsymbol{\pi}_D^L]u_z^L|| \leq C\mathrm{e}^{-\lambda[d^L_{\partial D}(z)]^2/4} \ ,$$

so away from the boundary the error is exponentially small. For compact $\bar{D}$ we have

$$\mathrm{tr}[(\boldsymbol{\pi}_D^L)^2 - \boldsymbol{\pi}_D^L] = \frac{|\partial D|_g}{|D|_g}\,\lambda^{-1/2}\,\mathrm{tr}[\boldsymbol{\pi}_D^L]\left(1 + O(\lambda^{-1})\right) \ .$$

Proof. The first relation follows immediately from Proposition 4.3.1.

To prove the second relation we write

$$\boldsymbol{\pi}_D^2 - \boldsymbol{\pi}_D = (\boldsymbol{\pi}_D - 1)\boldsymbol{\pi}_D = -\boldsymbol{\pi}_{\complement D}\boldsymbol{\pi}_D = -\left(\frac{\lambda}{2\pi}\right)^{2d}\int_{\complement D}\int_D |z\rangle\langle z, z'\rangle\langle z'|\ \mathrm{d}z\mathrm{d}z' \ ,$$

where $\complement D$ denotes the complement of D in T^*M.

Then by the completeness relation the trace of $(\boldsymbol{\pi}_D^L)^2 - \boldsymbol{\pi}_D^L$ is given by

$$\mathrm{tr}[(\boldsymbol{\pi}_D^L)^2 - \boldsymbol{\pi}_D^L] = -\left(\frac{\lambda}{2\pi}\right)^{2d}\int_{\complement D}\int_D |\langle z, z'\rangle|^2\ \mathrm{d}z'\mathrm{d}z \ .$$

Now

$$\left(\frac{\lambda}{2\pi}\right)^{d}\int_D |\langle z, z'\rangle|^2\ \mathrm{d}z'$$

is nothing but $\langle u_z^L, \boldsymbol{\pi}_D^L u_z^L\rangle$, a quantity which we have computed asymptotically in Proposition 4.3.2. Inserting that expression gives

$$\mathrm{tr}[(\boldsymbol{\pi}_D^L)^2 - \boldsymbol{\pi}_D^L] = -\left(\frac{\lambda}{2\pi}\right)^{d}\int_{\complement D}\frac{1}{2}\left[1 + \mathrm{erf}(-\sqrt{\lambda/2}\,d(z))\right]\ \mathrm{d}z(1 + O(1/\lambda)) \ ,$$

where $d(z)$ denotes the distance of ∂D to z. We now introduce new coordinates in a neighborhood of $\partial D = \partial \complement D$, such that

$$\mathrm{d}z = \mathrm{d}\mu_{\partial D}\, \mathrm{d}d \ ,$$

where $\mathrm{d}\mu_{\partial D}$ denotes the volume element on ∂D induced by the metric g. Then finally

$$\begin{aligned} \int_{D'} \frac{1}{2}\left[1+\operatorname{erf}(-\sqrt{\lambda/2}\, d(z))\right] \mathrm{d}z &= \int_{\partial D} \mathrm{d}\mu_{\partial D} \int_0^\infty \frac{1}{2}\left[1+\operatorname{erf}(-\sqrt{\lambda/2}\, d)\right] \mathrm{d}d \\ &= |\partial D|_g (2\pi\lambda)^{-1/2} \ , \end{aligned}$$

and with

$$\operatorname{tr}[\boldsymbol{\pi}_D^L] = \left(\frac{\lambda}{2\pi}\right)^d |D|_g \,(1+O(\lambda^{-1}))$$

the proof is complete. □

4.3.1 Stably invariant approximate projection operators

This section is devoted to the construction of an approximate projection operator associated with an invariant set in phase space, whose commutator with the Hamiltonian vanishes up to arbitrary order in λ. This is not possible for every D and we have to pose some conditions on D, the most important one being the stable invariance which we now define.

Definition 4.3.4. *Let $H \in C^\infty(T^*M, \mathbb{R})$ and let $D \subset T^*M$ be an open subset which is invariant under the Hamiltonian flow generated by H. D will be called **stably invariant** under the flow generated by H, if there exists a neighborhood $\mathcal{F} \subset C^\infty(T^*M,\mathbb{R})$ of H and a smooth family of embeddings*

$$\Phi : \mathcal{F} \times \partial D \to T^*M \ ,$$

such that for every $H' \in \mathcal{F}$, $\Phi(H') : \partial D \to T^*M$ is an embedding, $\Phi(H, \partial D) = \partial D$, and such that the image in T^*M,

$$\Phi(H', \partial D) \subset T^*M \ ,$$

is invariant under the Hamiltonian flow generated by H'.

Here $C^\infty(T^*M, \mathbb{R})$ is assumed to be equipped with the standart Fréchet topology.

So this definition means that we require stability under small perturbations, D should not only be invariant under the flow generated by H, but for small perturbations H' of H there should be a domain D' close to D which is invariant under the Hamiltonian flow generated by H'.

Example 4.3.5. If ∂D is a union of energy shells, then ∂D is stably invariant if the Hamiltonian vectorfield X_H is non-degenerate on ∂D, i.e. if H is a Morse function. This follows from the implicit function theorem.

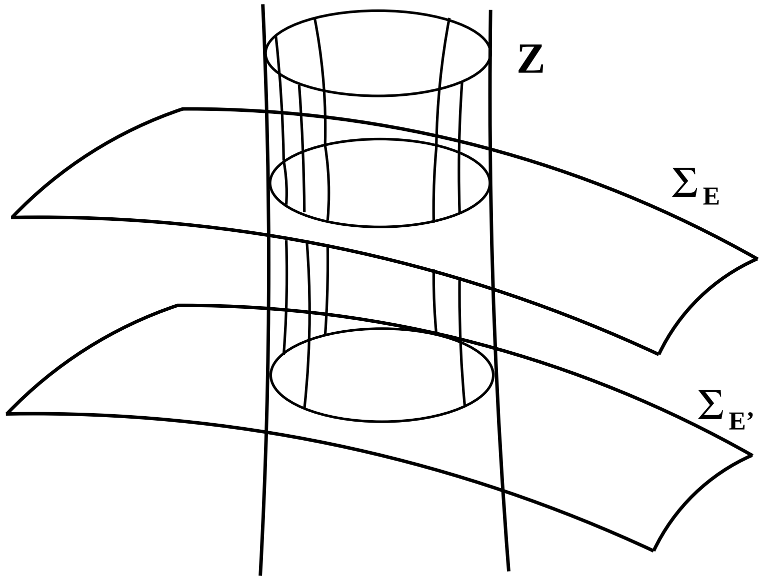

Figure 4.2: Sketch of a possible domain D allowed in Theorem 4.3.7. D is the intersection of the domain D_1 bounded by the two energy shells Σ_E and $\Sigma_{E'}$ with the interior D_2 of the orbit zylinder Z.

Example 4.3.6. If $\dim M = 2$ and ∂D is a union of invariant tori which satisfy a Diophantine condition, see e.g. [AKN97] and the discussion in Section 5.3, then ∂D is stably invariant. This follows from KAM Theory, see e.g. [AKN97].

The notion of stable invariance is further discussed in Section 5.3. The reason why this notion is important for us is that stable invariance guarantees the solvability of certain transport equations. In the construction of the approximate projection operators there will appear equations of the type,

$$\mathcal{L}_{X_H} a = b \tag{4.24}$$

on ∂D, with $b \in C^\infty(\partial D)$, and we need a solution $a \in C^\infty(\partial D)$. It is shown in Section 5.3 that a sufficient condition for the solvability of (4.24) is that the mean of b over ∂D vanishes, and that ∂D is stably invariant.

The domains D we consider can have piecewise smooth boundary, more precisely, we assume that D can be represented as the intersection of a finite number of invariant domains D_j which have smooth boundary in a neighborhood of D. An example is given by a domain D which is bounded by two energy shells and some families of invariant tori, see fig. 4.2.

Theorem 4.3.7. *Let $\mathcal{H}$ be a selfadjoint operator on $L^2(M)$ with Weyl symbol $H \in S^0(m_{a,b})$, and let $D \subset T^*M$ be an open subset of phase space which can be written as an intersection*

$$D = \bigcap_{j=1}^{J} D_j$$

of a finite number J of open subsets $D_j \in T^*M$ which have smooth boundary in a neighborhood of D and are invariant under the Hamiltonian flow generated by the principal symbol H_0 of $\mathcal{H}$. Assume furthermore that $\overline{D}$ is compact. Then there exists an approximate projection operator $\boldsymbol{\pi}_D^{(0)}$ associated with D such that

$$||[\mathcal{H}, \boldsymbol{\pi}_D^{(0)}]|| \leq C\lambda^{-3/2} .$$

If the D_j and hence D are furthermore stably invariant under the Hamiltonian flow generated by H_0, then there is for every $N \in \mathbb{N}$ an approximate projection operator $\boldsymbol{\pi}_D^{(N)}$ associated with D such that

$$||[\mathcal{H}, \boldsymbol{\pi}_D^{(N)}]|| \leq C_N\lambda^{-3/2-N} .$$

We recall that an approximate projection operator associated with D is an operator $\boldsymbol{\pi}_D$ which is microlocally 1 in D, and 0 in the interior of the complement of D.

The compactness assumption on $\overline{D}$ is not really necessary, but it facilitates the proof, since we don't need to prove any boundendess of solutions of transport equations at ∞.

The proof of this theorem will be rather long, and we will split it in several steps. We start by introducing suitable local coordinates.

Lemma 4.3.8. *Let X be a symplectic manifold and $S \subset X$ a submanifold of codimension 1 which is invariant under the Hamiltonian flow generated by $H \in C^\infty(X)$, and assume that the Hamiltonian vectorfield X_H is nondegenerate on S.*

We have to distinguish two cases.

(i) If H is constant on S then there exist local symplectic coordinates $z = (\xi, x) \in \mathbb{R}^d \times \mathbb{R}^d$ around $z_0 \in S$ on X, such that

$$H(z) - H(z_0) = x_1 ,$$

and S is determined by the condition $x_1 = 0$, $S = \{z \in \mathbb{R}^{2d} \, ; x_1 = 0\}$. This is the only case which can occur for $d = 1$.

(ii) If H is not constant on S, then there exist local symplectic coordinates $z = (\xi, x) \in \mathbb{R}^d \times \mathbb{R}^d$ on X around $z_0 \in S$, such that

$$H(z) - H(z_0) = x_2$$

and S is again given by $S = \{z \in \mathbb{R}^{2d} \, ; x_1 = 0\}$.

Proof. The first case is a standard result in symplectic geometry. By the nondegeneracy of X_H we can take $x_1 = H - H(z_0)$ as a new coordinate, which can according to [Hör85a, Theorem 21.1.6] be completed to a set of symplectic coordinates of X.

For the second case we start as in the first one by choosing symplectic coordinates in which

$$H(z) - H(z_0) = x_2 .$$

Now choose locally a boundary defining function f for S, i.e. a function which is zero on S and with $f' \neq 0$ in a neighborhood of S. Since $X_H = \partial_{\xi_2}$, and S is invariant under the flow generated by X_H, we can choose f to be independent of ξ_2, which means

$$\{H, f\} = 0 \ .$$

With [Hör85a, Theorem 21.1.6] we can extend the set of functions $x_1 = f$ and $x_2 = H$ therefore to a set of symplectic coordinates near z_0 in which S is given by $x_1 = 0$. □

We will apply this Lemma to the case that S is given by ∂D, where D and hence ∂D is invariant under the flow of the principal symbol H_0 of the given Hamiltonian $\mathcal{H}$. Notice that here we assume ∂D to be smooth. We will first compute the Weyl symbol of the approximate projection operator $\boldsymbol{\pi}_D$ in the coordinates close to z_0 introduced in Lemma 4.3.8.

Lemma 4.3.9. *In local symplectic coordinates $z = (\xi, x)$ such that D is given by $x_1 > 0$ the Weyl symbol of $\boldsymbol{\pi}_D$ is of the form*

$$w(\lambda, z) = \left(\frac{\lambda}{2\pi}\right)^{1/2} \sqrt{\alpha(z)} \int_0^\infty a(\lambda, z, x_1 - s) \mathrm{e}^{-\lambda\alpha(z)(x_1-s)^2} \, \mathrm{d}s \ , \tag{4.25}$$

where $a(\lambda, z, s) \sim \sum_{n\geq 0} \lambda^{-n} a_n(z, s)$, and

$$\sqrt{\alpha(z)} = \frac{1}{\sqrt{\det \mathbf{g}_{\partial D}}} > 0 \ ,$$

where $\mathbf{g}_{\partial D}$ denotes the Riemannian metric on ∂D induced by the metric $\mathbf{g}$ on T^*M. The amplitude $a(\lambda, z, s)$ furthermore satisfies the relations

$$a_0(z, 0) = 1$$

and

$$\sum_{k=0}^{m} \frac{1}{k!(2\alpha(z))^k} \, \partial_s^{2k} a_{m-k}(z, s)|_{s=0} = 0 \ , \quad m = 1, 2, \dots \ .$$

Proof. The Wigner function of the coherent state centered at $z' = (\xi', x')$ is of the form

$$W_{z'}(z) = \left(\frac{\lambda}{\pi}\right)^d b(\lambda, z'; z) \mathrm{e}^{-\lambda\varphi(z';z)}$$

with

$$\varphi(z'; z) = \langle z - z', \mathbf{g}(z')(z - z')\rangle + \tilde{r}(z'; z)$$

with $\tilde{r}(z';z) = O((z-z')^3)$, where $\mathbf{g}(z')$ is a nondegenerate positive symplectic matrix, and $b \in S(1)$ with

$$b(\lambda, z; z) = 1 + O(\lambda^{-1}) ,$$

see Proposition 3.3.16. The Weyl symbol of $\boldsymbol{\pi}_D$ is given by

$$\begin{aligned} w(\lambda, z) &= \int_0^\infty \int_{\mathbb{R}^{2d-1}} W_{z'}(z) \, \mathrm{d}\tilde{z}'\mathrm{d}x_1' \\ &= \left(\frac{\lambda}{\pi}\right)^d \int_0^\infty \int_{\mathbb{R}^{2d-1}} b(\lambda, z'; z)\mathrm{e}^{-\lambda\varphi(z';z)} \, \mathrm{d}\tilde{z}'\mathrm{d}x_1' \ , \end{aligned}$$

where $\tilde{z} = (\hat{z}, \xi_1)$ with $\hat{z} = (\xi_2, \cdots \xi_d, x_2 \cdots x_d)$ and D is locally defined by $x_1 \geq 0$. We will determine the inner integral by the method of stationary phase; notice that since $\mathbf{g}(z') = \mathbf{g}(z) + O(z-z')$ we have

$$\begin{aligned} \varphi(z';z) &= \langle z - z', \mathbf{g}(z)(z-z')\rangle + r(z';z) \\ &= \langle \tilde{z} - \tilde{z}', \tilde{\mathbf{g}}(z)(\tilde{z} - \tilde{z}')\rangle + 2\langle h(z), \tilde{z} - \tilde{z}'\rangle(x_1 - x_1') + g_0(z)(x_1 - x_1')^2 + r(z';z) \end{aligned}$$

with $r(z';z) = \tilde{r}(z';z) + O((z-z')^3) = O((z-z')^3)$, and where we have split $\mathbf{g}(z)$,

$$\mathbf{g}(z) = \begin{pmatrix} \tilde{\mathbf{g}}(z) & h(z) \\ h(z)^\dagger & g_0(z) \end{pmatrix}$$

according to the splitting of the coordinates $z = (\tilde{z}, x_1)$. The stationary point of the phase function as a function of $\tilde{z}'$ can now simply be determined to be

$$\tilde{z}_0' = \tilde{z} + \tilde{\mathbf{g}}(z)^{-1}h(z)(x_1 - x_1') ,$$

and the substitution $\tilde{z}' \mapsto \tilde{z}' + \tilde{z}_0'$ yields a phase function

$$\varphi(\tilde{z}', x_1'; z) = \langle \tilde{z}', \tilde{\mathbf{g}}(z)\tilde{z}'\rangle\rangle + [g_0(z) - \langle h(z), \tilde{\mathbf{g}}(z)^{-1}h(z)\rangle](x_1 - x_1')^2 + r(z' + z_0'; z)$$

with $z_0' = (\tilde{z}_0', 0)$. So we obtain for the inner integral

$$\begin{aligned} &\int b(\lambda, z'; z) \, \mathrm{e}^{-\lambda\varphi(z';z)} \, \mathrm{d}\tilde{z}' \\ &\qquad = \left(\frac{\pi}{\lambda}\right)^{d-1/2} \frac{1}{\sqrt{\det \tilde{\mathbf{g}}(z)}} \, a(\lambda, z, x_1' - x_1)\mathrm{e}^{-\lambda[g_0(z) - \langle h(z), \tilde{\mathbf{g}}(z)^{-1}h(z)\rangle](x_1 - x_1')^2} \end{aligned}$$

with

$$a(\lambda, z, x_1' - x_1) = \mathrm{e}^{\frac{1}{4\lambda}\langle \partial_{\tilde{z}'}, \tilde{\mathbf{g}}(z)^{-1}\partial_{\tilde{z}'}\rangle}\mathrm{e}^{-\lambda r'(z' + z_0'; z)}a(\lambda, z' + z_0'; z)|_{\tilde{z}'=0} \ ,$$

and so $a \in S(1)$ by the discussion following Theorem B.2.

Now we want to relate the two factors $\det \tilde{\mathbf{g}}(z)$ and $[g_0(z) - \langle h(z), \tilde{\mathbf{g}}(z)^{-1} h(z)\rangle]$ with each other. To this end we first note that

$$\mathbf{g} = \begin{pmatrix} \tilde{\mathbf{g}} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} I & \tilde{\mathbf{g}}^{-1} h \\ h^\dagger & g_0 \end{pmatrix}$$

and since for $\beta, \gamma \in \mathbb{R}^n$ and $\delta \in \mathbb{R}$ one has

$$\det \begin{pmatrix} I & \beta \\ \gamma^\dagger & \delta \end{pmatrix} = \delta - \langle \beta, \gamma \rangle \ ,$$

as one can show easily by induction, we obtain

$$1 = \det \mathbf{g} = \det \begin{pmatrix} \tilde{\mathbf{g}} & 0 \\ 0 & 1 \end{pmatrix} \det \begin{pmatrix} I & \tilde{\mathbf{g}}^{-1} h \\ h^\dagger & g_0 \end{pmatrix} = \det \tilde{\mathbf{g}} \ [g_0 - \langle h, \tilde{\mathbf{g}}^{-1} h \rangle] \ .$$

If we therefore define

$$\alpha(z) := \frac{1}{\det \tilde{\mathbf{g}}(z)} \ ,$$

we get $\alpha(z) > 0$ and

$$\alpha(z) = [g_0(z) - \langle h(z), \tilde{\mathbf{g}}(z)^{-1} h(z) \rangle] \ ,$$

and so the representation (4.25) is proven.

In order to obtain information on the amplitude a, we use the completeness relation for coherent states. For any $\varepsilon > 0$ we have for $x \geq \varepsilon$

$$\begin{aligned} w(\lambda, z) &= \left(\frac{\lambda}{2\pi}\right)^{1/2} \sqrt{\alpha(z)} \int_0^\infty a(\lambda, z, x_1 - s) \mathrm{e}^{-\lambda \alpha(z)(x_1 - s)^2/2} \ \mathrm{d}s \\ &= \left(\frac{\lambda}{\pi}\right)^d \int_{\mathbb{R}^{2d}} W_{z'}(z) \ \mathrm{d}z' + O(\lambda^{-\infty}) \\ &= 1 + O(\lambda^{-\infty}) \ . \end{aligned}$$

On the other hand, we get for $x \geq \varepsilon$ that

$$\left(\frac{\lambda}{2\pi}\right)^{1/2} \sqrt{\alpha(z)} \int_0^\infty a(\lambda, z, x_1 - s) \mathrm{e}^{-\lambda \alpha(z)(x_1 - s)^2/2} \ \mathrm{d}s = \mathrm{e}^{\frac{1}{2\lambda\alpha(z)} \partial_s^2} a(\lambda, z, s)|_{s=0} + O(\lambda^{-\infty}) \ ,$$

and comparing the two expressions we obtain

$$a_0(\lambda, z, 0) = 1$$

and

$$\sum_{k=0}^m \frac{1}{k!(2\alpha(z))^k} \partial_s^{2k} a_{m-k}(z, s)|_{s=0} = 0 \ .$$

□

We now have to study the asymptotic behavior of a function of the form (4.25). The factor $\alpha(z)$ can be thought of as a local rescaling of the semiclassical parameter λ. We will in the following study the case $\alpha = 1$, the general case then follows by the substitution $\lambda \to \alpha(z)\lambda$.

Lemma 4.3.10. *Let $b \in C^\infty(\mathbb{R})$ with $|b^{(k)}(s)| \leq C_k(1+s^2)^{m/2}$ for some fixed $m \in \mathbb{R}$ and all $k \in \mathbb{Z}_+$ and define*

$$F_k(\lambda, s) := \left(\frac{\lambda}{2\pi}\right)^{1/2} \int_0^\infty (s-s')^k \mathrm{e}^{-\lambda(s-s')^2/2}\, \mathrm{d}s' \ , \tag{4.26}$$

then we have for any $K \in \mathbb{N}$

$$\left(\frac{\lambda}{2\pi}\right)^{1/2} \int_0^\infty b(s-s')\mathrm{e}^{-\lambda(s-s')^2/2}\, \mathrm{d}s' = \sum_{k=0}^{K-1} \frac{b^{(k)}(0)}{k!} F_k(\lambda, s) + O(\lambda^{-K/2}) \ ,$$

where $b^{(k)}(0)$ denotes the k'th derivative of b at $s=0$.

Proof. The expansion is a simple consequence of the Taylor expansion of $b(s)$,

$$b(s-s') = \sum_{k=0}^{K-1} \frac{b^{(k)}(0)}{k!}(s-s')^k + (s-s')^K f_K(s,s')$$

where $f_K(s,s')$ is smooth and polynomially bounded by the conditions on b. Inserting this expansion into the integral and using

$$\begin{aligned}
&\left(\frac{\lambda}{2\pi}\right)^{1/2} \int_0^\infty (s-s')^K f_K(s,s')\mathrm{e}^{-\lambda(s-s')^2/2}\, \mathrm{d}s' \\
&\qquad = \lambda^{-K/2}\frac{1}{(2\pi)^{1/2}} \int_0^\infty (\sqrt{\lambda}s - s')^K f_K(s, s'/\sqrt{\lambda})\mathrm{e}^{-(\sqrt{\lambda}s-s')^2/2}\, \mathrm{d}s' \\
&\qquad = \lambda^{-K/2}\frac{1}{(2\pi)^{1/2}} \int_{-\sqrt{\lambda}s}^\infty (-s')^K f_K(s, s'/\sqrt{\lambda}+s)\mathrm{e}^{-s'^2/2}\, \mathrm{d}s'
\end{aligned}$$

gives the desired result, since

$$\begin{aligned}
\left|\int_{-\sqrt{\lambda}s}^\infty (-s')^K f_K(s, s'/\sqrt{\lambda}+s)\mathrm{e}^{-s'^2/2}\, \mathrm{d}s'\right| &\leq \int_{-\infty}^\infty |s'|^K |f_K(s, s'/\sqrt{\lambda}+s)| \mathrm{e}^{-s'^2/2}\, \mathrm{d}s' \\
&\leq C_K \ .
\end{aligned}$$

□

The functions $F_k(\lambda, s)$ provide a tool to express uniform asymptotic expansions close to the boundary ∂D. In the next lemma we collect some properties of these functions.

Lemma 4.3.11. *Let* $F_k(\lambda, s)$ *be defined by* (4.26), *then*

$$|F_k(\lambda, s)| \leq C\lambda^{-k/2} \ .$$

For $s < 0$ *we have*

$$F_k(\lambda, s) = O(\mathrm{e}^{-\lambda s^2/2})$$

and for $s > 0$

$$F_k(\lambda, s) = \begin{cases} O(\mathrm{e}^{-\lambda s^2/2}) & \text{for } k \text{ odd} \\ \frac{1\cdot 3\cdots(k-1)}{\lambda^{k/2}} + O(\mathrm{e}^{-\lambda s^2/2}) & \text{for } k \text{ even} \end{cases} .$$

Furthermore, one has

$$|s^m F_{2k+1}(\lambda, s)| \leq C\, \lambda^{-(k+1/2+m/2)} \ . \tag{4.27}$$

Explicit expressions can be obtained from

$$F_0(\lambda, s) = \frac{1}{2}[1 - \mathrm{erf}(\sqrt{\lambda/2}\, s)] \ , \quad F_1(\lambda, s) = \frac{1}{(\lambda 2\pi)^{1/2}}\, \mathrm{e}^{-\lambda s^2/2} \ ,$$

and

$$F_{k+1}(\lambda, s) - \frac{k}{\lambda}\, F_{k-1}(\lambda, s) = s^k F_1(\lambda, s) \ . \tag{4.28}$$

For odd $k = 2k' + 1$ *one has*

$$F_{2k'+1}(\lambda, s) = \sum_{l=0}^{k'} \frac{\alpha_l^{(k')}}{\lambda^{k'-l}}\, s^{2l}\, F_1(\lambda, s) \tag{4.29}$$

with $\alpha_l^{(k')} = \frac{2^{k'}k'!}{2^l l!}$, *and for even* $k = 2k'$

$$F_{2k'}(\lambda, s) = \frac{\beta_0^{(k')}}{\lambda^{k'}}\, F_0(\lambda, s) + \sum_{l=1}^{k'} \frac{\beta_l^{(k')}}{\lambda^{k'-l}}\, s^{2l-1}\, F_1(\lambda, s) \ ,$$

with $\beta_l^{(k')} = \frac{2^l l!(2k')!}{2^{k'}k'!(2l)!}$.

Proof. The asymptotic behavior for $s < 0$ is obvious. For the case $s > 0$ we use

$$\left(\frac{\lambda}{2\pi}\right)^{1/2} \int_0^\infty (s - s')^k \mathrm{e}^{-\lambda(s-s')^2/2}\, \mathrm{d}s' = \left(\frac{\lambda}{2\pi}\right)^{1/2} \int_{-\infty}^\infty (s - s')^k \mathrm{e}^{-\lambda(s-s')^2/2}\, \mathrm{d}s' - \left(\frac{\lambda}{2\pi}\right)^{1/2} \int_{-\infty}^0 (s - s')^k \mathrm{e}^{-\lambda(s-s')^2/2}\, \mathrm{d}s' \ .$$

The first integral can be computed explicitly, and the second can be estimated as in the case $s < 0$. The explicit expressions for $F_0(\lambda, s)$ and $F_1(\lambda, s)$ follow by direct computations.

A substitution $s' \mapsto s' + s$ yields

$$F_k(\lambda, s) = \left(\frac{\lambda}{2\pi}\right)^{1/2} \int_{-s}^{\infty} (-s')^k \mathrm{e}^{-\lambda s'^2/2} \, \mathrm{d}s'$$

and hence

$$\frac{\mathrm{d}F_k(\lambda, s)}{\mathrm{d}s} = -\left(\frac{\lambda}{2\pi}\right)^{1/2} s^k \mathrm{e}^{-\lambda s^2/2} = -\lambda \, s^k F_1(\lambda, s) \ .$$

On the other hand one has

$$\begin{aligned} \frac{\mathrm{d}F_k(\lambda, s)}{\mathrm{d}s} = \left(\frac{\lambda}{2\pi}\right)^{1/2} & \int_0^{\infty} k(s - s')^{k-1} \mathrm{e}^{-\lambda(s-s')^2/2} \, \mathrm{d}s' \\ & - \lambda \left(\frac{\lambda}{2\pi}\right)^{1/2} \int_0^{\infty} (s - s')^{k+1} \mathrm{e}^{-\lambda(s-s')^2/2} \, \mathrm{d}s' \\ = k F_{k-1}(\lambda, s) - \lambda F_{k+1}(\lambda, s) \ , & \end{aligned}$$

and comparing the two equations gives the recursion formula (4.28). The explicit expressions for $F_k(\lambda, s)$ for $k > 1$ can be checked by inserting them into the recursion formula. □

The recursion formula (4.28) can also be interpreted as providing an expansion of $s^k F_1(\lambda, s)$ into the set of functions $F_k(\lambda, s)$. By using Taylor expansion this can be used to expand the function $g(s)F_1(\lambda, s)$ for smooth $g(s)$ into a series $\sum_k a_k F_k(\lambda, s)$. We will state the result for arbitrary k in the next lemma.

Lemma 4.3.12. *Let $g \in C^\infty(\mathbb{R})$ with $|g^{(k)}(s)| \le C_k(1 + s^2)^{m/2}$ for some fixed $m \in \mathbb{R}$ and all $k \in \mathbb{Z}_+$, then*

$$g(s)F_1(\lambda, s) = \sum_{n=0}^{N-1} \frac{g^{(n)}(0)}{n!} \left[F_{n+1}(\lambda, s) - \frac{n}{\lambda} F_{n-1}(\lambda, s)\right] + O(\lambda^{-(N+1)/2}) \ .$$

More generally,

$$\begin{aligned} g(s)F_{2k+1}(\lambda, s) = & \sum_{n=0}^{N-1} \frac{g^{(n)}(0)}{n!} \sum_{l=0}^{k} \frac{\alpha_l^{(k)}}{\lambda^{k-l}} \left[F_{2l+n+1}(\lambda, s) - \frac{2l+n}{\lambda} F_{2l+n-1}(\lambda, s)\right] \\ & + O(\lambda^{-(N+1)/2}) \ , \end{aligned}$$

and

$$\begin{aligned} g(s)F_{2k}(\lambda, s) = & g(s) \frac{\beta_0^{(k)}}{\lambda^k} F_0(\lambda, s) \\ & + \sum_{n=0}^{N-1} \frac{g^{(n)}(0)}{n!} \sum_{l=1}^{k} \frac{\beta_l^{(k)}}{\lambda^{k-l}} \left[F_{2l+n+2}(\lambda, s) - \frac{2l+n+1}{\lambda} F_{2l+n}(\lambda, s)\right] \\ & + O(\lambda^{-(N+1)/2}) \ . \end{aligned}$$

Proof. We will show the case for odd k, the case of even k works similar. We write

$$\begin{aligned} g(s)F_{2k+1}(\lambda,s) &= \sum_{n=0}^{N-1} \frac{g^{(n)}(0)}{n!} s^n F_{2k+1}(\lambda,s) + r_N(s)F_{2k+1}(\lambda,s) \\ &= \sum_{n=0}^{N-1} \frac{g^{(n)}(0)}{n!} s^n F_{2k+1}(\lambda,s) + O(\lambda^{-(N+1)/2}) \end{aligned}$$

since $r_N(s) = O(s^N)$ and $s^N F_{2k+1}(\lambda,s) = O(\lambda^{-(N+1)/2})$. Now

$$\begin{aligned} s^n F_{2k+1}(\lambda,s) &= \sum_{l=0}^{k} \frac{\alpha_l^{(k)}}{\lambda^{k-l}}\, s^{2l+n}\, F_1(\lambda,s) \\ &= \sum_{l=0}^{k} \frac{\alpha_l^{(k)}}{\lambda^{k-l}} \left[F_{2l+n+1}(\lambda,s) - \frac{2l+n}{\lambda}\, F_{2l+n-1}(\lambda,s) \right] , \end{aligned}$$

and putting the equations together yields the result. □

Combining Lemmata 4.3.9 and 4.3.10, we get an asymptotic expansion of the symbol $w(\lambda,z)$

$$\begin{aligned} w(\lambda,z) &\sim \sum_n \frac{1}{\lambda^n} \left(\frac{\lambda}{2\pi}\right)^{1/2} \sqrt{\alpha(z)} \int_0^\infty a_n(z, x_1 - s) \mathrm{e}^{-\lambda\alpha(z)(x_1-s)^2/2}\, \mathrm{d}s \\ &\sim \sum_{n,k} \frac{1}{\lambda^n} \frac{1}{k!}\, a_n^{(k)}(z,0) F_k(\alpha(z)\lambda, x_1) \\ &= \sum_{n,k} \frac{1}{\lambda^n} \frac{1}{(2k)!}\, a_n^{(2k)}(z,0) F_{2k}(\alpha(z)\lambda, x_1) \\ &\qquad + \sum_{n,k} \frac{1}{\lambda^n} \frac{1}{(2k+1)!}\, a_n^{(2k+1)}(z,0) F_{2k+1}(\alpha(z)\lambda, x_1) \\ &= F_0(\alpha(z)\lambda, x_1) + \sum_{n,k} \frac{1}{\lambda^n} \frac{1}{(2k+1)!}\, a_n^{(2k+1)}(z,0) F_{2k+1}(\alpha(z)\lambda, x_1) \ . \end{aligned}$$

The functions $F_k(\alpha(z)\lambda, x_1)$ provide one way of studying uniform asymptotic expansions across a boundary. Since in the higher order terms of the asymptotic expansion only $F_k(\alpha(z)\lambda, x_1)$ with odd index occur, they are all concentrated in the vicinity of the boundary ∂D. It will be convenient to rewrite the expansion as

$$w(\lambda,z) = F_0(\alpha(z)\lambda, x_1) + \sum_{k=0}^{N-1} w_k(\lambda, z') x_1^k F_1(\alpha(z)\lambda, x_1) + R_K(z) F_1(\alpha(z)\lambda, x_1) \ ,$$

where $|R_K(z)| \leq C_K x_1^K$ and hence by Lemma 4.3.11

$$|R_K(z) F_1(\alpha(z)\lambda, x_1)| \leq C_K \lambda^{-(K+1)/2} \ ;$$

of course this is valid for every $K \in \mathbb{N}$. The functions $w_k(\lambda, z')$ then have an asymptotic expansion in powers of $1/\lambda$; for every $N \in \mathbb{N}$

$$w_k(\lambda, z') = \sum_{n=0}^{N-1} w_{k,n}(z')\lambda^{-k} + O(\lambda^{-N}) \ .$$

Our aim in the following now is to determine the functions $w_{k,n}(z')$ on ∂D such that the symbol of the commutator of $\mathcal{H}$ and $\boldsymbol{\pi}_D$ becomes as small in λ as one wishes.

Therefore, we first have to determine the symbol of the commutator of $\mathcal{H}$ with the Weyl quantization of a symbol of the form

$$\pi_{k+1}(z) := w_k(\lambda, z')x_1^k F_1(\alpha(z)\lambda, x_1)$$

for $k \in \mathbb{N}$, and with

$$\pi_0(z) = F_0(\alpha(z)\lambda, x_1) \ .$$

Since we have chosen our coordinates such that the principal symbol is linear, we first treat the case of a linear symbol.

Proposition 4.3.13. *Let $H_0(z) = \langle X_0, \mathcal{J}_0 z\rangle$ be given with X_0 constant, and assume that $H_0(z)$ does not depend on ξ_1. Then we have for $\pi_0(z) = F_0(\alpha(z)\lambda, x_1)$*

$$H_0\#\pi_0(z) - \pi_0\#H_0(z) = -\mathrm{i}x_1\left[\mathcal{L}_{X_0}\alpha(z)\right]F_1(\alpha(z)\lambda, x_1) \ ,$$

and for $\pi_{k+1}(z) = b_k(z')x_1^k F_1(\alpha(z)\lambda, x_1)$, with $b_k(z')$ smooth and with compact support,

$$\begin{aligned}[H_0\#\pi_{k+1} - \pi_{k+1}\#H_0](z) =& \frac{\mathrm{i}}{\lambda}\left[\mathcal{L}_{X_0}b_k(z')\right] x_1^k F_1(\alpha(z)\lambda, x_1) \\ & - \frac{\mathrm{i}}{\lambda}\left[\frac{1}{2}\frac{\left[\mathcal{L}_{X_0}\alpha(z)\right]}{\alpha(z)} + \lambda\left[\mathcal{L}_{X_0}\alpha(z)\right] x_1^2\right] b_k(z')x_1^k F_1(\alpha(z)\lambda, x_1) \ .\end{aligned}$$

Here the Lie-derivative $\mathcal{L}_{X_0}\alpha$ enters through the relation $\mathcal{L}_{X_0}\alpha = \{H_0, \alpha\}$.

Proof. By the linearity of $H_0(z)$ the product formula gives for any smooth function $a(z)$

$$H_0\#a - a\#H_0 = \frac{\mathrm{i}}{\lambda}\{H_0, a\} \ ,$$

and then the result follows by direct computation. The condition that $H_0(z)$ does not depend on ξ_1 implies that no derivative of a with respect to x_1 occurs. □

The leading part in λ of the symbol $[\mathcal{H}, \boldsymbol{\pi}_D]$ is therefore given by

$$-\mathrm{i}x_1\mathcal{L}_{X_0}\alpha(z)\left[1 + x_1\sum_{k=0}^{N} b_k(z')x_1^k + O(x_1^{N+2})\right]F_1(\alpha(z)\lambda, x_1) \ ,$$

for all $N \in \mathbb{N}$. If we expand $\alpha(z)$ in a Taylor series in x_1 around $x_1 = 0$,

$$\alpha(z) = \sum_n \frac{1}{n!}\alpha_n(z')x_1^n$$

with $\alpha_n(z') = \partial_{x_1}^n \alpha|_{x_1=0}$, then we see that in order that the leading term in λ of the commutator vanishes up to all orders in x_1, all the coefficients of the Taylor series of α have to satisfy the transport equation

$$\mathcal{L}_{X_0}\alpha_n = 0 \ .$$

This equation is always solved by a constant multiple of the canonical invariant Liouville density on ∂D, which in our local coordinates is just constant.

So we conclude that α has to be a function of x alone. In the case that the Hamiltonian is not constant on ∂D we can therefore choose $x\sqrt{\alpha(x)}$ as a new variable without changing any of the other assumptions. On the other hand , if the principal symbol is constant on ∂D we again choose $x\sqrt{\alpha(x)}$ as a new variable, but then we have to allow the Hamiltonian to be nonlinear, so we assume $H_0(z) = H_0(x)$.

Since we assume in Theorem 4.3.7 that $\overline{D}$ is compact, we can restrict ourselves to the case that $\mathcal{H}$ has a symbol H in $S(1)$. Because $\mathcal{H}\boldsymbol{\pi}_D$ is exponentially small in λ in the complement of $\overline{D}$ for every approximate projection operator $\boldsymbol{\pi}_D$ associated with D, the behavior of H outside D is not important for us.

Proposition 4.3.14. *For $H \in S(1)$ and for $\pi_0(z) = F_0(\lambda, x)$ we have*

$$H\#\pi_0(z) - \pi_0\#H(z) = \mathrm{i}\sum_{l=0}^{[L/2]-1}\frac{(-1)^l}{4^l(2l+1)!}\partial_\xi^{2l+1}\tilde{H}(\lambda, z, \xi, x)F_{2l+1}(\lambda, x) + r_L(\lambda, z)$$

for every $L \in \mathbb{N}$, where the remainder satisfies

$$|\partial_z^\alpha r_L(\lambda, z)| \leq C_{L,\alpha}\lambda^{-L/2+|\alpha|}$$

for any $\alpha \in \mathbb{Z}^{2d}$ and $\tilde{H}(\lambda, z, \xi, x) = \mathrm{e}^{\frac{1}{8\lambda}\partial_\xi^2}H(z', \xi, x)$.

Proof. We first treat the case $d = 1$ since it contains already the main difficulties; the general case will then be a simple consequence. We start with the first term. Let $z = (\xi, x)$, then it is given by $\pi_0(z) = F_0(\lambda, x)$, and we have to determine $H\#\pi_0(z)$. The integral form of the product formula for Weyl symbols then gives

$$\begin{aligned} H\#\pi_0(z) &= \left(\frac{\lambda}{\pi}\right)^2 \iint H(z + z')\pi_0(z + z'')\mathrm{e}^{2\mathrm{i}\lambda\langle z'', \mathcal{J}_0 z'\rangle}\,\mathrm{d}z'\mathrm{d}z'' \\ &= \left(\frac{\lambda}{2\pi}\right)^{1/2}\int_0^\infty \left(\frac{\lambda}{\pi}\right)^2 \iint H(z + z')\mathrm{e}^{-\lambda(x+x''-s)^2/2}\mathrm{e}^{2\mathrm{i}\lambda(\xi''x' - x''\xi')}\,\mathrm{d}z'\mathrm{d}z''\,\mathrm{d}s \ . \end{aligned}$$

Now the substitution $z' \mapsto z' + z_0^+$ with $z_0^+ = \frac{\mathrm{i}}{2}((x-s),0)$ leads to

$$H\#\pi_0(z) = \left(\frac{\lambda}{2\pi}\right)^{1/2} \int_0^\infty \left(\frac{\lambda}{\pi}\right)^2 \iint H(z+z'+z_0^+) \mathrm{e}^{-\lambda(s-x)^2/2} \mathrm{e}^{\mathrm{i}\lambda[2(\xi''x'-x''\xi')+\mathrm{i}x''^2/2]}\, \mathrm{d}z'\mathrm{d}z''\,\mathrm{d}s$$
$$= \left(\frac{\lambda}{2\pi}\right)^{1/2} \int_0^\infty \mathrm{e}^{-\lambda(s-x)^2/2} \left(\frac{\lambda}{\pi}\right)^2 \iint H(z+z'+z_0^+) \mathrm{e}^{\mathrm{i}\lambda\langle\hat{z},\mathbf{B}\hat{z}\rangle}\, \mathrm{d}z'\mathrm{d}z''\,\mathrm{d}s\ ,$$

with $\hat{z} = (z', z'')$ and

$$\mathbf{B} = \begin{pmatrix} 0 & \mathcal{J}_0 \\ -\mathcal{J}_0 & \frac{\mathrm{i}}{2}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \end{pmatrix} . \tag{4.30}$$

So by Lemma B.1 we get with

$$\det \mathbf{B} = 1\ , \qquad \mathbf{B}^{-1} = \begin{pmatrix} -\frac{\mathrm{i}}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} & -\mathcal{J}_0 \\ \mathcal{J}_0 & 0 \end{pmatrix}\ ,$$

that

$$H\#\pi_0(z) = \left(\frac{\lambda}{2\pi}\right)^{1/2} \int_0^\infty \mathrm{e}^{-\lambda(s-x)^2/2} \mathrm{e}^{\frac{\mathrm{i}}{4\lambda}[2\langle\partial_{z''},\mathcal{J}_0\partial_{z'}\rangle - \frac{\mathrm{i}}{2}\partial_{\xi'}^2]} H(z+z'+z_0^+)\big|_{z'=z''=0}\, \mathrm{d}s\ . \tag{4.31}$$

Since there is no z''-dependence we can determine the integrand very simply

$$\mathrm{e}^{\frac{\mathrm{i}}{4\lambda}[2\langle\partial_{z''},\mathcal{J}_0\partial_{z'}\rangle - \frac{\mathrm{i}}{2}\partial_{\xi'}^2]} H(z+z'+z_0^+)\big|_{z'=z''=0} = \mathrm{e}^{\frac{1}{8\lambda}\partial_\xi^2} H(z+z_0^+) = \tilde{H}(z+z_0^+)\ ,$$

where we have defined

$$\tilde{H}(z) := \mathrm{e}^{\frac{1}{8\lambda}\partial_\xi^2} H(z)\ .$$

A Taylor expansion of $\tilde{H}(z+z_0^+)$ around z_0^+ yields

$$\tilde{H}(z+z_0^+) = \sum_{l=0}^{L-1} \frac{1}{l!}\partial_\xi^l \tilde{H}(\xi,x) \left(\frac{\mathrm{i}}{2}\right)^l (x-s)^l + O((x-s)^L)\ ,$$

and inserting this into the integral then gives

$$H\#\pi_0(z) = \sum_{l=0}^{L-1} \frac{1}{l!}\partial_\xi^l \tilde{H}(\xi,x) \left(\frac{\mathrm{i}}{2}\right)^l F_l(\lambda,x) + O(\lambda^{-L/2})$$

for every $L \in \mathbb{N}$. In the same way we can determine $\pi_0 \# H(z)$ which yields

$$\pi_0 \# H(z) = \sum_{l=0}^{L-1} \frac{1}{l!} \partial_\xi^l \tilde{H}(\xi, x) \left(\frac{-\mathrm{i}}{2}\right)^l F_l(\lambda, x) + O(\lambda^{-L/2})$$

for every $L \in \mathbb{N}$. So putting both formulas together then gives for the symbol of the commutator

$$\begin{aligned} H \# \pi_0(z) - \pi_0 \# H(z) &= \sum_{l=0}^{L-1} \frac{1}{l!} \partial_\xi^l \tilde{H}(\xi, x) \left[\left(\frac{\mathrm{i}}{2}\right)^l - \left(\frac{-\mathrm{i}}{2}\right)^l\right] F_l(\lambda, x) + O(\lambda^{-L/2}) \\ &= \mathrm{i} \sum_{l=0}^{[L/2]-1} \frac{(-1)^l}{4^l (2l+1)!} \partial_\xi^{2l+1} \tilde{H}(\xi, x) F_{2l+1}(\lambda, x) + O(\lambda^{-L/2}) \end{aligned}$$

for every $L \in \mathbb{N}$. This completes the discussion for the case that $d = 1$. The general case $d \geq 1$ follows immediately by noticing that the product formula factorizes, hence all formulas remain the same, just with $H(\xi, x)$ now replaced by $H(z'; \xi, x)$.

□

Now we will study the commutator of $\mathcal{H}$ with the Weyl quantization of

$$\pi_{k+1}(z) = b_k(z) F_1(\lambda, x) \ .$$

Proposition 4.3.15. *Let $\mathcal{H}$ be a pseudodifferential operator in $\Psi^0(1)$ and*

$$\pi_{k+1}(z) = b_k(z) F_1(\lambda, x) \ ,$$

with $b_k \in S^0(1)$. Then the Weyl symbol of the product of $\mathcal{H}$ with the Weyl quantization of π_{k+1} is given by

$$H \# \pi_{k+1}(z) = \mathrm{e}^{\frac{\mathrm{i}}{2\lambda}\langle \partial_{z''}, \mathcal{J}_0 \partial_{z'} \rangle} \tilde{H}(z + z' + z_0^+) b(z + z'')|_{z'=z''=0} \, F_1(\lambda, x) \ ,$$

where $z_0^+ = \frac{\mathrm{i}}{2}(0; x, 0)$ and $\tilde{H}(z)$ denotes an almost analytic continuation of $\mathrm{e}^{\frac{1}{8\lambda}\partial_\xi^2} H(z)$. Similarly one has

$$\pi_{k+1} \# H(z) = \mathrm{e}^{-\frac{\mathrm{i}}{2\lambda}\langle \partial_{z''}, \mathcal{J}_0 \partial_{z'} \rangle} \tilde{H}(z + z' - z_0^+) b(z + z'')|_{z'=z''=0} \, F_1(\lambda, x) \ ,$$

and for the commutator one gets

$$\begin{aligned} & H \# \pi_{k+1}(z) - \pi_{k+1} \# H(z) \\ & \quad = 2\mathrm{i} \cos\left(\frac{1}{\lambda}\langle \partial_{z''}, \mathcal{J}_0 \partial_{z'} \rangle\right) \sin(x_1 \partial_{\xi_1'}) \tilde{H}(\lambda, z + z') b_k(z + z'')|_{z'=z''=0} \, F_1(\lambda, x) \\ & \qquad + 2\mathrm{i} \sin\left(\frac{1}{\lambda}\langle \partial_{z''}, \mathcal{J}_0 \partial_{z'} \rangle\right) \cos(x_1 \partial_{\xi_1'}) \tilde{H}(\lambda, z + z') b_k(z + z'')|_{z'=z''=0} \, F_1(\lambda, x) \ . \end{aligned}$$

Proof. The proof follows the same pattern as the proof of Proposition 4.3.14. The integral formula for the product gives

$$H\#\pi_{k+1}(z) = \left(\frac{\lambda}{\pi}\right)^d \iint H(z+z')b(z+z'')\,\frac{1}{(2\pi\lambda)^{1/2}}\,\mathrm{e}^{-\lambda(x+x'')^2/2}\mathrm{e}^{2\mathrm{i}\lambda\langle z'',J_0 z'\rangle}\,\mathrm{d}z'\mathrm{d}z''$$

and if make again a substitution $z' \mapsto z' + z_0^+$, now with $z_0^+ = \frac{\mathrm{i}}{2}(0; x_1, 0)$, we obtain

$$\begin{aligned}
H\#\pi_{k+1}(z) &= \left(\frac{\lambda}{\pi}\right)^d \iint H(z+z'+z_0^+)b(z+z'') \\
&\qquad\qquad \frac{1}{(2\pi\lambda)^{1/2}}\,\mathrm{e}^{-\lambda x^2/2}\mathrm{e}^{\mathrm{i}\lambda[2\langle z'',J_0 z'\rangle+\mathrm{i}x''^2/2]}\,\mathrm{d}z'\mathrm{d}z'' \\
&= \left(\frac{\lambda}{\pi}\right)^d \iint H(z+z'+z_0^+)b(z+z'')\mathrm{e}^{\mathrm{i}\lambda\langle\hat{z},\mathbf{B}\hat{z}\rangle}\,\mathrm{d}z'\mathrm{d}z''\,F_1(\lambda,x)\ ,
\end{aligned}$$

with $\hat{z} = (z', z'')$, and $\mathbf{B}$ the matrix (4.30). Therefore, we obtain in complete analogy with the previous case (4.31) that

$$\begin{aligned}
H\#\pi_{k+1}(z) &= \mathrm{e}^{\frac{\mathrm{i}}{4\lambda}[2\langle\partial_{z''},\mathcal{J}_0\partial_{z'}\rangle-\frac{\mathrm{i}}{2}\partial_{\xi'}^2]}H(z+z'+z_0^+)b(z+z'')|_{z'=z''=0}\,F_1(\lambda,x) \\
&= \mathrm{e}^{\frac{\mathrm{i}}{2\lambda}\langle\partial_{z''},\mathcal{J}_0\partial_{z'}\rangle}\tilde{H}(z+z'+z_0^+)b(z+z'')|_{z'=z''=0}\,F_1(\lambda,x)\ .
\end{aligned}$$

By a standard argument, scetched after Theorem B.2, it follows that the prefactor

$$a^{(+)}(\lambda,z) := \mathrm{e}^{\frac{\mathrm{i}}{2\lambda}\langle\partial_{z''},\mathcal{J}_0\partial_{z'}\rangle}\tilde{H}(z+z'+z_0^+)b(z+z'')|_{z'=z''=0}$$

is a symbol.

In the same way as for the first case, we get for the second product

$$\pi_{k+1}\#H(z) = a^{(-)}(\lambda,z)F_1(\lambda,x)\ ,$$

with

$$a^{(-)}(\lambda,z) = \mathrm{e}^{\frac{-\mathrm{i}}{2\lambda}\langle\partial_{z''},\mathcal{J}_0\partial_{z'}\rangle}\tilde{H}(z+z'-z_0^+)b(z+z'')|_{z'=z''=0}\ .$$

If we rewrite

$$\tilde{H}(z+z'\pm z_0^+) = \mathrm{e}^{\pm\mathrm{i}x_1\partial_{x_1'}}\tilde{H}(z+z')$$

we can write the commutator as

$$H\#\pi_{k+1} - \pi_{k+1}\#H = 2\mathrm{i}\sin\left(\frac{1}{\lambda}\langle\partial_{z''},\mathcal{J}_0\partial_{z'}\rangle + x_1\partial_{\xi_1'}\right)\tilde{H}(z+z')b(z+z'')|_{z'=z''=0}\,F_1(\lambda,x_1)\ ,$$

and expanding the sine gives the final result. □

In the course of the proof of our theorem we will have to solve a set of transport equations. Their solvability will then be assured by the following lemma. The solvability of general transport equations is discussed in detail in Section 5.3. There are two conditions which ensure the existence of a solution, the first one is the stability of ∂D under small perturbations of the Hamiltonian, and the second one is the vanishing of the integral of the inhomogeneity over ∂D. The first condition is assumed in the conditions of the theorem we set out to prove. The second one follows from the fact that the trace of a commutator vanishes, as the following lemma shows.

Lemma 4.3.16. *Assume that the symbol of $\mathcal{H}$ has compact support, and consider $\pi_0 := F_0(\lambda, x_1)$ and $\pi_1 := b(z)F_1(\lambda, x_1)$. Then all terms in the asymptotic series for $\lambda \to \infty$ and $x_1 \to 0$ of the symbol of the commutator*

$$H\#\pi_i - \pi_i\#H \sim \sum_{n,k} w_{n,k}(z')\frac{1}{\lambda^n}\, x_1^k\; F_1(\lambda, x)$$

satisfy

$$\int_{\partial D} w_{n,k}\; \mathrm{d}\mu_{\partial D} = 0\ .$$

Proof. Since the symbol of $\mathcal{H}$ has compact support, $\mathcal{H}$ is of trace class and we get on the one hand that

$$\mathrm{tr}[\mathcal{H}, \boldsymbol{\pi}_i] = 0\ ,$$

where $\boldsymbol{\pi}_i$ denotes the Weyl quantization of π_i. On the other hand the trace is given by the integral of the symbol of the commutator over phase space. With

$$\int x^k F_1(\lambda, x)\; \mathrm{d}x = C_k \lambda^{-1-k/2}$$

we therefore get

$$0 = \mathrm{tr}[\mathcal{H}, \boldsymbol{\pi}_i] \sim \sum_{n,k} C_k \int_{\partial D} w_{n,k}\; \mathrm{d}\mu\, \frac{1}{\lambda^{n+1+k/2}}\ .$$

In the case $i = 0$ we have $w_{0,0} = \partial_\xi H$ and $w_{n,k} = \partial_\xi H_{n,k}$, where $H_{n,k}$ consists of derivatives of H, so the leading term in λ gives

$$\int_{\partial D} \partial_\xi H\; \mathrm{d}\mu = 0\ ,$$

and since H is arbitrary, we can especially replace H by $H_{n,k}$ to obtain

$$\int_{\partial D} w_{n,k}\; \mathrm{d}\mu = \int_{\partial D} \partial_\xi H_{n,k}\; \mathrm{d}\mu = 0\ .$$

This can also be understood more geometrically, since ∂_ξ is the Hamiltonian vectorfield of the boundary-defining function, which is of course tangential to ∂D.

In the second case $i = 1$ we use the fact that b is arbitrary, so we consider the Taylor series of b around $x_1 = 0$ and by varying all coefficients independently, we obtain the result. □

We now need only one more ingredient for the proof of Theorem 4.3.7. The following lemma allows to estimate the remainder terms in our construction.

Lemma 4.3.17. *Let $a \in S^m(1)$ and denote by $\mathcal{A}_k$ the operator with Weyl symbol*

$$a_k(\lambda, z) = a(\lambda, z) x_1^k F_1(\lambda, x_1) .$$

Then the L^2-norm of $\mathcal{A}_k$ satisfies the estimate

$$||\mathcal{A}_k|| \leq C \lambda^{m - \frac{k+1}{2}} .$$

Proof. By the Calderon-Vaillancourt Theorem the norm of an operator $\mathcal{B}$ with Weyl symbol $b(\lambda, z)$ can be estimated by the first $2d + 1$ derivatives of the symbol,

$$||\mathcal{B}|| \leq C \sum_{|\alpha| \leq 2d+1} \sup_z |\partial_z^\alpha b(\lambda, z)| ,$$

see, e.g., [Fol89, Rob87]. If we make a Taylor expansion of $a(\lambda, z)$ around $x_1 = 0$, we get

$$a_k(\lambda, z) x_1^k F_1(\lambda, x_1) = \sum_{n=0}^{N-1} \frac{1}{n!} \partial_{x_1}^n a(\lambda, z', 0) x_1^{k+n} F_1(\lambda, x_1) + R_N(\lambda, z) F_1(\lambda, z)$$

with $R_N(\lambda, z) \in S^m(1)$ and $R(\lambda, z) = O(x_1^{k+N})$. Therefore we obtain with (4.27) from Lemma 4.3.11 and the Calderon-Vaillancourt Theorem that the Weyl quantization of the remainder term $R_N(\lambda, z) F_1(\lambda, z)$ can be estimated by

$$C \lambda^{2d+1+m-\frac{k+N+1}{2}} .$$

The terms in the Taylor series can be represented as Weyl symbols of the Anti-Wick quantization of a surface density on ∂D, and hence our general estimate on the norm of Anti-Wick operators can be applied, which yields an upper bound by

$$C \lambda^{m - \frac{k+n+1}{2}}$$

for the n'th term in the Taylor expansion. By choosing $N \geq 2(2d + 1)$ we are therefore done. □

We can now collect all the pieces together, to give a proof of Theorem 4.3.7

Proof of Theorem 4.3.7. We assume that the local coordinates have been chosen according to Lemma 4.3.8. Then we make an ansatz for the Weyl symbol of the approximate projection operator as

$$\pi^{(N)}(\lambda, z) = \pi_0(\lambda, z) + \sum_{n=0}^{N-1} \lambda^{-n}\pi_{n+1}(\lambda, z)$$

with

$$\pi_0(\lambda, z) = F_0(\lambda, x_1) \ , \quad \pi_{n+1}(\lambda, z) = b_n(z)F_1(\lambda, x_1)$$

where $b_n(z) \in S^0(1)$, and determine its commutator with $\mathcal{H}$. H has an asymptotic expansion

$$H(\lambda, z) \sim \sum_l \lambda^{-l} H_l(z) \ ,$$

and in our local coordinates $H_0(z)$ is linear and independent of ξ. Then we have

$$H_0\#\pi_0 - \pi_0\#H_0 = 0 \ ,$$

and so the leading contribution to the commutator with π_0 comes from the H_1 term, which is by Proposition 4.3.14 and with (4.29)

$$\frac{1}{\lambda}[H_1\#\pi_0 - \pi_0\#H_1] = \frac{\mathrm{i}}{\lambda}\sum_l \frac{(-1)^l}{4^l(2l+1)!}\,\partial_\xi^{2l+1} H_1 x_1^{2l}\, F_1(\lambda, x_1) + O(\lambda^{-2}) \ .$$

Lemma 4.3.17 therefore implies that

$$||[\mathcal{H}, \pi^{(0)}]|| \leq C\lambda^{-3/2} \ ,$$

and the first part of the theorem is proven for domains with smooth boundary.

The commutator of $\pi_1(z) = b_1(z)F_1(\lambda, x_1)$ with H_0 is

$$H_0\#\pi_1 - \pi_1\#H_0 = \frac{\mathrm{i}}{\lambda}\left[\mathcal{L}_{X_{H_0}} b_1(z)\right] F_1(\lambda, x_1) \ ,$$

and the leading part of the commutator of H_1 with π_1 is of the same order in λ, see Proposition 4.3.15,

$$\begin{aligned} H_1\#\pi_1 - \pi_1\#H_1 &= 2\mathrm{i}b_1(z)\sin(x_1\partial_{\xi_1})H_1(z)F_1(\lambda, x_1) + O(\lambda^{-1}) \\ &= \mathrm{i}\sum_l \frac{(-1)^l}{4^l(2l+1)!}(\partial_{\xi_1}^{2l+1} H_1)(z)b_1(z)x_1^{2l+1}F_1(\lambda, x_1) + O(\lambda^{-1}) \ . \end{aligned}$$

So the term of order $1/\lambda$ in the symbol of the commutator $[\mathcal{H}, \boldsymbol{\pi}^{(N)}]$ is given by

$$\left[\mathcal{L}_{X_0} b_1 + \sum_l \frac{(-1)^l}{4^l(2l+1)!}\partial_{\xi_1}^{2l+1} H_1 x_1^{2l+1} b_1 + \sum_l \frac{(-1)^l}{4^l(2l+1)!}\,\partial_\xi^{2l+1} H_1 x_1^{2l}\right] F_1(\lambda, x_1) \ , \quad (4.32)$$

and the conditions that it vanishes can be translated into a set of transport equations for b_1. To this end we expand $b_1(z)$ in a Taylor series in x_1 around $x_1 = 0$,

$$b_1(z) = \sum_k \frac{1}{k!} b_1^{(k)}(z') x_1^k$$

with $b_1^{(k)}(z') = \partial_{x_1}^k b_1(z', 0)$, and insert it into (4.32). Then the condition that (4.32) has to vanish in every power of x_1 gives a set of transport equations,

$$\begin{aligned} \mathcal{L}_{X_0} b_1^{(0)} + \partial_\xi H_1 &= 0 \\ \mathcal{L}_{X_0} b_1^{(1)} + \partial_\xi H_1 \, b_1^{(0)} &= 0 \\ \mathcal{L}_{X_0} b_1^{(2)} + \partial_\xi H_1 \, b_1^{(1)} - \frac{1}{4!} \partial_\xi^3 H_1 &= 0 \\ &\vdots \, . \end{aligned}$$

By Lemma 4.3.16 all these equations satisfy the quantization condition in Theorem 5.3.7, and hence all of them can be solved to give the Taylor series of b_1 around $x_1 = 0$. So by choosing $b_1 = b_{1,K_1}$ with

$$b_{1,K_1} = \sum_{k=0}^{K_1 - 1} \frac{1}{k!} b_1^{(k)}(z') x_1^k \, ,$$

we have obtained

$$H \# \pi^{(1)} - \pi^{(1)} \# H = \frac{\mathrm{i}}{\lambda} r_{K_1}(z) F_1(\lambda, x_1) + O(1/\lambda^2)$$

with

$$r_{K_1}(z) = O(x_1^{K_1}) \, .$$

Now we can add a further term $\pi_2 = \frac{1}{\lambda} b_2(z) F_1(\lambda, x_1)$ and choose $b_2(z)$ in the same way, such that the term in the commutator of order $1/\lambda^2$ vanishes up to order $x_1^{K_2}$. By repeating this procedure, after a finite number of steps we arrive at a function $\pi^{(N')}$ with

$$H \# \pi^{(N')} - \pi^{(N')} \# H = \mathrm{i} \sum_{k=1}^{N'} \frac{1}{\lambda^k} r_{K_k}(z) F_1(\lambda, x_1) + R_{N'}(\lambda, z)$$

where

$$r_{K_k}(z) = O(x_1^{K_k}) \, ,$$

and the overall remainder $R_{N'}(\lambda, z)$ satisfies

$$\partial_z^\alpha R_{N'}(\lambda, z) = O(\lambda^{-N'-1+|\alpha|})$$

for all $\alpha \in \mathbb{N}^{2d}$. By the theorem of Calderon-Vaillancourt the quantization of the remainder has therefore a norm which can be bounded by

$$C\lambda^{-N'+2d} ,$$

and the quantization of the terms $r_{K_k}(z)F_1(\lambda, x_1)$ have by Lemma 4.3.17 a norm which can be estimated by

$$C\lambda^{-K_k/2-1} .$$

Therefore, by choosing N' and the K_k large enough, we can make the commutator $[\mathcal{H}, \boldsymbol{\pi}^{(N')}]$ as small in λ as we wish. This completes the proof for the case that ∂D is smooth.

If D can be represented as an intersection of J, J finite, invariant domains D_j with smooth boundary,

$$D = \bigcap_{j\in J} D_j ,$$

then we take

$$\boldsymbol{\pi}_D^{(N)} := \prod_{j\in J} \boldsymbol{\pi}_{D_j}^{(N)} .$$

So with $||\boldsymbol{\pi}_{D_j}^{(N)}|| \leq C$ we obtain

$$||[\mathcal{H}, \boldsymbol{\pi}_D^{(N)}]|| \leq C^{J-1} \sum_{j\in J} ||[\mathcal{H}, \boldsymbol{\pi}_{D_j}^{(N)}]|| \leq C'\lambda^{-N} ,$$

and this proves the theorem for piecewise smooth boundary. □

Remark: Strictly speaking, we presented only the local part of the proof of Theorem 4.3.7, because we have been working in one fixed system of local coordinates. But the passage to a global proof follows from standart techniques by patching together different local solutions, using Fourier integral operators as quantizations of the symplectic coordinate transformations, see e.g. [Hör85b, Rob87, DS99].

4.4 Applications: Invariance and local quantum ergodicity

In this section we want to discuss two applications of the approximate projection operators that we have constructed.

In the first subsection we want to exploit the idea that a splitting of the classical phase space in several invariant subspaces of positive measure induces a corresponding asymptotic splitting of the quantum mechanical Hilbert space into approximately invariant subspaces. Of course these subspaces are determined by the approximate projection operators associated with the classical invariant domains.

In the second subsection we then derive a local quantum ergodicity theorem, which states that if the classical motion is ergodic on some invariant subset of phase space with positive measure, then almost all quantum mechanical eigenfunctions become equidistributed on that domain. The general question, wether these eigenfunctions are concentrated in that domain or its complement, will be discussed in Chapter 5. This is an open question. What we can show here is that the part of a wavefunction which is microlocally concentrated on an ergodic component becomes for almost all eigenfunctions locally constant on that part of phase space.

4.4.1 Almost invariant subspaces of the Hilbert space

Let $\mathcal{H}$ be a selfadjoint pseudodifferential operator on $L^2(M)$, with principal symbol H_0, which determines an Hamiltonian flow Φ^t on T^*M. In the theory of dynamical systems one often decomposes a system into its ergodic components, which form the elementary building blocks of the system. Since these different components do not interact with each other, one can determine the properties of the full system from the properties of its ergodic components. From the correspondence principle it seems natural to try a similar decomposition of the quantum mechanical Hilbert space into invariant subspaces, at least in the semiclassical limit. One of the first formulations of this idea on the level of eigenfunctions was given by Percival [Per73]. An extensive study and review of the properties of a quantum mechanical system with corresponding classical system of mixed type, i.e. with many invariant sets, has been undertaken in [BTU93].

A weak form of this decomposition can be achieved with the frequency set. Recall the definition of the space $H^0_\lambda(M)$, see Definition 3.4.10, which consists of all maps $\mathbb{R}^+ \to L^2(M)$, $\lambda \mapsto \psi(\lambda)$, which are uniformly bounded in λ. Of course we can identify $L^2(M)$ with the subspace of $H^0_\lambda(M)$ consisting of the λ-independent elements. To any subset $D \subset T^*M$ we can associate the subspace of $H^0_\lambda(M)$ consisting of those functions whose frequency set is contained in D,

$$H^0_{\lambda,D}(M) := \{\psi(\lambda) \in H^0_\lambda(M) \; ; \mathrm{FS}(\psi) \subset D\} \; .$$

It is clear that $H^0_{\lambda,D}(M)$ is a linear space and one easily sees that

$$\overline{H^0_{\lambda,D}(M)} = H^0_{\lambda,\overline{D}}(M) \; ,$$

where the bar denotes the closure. Hence, if D is closed, then $H^0_{\lambda,D}(M)$ is also closed. By the properties of the frequency set we furthermore know that

$$\langle \psi_1, \psi_2 \rangle = O(\lambda^{-\infty})$$

if $\psi_1 \in H^0_{\lambda,D_1}(M)$, $\psi_2 \in H^0_{\lambda,D_2}(M)$, and

$$D_1 \cap D_2 = \emptyset \; .$$

So the subspaces corresponding to disjoint sets in phase space are semiclassically orthogonal. By the general behavior of the frequency set under application by Fourier integral operators, we have for the time evolution operator $\mathcal{U}(t)$ that $\mathcal{U}(t)H^0_{\lambda,D}(M)\subset H^0_{\lambda,\Phi^t D}(M)$, and by multiplication with $\mathcal{U}(-t)$ we get the other inclusion, hence

$$\mathcal{U}(t)H^0_{\lambda,D}(M)=H^0_{\lambda,\Phi^t D}(M)$$

for finite times. Therefore, if D is invariant under the classical flow, the corresponding space $H^0_{\lambda,D}(M)$ is invariant under the quantum mechanical time evolution.

Next we want to estimate how large the space $H^0_{\lambda,D}(M)$ is. Of course its dimension will be ∞, but we can estimate the relative fraction of states up to a certain frequency, which live in that space. More precisely, let ρ_D be a smooth function, which is 1 on D and has support in a neighborhood of D. Let $\mathcal{H}$ be any selfadjoint pseudodifferential operator, such that D is contained in a compact union of energy shells of $\sigma(\mathcal{H})$, and denote by ψ_n and E_n the eigenfunctions and eigenenergies of $\mathcal{H}$. Then the number of eigenfunctions living semiclassically on D can be estimated by

$$\sum_n f(E_n)\langle\psi_n,\mathrm{Op}^{AW}[\rho_D]\psi_n\rangle$$

where $f\in C_0^\infty(\mathbb{R})$ satisfies $f(\sigma(\mathcal{H}))|_D\equiv 1$. By using the Szegö limit theorem, Theorem 4.2.3, we obtain that the relative number of states in $H^0_{\lambda,D}(M)$ is proportional to the volume of D.

A more explicit way of splitting the quantum mechanical Hilbert space into subspaces corresponding to classically invariant domains can be obtained by using the approximate projection operators constructed in Section 4.3.1. First we will study their time evolution. Since the domain D is invariant, we expect that the corresponding approximate projection operators are approximately invariant under time evolution.

Theorem 4.4.1. *Let D be an open subset of T^*M which is invariant under the time evolution generated by the principal symbol of $\mathcal{H}$. Assume furthermore that D satisfies the assumptions of Theorem 4.3.7 and let $\boldsymbol{\pi}_D^{(N)}$ be the operators constructed in that theorem. Then we have*

$$||\mathcal{U}^*(t)\boldsymbol{\pi}_D^{(0)}\mathcal{U}(t)-\boldsymbol{\pi}_D^{(0)}||\leq Ct\lambda^{-1/2}\ ,$$

and if D is stably invariant the stronger estimate

$$||\mathcal{U}^*(t)\boldsymbol{\pi}_D^{(N)}\mathcal{U}(t)-\boldsymbol{\pi}_D^{(N)}||\leq C_N t\lambda^{-1/2-N}\ ,$$

for any $N\in\mathbb{N}$ is valid.

Proof. We have

$$\begin{aligned}\mathcal{U}^*(t)\boldsymbol{\pi}_D^{(N)}\mathcal{U}(t)-\boldsymbol{\pi}_D^{(N)}&=\int_0^t\frac{\mathrm{d}}{\mathrm{d}s}\big(\mathcal{U}^*(s)\boldsymbol{\pi}_D^{(N)}\mathcal{U}(s)\big)\ \mathrm{d}s\\&=\mathrm{i}\lambda\int_0^t\mathcal{U}^*(s)[\mathcal{H},\boldsymbol{\pi}_D^{(N)}]\mathcal{U}(s)\ \mathrm{d}s\ ,\end{aligned}$$

and so

$$||\mathcal{U}^*(t)\boldsymbol{\pi}_D^{(N)}\mathcal{U}(t) - \boldsymbol{\pi}_D^{(N)}|| \leq \lambda t||[\mathcal{H}, \boldsymbol{\pi}_D^{(N)}]|| \ .$$

And since by Theorem 4.3.7 the commutator satisfies

$$||[\mathcal{H}, \boldsymbol{\pi}_D^{(N)}]|| \leq C_N \lambda^{-3/2-N} \ ,$$

the results follow. □

This result means that the image of $\boldsymbol{\pi}_D$, which consists of the states which semiclassically live on D, is almost invariant under time evolution, where the time up to which the theorem ensures that the state stays on D can scale like any power of λ. So compared with the timescales obtained for the time evolution of coherent states, see Theorem 3.5.7, we here have a much larger timescale.

4.4.2 Local quantum ergodicity

We have discussed in Section 2.3.1 the quantum ergodicity theorem on compact manifolds. A similar theorem in the semiclassical setting was proven by Helffer, Martinez and Robert in [HMR87]. Here we want to discuss a local version of quantum ergodicity. Assume $D \subset T^*M$ is an open subset which is invariant under the Hamiltonian flow, and on which in addition the flow is ergodic. In this case one would expect that in analogy with the quantum ergodicity theorem, the part of the eigenfunctions which live on D become semiclassically constant on D. This is indeed the case, as we will show in the next theorem.

We will choose a slightly broader setup. The reason is that it seems very likely that for typical systems, which have a mixed phase space, ergodic components do not seem to be of the simple type of an open set. One expects that typically on gets ergodic measures of a quite complicated and maybe even fractal structure, so we formulate the result for general measures whose Anti-Wick quantization approximately commutes with the Hamiltonian.

Theorem 4.4.2. *Let $\mathcal{H} \in \Psi^0(m_{a,b})$ be a selfadjoint operator such that the energy shell Σ_E of the principal symbol H_0 is compact for E. Assume that the restriction ν_E of the measure ν to the energy shell Σ_E is normalized and ergodic with respect to the Hamiltonian flow of H_0, and that*

$$||[\mathcal{H}, \mathrm{Op}^{AW}[\nu]]|| = o(\lambda^{-1}) \ . \tag{4.33}$$

Let for some $c > 0$, $I_c(E, \lambda) := [E - c/2\lambda, E - c/2\lambda]$ be the interval of width c/λ around E and denote by $N_I(\lambda) := \#\{E_n(\lambda) \in I_c(E, \lambda)\}$ the number of eigenvalues in $I_c(E, \lambda)$, then we have

$$\lim_{\lambda\to\infty} \frac{1}{N_I(\lambda)} \sum_{E_n(\lambda)\in I_c(E,\lambda)} \left|\langle\psi_n, \mathrm{Op}^{AW}[\nu]\mathcal{A}\psi_n\rangle - \langle\psi_n, \mathrm{Op}^{AW}[\nu]\psi_n\rangle\, \nu_E(\sigma(\mathcal{A})_E)\right| = 0 \ , \tag{4.34}$$

for every $\mathcal{A} \in \Psi^0(1)$, where $\sigma(\mathcal{A})_E$ denotes the restriction of $\sigma(\mathcal{A})$ to the energy shell Σ_E.

Proof. We will basically use the proof in [Col85], with some minor modifications. It has the advantage that we do not have to use powers of $\mathrm{Op}^{AW}[\nu]$, like $\mathrm{Op}^{AW}[\nu]^2$, which is necessary in the proof sketched after Theorem 2.3.1. We will assume that the observable $\mathcal{A}$ is given as the Anti-Wick quantization of some classical observable

$$\mathcal{A} = \mathrm{Op}^{AW}[a] \; .$$

Since the Weyl quantization and the Anti-Wick quantization of an element $a \in S^0(1)$ differ by a term of order λ^{-1} this choice doesn't affect the result. But since the Anti-Wick quantization preserves positivity and ν is assumed to be positive, the map

$$S^0(1) \ni a \mapsto \int a \, \mathrm{d}\nu_n := \langle \psi_n, \mathrm{Op}^{AW}[\nu] \, \mathrm{Op}^{AW}[a] \psi_n \rangle \in \mathbb{C}$$

is a positive distribution, hence a positive measure, for each eigenfunction.

Now the Szegö limit theorem, Theorem 4.2.3, gives

$$\lim_{\lambda \to \infty} \frac{1}{N_I(\lambda)} \sum_{E_n(\lambda) \in I_c(E,\lambda)} \langle \psi_n, \mathrm{Op}^{AW}[\nu] \, \mathrm{Op}^{AW}[a] \psi_n \rangle = \int_{\Sigma_E} a \, \mathrm{d}\nu_E =: \nu_E(a)$$

where ν_E denotes the restriction of ν to the energy shell Σ_E. So this means that the sequence

$$\frac{1}{N_I(\lambda)} \sum_{E_n(\lambda) \in I_c(E,\lambda)} \mathrm{d}\nu_n \; , \tag{4.35}$$

converges weakly to $\mathrm{d}\nu_E$ for $\lambda \to \infty$.

Now define

$$\mathcal{B}^T := \frac{1}{T} \int_0^T \mathcal{U}^*(t) \, \mathrm{Op}^{AW}[\nu] \big(\mathrm{Op}^{AW}[a] - \nu_E(a_E) \big) \mathcal{U}(t) \; \mathrm{d}t \; ,$$

and note that on the one hand

$$\langle \psi_n, \mathcal{B}^T \psi_n \rangle = \langle \psi_n, \mathrm{Op}^{AW}[\nu] \mathcal{A} \psi_n \rangle - \langle \psi_n, \mathrm{Op}^{AW}[\nu] \psi_n \rangle \, \nu_E(\sigma(\mathcal{A})_E) \; ,$$

and on the other hand we have by (4.33)

$$\mathcal{B}^T = \mathrm{Op}^{AW}[\nu] \mathcal{A}^T + o(1)$$

with

$$\mathcal{A}^T := \frac{1}{T} \int_0^T \mathcal{U}^*(t) \big(\mathrm{Op}^{AW}[a] - \nu_E(a_E) \big) \mathcal{U}(t) \; \mathrm{d}t \; .$$

If we define

$$a^T := \frac{1}{T} \int_0^T a \circ \Phi^t \; \mathrm{d}t - \nu_E(a_E) \; ,$$

we can rewrite this as

$$\mathcal{B}^T = \mathrm{Op}^{AW}[\nu]\,\mathrm{Op}^{AW}[a^T] + o(1)$$

and obtain

$$|\langle\psi_n, \mathcal{B}^T\psi_n\rangle| = \left|\int a^T \,\mathrm{d}\nu_n\right| + o(1) \leq \int |a^T| \,\mathrm{d}\nu_n + o(1) \ .$$

Summation over n then yields

$$\lim_{\lambda\to\infty}\frac{1}{N_I(\lambda)}\sum_{E_n(\lambda)\in I_c(E,\lambda)} \left|\langle\psi_n, \mathrm{Op}^{AW}[\nu]\mathcal{A}\psi_n\rangle - \langle\psi_n, \mathrm{Op}^{AW}[\nu]\psi_n\rangle\,\nu_E(\sigma(\mathcal{A})_E)\right| \leq \int |a^T| \,\mathrm{d}\nu_E \ ,$$

for every T. But by ergodicity of ν_E we have ν_E-almost everywhere that

$$a^T \to 0$$

for $T \to \infty$, and hence we can make

$$\int |a^T| \,\mathrm{d}\nu_E$$

as small as we wish by choosing T large enough. Therefore the relation (4.34) follows. □

Now one can use the standard arguments [Col85, Wal82] to show that one can extract a subsequence of density one which satisfies

$$\langle\psi_{n_j}, \mathrm{Op}^{AW}[\nu]\mathcal{A}\psi_{n_j}\rangle = \langle\psi_{n_j}, \mathrm{Op}^{AW}[\nu]\psi_{n_j}\rangle\nu_E(\sigma(\mathcal{A})) + o(1)$$

for every $\mathcal{A} \in \Psi^0(1)$. Notice that the factor $\langle\psi_{n_j}, \mathrm{Op}^{AW}[\nu]\psi_{n_j}\rangle$ does not depend on the observable $\mathcal{A}$. It measures the weight which the eigenfunction ψ_n has relative to ν.

The main application of this theorem we have in mind is of course the case that ν is the characteristic function of some open domain D on which the flow is ergodic. The term

$$0 \leq \langle\psi_n, \mathrm{Op}^{AW}[\chi_D]\psi_n\rangle \leq 1$$

can then be interpreted as measuring the relative fraction of the state ψ_{n_j} which lives in D, more explicitly

$$\langle\psi_n, \mathrm{Op}^{AW}[\chi_D]\psi_n\rangle = \int \chi_D(z) H_n^L(z) \,\mathrm{d}z \ ,$$

where $H_n^L(z)$ is the Husimi function of ψ_n. Since $H_n^L(z)$ is interpreted as a probability density, this expression gives the probability of finding the system in D when it is in the state ψ_n. It seems likely that generically almost all of the factors $\langle\psi_n, \mathrm{Op}^{AW}[\chi_D]\psi_n\rangle$ tend either to zero or to one. Hence the eigenfunctions would split into two subsequences, one of which is concentrated on D, and one is concentrated on the complement of D. Then our result would imply that the eigenfunctions in the subsequence localized on D are quantum ergodic on D, hence tend weakly to χ_D. We will discuss these points further in Chapter 5.

In the case at hand we obtain the slightly weaker result, that the part of the eigenfunction which is concentrated on D tends to a constant on D in the limit $\lambda \to \infty$.

Corollary 4.4.3. *Assume $\mathcal{H}$ satisfies the same conditions as in Theorem 4.4.2, and assume that $D \subset T^*M$ is an open domain with piecewise smooth boundary such that the flow is ergodic on $\Sigma_E \cap D$. Then there exists a sequence of subsequences*

$$\{E_{n_j}(\lambda)\} \subset \{E_n(\lambda) \in I_c(E, \lambda)\}$$

of density one, i.e.

$$\lim_{\lambda\to\infty} \frac{1}{N_I(\lambda)} |\{E_{n_j}(\lambda)\}| = 1 ,$$

such that for $\lambda \to \infty$

$$\langle \psi_{n_j}, \mathrm{Op}^{AW}[\chi_D]\mathcal{A}\psi_{n_j}\rangle = \langle \psi_{n_j}, \mathrm{Op}^{AW}[\chi_D]\psi_{n_j}\rangle \frac{1}{|\Sigma_E \cap D|} \int_{\Sigma_E\cap D} \sigma(\mathcal{A}) \, \mathrm{d}\mu_E + o(1) .$$

Since $\langle \psi_{n_j}, \mathrm{Op}^{AW}[\chi_D]\psi_{n_j}\rangle$ is bounded, we can furthermore choose subsequences $E_{n_{j_k}}(\lambda)$ for which

$$\lim_{\substack{k\to\infty\\ \lambda\to\infty}} \langle \psi_{n_{j_k}}, \mathrm{Op}^{AW}[\chi_D]\psi_{n_{j_k}}\rangle = \alpha ,$$

with $0 \leq \alpha \leq 1$, and then we have

$$\lim_{\substack{k\to\infty\\ \lambda\to\infty}} \langle \psi_{n_{j_k}}, \mathrm{Op}^{AW}[\chi_D]\mathcal{A}\psi_{n_{j_k}}\rangle = \alpha \int_{\Sigma_E\cap D} \sigma(\mathcal{A}) \, \mathrm{d}\mu_E .$$

In the case that the classical system is ergodic, we can take of course $D = T^*M$ and obtain the classical quantum ergodicity theorem in the formulation of [HMR87]. Unfortunately, this is the only case where examples of ergodicity are known. In the more general case of a Hamiltonian system which is not ergodic, no example has been constructed so far of an open ergodic subset. It seems that the dynamical structure is too complicated to allow such a simple type of ergodic subset. It seems much more likely that the ergodic components have a very intricate structure, maybe of some fractal nature. At least if one perturbes an integrable system, then KAM theory shows that the system stays integrable on a cantor like subset of phase space, and this suggests that the ergodic components, if there are any of positive measure, should have a fractal structure, too.

So one should consider the above results as first steps, which show what can be done in principle, but it seems that in order to be able to cover realistic situations some more work has to be done.

Chapter 5

Stable quasimodes

" ... to obtain positive results stating that this or that type of dynamical system must be accepted as one of the essential, not "exceptional", systems, that cannot be "neglected" from any sensible point of view (similar to the way in which we neglect sets of measure zero), we shall use the concept of stability in the sense of conservation of a given type of behavior of a dynamical system when there is a slight variation in the functions [defining the system]. *An arbitrary type of behavior of a dynamical system, for which there exists at least one example of its stable realization, must from this point of view be considered essential and may not be neglected."*

A. N. Kolmogorov in [Kol57], translation from [AM78].

Semiclassical methods can often be used to construct approximate solutions of the stationary Schrödinger equation, and in this chapter we want to study some of these approximate solutions and discuss their meaning. Such approximate solutions have been called quasimodes, and in the first section we discuss some basic properties of them. The most important one is the observation that quasimodes generally need not be close to eigenfunctions, but can be represented as a superposition of eigenfunctions with nearby eigenvalues. This implies that they are approximately invariant under the time evolution for long times, but one cannot deduce directly any information on the eigenfunctions themselves.

The known examples where quasimodes with a sufficiently small error term do not tend to eigenfunctions in the semiclassical limit are connected with discrete symmetries of the system. Since small perturbations generically destroy such symmetries, one might expect that for almost all perturbations of the original system quasimodes indeed converge to eigenfunctions in the semiclassical limit. These matters are discussed in Section 5.2 where more precise conjectures are formulated. The perturbations we consider are of lower order in the semiclassical parameter, which means that the classical system is not perturbed.

So one can view the perturbations as perturbations of the quantization. The appropriate notion of genericity in this context is then the topological one. This approach has some similarity with the ideas and results from the theory of decoherence. There it is shown that the coupling of a system to its environment leads to very fast decoherence, which means that mixed states tend to pure states, even if the coupling is very weak. In the semiclassical limit it could happen that pure quantum mechanical stationary states, i.e. they are pure in the set of invariant states, tend to classically mixed stationary states. The genericity conjecture implies that almost all perturbations would destroy this behavior, resulting in a pure classical invariant state as a quantum limit, where again pure is meant in the set of invariant classical sates (E.g. a delta function on an periodic orbit is pure in this sense, but not a delta function supported by two periodic orbits.)

In order that quasimodes become close to eigenfunctions under small perturbations, one has to demand that the quasimodes themselves are stable under these perturbations, and do not disappear. The notion of stability we introduce means that the quasimode can be extended to a family of quasimodes depending smoothly on the perturbation, and such that the order of the discrepancy does not change. Such quasimodes are called stable quasimodes and the remaining parts of this chapter are devoted to a study of the stability properties of quasimode constructions. In a nutshell, our main result is that quasimodes are stable if and only if the classical structure on which they are semiclassically concentrated is stable under small perturbations of the classical system.

In Section 5.3 as a preparation for the remaining part the solvability of certain transport equations is discussed. These transport equations occur in the construction of quasimodes, and their general solvability will be the main condition on the stability of the quasimodes. In the simple example of a transport equation on a Lagrangian torus we see that the general solvability is equivalent to a Diophantine condition on the frequencies of the flow on the torus. But by KAM theory this Diophantine condition in turn implies the stability of this torus under small perturbations of the classical system. We then use a linear response argument to give a direct proof, without refering to KAM theory, that stability of the classical invariant submanifold under small perturbations implies the general solvability of the transport equations.

In Section 5.4 we then study the construction of quasimodes associated with invariant tori and with elliptic orbits. The case of invariant tori is well known in the literature, and we only give a short review, where we put special emphasis on the fact that classical stability is necessary for the stability of the quasimodes.

The quasimodes associated with elliptic orbits are given by Lagrangian states associated with complex Lagrangian ideals, whose theory we developed in Chapter 3. We consider two approaches. The first one, due to [PU93], uses the time evolution of coherent states and allows a very simple construction of a quasimode with discrepancy of order $\lambda^{-3/2}$. In order to get smaller discrepancies we consider an approach using the local Birkhoff normal form; here we sketch a proof of the fact that if the orbit satisfies a non-resonance condition of order L, then one can construct a quasimode with discrepancy $O(\lambda^{-L})$. The non-resonance condition is exactly the condition of classical stability. The methods from Chapter 3 could probably be used to derive similar results near bifurcations and for other type of orbits, e.g., lower dimensional tori.

In the last section we finally discuss a different class of quasimodes which can be associated with every open stably invariant domain in phase space. Such kind of quasimodes have been considered by Shnirelman for the gaps between invariant tori in a KAM situation [Shn]. Their construction relies on the approximate projection operators of Chapter 4. The construction is not explicit, and in contrast to the quasimode constructions from Section 5.4 gives no formula for the eigenvalues. One only knows that they are concentrated in the given invariant domain, and that their relative number is bounded from below by the relative volume of the domain. But if the genericity conjecture of Section 5.2 were true, then we would obtain a proof that generically the set of eigenfunctions can be split into subsets of eigenfunctions concentrated on invariant domains in phase space, and thereby confirming the picture of Percival, [Per73].

In case that the flow on the invariant domain is ergodic, the local quantum ergodicity Theorem from Section 4.4.2 implies a quantum ergodicity Theorem for the quasimodes concentrated on the domain.

5.1 Preliminaries on quasimodes

Semiclassical constructions can often be used to obtain approximate solutions of the stationary Schrödinger equation, such approximate solutions have been called quasimodes.

Definition 5.1.1. *Let H be a Hilbert space and $\mathcal{H}$ a selfadjoint operator on H with domain $D(\mathcal{H})$. A pair (ψ, E) with $\psi \in D(\mathcal{H})$, $||\psi|| = 1$ and $E \in \mathbb{R}$ is called a **quasimode** with discrepancy δ, if*

$$(\mathcal{H} - E)\psi = r\ , \quad \text{with} \quad ||r|| \leq \delta\ . \tag{5.1}$$

One might hope that ψ is close to an eigenfunction with eigenvalue close to E, if δ is small enough. But this need not be true, generally only E is close to an eigenvalue.

Example 5.1.2. Take as quasimode a superposition of two eigenfunctions, $\psi = a_1\psi_1 + a_2\psi_2$, with $|a_1|^2 + |a_2|^2 = 1$. Then

$$(\mathcal{H} - E)\psi = (E_1 - E)a_1\psi_1 + (E_2 - E)a_2\psi_2 = r\ ,$$

and the remainder r can be estimated as

$$||r||^2 \leq (E_1 - E)^2 + (E_2 - E)^2\ .$$

So if E_1 and E_2 are close to E, $||r||$ will be small but ψ need not be close to an eigenfunction.

That approximate solutions of the Schrödinger equation need not be close to the true eigenfunctions has been pointed out by Arnold, [Arn72], who also invented the name quasimodes for them. In the following we review some well known properties of them, see [Col77, Laz93] for related material.

Proposition 5.1.3. *Assume that* (ψ, E) *is a quasimode of* $\mathcal{H}$ *with discrepancy* δ *and that the spectrum of* $\mathcal{H}$ *is discrete in a neighborhood of* $[E-\delta, E+\delta]$. *Then there is at least one eigenvalue of* $\mathcal{H}$ *in the interval*

$$[E-\delta, E+\delta] \ .$$

Proof. The proof follows from the well known estimate for the resolvent $R_{\mathcal{H}}(E) = (\mathcal{H} - E)^{-1}$,

$$||R_{\mathcal{H}}(E)|| \leq \frac{1}{\operatorname{dist}(E, \operatorname{spec}(\mathcal{H}))} \ , \tag{5.2}$$

where $\operatorname{spec}(\mathcal{H})$ denotes the spectrum of $\mathcal{H}$, and $\operatorname{dist}(E, \operatorname{spec}(\mathcal{H}))$ is the distance between E and the spectrum, see, e.g., [HS96]. Choose $E' \notin \operatorname{spec}(\mathcal{H})$, close to E, and apply $R_{\mathcal{H}}(E')$ to (5.1). This gives, together with the splitting $\mathcal{H} - E = (\mathcal{H} - E') + (E' - E)$,

$$R_{\mathcal{H}}(E')r = R_{\mathcal{H}}(E')(\mathcal{H} - E')\psi + (E' - E)R_{\mathcal{H}}(E')\psi \ ,$$

or

$$\psi = R_{\mathcal{H}}(E')r - (E' - E)R_{\mathcal{H}}(E')\psi \ . \tag{5.3}$$

Taking the norm of both sides, together with the resolvent estimate (5.2), leads to

$$1 \leq \frac{||r||}{\operatorname{dist}(E', \operatorname{spec}(\mathcal{H}))} + \frac{|E' - E|}{\operatorname{dist}(E', \operatorname{spec}(\mathcal{H}))} \ ,$$

and multiplying by $\operatorname{dist}(E', \operatorname{spec}(\mathcal{H}))$ yields finally

$$\operatorname{dist}(E', \operatorname{spec}(\mathcal{H})) \leq ||r|| + |E' - E| \ ,$$

which gives the lemma in the limit $E' \to E$. □

What the example 5.1.2 suggests is that a quasimode is a superposition of eigenfunctions whose eigenvalues are mainly in the interval $[E-\delta, E+\delta]$. The following proposition shows that this is true if the interval is far enough away from the remaining part of the spectrum.

Proposition 5.1.4. *Let* (ψ, E) *be a quasimode of* $\mathcal{H}$ *with discrepancy* δ, *and assume that the spectrum of* $\mathcal{H}$ *is discrete in a neighborhood of* $[E-\delta, E+\delta]$. *Denote the distance of* $[E-\delta, E+\delta]$ *to the part of* $\operatorname{spec}(\mathcal{H})$ *outside of* $[E-\delta, E+\delta]$ *by* ε. *Furthermore, let* π_2 *be the spectral projection corresponding to* $\operatorname{spec}(\mathcal{H}) \backslash \big([E-\delta, E+\delta] \cap \operatorname{spec}(\mathcal{H})\big)$, *then*

$$||\pi_2 \psi|| \leq \frac{\delta}{\varepsilon} \ .$$

Remark: Since π_2 is a projection one has the trivial inequality

$$||\pi_2 \psi|| \leq 1 \ ,$$

so the proposition becomes useful in the case that $\varepsilon > ||r||$.

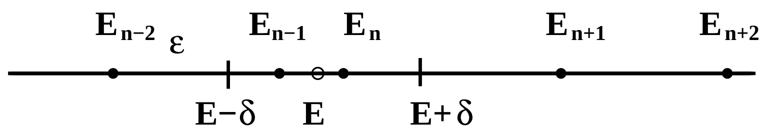

Figure 5.1: Illustration of the arrangement of the different quantities entering Proposition 5.1.4.

Proof. We again use the formula (5.3) now with $E' \in \mathbb{C}\setminus\operatorname{spec}(\mathcal{H})$, and divide through $(E'-E)$, which gives

$$\frac{1}{E'-E}\psi + R_{\mathcal{H}}(E')\psi = \frac{1}{E'-E}R_{\mathcal{H}}(E')r \ . \tag{5.4}$$

Let Γ be a circle in $\mathbb{C}$ around E with radius s larger than $||r||$ and smaller than $||r||+\varepsilon$. Integrating the left hand side of (5.4) along Γ gives

$$\frac{1}{2\pi\mathrm{i}}\int_\Gamma \left(\frac{1}{E'-E}\psi + R_{\mathcal{H}}(E')\psi\right)\,\mathrm{d}E' = \pi_2\psi \ ,$$

and for the right hand side one gets, using the parameterization $E' = E + s\mathrm{e}^{\mathrm{i}\varphi}$, with $||r|| < s < ||r|| + \varepsilon$, of Γ, the estimate

$$\left|\left|\frac{1}{2\pi\mathrm{i}}\int_\Gamma \frac{1}{E'-E}R_{\mathcal{H}}(E')r\,\mathrm{d}E'\right|\right| \leq \frac{1}{2\pi}\int_0^{2\pi} ||R_{\mathcal{H}}(E+s\mathrm{e}^{\mathrm{i}\varphi})r||\,\mathrm{d}\varphi < \frac{||r||}{\varepsilon} \ .$$

□

The conclusion of our discussion of quasimodes up to now is that in general they allow to draw conclusions about the spectrum, but not on the eigenfunctions. From Proposition 5.1.4 it follows that if we were able to give lower bounds on the spacings between adjacent eigenvalues, and construct quasimodes with discrepancy much smaller than these spacings, then these quasimodes would be close to eigenfunctions.

From the practical point of view, quasimodes are as important as eigenfunctions, since in typical experimental situations where the energy resolution is not infinitely sharp, one cannot distinguish between eigenfunctions and quasimodes. From this point of view, their most striking property is their almost invariance under time evolution. We will state the result in the semiclassical λ-dependent case.

Theorem 5.1.5. *Let $\mathcal{H}$ be a semiclassical Hamiltonian, (ψ, E) a quasimode of $\mathcal{H}$ with discrepancy δ and $\mathcal{U}(t) = \mathrm{e}^{-\mathrm{i}\lambda t\mathcal{H}}$ the time evolution operator, then*

$$||\mathcal{U}(t)\psi - \mathrm{e}^{-\mathrm{i}t\lambda E}\psi|| \leq \lambda t\delta$$

Proof. We have

$$\begin{aligned}\mathcal{U}(t)\psi - \mathrm{e}^{-\mathrm{i}t\lambda E}\psi &= \mathrm{e}^{-\mathrm{i}t\lambda E}[\mathrm{e}^{\mathrm{i}t\lambda E}\mathcal{U}(t)\psi - \psi] \\ &= -\mathrm{i}\lambda \mathrm{e}^{-\mathrm{i}t\lambda E}\int_0^t \frac{\mathrm{i}}{\lambda}\partial_{t'}\left(\mathrm{e}^{\mathrm{i}t'\lambda E}\mathcal{U}(t')\psi\right)\,\mathrm{d}t' \\ &= -\mathrm{i}\lambda \mathrm{e}^{-\mathrm{i}t\lambda E}\int_0^t \mathrm{e}^{\mathrm{i}t'\lambda E}\mathcal{U}(t')(H-E)\psi\,\mathrm{d}t'\end{aligned}$$

and taking the norm of both sides gives the desired estimate. □

So if the discrepancy is sufficiently small, the state ψ remains stationary for a fairly long time. Especially, if we have

$$\delta \leq C_N \lambda^{-N} ,$$

as will be the case for many quasimode constructions, then the state ψ remains almost stationary for $t \leq T_\varepsilon^*$ with

$$T_\varepsilon^* \sim \lambda^{N-1-\varepsilon}$$

for every $\varepsilon > 0$.

5.2 Small perturbations and genericity

We have learned in the last subsection, that the main obstruction for a sufficiently good quasimode to be close to an eigenfunction is the possibility of quasi-degeneracies of eigenvalues, i.e. the existence of consecutive eigenvalues whose distance is much smaller than the mean level spacing.

A typical example where such a behavior occurs is the symmetric double well potential. This is a one dimensional system with Hamiltonian

$$\mathcal{H} = -\frac{1}{\lambda^2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$$

where, e.g.,

$$V(x) = x^4 - x^2 .$$

Here the eigenfunctions occur in pairs of symmetric and antisymmetric functions whose eigenvalues are almost degenerate, the distance between them is of order $\mathrm{e}^{-c\lambda}$, see, e.g., [HS96]. Therefore, suitable superpositions of the even and odd eigenfunctions produce quasimodes concentrated in one well with a very small discrepancy. Nevertheless they are obviously not close to the eigenfunctions. The special structure of the eigenfunctions is of course related to the symmetry. Simon has shown in [Sim85] that if one perturbes the potential slightly, in a way which breaks the symmetry, then the structure of the eigenfunctions changes immediately; they are then all concentrated in one well only.

This example suggests that even if a quasimode is not close to an eigenfunction it might be close to an eigenfunction of a small perturbation of the system. We will develop this idea somewhat further now.

First of all, we do not want to change the classical limit, so we will study perturbations with semiclassically small operators. So let $\mathcal{H} \in \Psi^0(m_{a,b})$ be selfadjoint, then we will study perturbations of the form

$$\mathcal{H} + \lambda^{-m}\mathcal{A} ,$$

with $\mathcal{A} \in \Psi^0_{\mathbb{R}}(1)$ and $m > 0$. The subscript $\mathbb{R}$ denotes that the symbol of $\mathcal{A}$ should be real valued, then $\mathcal{H} + \lambda^{-m}\mathcal{A}$ is selfadjoint since $\mathcal{A}$ is bounded and symmetric.

If we now study quasimodes for such families of Hamiltonians, we get an additional condition, namely that a quasimode for $\mathcal{H}$ can be extended smoothly to a quasimode for $\mathcal{H} + \lambda^{-m}\mathcal{A}$ for all $\mathcal{A}$. Such a quasimode will be called stable.

Definition 5.2.1. *Let $\mathcal{H} \in \Psi^0(m_{a,b})$ be selfadjoint. A quasimode (E, ψ) with discrepancy of order λ^{-N}*

$$||(\mathcal{H} - E)\psi|| \leq C_N\lambda^{-N}$$

is called a ***stable quasimode****, if it can be extended to a family of quasimodes*

$$\mathcal{A} \mapsto (E(\mathcal{A}), \psi(\mathcal{A}))$$

with discrepancy of order λ^{-N}

$$||((\mathcal{H} + \lambda^{-m}\mathcal{A}) - E(\mathcal{A}))\psi(\mathcal{A})|| \leq C_N(\mathcal{A})\lambda^{-N}$$

for all $\mathcal{A} \in \Psi^0_{\mathbb{R}}(1)$, and if

$$||\psi(\mathcal{A}) - \psi(\mathcal{A}')|| \leq C\lambda^{-m}||\mathcal{A} - \mathcal{A}'|| .$$

We will study a number of explicit examples of quasimode constructions in the next sections and find that there exist quasimodes which are stable, and quasimodes which are not stable. Roughly speaking, it turns out that quasimodes concentrated on classical structures which themselves are stable under small perturbations of the classical system turn out to be stable.

A further reason for believing that small perturbations can lead to the convergence of quasimodes to eigenfunctions is that quasidegeneracies of eigenvalues are unstable under small perturbations.

Example 5.2.2. As a model to study the effect of a perturbation on two quasi-degenerate eigenvalues we consider the case of a two by two matrix,

$$\mathcal{H} = \begin{pmatrix} E_0 + \delta/2 & 0 \\ 0 & E_0 - \delta/2 \end{pmatrix}$$

and a perturbation

$$A = \frac{1}{2}\begin{pmatrix} 0 & \alpha \\ \alpha^* & 0 \end{pmatrix} .$$

Then the eigenvalues of $\mathcal{H} + A$ are easily computed to be

$$E_\pm = E_0 \pm \sqrt{\delta^2/4 + |\alpha|^2/4} ,$$

hence the difference between the two eigenvalues is given by

$$E_+ - E_- = \sqrt{\delta^2 + |\alpha|^2} \geq |\alpha| .$$

So a perturbation which has non-vanishing off-diagonal matrix elements will remove a quasi-degeneracy. This is essentially the example von Neuman and Wigner used to study avoided crossings, [vNW29].

Unfortunately, it is not easy to extend the previous example of a two-level system to an infinite dimensional system. The problem is that at the same time when one removes a quasi-degeneracy with a small perturbation, one might create a new one somewhere else in the spectrum, and this is hard to control.

By Weyl's law we have for the spectral counting functions of a selfadjoint operator $\mathcal{H} \in \Psi^0(m_{a,b})$

$$N(\lambda) = c_d\lambda^d + O(\lambda^{d-1})$$

and therefore we can have clusters of eigenvalues which contain up to $O(\lambda^{d-1})$ eigenvalues.

Now we have

Lemma 5.2.3. *Let $E_n(\mathcal{A})$ be a continuous family of eigenvalues of $\mathcal{H} + \lambda^{-m}\mathcal{A}$, then*

$$|E_n(\mathcal{A}) - E_n(0)| \leq \lambda^{-m}||\mathcal{A}|| .$$

Proof. Consider $\mathcal{H}_\varepsilon := \mathcal{H} + \varepsilon\lambda^{-m}\mathcal{A}$, and let

$$\mathcal{H}_\varepsilon\psi(\varepsilon) = E(\varepsilon)\psi(\varepsilon) ,$$

with $||\psi(\varepsilon)|| = 1$. By the Feynman Hellmann theorem we have

$$\frac{\mathrm{d}E(\varepsilon)}{\mathrm{d}\varepsilon} = \lambda^{-m}\langle\psi(\varepsilon), \mathcal{A}\psi(\varepsilon)\rangle ,$$

and integration gives

$$E_n(\mathcal{A}) - E_n(0) = \lambda^{-m}\int_0^1 \langle\psi(\varepsilon), \mathcal{A}\psi(\varepsilon)\rangle \,\mathrm{d}\varepsilon ,$$

and so the result follows. □

This result tells us that in order to straighten out a cluster of eigenvalues of order $O(\lambda^{d-1})$ we need at least a perturbation of order λ^{-1}.

Given an interval $I = [\alpha, \beta]$ such that the spectrum of $\mathcal{H}$ is discrete in I and let us denote the smallest level spacing by

$$s_I^{\min}(\mathcal{H}, \lambda) := \inf\{|E_n(\lambda) - E_m(\lambda)| \ ; n \neq m,\ E_n(\lambda), E_m(\lambda) \in I\} \ .$$

From Weyl's law we know that

$$\limsup_{\lambda\to\infty} s_I^{\min}(\mathcal{H}, \lambda)\lambda^d \leq C \ ,$$

and in order to get information on quasimodes we need a lower bound on $s_I^{\min}(\mathcal{H}, \lambda)$. For $\delta > 0$ denote by $\Sigma_\delta^0(\mathcal{H})$ the set of $\mathcal{A} \in \Psi^0(1)$ such that

$$\liminf_{\lambda\to\infty} s_I^{\min}(\mathcal{H} + \lambda^{-1}\mathcal{A}, \lambda)\lambda^{d+\delta} \geq \varepsilon \tag{5.5}$$

for some $\varepsilon > 0$.

We will conjecture that (5.5) is the generic behavior, so we first have to discuss the notion of genericity which is appropriate in this context. Let X be a complete metriziable space, e.g., a Frechet space or a Banach space. A subset $Y \subset X$ is said to be a set of second Baire category in X if it can be represented as a countable intersection

$$Y = \bigcap_{l\in\mathbb{N}} Y_l$$

of dense open subsets $Y_l \subset X$. A property is said to be generically true, if it is true on a set of second Baire category, see, e.g., [AR67] for more details.

Conjecture 5.2.4. *Let $\mathcal{H} \in \Psi^0(m_{a,b})$ be selfadjoint, and assume that $H_0^{-1}([\alpha, \beta])$ is compact, where H_0 denotes the principal symbol of $\mathcal{H}$. Then the set $\Sigma_\delta^0(\mathcal{H})$ of perturbations satisfying* (5.5) *is of second Baire category in $\Psi^0(1)$ for any $\delta > 0$.*

This conjecture would of course imply that every stable quasimode with discrepancy $o(\lambda^{-d-\delta})$ would converge to an eigenfunction.

Conjecture 5.2.5. *Let $\mathcal{H} \in \Psi^0(m_{a,b})$ be selfadjoint and assume that $H_0^{-1}([\alpha, \beta])$ is compact, where H_0 denotes the principal symbol of $\mathcal{H}$. Let (ψ, E) be a stable quasimode with discrepancy*

$$O(\lambda^{-d-\delta})$$

for some $\delta > 0$. Then the set $Q_\delta^0(\mathcal{H})$ of perturbations for which $\psi(\mathcal{A})$ converges to an eigenfunction is of second Baire category in $\Psi^0(1)$.

As we mentioned already, Conjecture 5.2.4 implies Conjecture 5.2.5. But as the example of the double well potential shows, there can be more perturbations for which quasimodes tend to eigenfunctions, than for which quasi-degeneracies are removed. So even if Conjecture 5.2.4 is wrong, Conjecture 5.2.5 could still be true.

In the literature there exist some studies on general generic properties of eigenfunctions and eigenvalues. In [Uhl72, Uhl76, Alb78] it was shown that certain properties of eigenfunctions and eigenvalues are generic, for instance that critical points of eigenfunctions are simple and some facts on nodal lines. In particular, it is shown that generically eigenvalues are simple, which can be viewed as a first step towards a proof of conjecture 5.2.4.

In [AK99] a result very similar to Conjecture 5.2.5 is proven. There a Schrödinger operator on $\mathbb{R}^d$ with smooth periodic potential is considered. This is by Bloch theory equivalent to a family of operators on the torus indexed by the Bloch vector, which determines the subprincipal symbol. For large energies the potential can be considered as a small perturbation of the free particle, and so one is in a KAM situation with plenty of quasimodes. They showed then that for a set of Bloch vectors of full measure in the Brillouin-zone quasimodes converge to eigenfunctions semiclassically.

The idea of genericity of stable properties in the above sense is close in spirit to the ideas and results in the theory of decoherence, see, e.g., [GJK$^+$96]. The theory of decoherence attempts to explain the fact that although in quantum mechanics entangled states between different subsystems are possible, they are not observed on a macrscopic level. This phenomenon is explained by the coupling to the environment, which induces a rapid decay of coherence. What is especially remarkable, is that already a very weak coupling to the environment is sufficient to destroy coherence effects. In order to make the analogy with our situation clearer, we consider for a given Hamiltonian the set of invariant states in quantum mechanics and in classical mechanics. In a situation like the symmetric double well potential, we find that the quantum mechanically pure states, the eigenfunctions, tend in the semiclassical limit to classical states which are not pure, but are sums of two pure states (pure in the convex set of invariant states) which are concentrated in each well. This would mean that even in the classical limit the particle remains to be in both wells with equal probability. But by the result of Simon, stating that by a small perturbation the eigenfunctions become semiclassically concentrated in one well, the classical limits are therefore pure, too. So a small perturbation of the Hamiltionian has a similar effect as a weak coupling to some environment, and so from the theory of decoherence we expect that the semiclassically observable quantities are the ones which are stable under small perturbations, which by our conjectures should in turn be the generic properties of a system.

Motivated by Conjectures 5.2.4, 5.2.5, and by the general philosophy expressed in the citation of Kolomogorov at the beginning of this chapter, that properties which are stable under small perturbations are the essential ones from a physical pint of view, we will study a number of quasimode constructions in the following sections more closely. Our emphasis will thereby be on the question of stability or non-stability of these quasimodes.

5.3 Solvability of transport equations

In this section we want to discuss the solvability of certain transport equations which occur in semiclassical constructions of quasimodes and approximate projection operators. The main result of our discussion will be that the solvability of the transport equations is closely related to the stability of the underlying classical structures under small perturbations.

Let X be a symplectic manifold, H a smooth function on X, and X_H the corresponding Hamiltonian vectorfield. Let $S \subset X$ be a compact submanifold of X without boundary, which is invariant under the Hamiltonian vectorfield, i.e.

$$X_H(s) \in T_sS \text{ for all } s \in S \ ,$$

and on which H is nondegenerate, i.e.

$$X_H(s) \neq 0 \text{ for all } s \in S \ .$$

The question we want to study is, for which $b \in C^\infty(S)$ does the equation

$$X_H a = b \tag{5.6}$$

on S has a solution $a \in C^\infty(S)$. This is the general form to which the usual transport equations can be reduced. E.g., the equation $X_H f = fb$ is reduced by the substitution $f = \exp(a)$ to this form.

One can easily give a necessary condition on b for the existence of a solution a, which in practice will occur as a higher order quantization condition. Recall that the Liouville density $\mathrm{d}\mu$ on X induces an invariant density on S which we will denote by $\mathrm{d}\mu_S$.

Lemma 5.3.1. *If the equation* (5.6) *is solvable then*

$$\int_S b\, \mathrm{d}\mu_S = 0 \ . \tag{5.7}$$

Proof. The result is a simple consequence of Stokes theorem, and the fact that S has no boundary. Since $\mathrm{d}\mu_S$ is invariant under the Hamiltonian flow we have

$$\mathcal{L}_{X_H} a\, \mathrm{d}\mu_S = (X_H a)\, \mathrm{d}\mu_S = b\, \mathrm{d}\mu_S \ ,$$

and integrating this equation yields

$$\int_S b\, \mathrm{d}\mu_S = \int_S \mathcal{L}_{X_H} a\, \mathrm{d}\mu_S = 0 \ .$$

□

Before proceeding further we want to study two examples which will contain already the typical features of the general problem.

Example 5.3.2. Let us assume that X is two dimensional, then the invariant submanifolds are just the lines of constant energy, so assume that

$$S = \{x \in X\ ,\ H(x) = 1\}$$

is compact and non-degenerate. The Hamiltonian flow then is periodic on S, and we can choose the time $t \in [0, T)$, where T is the period, as new coordinate on S. In this coordinate the Hamiltonian vectorfield is given by $\frac{\mathrm{d}}{\mathrm{d}t}$ and the invariant density on S is $\mathrm{d}\mu_S = \mathrm{d}t$. The general transport equation now reads

$$\frac{\mathrm{d}a}{\mathrm{d}t} = b\ .$$

The functions on S can be represented by periodic functions on $\mathbb{R}$ with period T, and if we insert for a and b their Fourier series,

$$a(t) = \sum_{n\in\mathbb{Z}} a_n \mathrm{e}^{2\pi \mathrm{i} nt/T}\ , \qquad b(t) = \sum_{n\in\mathbb{Z}} b_n \mathrm{e}^{2\pi \mathrm{i} nt/T}\ ,$$

then we obtain

$$\sum_{n\in\mathbb{Z}} \left[\frac{2\pi \mathrm{i} n}{T} a_n - b_n\right] \mathrm{e}^{2\pi n \mathrm{i} t/T} = 0\ .$$

So we see that if the condition

$$b_0 = 0 \tag{5.8}$$

is fulfilled, the choice

$$a_n = \frac{T}{2\pi \mathrm{i} n} b_n$$

for $n \neq 0$ determines a solution of the transport equation. Since

$$b_0 = \frac{1}{T}\int_0^T b(t)\ \mathrm{d}t\ ,$$

we see that the condition (5.8) is exactly the condition (5.7) from Lemma 5.3.1. So in this case no other conditions on the solvability appear.

Example 5.3.3. : The second case we want to study is that X is 4-dimensional and S is a 2-dimensional torus on which the motion is quasi-periodic. This is a typical structure which appears in integrable systems and in small perturbations thereof. These tori serve as semiclassical supports of quasimodes which can be constructed on them if certain conditions are fulfilled, one of them being the solvability of a transport equation. One can choose action-angle coordinates on X in a neighborhood of the torus S, such that $\varphi = (\varphi_1, \varphi_2) \in$

$[0, 2\pi) \times [0, 2\pi)$ parameterize S and the restriction of the Hamiltonian vectorfield to S is given by

$$X_H = \langle k, \nabla_\varphi \rangle = k_1 \frac{\partial}{\partial \varphi_1} + k_2 \frac{\partial}{\partial \varphi_2} \ ,$$

with $k = (k_1, k_2) \in \mathbb{R}^2$ being the frequency vector, see, e.g., [Laz93]. The invariant measure on S is of course given by $\mathrm{d}\mu_S = \mathrm{d}\varphi_1 \mathrm{d}\varphi_2$. We will again expand the functions b and a in a Fourier series,

$$a(\varphi) = \sum_{n \in \mathbb{Z}^2} a_n \mathrm{e}^{\mathrm{i}\langle n, \varphi \rangle} \ , \qquad b(\varphi) = \sum_{n \in \mathbb{Z}^2} b_n \mathrm{e}^{\mathrm{i}\langle n, \varphi \rangle} \ ,$$

and then the transport equation reads

$$\sum_{n \in \mathbb{Z}^2} \big[\mathrm{i}\langle k, n \rangle a_n - b_n\big] \mathrm{e}^{\mathrm{i}\langle n, \varphi \rangle} = 0 \ .$$

Of course all coefficients have to vanish simultaneously in order that the transport equation is fulfilled, so we get

$$\mathrm{i}\langle k, n \rangle a_n - b_n = 0$$

for all $n \in \mathbb{Z}^2$. The equation for $n = 0$, $b_0 = 0$, is the now again the condition from Lemma 5.3.1, since

$$b_0 = \int_S b(\varphi) \ \mathrm{d}\mu_S \ .$$

The equations for $n \neq 0$ can only be solved for those $n \in \mathbb{Z}^2$ for which

$$\langle k, n \rangle \neq 0 \ ,$$

where we get

$$a_n = \frac{1}{\mathrm{i}\langle k, n \rangle} b_n \ .$$

So if the frequencies are linearly dependent over $\mathbb{Z}$, then the transport equation is not solvable for all inhomogeneities b which have mean zero. But even if the frequencies are linearly independent we have to assure that the the scalar product $\langle k, n \rangle$ stays sufficiently far away from zero, in order that the resulting function a is smooth. Recall that smoothness of a is equivalent to the condition that

$$|a_n| \leq C_N (1 + |n|)^{-N}$$

for all $N \in \mathbb{N}$. Therefore, we must assume that $1/|\langle k, n\rangle|$ grows at most polynomially in $|n|$, i.e. there should exist constants $C_K > 0$ and $K \in \mathbb{R}^+$ such that

$$\frac{1}{|\langle k, n\rangle|} \leq C_K(1 + |n|)^K$$

for all $n \in \mathbb{Z}^2$. This is a so called Diophantine condition, which is more frequently stated in the form

$$|\langle k, n\rangle| \geq C'_K(1 + |n|)^{-K} ,$$

for $n \neq 0$. So the validity of a Diophantine condition on the frequency vector k is a necessary and sufficient condition for the transport equation to have smooth solutions a for all smooth functions b which satisfy the quantization condition (5.7).

Of course, the results of our discussion remain valid in arbitrary dimensions; we collect them in the following theorem.

Theorem 5.3.4. *Let X be a $2d$-dimensional symplectic manifold, H a smooth real valued function on X, and S a d-dimensional Lagrangian torus in X which is invariant under the Hamiltonian vectorfield X_H. Let us choose action-angle coordinates in a neighborhood of S such that the vectorfield is $X_H = \langle k, \nabla_\varphi\rangle$, with a constant frequency vector $k \in \mathbb{R}^d$. Then the transport equation*

$$X_H a = b$$

has for every $b \in C^\infty(S)$ which satisfies the condition (5.7) a smooth solution $a \in C^\infty(S)$, if and only if the frequency-vector satisfies a Diophantine condition, i.e. there exist constants $C > 0$ and $K > 0$ with

$$|\langle k, n\rangle| \geq C(1 + |n|)^{-K} ,$$

for all $n \in \mathbb{Z}^d\backslash\{0\}$.

This example of invariant tori suggests an important idea. The Diophantine condition on the frequency-vector is the same condition which appears in KAM-Theory, see, e.g., [Laz93, AKN97]. The main result of KAM-Theory is that a torus whose frequency-vector satisfies a Diophantine condition is stable under small perturbation of the Hamilton function. This means that for all sufficiently small perturbations of the Hamilton function, there is an invariant torus close to the original one. So the idea which emerges from our discussion is that for a general invariant submanifold S, the stability of S under small perturbations of the Hamilton function ensures the solvability of the transport equation on S, up to the universal obstruction (5.7).

In order to develop this idea further we first have to make the notion of stability of an invariant submanifold under small perturbations more precise.

Definition 5.3.5. *Let X be a symplectic manifold, H a real valued smooth function on X and $S_0 \subset X$ a compact submanifold without boundary which is invariant under the Hamiltonian flow of H, and on which the Hamiltonian vectorfield is non-degenerate. We call S_0* ***stably invariant****, if there exists a manifold S and a neighborhood $F \subset C^\infty(X)$ of H together with a smooth family of embeddings*

$$\Phi : F \times S \to X \ ,$$

such that $\Phi(H, S) = S_0$, and for every $\tilde{H} \in F$ $S_{\tilde{H}} := \Phi(\tilde{H}, S)$ is invariant under the Hamiltonian flow generated by $\tilde{H}$.

Examples 5.3.6:

- By KAM-theory any invariant torus whose frequencies satisfies a Diophantine condition are stably invariant.
- Any compact energy surface on which the Hamiltonian vectorfield is nondegenerate is stably invariant.

For a stably invariant S_0, each $S_{\tilde{H}}$ carries an invariant density $\mu_{S_{\tilde{H}}}$, which we can pull back to the manifold S,

$$\mu_{\tilde{H}} := \Phi_{\tilde{H}}^* \mu_{S_{\tilde{H}}} \ , \tag{5.9}$$

and similarly the Hamiltonian vectorfields $X_{\tilde{H}}$ can be pulled back to S,

$$\tilde{X}_{\tilde{H}} := \Phi_{\tilde{H}}^* X_{\tilde{H}} \ . \tag{5.10}$$

The invariance of $\mu_{S_{\tilde{H}}}$ means that

$$\mathcal{L}_{\tilde{X}_{\tilde{H}}} \mu_{\tilde{H}} = 0 \tag{5.11}$$

for all $\tilde{H} \in F$. Now, by differentiating this equation with respect to $\tilde{H}$ at $\tilde{H} = H$ we can get solutions to certain inhomogeneous transport equations. What we then have to show is that the inhomogeneities obtained in this way cover all smooth densities which satisfy the universal condition (5.7). This is a kind of linear response theory.

Theorem 5.3.7. *Let X be a symplectic manifold, H a smooth real valued function on X and S a submanifold which is invariant under the Hamiltonian flow generated by H and on which the Hamiltonian vectorfield X_H is nondegenerate. If S is stably invariant in the sense of Definition 5.3.5, and S is either a Lagrangian submanifold, or has codimension 1, then the transport equation on S*

$$X_H a = b$$

has for every $b \in C^\infty(S)$ which satisfies

$$\int_S b \ \mu_S = 0 \tag{5.12}$$

a solution $a \in C^\infty(S)$.

Proof. We will first study the consequence of the condition on b more closely. By choosing an orientation on S, we can interpret $b\ \mathrm{d}\mu_S$ as a differential form on S (If S is not orientable, we still can interpret $b\ \mathrm{d}\mu_S$ as a differential form. However, its coefficients are sections in the line bundle which is associated with the orientation covering). Now by Poincaré duality, see, e.g., [BT82], it follows that for a closed compact S and a $\dim S$-form ω the equation

$$\int_S \omega = 0$$

implies that there exists a $(\dim S - 1)$-form σ with $\omega = \mathrm{d}\sigma$. Hence the condition 5.12 implies that there exists a $(\dim S - 1)$-form σ_b with

$$b\ \mu_S = \mathrm{d}\sigma_b\ .$$

This will allow us to localize the problem.

Now let $H_1 \in C^\infty(X)$ be a perturbation term and let us study

$$\tilde{H} = H_0 + \varepsilon H_1\ ,$$

which will be in F for for sufficiently small ε. Let us expand the quantities (5.9), (5.10) and the equation (5.11) in ε,

$$\mu_{\tilde{H}} = \mu_0 + \varepsilon\mu_1 + O(\varepsilon^2)\ ,$$
$$\tilde{X}_{\tilde{H}} = X_0 + \varepsilon X_1 + O(\varepsilon^2)\ ,$$

and

$$\mathcal{L}_{X_0}\mu_0 + \varepsilon(\mathcal{L}_{X_0}\mu_1 + \mathcal{L}_{X_1}\mu_0) + O(\varepsilon^2) = 0\ .$$

So with $X_0 = X_{H_0}$, $\mu_0 = \mu_S$ and Cartan's equation $\mathcal{L}_X = \mathrm{d}\iota_X + \iota_X\mathrm{d}$, where ι_X denotes the contraction with X, we obtain the equation

$$\mathcal{L}_{X_{H_0}}\mu_1 = -\mathcal{L}_{X_1}\mu_0 = -\mathrm{d}\iota_{X_1}\mu_0\ .$$

So if we can find for any $(\dim S - 1)$-form σ a perturbation H_1 such that

$$-\iota_{X_1}\mu_0 = \sigma + \mathrm{d}\omega$$

for some $(\dim S - 2)$-form ω, then we are done. But this is a local problem and basically linear.

Let us now come to the two special cases. We start with the case that $\dim S = \dim X - 1$. We can introduce local coordinates $z = (\hat{z}; \xi, x)$ such that S is defined by $x = 0$ and ξ is symplectically dual to x, where $\hat{z}$ are symplectic coordinates in $\mathbb{R}^{2d-2}$. That S is invariant under the flow generated by H_0 means that $H'_{0_\xi} = 0$. For a sufficiently small perturbation

$$H_\varepsilon(z) = H_0(\hat{z}, x) + \varepsilon H_1(\hat{z}, \xi, x)$$

we can write S_ε as a graph

$$S_\varepsilon = \{(\hat{z}; \xi, f_\varepsilon(\hat{z}, \xi))\}$$

with $f_\varepsilon(\hat{z}, \xi) = O(\varepsilon)$. Therefore, we get that

$$\Phi_\varepsilon^* = (I_{2d-1}, f_\varepsilon') ,$$

where f_ε' denotes the gradient with respect to $(\hat{z}, \xi)$. The Hamiltonian vectorfield on S_ε is

$$X_{H_\varepsilon} = X_{H_0}(\hat{z}; f_\varepsilon) + \varepsilon X_{H_1}(\hat{z}; \xi, f_\varepsilon) ,$$

and therefore

$$\Phi_\varepsilon^* X_{H_\varepsilon} = X_{H_0}(\hat{z}; f_\varepsilon) + \varepsilon \left[\hat{X}_{H_1}(\hat{z}; \xi, 0) + {H_1}'_x(\hat{z}; \xi, 0)\partial_\xi \right] + O(\varepsilon^2) ,$$

where $\hat{X}_{H_1}$ denotes the part of X_{H_1} in the symplectic subspace spanned by $\hat{z}$. Hence we get

$$X_1(\hat{z}; \xi) = \hat{X}_{H_1}(\hat{z}; \xi, 0) + {H_1}'_x(\hat{z}; \xi, 0)\partial_\xi .$$

Since the invariant density on S is $\mathrm{d}\hat{z} \wedge \mathrm{d}\xi$ and $\mathcal{L}_{\hat{X}_{H_1}} \mathrm{d}\hat{z} = 0$, we obtain

$$\mathcal{L}_{Y_0'} \mathrm{d}\hat{z} \wedge \mathrm{d}\xi = {H_1}''_{x,\xi}(\hat{z}; \xi, 0)\mathrm{d}\hat{z} \wedge \mathrm{d}\xi = \mathrm{d}\big({H_1}'_x \mathrm{d}\hat{z}\big) ,$$

so we have found that we can take

$$\sigma = {H_1}'_x \mathrm{d}\hat{z} .$$

Now we will study the case that S is Lagrangian. We choose local coordinates $(\xi, x) \in \mathbb{R}^d \oplus \mathbb{R}^d$ such that S is given by $x = 0$, and the Hamiltonian is $H_0(\xi, x) = \langle k, x \rangle$ with $k \in \mathbb{R}^d$ constant. We furthermore choose a family of perturbations of the form

$$H_\varepsilon(z) = \langle k, x \rangle + \varepsilon H_1(\xi, x) ,$$

and for sufficiently small ε, S_ε can be represented with a generating function,

$$S_\varepsilon = \{(\xi, \varphi(\varepsilon, \xi)')\} ,$$

with $\varphi(\varepsilon, \xi)' = O(\varepsilon)$. Then the linearized embedding is given by

$$\Phi_\varepsilon^* = (I_d, \varphi(\varepsilon, \xi)'') ,$$

and the Hamiltonian vectorfield on S_ε

$$X_{H_\varepsilon} = \langle k, \partial_\xi \rangle + \varepsilon \left[\langle \partial_x H_1(\xi, x), \partial_\xi \rangle - \langle \partial_\xi H_1(\xi, x), \partial_x \rangle \right] ,$$

and therefore

$$\Phi_\varepsilon^* X_{H_\varepsilon} = \langle k, \partial_\xi \rangle + \varepsilon \langle \partial_x H_1(\xi, 0), \partial_\xi \rangle + O(\varepsilon^2) .$$

So we have $X_1 = \partial_x H_1(\xi, 0)$, and this can be arbitrary. □

We have until now only discussed the existence of a solution to the transport equation, and not the uniqueness of the solution, if it exists. Since the difference of two solutions of the inhomogeneous transport equation is always a solution of the homogeneous transport equation, the dimension of space of solutions ist determined by the set of solutions of the homogeneous transport equation. The space of solutions is always at least one dimensional, since any constant multiple of the invariant measure is as well a solution. In the case of the Lagrangian tori which satisfy a Diophantine condition, these are all solutions, since the flow on the torus is uniquely ergodic then.

5.4 Construction of quasimodes

5.4.1 Quasimodes concentrated on invariant tori

In this subsection we will discuss some aspects of quasimode constructions on invariant tori, mainly with respect to the question of stability. Collecting the results from Section 3.1 and Section 5.3 we immediately get the following result.

Theorem 5.4.1. *Let $\mathcal{H} \in \Psi^0(m_{a,b})$ be a selfadjoint operator with principal symbol H_0. Assume that there exists an Lagrangian torus Λ which is invariant under the Hamiltonian flow Φ^t generated by H_0 and which satisfies the quantization condition* (3.13)

$$\frac{1}{2\pi}\Big(\lambda\Theta + \frac{\pi}{4}\alpha\Big) \in H^1(\Lambda, \mathbb{Z}) \ .$$

Then there exists a stable quasimode $(\psi(\mathcal{A}), E(\mathcal{A}))$ concentrated on Λ,

$$||[(\mathcal{H} + \lambda^{-1}\mathcal{A})\psi(\mathcal{A}) - E(\mathcal{A})\psi(\mathcal{A})|| \leq C(\mathcal{A})\lambda^{-2}$$

for all $\mathcal{A} \in \Psi^0(1)$, if and only if the frequency vector k of the flow on Λ satisfies the Diophantine condition

$$|\langle k, n\rangle| \geq C_k(1 + |n|)^{-K}$$

for some $C_K, K > 0$.

This theorem is an immediate consequence of the results of Section 3.1, especially equations (3.13), (3.15) and (3.16), and the discussion of the solvability of the transport equation (3.15) in example 5.3.3.

The main point we want to stress in this theorem is that if the Diophantine condition is not fulfilled, so if the frequencies are for instance linearly dependent over $\mathbb{Z}$, then there exist no stable quasimodes concentrated on Λ. Of course, this raises the question what happens with eigenfunctions or quasimodes concentrated on a rational torus when we add a small perturbation. If the subprincipal symbol of $\mathcal{H}$ is zero, which is for instance the case if we consider the Laplacian on some Riemannian manifold, and if $\mathcal{A} = 0$, then the transport equation can be trivially solved, and we get a quasimode of discrepancy $\sim \lambda^{-2}$.

The question how such states react to small perturbations have been studied for a class of systems in [FKT90, FKT91].

If the Diophantine condition on the torus is fulfilled, then Theorem 5.4.1 can be strengthend in at least two directions. First, the construction in Section 3.1 can be continued in order to compute higher order terms of the quasimode, and therefore we can obtain a discrepancy of order λ^{-N} for any $N \in \mathbb{N}$. Secondly, a more important observation [Col77, Laz93] is that we can relax the quantization condition. It is sufficient that there exists a $\delta(\lambda)$ with

$$\frac{1}{2\pi}\Big(\lambda\Theta + \frac{\pi}{4}\alpha\Big) - \delta(\lambda) \in H^1(\Lambda, \mathbb{Z}) \ ,$$

and

$$\delta(\lambda) = O(\lambda^{-\alpha})$$

for some $\alpha > 0$. Then the remaining constructions can be adapted to yield quasimodes with discrepancy of order λ^{-N} for any $N \in \mathbb{N}$. This is especially important in the case of a slightly perturbed integrable system, where by KAM theory a cantor set of invariant tori has survived, but maybe not the one satisfying a quantization condition, but some nearby ones.

5.4.2 Quasimodes concentrated on closed orbits

We will now discuss the construction of quasimodes concentrated on elliptic orbits. We will be sketchy, and mostly indicate the main ideas. The possibility of constructing quasimodes on elliptic periodic orbits is well known, see the part of Babich in [Fed99], for an overview of the work by the Russian school, and [GW76b, GW76a, Ral76, Ral79, PU93] for some other works.

We can use the results on the time evolution of coherent states to construct approximate solutions to the stationary Schrödinger equation which are concentrated on a periodic orbit. The basic idea is simply to launch a coherent state on the orbit and average over the time evolution. This is expected to yield an approximately invariant state, see also [PU93].

So let $\mathcal{H} \in \Psi^0(m_{a,b})$ be selfadjoint with principal symbol H_0 and choose $\psi \in L^2(M)$ with $\mathrm{FS}(\psi) = \{z\}$, where $z \in T^*M$ is periodic under the Hamiltonian flow generated by H_0 with period T. We associate with ψ a state

$$\psi_E := \frac{1}{T}\int_0^T \mathrm{e}^{\mathrm{i}\lambda t E}\mathcal{U}(t)\psi \ \mathrm{d}t \ , \tag{5.13}$$

where $E = H(z)$. Then we obtain

$$\begin{aligned}(\mathcal{H} - E)\psi_E &= \frac{1}{T}\int_0^T (\mathcal{H} - E)\mathrm{e}^{\mathrm{i}\lambda t E}\mathcal{U}(t)\psi \; \mathrm{d}t \\ &= \frac{1}{T}\int_0^T \frac{\mathrm{i}}{\lambda}\frac{\mathrm{d}}{\mathrm{d}t}\big(\mathrm{e}^{\mathrm{i}\lambda t E}\mathcal{U}(t)\psi\big) \; \mathrm{d}t \\ &= \frac{\mathrm{i}}{T\lambda}\big[\mathrm{e}^{\mathrm{i}\lambda T E}\mathcal{U}(T)\psi - \psi\big] \; ,\end{aligned}$$

and so our aim will be to choose the state ψ appropriately in order that the right-hand side becomes small. If we choose ψ to be a coherent state centered at z, $\psi = u_z^L(\lambda)$, then by Theorem 3.5.7 and Theorem 3.5.1 we have

$$\mathcal{U}(T)\psi = \mathrm{e}^{\mathrm{i}(\lambda\gamma(T)+\sigma(T))}u_{z(T)}^{\mathcal{S}(T)L}(\lambda) + O(\lambda^{-1/2}) \; ,$$

and hence with $z(T) = z$,

$$\mathrm{e}^{\mathrm{i}\lambda T E}\mathcal{U}(T)\psi - \psi = \mathrm{e}^{\mathrm{i}(\lambda[\gamma(T)+TE]+\sigma(T))}u_z^{\mathcal{S}(T)L}(\lambda) - u_z^L(\lambda) + O(\lambda^{-1/2}) \; .$$

So we get the two conditions

$$\mathcal{S}(T)L = L \tag{5.14}$$

and

$$\lambda[\gamma(T) + TE] + \sigma(T) = 2\pi k \; , \qquad k \in \mathbb{Z} \; ; \tag{5.15}$$

when these are fulfilled we have

$$||(\mathcal{H} - E)\psi_E|| = O(\lambda^{-3/2}) \; .$$

With

$$\gamma(T) = \int_0^T \big(\langle p, \dot{q}\rangle - H(p,q)\big) \; \mathrm{d}t = \int_{\gamma(E)} \langle p, \mathrm{d}q\rangle - ET$$

we can rewrite the second condition (5.15) as

$$\lambda\int_{\gamma(E)} \langle p, \mathrm{d}q\rangle + \sigma_{\gamma(E)} = 2\pi k \; , \qquad k \in \mathbb{Z} \; , \tag{5.16}$$

which has exactly the form of a Bohr-Sommerfeld quantization condition. This condition restricts the set of λ values to a sequence

$$\{\lambda_k(E)\}_{k\in\mathbb{N}}$$

satisfying (5.16). The only new thing compared to WKB and EBK quantization which appears here is that the Maslov index $\sigma_{\gamma(E)}$ is not an integer multiple of $\pi/4$, but can take arbitrary values in $\mathbb{R}$.

We will now study the first condition (5.14) more closely. It will turn out that this is the crucial condition which allows only elliptic orbits to be quantized in this way. The Lagrangian plane L defines the coherent state, hence it has to be positive, so the symplectic map $\mathcal{S}(T) : T_zT^*M \to T_zT^*M$ must leave a positive Lagrangian plane invariant. By the general classification of linear symplectic maps it follows that $\mathcal{S}(T)$ must be conjugated to an orthogonal matrix then, and has therefore only eigenvalues of modulus one, so the orbit is elliptic.

From a more general point of view, we can study the normal forms of the map $\mathcal{S}(T)$ for an arbitrary periodic orbit. There is always one invariant two dimensional symplectic eigenspace, spanned by the direction of the Hamiltonian vectorfield, and the direction perpendicular to the energy shell. So we can bring $\mathcal{S}(T)$ into a normal form

$$\mathcal{S}(T) = \begin{pmatrix} \begin{smallmatrix} 1 & u \\ 0 & 1 \end{smallmatrix} & 0 \\ 0 & \mathcal{S}_P \end{pmatrix} . \tag{5.17}$$

Lemma 5.4.2. *Let $\mathcal{S}$ be a symplectic matrix of the form* (5.17) *and let L be a positive Lagrangian plane with*

$$\mathcal{S}L = L ,$$

then $u = 0$ and all eigenvalues of $\mathcal{S}_P$ have modulus one.

We summarize the results of this simple approach in the following theorem.

Theorem 5.4.3. *Let $\mathcal{H} \in \Psi^0(m_{a,b})$ be selfadjoint, and assume that $z \in T^*M$ is periodic with period T under the Hamiltonian flow generated by the principal symbol H_0 of $\mathcal{H}$, and let $E = H_0(z)$. If the orbit through z is elliptic and the Poincaré map is of the form* (5.17) *with $u = 0$, then the state* (5.13) *with $\psi = u_z^L$ satisfies*

$$||(\mathcal{H} - E)\psi_E|| = O(\lambda^{-3/2}) ,$$

if $\mathcal{S}(T)L = L$ and λ satisfies the quantization condition

$$\lambda \int_{\gamma(E)} \langle p, \mathrm{d}q\rangle + \sigma_{\gamma(E)} = 2\pi k , \qquad k \in \mathbb{Z} .$$

The discrepancy of this quasimode construction is quite large, and one can improve the result by considering higher order terms in the time evolution, see Theorem 3.5.9. This would then lead to transport equations, whose solvability will pose additional conditions on the orbit.

But in order to follow this approach further we would have to make the higher order terms in the time evolution more explicit. Since we want to avoid this, we will now sketch a different approach to the construction of quasimodes concentrated on elliptic orbits, which is based on local normal forms of the Hamiltonian near the orbit, and is closer to our approach to derive quasimodes concentrated on invariant tori.

It is useful to choose appropriate local coordinates around the given periodic orbit γ. In the neighborhood of the orbit one can always choose coordinates $(h, s; p, q) \in I \times [0, T] \times U \subset \mathbb{R} \times [0, L] \times \mathbb{R}^{2d-2}$ such that the orbit is given by $h = 0, p = q = 0$, T is the period of the orbit, and the Hamilton function is of the form

$$H_0(h, s, p, q) = f(h) + \sum_{j=1}^{d-1} \frac{\omega_j}{2}(p_j^2 + q_j^2) \ , + \Psi_3(h, s; p, q) \tag{5.18}$$

where $\Psi_3(h, s; p, q)$ is a function which is T-periodic in s and of third order in p and q, see, e.g., [AKN97]. The constants ω_j are called characteristic frequencies of the orbit. One says that the characteristic frequencies ω_j satisfy a resonance condition of order l, if there exist $k_1, k_2, \dots, k_d \in \mathbb{Z}$ with

$$k_1\omega_1 + k_2\omega_2 + \dots + k_{d-1}\omega_{d-1} + k_d = 0$$

and $|k_1| + |k_2| + \dots + |k_d| = l$. If the characteristic frequencies of an elliptic orbit do not satisfy a resonance condition of order l for all $l \leq L$, then the orbit is called nonresonant up to order L. Under this condition one can find local symplectic coordinates near the orbit in which the Hamilton function is in Birkhoff normal form of degree L, which means that

$$H_0(h, s, p, q) = f(h) + H_0^{(L)}(p, q) + \Psi_{L+1}(h, s; p, q) \ , \tag{5.19}$$

where $\Psi_{L+1}(h, s; p, q) = O((|p| + |q|)^{L+1})$ and $H_0^{(L)}(p, q)$ is polynomial of degree $[L/2]$ in the variables $\rho_j := p_j^2 + q_j^2$, and whose lowest order term is again given by

$$\sum_{j=1}^{d-1} \frac{\omega_j}{2}(p_j^2 + q_j^2) \ .$$

Since by the theory of Fourier integral operators we can quantize canonical transformations, we can map the eigenvalue problem microlocally near the elliptic orbit to an eigenvalue problem with the operator given by the Hamiltonian in Birkhoff normal form plus higher order corrections due to subprincipal and higher terms in λ.

In order to simplify the following discussions, we will assume that $f(h)$ is linear in h,

$$f(h) = h \ , \tag{5.20}$$

which means that the period is constant on the orbit cylinder through the periodic orbit. For instance if the system is scaling this is the case for all orbits. Compared to the previous discussion, this is equivalent to the condition $u = 0$ in (5.17).

We first discuss the case that the remainder $\Psi_3(h, s; p, q)$ in (5.18) vanishes and no higher order terms in λ are present. Then the corresponding Hamilton operator is given by

$$\mathcal{H} = \frac{1}{\mathrm{i}\lambda}\partial_s + \sum_{j=1}^{d-1}\frac{\omega_j}{2}\bigg(-\frac{1}{\lambda^2}\partial_{q_j}^2 + q_j^2\bigg) .$$

If we insert the ansatz

$$\psi_E(s,q) = \frac{1}{L^{1/2}}\bigg(\frac{\lambda}{\pi}\bigg)^{(d-1)/4} \mathrm{e}^{\mathrm{i}\lambda[\phi(s)+\mathrm{i}\sum_j q_j^2/2]} ,$$

where the prefactor ensures normalization, into the stationary Schrödinger equation, we get with

$$\bigg(-\frac{1}{\lambda^2}\partial_{q_j}^2 + q_j^2\bigg)\psi_E(s,q) = \frac{1}{\lambda}\psi_E(s,q)$$

that

$$(\mathcal{H}-E)\psi_E(s,q) = \bigg[\phi'(s) + \frac{1}{\lambda}\sum_{j=1}^{d-1}\frac{\omega_j}{2} - E\bigg]\psi_E(s,q) .$$

And in order that the right-hand side vanishes, we have to set

$$\phi(s) = \bigg(E - \frac{1}{\lambda}\sum_{j=1}^{d-1}\frac{\omega_j}{2}\bigg)s$$

and thus have obtained a solution of the Schrödinger equation. Only one condition remains because the solution $\psi_E(s,q)$ has to be periodic in s with period T, and in order to ensure this we have to require that

$$\lambda\bigg(E - \frac{1}{\lambda}\sum_{j=1}^{d-1}\frac{\omega_j}{2}\bigg)T = 2\pi k$$

for $k \in \mathbb{Z}$. This is the quantization condition by which a discrete set of eigenvalues is selected. In order to compare this condition with (5.15), we use that with our choice, (5.20), of $f(h)$ we have for the reduced action

$$S = \int_0^T h \,\mathrm{d}t = hT = ET ,$$

and furthermore the Maslov index is given by $\sum_{j=1}^{d-1}\frac{\omega_j}{2}T$, so the two conditions indeed coincide.

Higher order terms in the Hamiltonian can now be considered by modifying the ansatz appropriately,

$$\psi_E(s,q) = \frac{1}{L^{1/2}}\left(\frac{\lambda}{\pi}\right)^{(d-1)/4} a(\lambda,s,q)\mathrm{e}^{\lambda\mathrm{i}[\phi(s)+\mathrm{i}\sum_j q_j^2/2]} .$$

Let us denote the quantizations of the monomials $(p_j^2+q_j^2)$ in the Birkhoff normal form by

$$\mathcal{P}_j := -\frac{1}{\lambda^2}\,\partial_{q_j}^2 + q_j^2 ,$$

then we have

$$\mathcal{P}_j a\mathrm{e}^{\lambda\mathrm{i}[\phi(s)+\mathrm{i}\sum_j q_j^2/2]} = \left[-\frac{1}{\lambda^2}\,\partial_{q_j}^2 a + \frac{2}{\lambda} q_j\partial_{q_j} a + \frac{1}{\lambda} a\right]\mathrm{e}^{\lambda\mathrm{i}[\phi(s)+\mathrm{i}\sum_j q_j^2/2]} .$$

By iteration we see that

$$\mathcal{P}_{j_1}\cdots\mathcal{P}_{j_l} a\mathrm{e}^{\lambda\mathrm{i}[\phi(s)+\mathrm{i}\sum_j q_j^2/2]} = \left[\frac{1}{\lambda^k}(a+O(q)) + O(\lambda^{-k-1})\right]\mathrm{e}^{\lambda\mathrm{i}[\phi(s)+\mathrm{i}\sum_j q_j^2/2]} ,$$

for every $k\in\mathbb{N}$.

If we now apply the full Hamiltonian to the modified ansatz, and make for the energy an ansatz as an asymptotic series $E = E_0 + \frac{1}{\lambda}E_1\cdots$, we obtain

$$\begin{aligned}(\mathcal{H} - E_0 - \lambda^{-1}E_1)\psi_E(s,q) = \Bigg[&\partial_s\phi\, a + \frac{1}{\mathrm{i}\lambda}\partial_s a + \sum_{j=1}^{d-1}\frac{\omega_j}{2}\left(\frac{2}{\lambda}\, q_j\partial_j a + \frac{1}{\lambda}\, a\right)\\ &+ \frac{1}{\lambda}H_1 a - E_0 a - \frac{1}{\lambda}E_1 + O(\lambda^{-2})\Bigg]\mathrm{e}^{\lambda\mathrm{i}[\phi(s)+\mathrm{i}\sum_j q_j^2/2]} ,\end{aligned}$$

and if λ and E_0 satisfy the quantization condition, only terms of order λ^{-1} remain ,

$$\frac{1}{\mathrm{i}}\partial_s a + \sum_{j=1}^{d-1}\omega_j q_j\partial_j a + (H_1 - E_1)a = 0 .$$

This is a transport equation for a half-density in the tangent planes of the complex Lagrangian ideal, and it is solvable if the ideal is stably invariant and if the higher order quantization condition,

$$E_1 = \frac{1}{L}\int_0^L H_1\ \mathrm{d}s ,$$

is fulfilled. In a similar way higher order contributions can be treated, and in this way one could prove the following result.

Theorem 5.4.4. *Let $\mathcal{H} \in \Psi^0(m_{a,b})$ be selfadjoint, and assume that γ is an elliptic orbit of the Hamiltonian flow generated by the principal symbol of $\mathcal{H}$. If the principal symbol has a local normal form* (5.19)*, with linear f,* (5.20)*, and if the characteristic frequencies do not satisfy a resonance condition up to order L, then one can construct a quasimode of order λ^{-L} concentrated on γ,*

$$||(\mathcal{H} - E(\lambda))\psi|| = O(\lambda^{-L}) \ ,$$

where in Birkhoff coordinates

$$\psi = a(\lambda, s, q)\mathrm{e}^{\mathrm{i}\lambda[\phi(s)+\mathrm{i}\sum_j q_j^2/2]} \ ,$$

and

$$E = E_0 + \lambda^{-1}E_1 + \lambda^{-2}E_2 + \cdots \ ,$$

with

$$\lambda\left(E_0 - \frac{1}{\lambda}\sum_{j=1}^{d-1}\frac{\omega_j}{2}\right)L = 2\pi k$$

for $k \in \mathbb{Z}$ and

$$E_1 = \frac{1}{L}\int_0^L H_1 \ \mathrm{d}s \ .$$

So for nonresonant elliptic orbits quasimodes of arbitrary order can be constructed. The question remains what happens for resonant orbits. They play an important role when on studies families of systems since under a change of the parameters of a system typically bifurcations of orbits occur, where orbits become resonant and then bifurcate into new orbits. In fact this is the basic mechanism how elliptic periodic orbits vanish and hyperbolic ones appear in the passage from a system with mixed phase space to a hyperbolic system. The general methods developed in Chapter 3 should allow similar studies of quasimodes near bifurcations and on lower dimensional tori.

5.5 Quasimodes associated with invariant sets in phase space

In this section we will use the approximate projection operators of Chapter 4.3.1 to construct quasimodes concentrated on stably invariant subsets of phase space. A similar construction in a KAM situation has been done by Shnirelman in [Shn].

The main idea is fairly simple. Given an invariant open domain D in phase space, then the techniques of Chapter 4.3.1 allow to associate an approximate projection operator $\boldsymbol{\pi}_D$

with it, which approximately commutes with the Hamilton operator $\mathcal{H}$. In order to clarify the main idea, imagine for a moment that it commutes exactly,

$$[\mathcal{H}, \boldsymbol{\pi}_D] = 0 \ .$$

Then we could choose an orthonormal basis of joint eigenfunctions ψ_n of both operators, i.e.

$$\mathcal{H}\psi_n = E_n\psi_n \quad \text{and} \qquad \boldsymbol{\pi}_D\psi_n = \varepsilon_n\psi_n \ ,$$

and since $\boldsymbol{\pi}_D$ is an approximate projection operator its eigenvalues ε_n cluster around 0 and 1. Clearly the eigenfunctions corresponding to $\varepsilon_n \approx 1$ are concentrated in D, whereas the ones corresponding to $\varepsilon_n \approx 0$ are concentrated in the complement of D. The Szegö limit theorem, Theorem 4.2.3, allows, furthermore, to determine the asymptotic number $N_D(\lambda)$ of eigenfunctions concentrated in D. Since

$$\sum_{E_n\in I} \langle \psi_n, \boldsymbol{\pi}_D\psi_n\rangle = \sum_{E_n\in I} \varepsilon_n \sim N_D(\lambda) \ ,$$

we get

$$\lim_{\lambda\to\infty} \frac{N_D(\lambda)}{N(\lambda)} = \frac{\mathrm{vol}(D\cap\Sigma_E)}{\mathrm{vol}(\Sigma_E)} \ .$$

Hence the fraction of eigenfunctions which is concentrated in D is proportional to the volume of D. This construction breaks down if $\mathcal{H}$ and $\boldsymbol{\pi}_D$ no longer commute.

The construction of approximate projection operators associated with open stably invariant sets gives immediately the existence of quasimodes concentrated on these sets.

Theorem 5.5.1. *Let $\mathcal{H} \in \Psi^0(m_{a,b})$ be a selfadjoint operator with principal symbol H_0 and let $D \subset T^*M$ be an open stably invariant subset whose closure is compact. Then*

$$||(\mathcal{H} - E_n)\boldsymbol{\pi}_D^{(N)}\psi_n|| \leq C_N\lambda^{-3/2-N} \ .$$

Proof. In fact this is a corollary of Theorem 4.3.7; we have

$$[\mathcal{H}, \boldsymbol{\pi}_D^{(N)}]\psi_n = (\mathcal{H} - E_n)\boldsymbol{\pi}_D^{(N)}\psi_n \ ,$$

and so with $||\psi_n|| = 1$ we get

$$||(\mathcal{H} - E_n)\boldsymbol{\pi}_D^{(N)}\psi_n|| = ||[\mathcal{H}, \boldsymbol{\pi}_D^{(N)}]\psi_n|| \leq ||[\mathcal{H}, \boldsymbol{\pi}_D^{(N)}]|| \ ,$$

and the commutator was estimated in Theorem 4.3.7. □

In order to estimate how many quasimodes we obtain from this result, we have to estimate $||\boldsymbol{\pi}_D^{(N)}\psi_n||$ from below, because if the norm tends to zero sufficiently fast, then the estimate in the theorem is trivially fulfilled.

By the Szegö limit theorem we have

$$\lim_{\lambda\to\infty} \frac{1}{N_I} \sum_{E_n \in I} ||\boldsymbol{\pi}_D^{(N)} \psi_n||^2 = \frac{\mathrm{vol}(D \cap \Sigma_E)}{\mathrm{vol}\, \Sigma_E} \;, \tag{5.21}$$

with $I = [E - \alpha/\lambda, E + \alpha/\lambda]$ and $N_I := \#\{E_n \in I\}$. This formula allows us to derive some simple estimates on the number of eigenfunctions which are concentrated entirely in D or living partly in D, respectively.

If ψ_n is concentrated in D, then $\boldsymbol{\pi}_D \psi_n - \psi_n \to 0$ for $\lambda \to \infty$ and hence

$$||\boldsymbol{\pi}_D \psi_n|| \to 1 \;, \quad \text{for } \lambda \to \infty \;.$$

Therefore, (5.21) yields an upper bound for the number

$$N_I^{\mathrm{int}}(D) := \#\{E_n \in I \,;\, \boldsymbol{\pi}_D \psi_n = \psi_n + o(1)\} \;,$$

$$\lim_{\lambda\to\infty} \frac{N_I^{\mathrm{int}}(D)}{N_I} \leq \frac{\mathrm{vol}(D \cap \Sigma_E)}{\mathrm{vol}\, \Sigma_E} \;.$$

On the other hand, we can estimate for every $1 > \delta > 0$ the number of eigenfunctions with $||\boldsymbol{\pi}_D \psi_n|| \geq \delta$,

$$N_I^{\mathrm{tot}}(D, \delta) := \#\{E_n \in I \,;\, ||\boldsymbol{\pi}_D \psi_n|| \geq \delta\} \;,$$

i.e. the ones of which at least a part of relative fraction δ lives on D, from below by

$$\lim_{\lambda\to\infty} \frac{N_I^{\mathrm{tot}}(D, \delta)}{N_I} \geq \frac{\mathrm{vol}(D \cap \Sigma_E)}{\mathrm{vol}\, \Sigma_E} \;.$$

The eigenfunctions which satisfy $||\boldsymbol{\pi}_D \psi_n|| \geq \delta$ for a $\delta > 0$, can of course be used to define quasimodes

$$\phi_n := \frac{1}{||\boldsymbol{\pi}_D^{(N)} \psi_n||} \boldsymbol{\pi}_D^{(N)} \psi_n \;,$$

which satisfy by Theorem 5.5.1

$$||(\mathcal{H} - E_n)\phi_n|| \leq \delta^{-1} C_N \lambda^{-3/2-N} \;,$$

and are normalized. By the previous discussion we have a lower bound on their number. But apart from this not very much information can be extracted from them which goes beyond the general time evolution estimates for states concentrated in D. In contrast to the explicit quasimode constructions in the last section, we get no further information on the eigenvalues, nor do we have an explicit formula for the quasimodes.

But if the flow on $D \cap \Sigma_E$ is ergodic, then the local quantum ergodicity theorem implies quantum ergodicity for the quasimodes.

Theorem 5.5.2. *Let $\mathcal{H} \in \Psi^0(m_{a,b})$ be selfadjoint, and assume D is an invariant open domain which is stably invariant under the flow generated by the principal symbol H_0 of $\mathcal{H}$. Let $\boldsymbol{\pi}_D^{(N)}$ be the approximate projection operator constructed in Theorem 4.3.7 and define*

$$\phi_{n_j} := \frac{1}{||\boldsymbol{\pi}_D^{(N)}\psi_{n_j}||}\,\boldsymbol{\pi}_D^{(N)}\psi_{n_j}$$

for the subsequence ψ_{n_j} of eigenfunctions which satisfy $||\boldsymbol{\pi}_D^{(N)}\psi_{n_j}|| \geq \delta$ for some fixed $\delta > 0$. If the flow is ergodic on $D \cap \Sigma_E$, then

$$\lim_{\lambda\to\infty} \frac{1}{N_I} \sum_{E_{n_j}\in I} |\langle \phi_{n_j}, \mathcal{A}\phi_{n_j}\rangle - \overline{\sigma(\mathcal{A})}^D| = 0 \tag{5.22}$$

for all $\mathcal{A} \in \Psi^0(1)$, and where $\overline{\sigma(\mathcal{A})}^D := \frac{1}{\mathrm{vol}(D\cap\Sigma_E)}\int_{D\cap\Sigma_E} \sigma(\mathcal{A})\,\mathrm{d}\mu_E$.

As in the standard quantum ergodicity theorem, it follows from (5.22) that almost all quasimodes concentrated on $D \cap \Sigma_E$ tend to be equidistributed on $D \cap \Sigma_E$.

Proof. We will use Theorem 4.4.2 with $\mathrm{Op}^{AW}[\nu] = \boldsymbol{\pi}_D^{(N)}$. Define

$$\mathcal{B}_{\mathcal{A}} := \boldsymbol{\pi}_D\mathcal{A}\boldsymbol{\pi}_D - \boldsymbol{\pi}_D\mathcal{A}$$

then by Theorem 4.2.3 we have

$$\lim_{\lambda\to\infty} \frac{1}{N_I} \sum_{E_n\in I} \langle \psi_n, |\mathcal{B}_{\mathcal{A}}|\psi_n\rangle = 0\ ,$$

and using this relation with $\mathcal{A}$ and $\mathcal{A} = 1$ we obtain

$$\begin{aligned}
&\lim_{\lambda\to\infty} \frac{1}{N_I} \sum_{E_{n_j}\in I} |\langle \phi_{n_j}, \mathcal{A}\phi_{n_j}\rangle - \overline{\sigma(\mathcal{A})}^D| \\
&\leq \lim_{\lambda\to\infty} \frac{1}{N_I} \sum_{E_{n_j}\in I} \frac{1}{||\boldsymbol{\pi}_D\psi_{n_j}||^2} |\langle \boldsymbol{\pi}_D\psi_{n_j}, \mathcal{A}\boldsymbol{\pi}_D\psi_{n_j}\rangle - \langle \boldsymbol{\pi}_D\psi_{n_j}, \boldsymbol{\pi}_D\psi_{n_j}\rangle\overline{\sigma(\mathcal{A})}^D| \\
&\leq \frac{1}{\delta}\lim_{\lambda\to\infty} \frac{1}{N_I} \sum_{E_{n_j}\in I} |\langle \boldsymbol{\pi}_D\psi_{n_j}, \mathcal{A}\boldsymbol{\pi}_D\psi_{n_j}\rangle - \langle \boldsymbol{\pi}_D\psi_{n_j}, \boldsymbol{\pi}_D\psi_{n_j}\rangle\overline{\sigma(\mathcal{A})}^D| \\
&\leq \frac{1}{\delta}\lim_{\lambda\to\infty} \frac{1}{N_I} \sum_{E_n\in I} |\langle \psi_n, \boldsymbol{\pi}_D\mathcal{A}\psi_n\rangle - \langle \psi_n, \boldsymbol{\pi}_D\psi_n\rangle\overline{\sigma(\mathcal{A})}^D| = 0
\end{aligned}$$

□

If Conjecture 5.2.5 were true, then we would get as a corollary of Theorem 5.5.1 that generically a subsequence of eigenfunctions of density $\frac{\mathrm{vol}(D\cap\Sigma_E)}{\mathrm{vol}(\Sigma_E)}$ is semiclassically concentrated on each stably invariant domain D. This would be a rigorous confirmation of the general believe, going back at least to Percival [Per73], that the set of eigenfunctions split into subsets living semiclassically in the different invariant regions in phase space.

Appendix A

Densities and half-densities

In microlocal analysis and in semiclassics it is often useful to work with densities and half-densities instead of functions. We will here collect some of their properties and indicate some applications, mainly taken from [BW97, GS77, Hör85a].

A.1. Definition. *Let E be a vector space (over $\mathbb{R}$ or $\mathbb{C}$) and α a complex number. An α-density ν on E is a map*

$$\underbrace{E \times E \times \cdots \times E}_{\dim E \text{ times}} \longrightarrow \mathbb{C}$$
$$\hat{e} = (e_1, \dots, e_d) \mapsto \nu(e)$$

which satisfies for every $A \in \mathrm{GL}(E)$

$$\nu(A\hat{e}) = |\det A|^{\alpha} \nu(\hat{e}) \;, \tag{A.1}$$

where $A\hat{e} = (Ae_1, \dots, Ae_d)$. The space of α-densities on E will be denoted by $\Omega_\alpha(E)$.

It is clear that $\nu(\hat{e}) = 0$ if the vectors $(e_1, \dots, e_d)$ are linearly dependent, i.e. if they do not form a basis of E, because then they can be written as the image of a basis $\hat{f}$ under a degenerate map $A \in \mathrm{GL}(E)$, $\hat{e} = A\hat{f}$, and then (A.1) gives $\nu(\hat{e}) = \nu(A\hat{f}) = |\det A|^{\alpha}\nu(\hat{f}) = 0$ since $\det A = 0$. Since $\mathrm{GL}(E)$ acts transitively on the set of bases of E, the space of α-densities on E is one-dimensional. The 1-densities can be thought of as giving an assignment of volume to the parallel-epiped spanned by a basis.

We will summarize some properties of α-densities in the following lemma.

A.2. Lemma. *(1) Let $\nu \in \Omega_\alpha(E)$, then for $\beta \in \mathbb{C}$ $\nu^\beta \in \Omega_{\alpha\beta}(E)$.*

(2) A linear map $T : E \to E^*$ induces an α-density on E given by

$$\nu_T(\hat{e}) := |\det\langle Te_i, e_j\rangle|^{\alpha/2} \;,$$

hence every bilinear form ω on E induces an α-density on E. In particular, it follows that every symplectic vector space carries a natural 1-density.

(3) *Multiplication of densities is defined by multiplication of their values and hence gives a map*

$$\Omega_\alpha(E) \times \Omega_\beta(E) \to \Omega_{\alpha+\beta}(E) \ .$$

(4) *An isomorphism* $A : E \to F$ *induces an isomorphism on* α*-densities,* $A_* : \Omega_\alpha(E) \to \Omega_\alpha(F)$*, defined as*

$$A_*\nu(\hat{f}) := \nu(A^{-1}\hat{f}) \ .$$

(5) *There is a natural map*

$$\Omega_\alpha(E) \to \Omega_{-\alpha}(E^*) \ ,$$

defined by associating to each basis $\hat{e}$ *its dual basis* $\hat{e}^*$*.*

(6) *More generally, every exact sequence of vector spaces*

$$0 \to F \to E \to G \to 0$$

defines a natural isomorphism

$$\Omega_\alpha(F) \otimes \Omega_\alpha(G) \backsimeq \Omega_\alpha(E) \ .$$

Proof. (1) to (4) are obvious. To show (5), let $\nu \in \Omega_\alpha(E)$ and let $\hat{e^*}$ be a basis of E^*. We claim that $\nu^* \in \Omega_{-\alpha}$ where ν^* is defined by

$$\nu^*(\hat{e^*}) := \nu(\hat{e}) \ .$$

The dual basis is defined by $\langle e_i^*, e_j\rangle = \delta_{ij}$ and therefore, if $A^* : E^* \to E^*$ is dual to $A : E \to E$ in the sense that $\langle A^*e, Af\rangle = \langle e, f\rangle$ for all $e, f \in E$, then $\det A = (\det A^*)^{-1}$, hence

$$\nu^*(A^*\hat{e^*}) = |\det A^*|^{-\alpha}\nu^*(\hat{e^*})$$

for all $A^* \in \mathrm{GL}(E^*)$.

□

Let M be a C^∞ manifold, then the bundle of α-densities on M is given by assigning to each tangentspace T_xM the space of α-densities $\Omega_\alpha(T^*M)$; we will denote this bundle by $\Omega_\alpha(M)$. The sections of this bundle will be called α-densities on M. Let $u(x)$ be such a section, then under a change of coordinates $x \mapsto y(x)$, it becomes multiplied by a factor

$$\left|\det \frac{\partial y_i}{\partial x_j}\right|^\alpha \ .$$

For 1-densities the integral is defined naturally: let $M \to U$ be a chart, and let $|\mathrm{d}x|$ be the Lebesgue-density in this local coordinates. Every density with support in U can then be written as $u(x)|\mathrm{d}x|$ and the integral is defined as

$$\int u(x)\ \mathrm{d}x\ .$$

The transformation properties of 1-densities ensures that this is well defined. Since 1-densities can be integrated, we get a natural duality between α-densities and $(1-\alpha)$-densities. The set of 1/2-densities therefore carries a natural pre-Hilbert space structure, and its completion defines an intrinsic Hilbert space on every manifold.

The theory of distributions naturally leads as well to densities. If we define a space of distributions on a manifold as the dual-space to the smooth functions, then we have a natural embedding of the smooth 1-densities with compact support into this distribution space. Therefore it is natural to call these distributions generalized 1-densities. On the other hand, we can look at the dual space to the smooth 1-densities, this will have embedded the smooth functions in a natural way. Now, if one wants to have dual objects with the same transformation properties, it is again natural to consider 1/2-densities.

Appendix B

Gauss transforms

In semiclassics one often has to treat integrals of the form

$$\int e^{-\langle x,Qx\rangle/2} f(x)\ \mathrm{d}x\ ,$$

where Q is a symmetric nondegenerate quadratic form with $\operatorname{Re} Q \geq 0$, and f some smooth function. The basic trick leading to an asymptotic evaluation of such an integral is the use of the Fouriertransformation, which gives for smooth and sufficiently fast decaying functions f the following result.

B.1. Lemma. *Let Q be a quadratic nondegenerate $d \times d$ matrix such that $\operatorname{Re}(\langle x, Qx\rangle) \geq 0$, and let $f \in \mathcal{S}(\mathbb{R}^d)$ then*

$$\int e^{-\langle x,Qx\rangle/2} f(x)\ \mathrm{d}x = \frac{1}{\sqrt{\det(Q/2\pi)}} e^{-\langle D_x, Q^{-1}D_x\rangle/2} f(x)|_{x=0}\ , \tag{B.1}$$

where the operator $e^{-\langle D_x, Q^{-1}D_x\rangle/2}$ is defined by $e^{-\langle D_x, Q^{-1}D_x\rangle/2} e^{i\langle x,\xi\rangle} = e^{-\langle \xi, Q^{-1}\xi\rangle/2} e^{i\langle x,\xi\rangle}$.

Proof. The proof just follows from the formula for the Fourier transform of a Gaussian function. Using

$$e^{-\langle x,Qx\rangle/2} = \frac{1}{(2\pi)^d} \frac{1}{\sqrt{\det(Q/2\pi)}} \int e^{-\langle \xi, Q^{-1}\xi\rangle/2} e^{i\langle x,\xi\rangle}\ \mathrm{d}\xi\ ,$$

see Theorem D.2, and the Fourier inversion formula, one gets

$$\begin{aligned}\int \mathrm{e}^{-\langle x,Qx\rangle/2} f(x)\ \mathrm{d}x &= \frac{1}{(2\pi)^d}\frac{1}{\sqrt{\det(Q/2\pi)}}\iint \mathrm{e}^{-\langle \xi,Q^{-1}\xi\rangle/2}\mathrm{e}^{\mathrm{i}\langle x,\xi\rangle} f(x)\ \mathrm{d}x\mathrm{d}\xi \\ &= \frac{1}{\sqrt{\det(Q/2\pi)}}\int \mathrm{e}^{-\langle \xi,Q^{-1}\xi\rangle/2}\check{f}(\xi)\ \mathrm{d}\xi \\ &= \frac{1}{\sqrt{\det(Q/2\pi)}}\int \mathrm{e}^{-\langle D_x,Q^{-1}D_x\rangle/2}\mathrm{e}^{-\mathrm{i}\langle x,\xi\rangle}\check{f}(\xi)\ \mathrm{d}\xi|_{x=0} \\ &= \frac{1}{\sqrt{\det(Q/2\pi)}}\mathrm{e}^{-\langle D_x,Q^{-1}D_x\rangle/2}\int \mathrm{e}^{-\mathrm{i}\langle x,\xi\rangle}\check{f}\ \mathrm{d}\xi|_{x=0} \\ &= \frac{1}{\sqrt{\det(Q/2\pi)}}\left[\mathrm{e}^{-\langle D_x,Q^{-1}D_x\rangle/2} f\right](0)\ .\end{aligned}$$

□

In order to make use of the formula (B.1) one would like to develop the exponential into a series, to get

$$\frac{1}{\sqrt{\det(Q/2\pi)}}\mathrm{e}^{-\langle D_x,Q^{-1}D_x\rangle/2} f(x)|_{x=0} = \frac{1}{\sqrt{\det(Q/2\pi)}}\sum_{j=0}^{\infty}\frac{1}{j!}\left[-\langle D_x,Q^{-1}D_x\rangle/2\right]^j f(0)\ .$$

In order to make sense of this series, and to extend the range of functions f for which it is valid, one needs estimates on the remainder term if one truncates the sum. The following result is quoted from [Hör83, Lemma 7.6.4 and Theorem 7.6.5].

B.2. Theorem. *Let* $\mathrm{Re}\, Q^{-1} \geq 0$ *and* $||Q^{-1}|| \leq 1$, *and let* s *be an integer* $> d/2$. *Then we have for any integer* $k \geq s$ *that* $\mathrm{e}^{-\langle D_x,Q^{-1}D_x\rangle/2} f(x)$ *is continuous and*

$$\left|\mathrm{e}^{-\langle D_x,Q^{-1}D_x\rangle/2} f(x) - \sum_{j<k}\frac{1}{j!}\left[-\langle D_x,Q^{-1}D_x\rangle/2\right]^j f(x)\right| \leq C_k ||Q^{-1}||^k \sum_{|\alpha|\leq s+2k}\sup|D^\alpha f|$$

if $f \in C^{s+2k}$ *such that the right-hand side is finite. At Euclidean distance* $d(x)$ *from* $\mathrm{supp}\, f$ *greater than* 1, *the bound*

$$\left|\mathrm{e}^{-\langle D_x,Q^{-1}D_x\rangle/2} f(x)\right| \leq C_k ||Q^{-1}||^k d(x)^{-(k-s)} \sum_{|\alpha|\leq s+2k}\sup|D^\alpha f|$$

is valid.

In the applications, Q will often be of the form $Q = \lambda B$ with $\lambda \in \mathbb{R}$ and one is looking for the limit $\lambda \to \infty$. Then we have $||Q^{-1}|| = \lambda^{-1}||B^{-1}||$ and the formulas can be read as asymptotic expansions for $\lambda \to \infty$.

These estimates are the basis of many results in the theory of pseudodifferential operators, where many results e.g., the product formula, are given in terms of Gaussian integrals containing symbols, and the above estimates then show that these integral formulas define again symbols.

As an example, assume that $a \in S^0(1)$, i.e. there exist for every $\alpha \in \mathbb{Z}_+^d$ a constant C_α with

$$|\partial_x^\alpha a(\lambda, x)| \leq C_\alpha \ ,$$

and consider the integral

$$b(x) := \left(\frac{\lambda}{2\pi}\right)^{d/2} \int \mathrm{e}^{\lambda \mathrm{i}\langle x, Bx\rangle/2} a(x) \ \mathrm{d}x \ ,$$

where B is non-degenerate and has positive imaginary part. Then it follows from Theorem B.2 that $b \in S^0(1)$ and that the corresponding expansion obtained by expanding the exponential function defines an asymptotic expansion of b in $S^0(1)$.

Appendix C

The Malgrange preparation theorem

Let $f(t)$ be a C^∞-function of $t \in \mathbb{R}$ which has a multiple zero at $t = 0$:

$$f(0) = f'(0) = \cdots = f^{(k-1)}(0) = 0 \ , \quad f^{(k)}(0) \neq 0 \ .$$

Then it follows from Taylor's formula that there is a smooth function $c(t)$ with $c(0) \neq 0$, such that in a neighborhood of $t = 0$

$$f(t) = c(t) t^k \ .$$

Given an arbitrary C^∞ function $g(t)$, we want to study the question to what extent it can be written as a multiple of $f(t)$. The Taylor expansion gives $g(t) = \sum_{j=0}^{k-1} t^j r_j + r(t)$ with $r(t) = O(t^k)$, which means that $q(t) := r(t)/f(t)$ is well defined and bounded in a neighborhood of $t = 0$. Hence we can represent any $g(t) \in C^\infty(\mathbb{R})$ in a neighborhood of $t = 0$ as

$$g(t) = q(t) f(t) + \sum_{j=0}^{k-1} t^j r_j \ ,$$

with $q(t)$ locally in $C^\infty(\mathbb{R})$, that means we can divide $g(t)$ by $f(t)$ modulo a remainder which is a polynomial in t of order $k-1$.

All this is trivial, but the situation becomes more complicated if the function f depends on parameters $x \in \mathbb{R}^d$; then the corresponding result is known as the Malgrange preparation theorem. We quote here from [Hör83, chapter 7.5].

C.1. Theorem. *Let $f(t,x)$ be a C^∞ function of $(t,x) \in \mathbb{R}^{1+d}$ near $(0,0)$, which has a multiple zero as a function of t at $(t,x) = (0,0)$, i.e.*

$$f = \partial f/\partial t = \cdots = \partial^{k-1} f/\partial t^{k-1} = 0 \ , \quad \partial^k f/\partial t^k \neq 0 \ \textit{at} \ (0,0) \ .$$

Then there exists a factorization

$$f(t,x) = c(t,x)(t^k + a_{k-1}(x) t^{k-1} + \cdots + a_0(x)) \ , \tag{C.1}$$

where a_j and c are C^∞ functions near 0 *and* $(0,0)$ *respectively, with* $c(0,0) \neq 0$ *and* $a_j(0) = 0$. *When f is real the factorization can be chosen real. Furthermore, if f is real-valued there exists a real-valued C^∞ function $T(t,x)$ with*

$$T = 0 \ , \quad \partial T/\partial t > 0 \quad \text{at } (0,0) \ ,$$

and C^∞ functions $a_j(x)$ vanishing at 0 *such that*

$$f(t,x) = T^k/k + \sum_{j=0}^{k-2} a_j(x) T^j \ ,$$

in a neighborhood of $(0,0)$.

If $g(t,x)$ is a C^∞ function in a neighborhood of $(0,0)$ *then*

$$g(t,x) = q(t,x) f(t,x) + \sum_{j=0}^{k-1} t^j r_j(x) \ ,$$

where q and r_j are C^∞ functions in a neighborhood of $(0,0)$ *and* 0.

We will mainly need an extension of this theorem to several t variables in the case $k=1$, see [Hör83, chapter 7.5].

C.2. Theorem. *Let $f_j(t,x)$, $j = 1, \dots, m$, be complex valued C^∞ functions in a neighborhood of* $(0,0)$ *in* $\mathbb{R}^{m+d}$ *with* $f_j(0,0) = 0$, $j = 1, \dots, m$, *and* $\det \partial f_j(0,0)/\partial t_k \neq 0$. *If $g \in C^\infty$ in a neighborhood of* $(0,0)$ *we can then find $q_j(t,x) \in C^\infty$ at* $(0,0)$ *and $r(x) \in C^\infty$ at* 0 *so that*

$$g(t,x) = \sum_{j=1}^{m} q_j(t,x) f_j(t,x) + r(x) \ . \tag{C.2}$$

It is useful to introduce at this place the ideal $I(f_1, \dots, f_m)$ of functions generated by the $f_j(t,x)$, $j = 1, \dots, m$. This is the set of all C^∞ functions g in a neighborhood of 0 which are multiples of the f_j,

$$g(t,x) = \sum_{j=1}^{k} q_j(t,x) f_j(t,x) \ ,$$

for some $q_j \in C^\infty$ in a neighborhood of 0. It is easy to see, [Hör83, Lemma 7.5.8], that if $F_1, \dots, F_m \in I(f_1, \dots, f_m)$ and $\mathrm{d}F_1, \dots, \mathrm{d}F_m$ are linearly independent at 0, $F_1 = \dots = F_m = 0$ at 0, then

$$I(F_1, \dots, F_m) = I(f_1, \dots, f_m) \ .$$

A natural way how ideals appear is, e.g., as vanishing ideals of submanifolds. Let M be a C^∞-manifold and $\Lambda \subset M$ be a smooth submanifold, the vanishing ideal of Λ is defined as the set of smooth functions on M which vanish on Λ

$$I_\Lambda := \{f \in C^\infty(M) \text{ with } f|_\Lambda = 0\} .$$

Locally every submanifold of codimension m can be represented as the set of common zeros of m real-valued functions f_j with $\mathrm{d}f_1, \dots, \mathrm{d}f_m$ linearly independent on Λ. According to Theorem (C.2) one can represent every $g \in C^\infty(M)$ in a neighborhood of some point on Λ as $g = \sum_j q_j f_j + r$ and $g \in I_\Lambda$ is equivalent to $r = 0$, hence

$$I_\Lambda = I(f_1, \dots, f_m) .$$

For a general g the remainder r in the representation (C.2) is equal to the restriction of g to Λ. If one chooses local coordinates $(t, x) \in \mathbb{R}^{m+d}$ on M such that the projection of Λ to the set $\{(0, x)\ x \in \mathbb{R}^d\}$ is locally bijective, then Λ can be represented as $\{T(x), x\}$ for some C^∞ functions $T = (T_1, \dots, T_m)$ and the vanishing ideal is locally generated by the functions $t_j - T_j(x)$, $j = 1, \dots, m$,

$$I_\Lambda = I(t_1 - T_1, \dots, t_m - T_m) . \tag{C.3}$$

By fixing the coordinates the functions are fixed, too.

So one can identify the set of real-valued ideals in $C^\infty(M)$ with the set of smooth submanifolds of M. In analogy with this we will think of the complex valued ideals as complex submanifolds of M. In analogy with the real valued case there is a similar way as (C.3) to generate such an ideal locally.

C.3. Theorem. *If $f_1, \dots, f_m$ satisfy the hypotheses in Theorem C.2, then*

$$I(f_1, \dots, f_m) = I(t_1 - T_1(x), \dots, t_m - T_m(x)) \tag{C.4}$$

for some $T_j(x) \in C^\infty$ vanishing at 0.

In the real valued case the functions $T_j(x)$ are uniquely determined; this is no longer the case in the complex valued case. If we have a different set of $T_j'(x)$ with (C.4) then $T_j - T_j' \in I(t_1 - T_1(x), \dots, t_m - T_m(x))$, so we need to know how large this class of functions can be.

C.4. Theorem. *If $I = I(t_1 - T_1(x), \dots, t_m - T_m(x))$, where $T_1(0) = \dots = T_m(0) = 0$, and if $R(x) \in C^\infty$ then the following conditions are equivalent:*

(i) $R \in I$ *at* $(0, 0)$.

(ii) $|R(x)| \leq C_N |\operatorname{Im} T(x)|^N$, *for* $N = 1, 2, \dots$ *in a neighborhood of* 0.

(iii) *$R \in I^\infty = \bigcap I^N$ at $(0,0)$. More precisely, there is a neighborhood V of $(0,0)$ and functions $q_\alpha \in C^\infty(\mathbb{R}^{m+d})$ such that for every N*

$$R(x) = \sum_{|\alpha|=N} q_\alpha(t,x)(t - T(x))^\alpha/\alpha! \ , \quad (t,x) \in V \ .$$

In accordance with the interpretation of the ideal $I(f_1, \ldots, f_m)$ as a kind of complex submanifold, we will think of the remainder r in the representation (C.2) of an arbitrary function g as the restriction of g to $I(f_1, \ldots, f_m)$. For a general complex ideal $I(f_1, \ldots, f_m)$ this restriction r is not unique, but by Theorem C.4 we know that if r' is another function satisfying (C.2) for the same g, then

$$|r(x) - r'(x)| \le C_N |\operatorname{Im} T(x)|^N \ ,$$

for all $N \in \mathbb{N}$. So r is unique at the zero-set of I and the difference between two different remainders r and r' is flat on the zero set of I.

There is a close relationship of the preceeding constructions with the theory of almost analytic extensions. Assume that the functions $f_j(t,x)$, $j = 1, \ldots, m$, satisfy the hypotheses of Theorem C.2, then if the functions f_j are real valued the set

$$\{(t,x)\,;\ f_j(t,x) = 0\ ,\ j = 1, \ldots, m\}$$

is a submanifold of codimension m of $\mathbb{R}^{m+d}$ in a neighborhood of $(0,0)$. If in case that the f_j are complex valued we choose almost analytic extensions $\tilde{f}_j(t,x)$, $j = 1, \ldots, m$, then the set

$$\Lambda^{\mathbb{C}} := \{(t,x) \in \mathbb{C}^{m+d}\,;\ \tilde{f}_j(t,x) = 0\ ,\ j = 1, \ldots, m\} \ ,$$

is a complex submanifold of codimension m of $\mathbb{C}^{m+d}$ in a neighborhood of $(0,0)$. It depends of course on the choice of the almost analytic extensions. The equations $\tilde{f}_j(t,x) = 0$, $j = 1, \ldots, m$, can be solved in a neighborhood of $(0,0)$ to give a function $\tilde{t}(x)$, so that $\Lambda^{\mathbb{C}}$ is given by

$$\{(\tilde{t}(x), x)\,;\ x \in \mathbb{C}^d\} \ .$$

Hence the restriction of a function $g \in C^\infty(\mathbb{R}^{m+d})$ is given as $\tilde{g}(\tilde{t}(x), x)$, where $\tilde{g}$ denotes an almost analytic extension of g. But if we take an almost analytic extension of (C.2) and restrict it to $\Lambda^{\mathbb{C}}$, we get

$$\tilde{g}(\tilde{t}(x), x) = r(x) \ , \tag{C.5}$$

so we see that the apparatus connected with the Malgrange preparation Theorem allows to replace part of the almost analytic machinery.

In the applications there often appears the case that a function $f(x,y) \in C^\infty$ is given with

$$\operatorname{Im} f \ge 0\ , \quad \operatorname{Im}(0,0) = 0\ , \quad f'_x(0,0) = 0\ , \quad \det f''_{xx}(0,0) \ne 0\ , \tag{C.6}$$

and that one has to study the ideal generated by the derivatives $\partial f/\partial x_i$. By Theorem C.3 there exist $X_j(y) \in C^\infty$ near 0 with

$$I(\partial f/\partial x_1, \ldots, \partial f/\partial x_d) = I(x_1 - X_1(y), \ldots, x_d - X_d(y)) \; .$$

If $X(y) = (X_1(y), \cdots, X_d(y))$ is real valued, then f has a critical point at $X(y)$. Therefore, we will think of a complex valued $X(y) \in \mathbb{C}^d$ as a critical point of f which has moved to the complex plane. This interpretation can be made even more natural, when one takes an almost analytic extension of f. This will then really have a critical point at some $X(y)$.

By Theorem C.2 we can represent f as

$$f(x,y) = f^0(y) + \sum_j f_j(x,y)(x_j - X_j(y)) \; ,$$

and if we apply the same Theorem to the $f_j(x,y)$, $f_j(x,y) = f^j(y) + \sum_i f_{i,j}(x,y)(x_i - X_i(y))/2$, we get

$$f(x,y) = f^0(y) + \sum_j f^j(y)(x_j - X_j(y)) + \sum_{ij} f_{i,j}(x,y)(x_i - X_i(y))(x_j - X_j(y))/2 \; ,$$

and by iterating this procedure we arrive at

$$f(x,y) = \sum_{|\alpha| \le N} f^\alpha(y)(x - X(y))^\alpha/\alpha! \mod I^N \; . \tag{C.7}$$

This can be thought of as the Taylor expansion of f around the critical point $X(y)$ and since we get by taking derivatives of (C.7) that

$$\partial_x^\alpha f(x,y) - f^\alpha(y) \in I \; ,$$

the functions $f^\alpha(y)$ in (C.7) can be thought of as the derivatives of f at the critical point. Especially for $|\alpha| = 1$ we get by (C.6) $f^\alpha(y) \in I$, and hence by Theorem C.4 $f^\alpha(y) \in I^\infty$, and therefore we have

$$f(x,y) = f^0(y) + \sum_{2 \le |\alpha| \le N} f^\alpha(y)(x - X(y))^\alpha/\alpha! \mod I^N \; . \tag{C.8}$$

It will be important in the applications to ensure that the value $f^0(y)$ of f at the critical point has a positive imaginary part.

C.5. Lemma. *Under the hypotheses* (C.6) *there exists a constant* $C > 0$ *such that in a neighborhood of* 0

$$\operatorname{Im} f^0(y) \ge C |\operatorname{Im} X(y)|^2 \; .$$

Appendix D

The method of stationary phase

The method of stationary phase lies at the heart of all of semiclassics. Its general aim is to determine the asymptotic behavior of integrals of the form

$$\int e^{i\lambda f(x)} u(x) \, dx$$

in the limit $\lambda \to \infty$, where f and u are sufficiently smooth and $\operatorname{Im} f \geq 0$. We will collect here the main results, which are all quoted from [Hör83, chapter7.7].

The principal idea is that the main contributions to the integral come from the points where f is stationary and $\operatorname{Im} f = 0$. We first give an estimate for the case that there are no such points in the support of u. This is a non-stationary phase theorem.

D.1. Theorem. *Let $K \subset \mathbb{R}^d$ be a compact set, X an open neighborhood of K and j, k non-negative integers. If $u \in C_0^k(K)$, $f \in C^{k+1}(X)$ and $\operatorname{Im} f \geq 0$ in X, then*

$$\lambda^{j+k} \left| \int e^{i\lambda f(x)} (\operatorname{Im} f(x))^j u(x) \, dx \right| \leq C \sum_{|\alpha| \leq k} \sup |D^\alpha u| (|f'|^2 + \operatorname{Im} f)^{|\alpha|/2-k} , \quad \lambda > 0 . \tag{D.1}$$

Here C is bounded when f stays in a bounded set in $C^{k+1}(X)$. When f is real valued, the estimate (D.1) *reduces to*

$$\lambda^k \left| \int e^{i\lambda f(x)} u(x) \, dx \right| \leq C \sum_{|\alpha| \leq k} \sup |D^\alpha u| |f'|^{|\alpha|-2k} , \quad \lambda > 0 .$$

From the estimate (D.1) we see that the integral decreases faster than any power of $1/\lambda$ for $\lambda \to \infty$ as long as there is no point x with $f'(x) = 0$ and $\operatorname{Im} f(x) = 0$ in the support of u. The stationary phase formula describes what happens when such a point is in the support of u.

Before coming to the general result we want to treat the simplest case that the Taylor-series of the phase function terminates after the quadratic part which is assumed to be non-degenerate, and the amplitude is constant. Then the result is just the well known formula for the Fourier-transform of a Gaussian, see, e.g., [Hör83].

D.2. Theorem. *Let B be a non-singular symmetric $d \times d$ matrix with $\operatorname{Im} B \geq 0$, then*

$$\int e^{i\langle Bx,x\rangle/2} e^{i\langle x,\xi\rangle} \, dx = [\det(B/(2\pi i))]^{-1/2} e^{-i\langle B^{-1}\xi,\xi\rangle/2} \ .$$

The branch of the square root is defined by demanding continuity and $[\det(B/(2\pi i))]^{1/2} > 0$ if B/i is real, note that $-B^{-1}$ satisfies $\operatorname{Im} -B^{-1} \geq 0$ too.

We want to make the definition of the square-root more explicit. First notice that since the set of non-singular symmetric B with $\operatorname{Im} B \geq 0$ is contractible, the branch of the square root is well defined. Now let b_j, $j = 1, \ldots, d$, be the eigenvalues of B and let $b_j = r_j e^{i\varphi_j}$, $j = 1, \ldots, d$, be their polar decomposition. Then $\operatorname{Im} B \geq 0$ implies that $\varphi_j \in [0, \pi]$, hence we get

$$[\det(B/i)]^{1/2} = [|\det B|]^{1/2} \ e^{i\frac{1}{2}\sum_j(\varphi_j - \pi/2)}$$

as the branch which is positive for $\operatorname{Re} B = 0$. In the special case that $\operatorname{Im} B = 0$ one has $\varphi_j = 0$ if $b_j > 0$, or $\varphi_j = \pi$ if $b_j < 0$, and we get

$$\sum_j (\varphi_j - \pi/2) = -\frac{\pi}{2}\sum_j \operatorname{sign} b_j = -\frac{\pi}{2}\operatorname{sign} B \ .$$

In analogy with this case we will sometimes also call the quantity

$$\operatorname{sign}_+ B := -\frac{2}{\pi}\sum_j (\varphi_j - \pi/2) \tag{D.2}$$

the signature of B. The plus-sign indicates that it is the extension of the signature to matrices with positive imaginary part. There is an analogous definition for matrices with negative imaginary part. Although this quantity appears always implicitly when Gaussian integrals are discussed, it was introduced explicitly in [RZ84] in order to give a systematic study of the Maslov-bundle in the complex case, and for the same reason we introduce it here as well, see section 3.4.3. So with this notation we have

$$[\det(B/(2\pi i))]^{-1/2} = (2\pi)^{d/2}\frac{e^{i\pi \operatorname{sign}_+ B/4}}{\sqrt{|\det B|}} \ . \tag{D.3}$$

Coming back to the general case, the basic result is:

D.3. Theorem. *Let $K \subset \mathbb{R}^d$ be a compact set, X an open neighborhood of K and k a non-negative integer. If $u \in C_0^{2k}(K)$, $f \in C^{3k+1}(X)$ and $\operatorname{Im} f \geq 0$ in X, $\operatorname{Im} f(x_0) = 0$, $f'(x_0) = 0$, $\det f''(x_0) \neq 0$, $f' \neq 0$ in $K \backslash \{x_0\}$, then*

$$\left| \int e^{i\lambda f(x)} u(x) \, dx - e^{i\lambda f(x_0)} \left[\det(\lambda f''(x_0)/2\pi i)\right]^{-1/2} \sum_{j<k} \lambda^{-j} L_j u \right| \leq C\lambda^{-k} \sum_{|\alpha|\leq 2k} \sup |D^\alpha u| \ , \tag{D.4}$$

for $\lambda > 0$. Here C is bounded when f stays in a bounded set in $C^{3k+1}(X)$ and $|x-x_0|/f'(x)$ has a uniform bound. With

$$g_{x_0}(x) := f(x) - f(x_0) - \langle f''(x_0)(x-x_0), (x-x_0)\rangle/2$$

which vanishes to third order at x_0, we have

$$L_j u = \sum_{\nu-\mu=j} \sum_{2\nu \geq 3\mu} \frac{\langle f''(x_0)^{-1} D, D\rangle^{\nu} [g_{x_0}{}^{\mu} u]}{\mathrm{i}^j 2^{\nu} \mu! \nu!}(x_0) \ .$$

This is a differential operator of order $2j$ acting on u at x_0. The coefficients are rational homogeneous functions of degree $-j$ in $f''(x_0), \dots, f^{(2j+2)}(x_0)$ with denominator $(\det f''(x_0))^{3j}$. In every term the total number of derivatives of u and of f'' is at most $2j$.

The branch of the square-root $[\det(\lambda f''(x_0)/2\pi\mathrm{i})]^{-1/2}$ is the same as discussed before. Explicitly we have with (D.2)

$$[\det(\lambda f''(x_0)/2\pi\mathrm{i})]^{-1/2} = \left(\frac{2\pi}{\lambda}\right)^{d/2} \frac{\mathrm{e}^{\mathrm{i}\frac{\pi}{4}\,\mathrm{sign}_+ f''(x_0)}}{\sqrt{|\det f''(x_0)|}} \ . \tag{D.5}$$

In most applications one only needs the leading term in the asymptotic expansion. This gives

$$\int \mathrm{e}^{\mathrm{i}\lambda f(x)} u(x)\ \mathrm{d}x = \left(\frac{2\pi}{\lambda}\right)^{d/2} \mathrm{e}^{\mathrm{i}\lambda f(x_0)} \frac{1}{\sqrt{\det(-\mathrm{i} f''(x_0))}}\, u(x_0) + O(\lambda^{d/2-1}) \ ,$$

and the square-root can be written as just shown in (D.5).

Often f and u depend on additional parameters $y \in \mathbb{R}^m$ and this can cause problems. The simplest case is that $f(x,y)$ is real valued and nondegenerate at $x = 0$ for some value of the external parameter which we will assume to be $y = 0$, i.e.

$$f'_x(0,0) = 0 \quad \text{and} \quad \det f''_{x,x}(0,0) \neq 0 \ . \tag{D.6}$$

Then by the implicit function theorem the equation

$$f'_x(x,y) = 0 \tag{D.7}$$

has in a neighborhood of $(0,0)$ a smooth solution $x(y)$ with $x(0) = 0$. Then Theorem D.3 is true with x_0 replaced by $x(y)$ and for $u(x,y)$ supported in a sufficiently small neighborhood of $(0,0)$. Explicitly we have in leading order

$$\int \mathrm{e}^{\mathrm{i}\lambda f(x,y)} u(x,y)\ \mathrm{d}x = \left(\frac{2\pi}{\lambda}\right)^{d/2} \frac{\mathrm{e}^{\mathrm{i}\frac{\pi}{4}\,\mathrm{sign}\, f''(x(y),y)}}{\sqrt{|\det f''(x(y),y)|}}\, \mathrm{e}^{\mathrm{i}\lambda f(x(y),y)} + O(\lambda^{-d/2-1}) \ . \tag{D.8}$$

The problem which appears when the phase function is complex-valued and depends on a parameter $y \in \mathbb{R}^m$ is that the equation (D.7) does not necessarily have a solution $y(x)$. Take as example the integral

$$\left(\frac{\lambda}{2\pi}\right)^{d/2} \int \mathrm{e}^{\mathrm{i}\lambda(\langle x,y\rangle + \frac{\mathrm{i}}{2}\langle x,x\rangle)}\, \mathrm{d}x = \mathrm{e}^{-\lambda\langle y,y\rangle} ,$$

where the phase function is

$$f(x,y) = \langle x,y\rangle + \frac{\mathrm{i}}{2}\langle x,x\rangle .$$

Then the only stationary point of f with $\operatorname{Im} f(x,y) = 0$ is given by $x = 0$ at $y = 0$, so we know by the non-stationary phase Theorem D.1 that for $y \neq 0$ the integral is $O(\lambda^{-\infty})$, and by the stationary phase Theorem D.3 we know that for $y = 0$ it is asymptotically equal to 1. Now it is clearly desirable to have a formula which describes the transition between these two asymptotic regimes. The stationary phase condition

$$f'_x(x,y) = y + \mathrm{i}x = 0$$

has even a solution for $y \neq 0$, namely $x(y) = \mathrm{i}y$, but it is complex. This is the phenomenon which generally appears when one has parameter-dependent complex-valued phase functions: the stationary points become complex when the parameter is varied. If we insert the complex solution $x(y)$ naively in the equation (D.8) for the real valued case, we get

$$\left(\frac{\lambda}{2\pi}\right)^{d/2} \int \mathrm{e}^{\mathrm{i}\lambda(\langle x,y\rangle + \frac{\mathrm{i}}{2}\langle x,x\rangle)}\, \mathrm{d}x = \mathrm{e}^{-\lambda\langle y,y\rangle} + O(\lambda^{-1}) ,$$

which is indeed the correct result.

This example suggests that we should modify the stationary phase formulas such that we can take the passage of stationary points to the complex into account. If $f \in C^\infty$ is not real analytic this can not be done directly, but we can use the apparatus of almost analytic extensions, which provide a way to pass to the complex. So for $f \in C^\infty$ we choose an almost analytic extension $\tilde{f}$. Then under the conditions (D.6) the equation

$$\tilde{f}'(x,y) = 0 \tag{D.9}$$

will locally have a unique solution $\tilde{x}(y) \in \mathbb{C}^d$ with $\tilde{x}(0) = 0$. It turns out that if we choose in the formula (D.4) almost analytic extensions for all quantities and insert $\tilde{x}(y)$ for x_0, this gives indeed the correct result.

D.4. Theorem. *Let $f(x,y)$ be a complex valued C^∞ function in a neighborhood of* $(0,0)$ *in $\mathbb{R}^{d+m}$, satisfying* (D.6)*, let $\tilde{f}$ be an almost analytic extension of f, and $\tilde{x}(y)$ be the solution of* (D.9)*. Then for $u \in C^\infty$ with support in a neighborhood of* $(0,0)$

$$\left| \int \mathrm{e}^{\mathrm{i}\lambda f(x,y)} u(x,y)\, \mathrm{d}x - \mathrm{e}^{\mathrm{i}\lambda \tilde{f}(\tilde{x}(y),y)} \left[\det(\lambda \tilde{f}''(\tilde{x}(y),y)/2\pi\mathrm{i})\right]^{-1/2} \sum_{j<k} \lambda^{-j} \widetilde{L_j u} \right| \leq C\lambda^{-k-d/2} , \tag{D.10}$$

for $\lambda > 0$, where $\widetilde{L_j u}$ denotes the almost analytic continuation of the expression in Theorem D.3 evaluated at $\tilde{x}(y)$.

One can avoid the use of almost analytic extensions if one uses the Malgrange preparation theorem. If we introduce the ideal generated by the derivatives of the phase function,

$$I(\partial f/\partial x_1, \dots , \partial f/\partial x_d) \ ,$$

then the discussion at the end of Appendix C shows that we can replace $\tilde{f}(\tilde{x}(y), y)$ by $f^0(y) = f(x, y) \mod I$. More precisely, f^0 is determined by the representation in Theorem C.2,

$$f(x, y) = \sum_j q_j(x, y)\partial f/\partial x_j + f^0(y) \ .$$

Similarly one can replace all other almost analytically continued functions in (D.10) by their representatives modulo the ideal I.

If one wants to determine the first terms of the asymptotic approximation in practice, one has to find a way to deal practically with the almost analytic extensions. Fortunately it turns out that it is sufficient to manipulate Taylor expansions, i.e. polynomials or formal power-series. Let

$$\sum_{\alpha,\beta} f_{\alpha,\beta} x^\alpha y^\beta$$

be the Taylor series of $f(x, y)$ around $(0, 0)$, viewed as a formal power series, and make an ansatz for $x(y)$ as a formal power series, too,

$$x(y) = \sum_\gamma x_\gamma y^\gamma \ .$$

Then the equations $f'_{x_i} = 0$, $i = 1, \dots , d$, for these formal power series read

$$\sum_{\alpha>0,\beta} f_{\alpha,\beta}\alpha_i \Big(\sum_\gamma x_\gamma y^\gamma\Big)^{\alpha-\delta_i} y^\beta = 0 \ ,$$

where $\delta_i = (0, \dots , 1, \dots , 0)$ with the one on the i'th place. Equating now equal powers of y gives a set of equations for x_γ in terms of the $f_{\alpha,\beta}$ which can be solved recursively.

We will determine the leading order contributions; the Taylor series for $f'_x(x, y)$ around $(0, 0)$,

$$f'_x(x, y) = f'_x(0, 0) + f''_{x,y}(0, 0)y + f''_{x,x}(0, 0)x + \cdots \ ,$$

together with the condition $f'_x(0, 0) = 0$ gives that

$$x(y) = -[f''_{x,x}(0, 0)]^{-1} f''_{x,y}(0, 0)y + O(y^2) \ .$$

For the phase-function $f(x(y),y)$ we then get

$$\begin{aligned}
f(x(y),y) = f(0,0) &+ \langle f'_x(0,0), \frac{\partial x}{\partial y} y\rangle + \langle f'_y(0,0), y\rangle \\
&+ \frac{1}{2}[\langle y, f''_{y,y} y\rangle + \langle \frac{\partial x}{\partial y} y, f''_{x,y} y\rangle + \langle y, f''_{y,x} \frac{\partial x}{\partial y} y\rangle + \langle \frac{\partial x}{\partial y} y, f''_{y,y} \frac{\partial x}{\partial y} y\rangle] + O(y^3) \\
&= f(0,0) + \langle f'_y(0,0), y\rangle + \frac{1}{2}\langle y, [f''_{y,y} - f''_{y,x}[f''_{x,x}]^{-1} f''_{x,y}] y\rangle + O(y^3) \ ,
\end{aligned}$$

where the second-order derivatives are taken at $(0,0)$. Notice that since $\operatorname{Im} f \geq 0$ and $\operatorname{Im} f(0,0) = 0$ we must have

$$\operatorname{Im} f'_y(0,0) = 0 \ ,$$

and furthermore

$$\operatorname{Im}[f''_{y,y} - f''_{y,x}[f''_{x,x}]^{-1} f''_{x,y}] \geq 0 \ .$$

For the case that the imaginary part is strictly positive we will give an explicit formula for the leading part of the asymptotic expansion in the stationary phase theorem. By Lemma 3.2.6 we then have

$$\mathrm{e}^{\mathrm{i}\lambda \tilde{f}(\tilde{x}(y),y)} - \mathrm{e}^{\mathrm{i}\lambda(f(0,0) + \langle f'_y(0,0),y\rangle + \frac{1}{2}\langle y,[f''_{y,y} - f''_{y,x}[f''_{x,x}]^{-1} f''_{x,y}]y\rangle)} = O(\lambda^{-3/2}) \ ,$$

and

$$\mathrm{e}^{\mathrm{i}\lambda \tilde{f}(\tilde{x}(y),y)} \left(\frac{\tilde{u}(\tilde{x}(y),y)}{[\det(\lambda \tilde{f}''(\tilde{x}(y),y)/2\pi \mathrm{i})]^{1/2}} - \frac{u(0,0)}{[\det(\lambda f''(0,0)/2\pi \mathrm{i})]^{1/2}} \right) = O(\lambda^{-1/2}) \ ,$$

hence we get

$$\int \mathrm{e}^{\mathrm{i}\lambda f(x,y)} u(x,y) \ \mathrm{d}x = \frac{u}{[\det(\lambda f''/2\pi \mathrm{i})]^{1/2}} \, \mathrm{e}^{\mathrm{i}\lambda(f + \langle f'_y, y\rangle + \frac{1}{2}\langle y,[f''_{y,y} - f''_{y,x}[f''_{x,x}]^{-1} f''_{x,y}]y\rangle)} (1 + O(\lambda^{-1/2})) \ ,$$

where on the right hand side u, f and all derivatives of f are taken at $(0,0)$. When one takes higher order terms in the Taylor expansions of u and f into account, one systematically gets explicit formulas for arbitrary order terms in the asymptotic expansion. If the imaginary part of the quadratic form $[f''_{y,y} - f''_{y,x}[f''_{x,x}]^{-1} f''_{x,y}]$ is not strictly positive, one can choose a splitting $y = (y', y'')$ such that the imaginary part vanishes on the y' subspace and is strictly positive on the y'' subspace. Then we can view y' as a parameter as in the real case and perform the above calculations only with respect to y''.

Until now we have only discussed the case that the stationary point is nondegenerate, i.e. the matrix of second derivatives of the phase function is non-degenerate at the stationary point. The inclusion of higher order stationary points poses no essential difficulty. The characteristic phenomenon which appears is that the leading term has other powers of λ. As an example consider the simple case that $x \in \mathbb{R}$ and $f(x) = x^k$, $k \in \mathbb{N}$. Then for $u \in C_0^\infty(\mathbb{R})$ we get

$$\int e^{i\lambda x^k} u(x)\, dx = \begin{cases} \lambda^{-1/k} 2\Gamma(1/k)\sin((1-1/k)\pi/2)/k\, u(0) + O(\lambda^{-2/k}) & \text{if } k \text{ is odd} \\ \lambda^{-1/k} 2\Gamma(1/k) e^{ik\pi/2}/k\, u(0) + O(\lambda^{-3/k}) & \text{if } k \text{ is even} \end{cases} ;$$

a complete asymptotic expansion is contained in [Hör83]. With the standard techniques used in the proof of the stationary phase formula the general multi-dimensional case can be reduced to these examples.

The situation becomes more complicated if additional parameters are present, and one needs uniform asymptotic expansions. The problem is that a slight perturbation of a phase-function with degenerate critical point will generically produce a phase-function with non-degenerate critical point. Therefore, if we have a family of phase-functions we expect them to be degenerate only at isolated points of the parameter space. A simple example is given by the function

$$f(x,y) = \frac{1}{3}x^3 + yx ,$$

with $x \in \mathbb{R}$ and $y \in \mathbb{R}$. Then the stationary points are given by

$$\begin{aligned} &\sqrt{y}\ , \quad -\sqrt{y} \qquad \text{if}\, y \le 0 \ , \\ &i\sqrt{|y|}\ , \quad -i\sqrt{|y|} \qquad \text{if}\, y \ge 0 \ , \end{aligned} \tag{D.11}$$

so for $y < 0$ we have two non-degenerate stationary points, for $y = 0$ we have a degenerate critical point and for $y > 0$ the critical points have moved to the complex, hence there is no stationary point. The first case we look at is that the amplitude u is constant. Then the integral gives the well-known Airy-function

$$\int e^{i\lambda(x^3/3+yx)}\, dx = \lambda^{-1/3}\, \mathrm{Ai}(\lambda^{2/3}y) \ .$$

The asymptotic expansion of $\mathrm{Ai}(x)$ in the two regions $x > 0$ and $x < 0$, see, e.g.,[AS84], gives the expected behavior of the integral,

$$\lambda^{-1/3}\,\mathrm{Ai}(\lambda^{2/3}y) \sim \begin{cases} \frac{1}{\sqrt{\pi\lambda}\, y^{1/4}} \sin(2\lambda y^{3/2}/3 + \pi/4) & \text{if } y > 0 \\ \frac{1}{\sqrt{2\pi\lambda}\, y^{1/4}} e^{-2\lambda y^{3/2}/3} & \text{if } y < 0 \end{cases} ,$$

therefore the Airy-function describes the transition between these two asymptotic regimes while passing the degenerate stationary point at $y = 0$.

Let us now discuss the more general case that an amplitude-function $u(x,y) \in C^\infty$ with compact support close to $(0,0)$ is present,

$$\int u(x,y) e^{i\lambda[x^3/3+yx+b(y)]}\, dx \ .$$

By Theorem C.1 we can divide $u(x,y)$ by x^2+y,

$$u(x,y) = u_0(y) + u_1(y)x + (x^2+y)g(x,y) \ . \tag{D.12}$$

Inserting this relation into the integral and using

$$(x^2+y)\mathrm{e}^{\mathrm{i}\lambda[x^3/3+yx+b(y)]} = \frac{1}{\mathrm{i}\lambda}\frac{\partial}{\partial x}\mathrm{e}^{\mathrm{i}\lambda[x^3/3+yx+b(y)]}$$

we get with partial integration

$$\begin{aligned}\int u(x,y)\mathrm{e}^{\mathrm{i}\lambda[x^3/3+yx+b(y)]}\,\mathrm{d}x = \mathrm{e}^{\mathrm{i}\lambda b(y)}\Big(\int \mathrm{e}^{\mathrm{i}\lambda[x^3/3+yx]}\,\mathrm{d}x u_0(y) + \int x\mathrm{e}^{\mathrm{i}\lambda[x^3/3+yx]}\,\mathrm{d}x u_1(y)\\ + \int g(x,y)\frac{1}{\mathrm{i}\lambda}\frac{\partial}{\partial x}\mathrm{e}^{\mathrm{i}\lambda[x^3/3+yx]}\,\mathrm{d}x\Big)\\ = \mathrm{e}^{\mathrm{i}\lambda b(y)}\Big(\lambda^{-1/3}\,\mathrm{Ai}(\lambda^{2/3}y)u_0(y) + \lambda^{-2/3}\,\mathrm{Ai}'(\lambda^{2/3}y)u_1(y)\\ + \frac{\mathrm{i}}{\lambda}\int \frac{\partial g(x,y)}{\partial x}\mathrm{e}^{\mathrm{i}\lambda[x^3/3+yx]}\,\mathrm{d}x\Big) \ .\end{aligned}$$

The integral in the last line is of the same form as the one we started with, with u replaced by $\partial g/\partial x$, so by iterating this procedure we arrive at a representation

$$\int u(x,y)\mathrm{e}^{\mathrm{i}\lambda[x^3/3+yx+b(y)]}\,\mathrm{d}x = \mathrm{e}^{\mathrm{i}\lambda b(y)}\Big(\lambda^{-1/3}\,\mathrm{Ai}(\lambda^{2/3}y)u_0(\lambda,y) + \lambda^{-2/3}\,\mathrm{Ai}'(\lambda^{2/3}y)u_1(\lambda,y)\Big) \ ,$$

with

$$u_j(\lambda,y) \sim \sum_{\nu=0}^{\infty} u_{j,\nu}(y)\lambda^{-\nu} \ .$$

The drawback of this method is that we do not know the functions u_j explicitly. From (D.12) and the equations one obtains by differentiating on that one can determine the terms of the Taylor-expansion of $u_j(y)$. For the first two terms we get

$$\begin{aligned}u_0(y) &= u(0,0) + (\partial u/\partial y(0,0) - \partial^2 u/\partial x^2(0,0)/2)y + O(y^2)\\ u_1(y) &= \partial u/\partial x(0,0) + (\partial^2 u/\partial x\partial y(0,0) - \partial^3 u/\partial x^3(0,0)/6)y + O(y^2) \ ,\end{aligned}$$

and this can be continued.

So far we have discussed the case that the phase-function is of the special form $x^3/3 + yx + b(y)$. We now sketch how one can reduce the general case of a phase-function $f(x,y)$ which has a second order zero as a function of x at $(0,0)$. So assume that $\partial_x f(0,0) = 0$ and $\partial_x^2 f(0,0) = 0$, but $\partial_x^3 f(0,0) \neq 0$, then by Theorem C.1, with $k = 3$, there exists a function $T(x,y)$ with $T(0,0)=0$ and $\partial T/\partial x(0,0)>0$ and C^∞ functions $a(y)$, $b(y)$ with $a(0)=0$, such that

$$f(x,y)=T^3/3+a(y)T+b(y)\ .$$

By taking T as a new variable in the integral one can reduce the general case to the special case discussed before. This procedure can as well be applied in d dimension. The general result for a third order stationary point is, quoted from [Hör83]:

D.5. Theorem. *Let $f(x,y)$ ba real valued C^∞ function near 0 in $\mathbb{R}^{d+m}$ such that*

$$f'_x(0,0)=0\ ,\quad \operatorname{rank} f''_{x,x}(0,0)=d-1\ ,$$
$$\langle X,\partial/\partial x\rangle^3 f(0,0)\neq 0\quad \textit{if}\ 0\neq X\in \operatorname{Ker} f''_{x,x}(0,0)\ .$$

Then there exist real valued C^∞ functions $a(y)$, $b(y)$ near 0 such that $a(0)=0$, $b(0)=f(0,0)$ and

$$\int u(x,y)\mathrm{e}^{\mathrm{i}\lambda f(x,y)}\,\mathrm{d}x\sim \mathrm{e}^{\mathrm{i}\lambda b(y)}\lambda^{-(d-1)/2}\Big(\lambda^{-1/3}\operatorname{Ai}(a(y)\lambda^{2/3})\sum_{\nu=0}^{\infty}u_{0,\nu}(y)\lambda^{-\nu}$$
$$+\lambda^{-2/3}\operatorname{Ai}'(a(y)\lambda^{2/3})\sum_{\nu=0}^{\infty}u_{1,\nu}(y)\lambda^{-\nu}\Big)\ ,$$

provided that $u\in C_0^\infty$ with support close enough to 0; here $u_{j,\nu}\in C_0^\infty$.

The case that one has critical points of order $k-1>2$ is treated in the same way as the second order case. One first uses the Malgrange preparation theorem, Theorem C.1, to reduce the phase function to a polynomial of order k, and then the general asymptotic expansion can be represented in terms of a special function, which is determined by this polynomial, as a phase-function. For a more detailed description we refer to [Dui74, AGV88]. The general problem with higher order degeneracies is that the higher the order of it is, the less is known about the special functions appearing in the asymptotic expansions. The properties of the Airy function are very well known. The function appearing in the next order is called Pearcy's-integral, which is already less intensively studied and in higher orders even less is known.

Bibliography

[ABS94] R. Aurich, J. Bolte, and F. Steiner, *Universal signatures of quantum chaos*, Phys. Rev. Lett. **73** (1994), 1356.

[ABS97] R. Aurich, A. Bäcker, and F. Steiner, *Mode fluctuations as fingerprints of chaotic and non-chaotic systems*, Int. J. Mod. Phys. B **11** (1997), 805–849.

[AGV88] V. I. Arnold, S. M. Gusein-Zade, and A. N. Varchenko, *Singularities of differentiable mappings I-II*, Birkhäuser, Boston, 1985-88.

[AK99] J. Asch and A. Knauf, *Quantum transport on KAM tori*, Comm. Math. Phys. **205** (1999), no. 1, 113–128.

[AKN97] V. I. Arnold, V. V. Kozlov, and A. I. Neishtadt, *Mathematical aspects of classical and celestial mechanics*, Springer-Verlag, Berlin, 1997.

[Alb78] J. A. Albert, *Generic properties of eigenfunctions of elliptic partial differential operators*, Trans. Amer. Math. Soc. **238** (1978), 341–354.

[AM78] R. Abraham and J. Marsden, *Foundations of mechanics*, Addison-Wesley, Redwood City, California, 1978.

[AR67] R. Abraham and J. Robbin, *Transversal mappings and flows*, W. A. Benjamin, Inc., New York-Amsterdam, 1967.

[Arn72] V. I. Arnold, *Modes and quasimodes*, Funkcional. Anal. i Priložen. **6** (1972), no. 2, 12–20, English transl.:Functional Anal. Appl. 6 (1972).

[Arn78] V. I. Arnold, *Mathematical methods of classical mechanics*, Springer, New York, 1978.

[AS84] M. Abramowitz and I.A. Stegun, *Pocketbook of mathematical functions*, Harri Deutsch, Thun Frankfurt/Main, 1984.

[AT98] R. Aurich and M. Taglieber, *On the rate of quantum ergodicity on hyperbolic surfaces and for billiard*, Physica D **118** (1998), 84–102.

[Bäc98] A. Bäcker, *Classical and quantum chaos in billiards*, Ph.D. thesis, Universität Ulm, 1998.

[BB72] R. Balian and C. Bloch, *Distribution of eigenfrequencies for the wave equation in a finite domain. III. Eigenfrequency density oscillations*, Ann. Physics **69** (1972), 76–160.

[BBR96] P. Boggiatto, E. Buzano, and L. Rodino, *Global hypoellipticity and spectral theory*, Akademie Verlag, Berlin, 1996.

[BDB00] F. Bonechi and S. De Bièvre, *Exponential mixing and* $|\ln\hbar|$ *time scales in quantized hyperbolic maps on the torus*, Comm. Math. Phys. **211** (2000), no. 3, 659–686.

[BDD$^+$00] L. A. Bunimovich, S. G. Dani, R. L. Dobrushin, M. V. Jakobson, I. P. Kornfeld, N. B. Maslova, Ya. B. Pesin, Ya. G. Sinai, J. Smillie, Yu. M. Sukhov, and A. M. Vershik, *Dynamical systems, ergodic theory and applications*, revised ed., Springer-Verlag, Berlin, 2000, Edited and with a preface by Sinai, Translated from the Russian, Mathematical Physics, I.

[Ber71] F. A. Berezin, *Wick and Anti-Wick symbols of operators* (russian), Mat. Sb. (N.S.) **86(128)** (1971), 578–610.

[Bér77a] P. H. Bérard, *On the wave equation on a compact Riemannian manifold without conjugate points*, Math. Z. **155** (1977), 249–276.

[Ber77b] M. V. Berry, *Regular and irregular semiclassical wavefunctions*, J. Phys. A **10** (1977), 2083–2091.

[Ber85] M. V. Berry, *Semiclassical theory of spectral rigidity*, Proc. R. Soc. London **A400** (1985), 229–251.

[Bes78] A. Besse, *Manifolds all of whose geodesics are closed*, Ergebnisse der Mathematik und ihrer Grenzgebiete, vol. 93, Springer, New York, 1978.

[BGP99] D. Bambusi, S. Graffi, and T. Paul, *Long time semiclassical approximation of quantum flows: a proof of the Ehrenfest time*, Asymptot. Anal. **21** (1999), no. 2, 149–160.

[BGS84] O. Bohigas, M.-J. Giannoni, and C. Schmit, *Characterization of chaotic quantum spectra and universality of level fluctuation laws*, Phys. Rev. Lett. **52** (1984), no. 1, 1–4.

[Ble99] P. Bleher, *Trace formula for quantum integrable systems, lattice-point problem, and small divisors*, Emerging applications of number theory (Minneapolis, MN, 1996), IMA Vol. Math. Appl., vol. 109, Springer, New York, 1999, pp. 1–38.

[BO95] U. Bunke and M. Olbricht, *Selberg zeta and theta functions*, Mathematical Research, vol. 83, Akademie Verlag, Berlin, 1995.

[BR79] O. Bratteli and D. W. Robinson, *Operator algebras and quantum statistical mechanics*, vol. 1, Springer, 1979.

[BSS97] A. Bäcker, R. Schubert, and P. Stifter, *On the number of bouncing-ball modes in billiards*, J. Phys. A. **30** (1997), 6783–6795.

[BSS98] A. Bäcker, R. Schubert, and P. Stifter, *Rate of quantum ergodicity in Euclidean billiards*, Phys. Rev E **57** (1998), 5425–5447.

[BT82] R. Bott and L. W. Tu, *Differential forms in algebraic topology*, Springer, New York, 1982.

[BTU93] O. Bohigas, S. Tomsovic, and D. Ullmo, *Manifestations of classical phase space structures in quantum mechanics*, Phys. Rep. **223** (1993), no. 2, 43–133.

[BU91] R. Brummelhuis and A Uribe, *A semiclassical trace formula for Schrödinger operators*, Comm. Math. Phys. **136** (1991), 567–584.

[BW97] S. Bates and A. Weinstein, *Lectures on the geometry of quantization*, Berkeley Mathematics Lecture Notes, vol. 8, AMS, Providence, 1997.

[Cha74] J. Chazarain, *Formules de Poisson pour le variétés riemannienes*, Invent. Math. **24** (1974), 65–82.

[Cha80] J. Chazarain, *Spectre d'un Hamiltonien quantique et mécanique classique*, Comm. in P.D.E. **5** (1980), no. 6, 595–644.

[Cha93] I. Chavel, *Riemannian geometry—a modern introduction*, Cambridge Tracts in Mathematics, vol. 108, Cambridge University Press, Cambridge, 1993.

[CLM94] S. E. Cappell, R. Lee, and E. Y. Miller, *On the Maslov index*, Comm. Pure Appl. Math. **47** (1994), 121–186.

[Col73] Y. Colin de Verdière, *Spectre du Laplacien et longeurs des géodésiques périodiques I* & *II*, Compos. Math. **27** (1973), 83–106, 159–184.

[Col77] Y. Colin de Verdière, *Quasi-modes sur les variétés riemanniennes*, Inv. Math. **43** (1977), 15–52.

[Col85] Y. Colin de Verdière, *Ergodicité et fonctions propres du laplacien*, Commun. Math. Phys. **102** (1985), 111–134.

[Com74] L. Comtet, *Advanced combinatorics*, enlarged ed., D. Reidel Publishing Co., Dordrecht, 1974, The art of finite and infinite expansions.

[Com92] M. Combescure, *The squeezed state approach of the semiclassical limit of the time-dependent Schrödinger equation*, J. Math. Phys. **33** (1992), no. 11, 3870–3880.

[CR95] M. Combescure and D. Robert, *Semiclassical sum rules and generalized coherent states*, J. Math. Phys. **36** (1995), no. 12, 6596–6610.

[CR97] M. Combescure and D. Robert, *Semiclassical spreading of quantum wave packets and applications near unstable fixed points of the classical flow*, Asymptot. Anal. **14** (1997), no. 4, 377–404.

[CV90] P. Cartier and A. Voros, *Une nouvelle interprétation de la formule des traces de Selberg*, The Grothendieck Festschrift, Progress in Math., vol. 87, Birkhäuser, 1990, pp. 1–67.

[DG75] J. J. Duistermaat and V. W. Guillemin, *The spectrum of positive elliptic operators and periodic bicharacteristics*, Invent. Math. **29** (1975), 39–79.

[Dir58] P. A. M. Dirac, *The principles of quantum mechanics*, Oxford University Press, Oxford, 1958.

[DKV79] J. J Duistermaat, J. A. C. Kolk, and V. S. Varadarajan, *Spectra of compact locally symmetric manifolds of negative curvature*, Invent. Math **52** (1979), 27–93.

[Don78] H. Donnelly, *On the wave equation asymptotics of a compact negatively curved surface*, Invent. Math. **45** (1978), 115–137.

[DS76] J. J. Duistermaat and I. M. Singer, *Order-preserving isomorphisms between algebras of pseudodifferential operators*, Comm. Pure Appl. Math. **29** (1976), 39–47.

[DS99] M. Dimassi and J. Sjöstrand, *Spectral asymptotics in the semi-classical limit*, Cambridge University Press, Cambridge, 1999.

[Dui73] J. J. Duistermaat, *Fourier integral operators*, Courant Institute, New York, 1973, lecture note.

[Dui74] J. J. Duistermaat, *Oscillatory integrals, Lagrange immersions and unfolding of singularities*, Comm. Pure Appl. Math. **27** (1974), 207–281.

[Dui76] J. J. Duistermaat, *On the Morse index in variational calculus*, Adv. Math. **21** (1976), 173–195.

[EFK+95] B. Eckhardt, S. Fishman, J. Keating, O. Agam, J. Main, and K. Müller, *Approach to ergodicity in quantum wave functions*, Phys. Rev. E **52** (1995), 5893–5903.

[Ego69] Ju. V. Egorov, *The canonical transformations of pseudo-differential operators*, Uspehi Mat. Nauk **25** (1969), no. 5, 235–236.

[Fal90] K. Falconer, *Fractal geometry*, John Wiley & Sons Ltd., Chichester, 1990, Mathematical foundations and applications.

[Fal97] K. Falconer, *Techniques in fractal geometry*, John Wiley & Sons Ltd., Chichester, 1997.

[Fed99] *Partial differential equations. V*, Springer-Verlag, Berlin, 1999, Asymptotic methods for partial differential equations, A translation of *Current problems in mathematics. Fundamental directions. Vol. 34* (Russian), Akad. Nauk SSSR, Vsesoyuz. Inst. Nauchn. i Tekhn. Inform., Moscow, 1988 [MR 91e:35002], Translation by J. S. Joel and S. A. Wolf, Translation edited by M. V. Fedoryuk.

[Fef83] C. L. Fefferman, *The uncertainty principle*, Bull. Am. Math. Soc. **9** (1983), no. 2, 129–206.

[FFG97] C. Fefferman, J. Fröhlich, and G. Graf, *Stability of ultraviolet-cutoff quantum electrodynamics with non-relativistic matter*, Comm. Math. Phys. **190** (1997), no. 2, 309–330.

[FGLS96] B. Fedosov, F. Golse, E. Leichtnam, and E. Schrohe, *The noncommutative residue for manifolds with boundary*, J. Funct. Anal. **142** (1996), no. 1, 1–31.

[FKT90] J. Feldman, H. Knörrer, and E. Trubowitz, *The perturbatively stable spectrum of a periodic Schrödinger operator*, Invent. Math. **100** (1990), no. 2, 259–300.

[FKT91] J. Feldman, H. Knörrer, and E. Trubowitz, *Perturbatively unstable eigenvalues of a periodic Schrödinger operator*, Comment. Math. Helv. **66** (1991), no. 4, 557–579.

[Foc59] V. A. Fock, *On the canonical transformation in classical and quantum mechanics*, Vestnik Leningr. Univ. sep. Phys. Chem. **16** (1959), 67–10.

[Fol89] G. B. Folland, *Harmonic analysis in phase space*, Annals of Mathematics Studies, vol. 122, Princeton University Press, Princeton, 1989.

[GJK+96] D. Giulini, E. Joos, C. Kiefer, J. Kupsch, I. O. Stamatescu, and H. D. Zeh, *Decoherence and the Appearence of a Classical World in Quantum Theory*, Springer, Berlin, 1996.

[GL93] P. Gérard and E. Leichtnam, *Ergodic properties of eigenfunctions for the Dirichlet problem*, Duke Math. J. **71** (1993), 559–607.

[GS77] V. W. Guillemin and S. Sternberg, *Geometric asymptotics*, Math. Surveys, vol. 14, AMS, Providence, 1977.

[GS94] A. Grigis and J. Sjöstrand, *Microlocal analysis for differential operators*, London Mathematical Society Lecture Note Series, vol. 196, Cambridge University Press, Cambridge, 1994.

[GU89] V. Guillemin and A. Uribe, *Circular symmetry and the trace formula*, Inv. Math. **96** (1989), 385–423.

[Gui77] V. Guillemin, *Lectures on spectral theory of elliptic operators*, Duke Math. Journal **44** (1977), 485–517.

[Gui79] V. Guillemin, *Some classical theorems in spectral theory revisited*, Seminar on Singularities of Solutions of Linear Partial Differential Equations, Ann. Math. Stud., vol. 91, Princeton University Press, Princeton, 1979, pp. 219–259.

[Gui85] V. Guillemin, *A new proof of Weyl's formula on the asymptotic distribution of eigenvalues*, Adv. in Math. **55** (1985), 131–160.

[Gui93] V. Guillemin, *Wave trace invariants and a theorem of Zelditch*, Duke Math. Journal, Int. Res. Notices **12** (1993), 303–308.

[Gui94] V. Guillemin, *25 years of Fourier integral operators*, Mathematics Past and Present. Fourier Integral Operators (J. Brüning and V. Guillemin, eds.), Springer, 1994, pp. 1–21.

[Gui96] V. Guillemin, *Wave-trace invariants*, Duke Math. J. **83** (1996), no. 2, 287–352.

[Gut71] M. C. Gutzwiller, *Periodic orbits and classical quantization conditions*, J. Math. Phys. **44** (1971), 343.

[GW76a] V. Guillemin and A. Weinstein, *Correction and addendum: "Eigenvalues associated with a closed geodesic" (Bull. Amer. Math. Soc.* **82** *(1976), no. 1, 92–94)*, Bull. Amer. Math. Soc. **82** (1976), no. 6, 966.

[GW76b] V. Guillemin and A. Weinstein, *Eigenvalues associated with a closed geodesic*, Bull. Amer. Math. Soc. **82** (1976), no. 1, 92–94.

[HB92] D. R. Heath-Brown, *The distribution and moments of the error term in the Dirichlet divisor problems*, Acta Arith. **60** (1992), no. 4, 389–415.

[Hej76] D. A. Hejhal, *The Selberg trace formula and the Riemann zeta function*, Duke Math. Journal **43** (1976), 441–482.

[Hel97] B. Helffer, *h-pseudodifferential operators and applications: An introduction*, In Rauch and Simon [RS97], pp. 1–50.

[HJ99] G. A. Hagedorn and A. Joye, *Semiclassical dynamics with exponentially small error estimates*, Comm. Math. Phys. **207** (1999), no. 2, 439–465.

[HMR87] B. Helffer, A. Martinez, and D. Robert, *Ergodicité et limite semi-classique*, Commun. Math. Phys. **109** (1987), 313–326.

[Hör68] L. Hörmander, *The spectral function of an elliptic operator*, Acta Math. **121** (1968), 193–218.

[Hör71] L. Hörmander, *Fourier integral operators I*, Acta Math. **127** (1971), 79–183.

[Hör79] L. Hörmander, *On the asymptotic distribution of the eigenvalues of pseudodifferential operators in* $\mathbb{R}^n$., Ark. Mat. **17** (1979), 297–313.

[Hör83] L. Hörmander, *The analysis of linear partial differential operators I*, Springer, Berlin, Heidelberg, 1983.

[Hör85a] L. Hörmander, *The analysis of linear partial differential operators III*, Springer, Berlin, Heidelberg, 1985.

[Hör85b] L. Hörmander, *The analysis of linear partial differential operators IV*, Springer, Berlin, Heidelberg, 1985.

[Hör85] L. Hörmander, *The analysis of linear partial differential operators I-IV*, Springer, Berlin, Heidelberg, 1983-85.

[HS96] P. D. Hislop and I. M. Sigal, *Introduction to spectral theory*, Springer-Verlag, New York, 1996, With applications to Schrödinger operators.

[HST01] F. Hövermann, H. Spohn, and S. Teufel, *Semiclassical limit for the Schrödinger equation with a short scale periodic potential*, Comm. Math. Phys. **215** (2001), no. 3, 609–629.

[Hux93] M. N. Huxley, *Exponential sums and lattice points*, Proc. London Math. Soc. **66** (1993), 279–301.

[Ivr98] V. Ivrii, *Microlocal analysis and precise spectral asymptotics*, Springer-Verlag, Berlin, 1998.

[Jak97] D. Jakobson, *Equidistribution of cusp forms on* $PSL_2(\mathbf{Z})\backslash PSL_2(\mathbf{R})$, Ann. Inst. Fourier (Grenoble) **47** (1997), no. 3, 967–984.

[Kas89] C. Kassel, *Le résidue non commutatif*, Astérisque **177-178** (1989), 199–229, Séminaire Bourbaki, 41éme année, Exposé no. 708.

[KN65] J. J. Kohn and L. Nirenberg, *An algebra of pseudodifferential operators*, Commun. Pure Apl. Math. **18** (1965), 269–305.

[Kol57] A. N. Kolmogorov, *Théorie générale des systèmes dynamiques et mécanique classique*, Proceedings of the International Congress of Mathematicians, Amsterdam, 1954, Vol. 1, Erven P. Noordhoff N.V., Groningen, 1957, pp. 315–333.

[Laz93] V. F. Lazutkin, *KAM theory and semiclassical approximations to eigenfunctions*, Springer, Berlin, 1993.

[Lit86] R. G. Littlejohn, *The semiclassical evolution of wave packets*, Phys. Rep. **138** (1986), no. 4-5, 193–291.

[LM87] P. Libermann and C. M. Marle, *Symplectic geometry and analytical mechanics*, Reidel, Dordrecht, 1987.

[LS95] W. Luo and P. Sarnak, *Quantum ergodicity of eigenfunctions on* $PSL_2(\mathbb{Z})\backslash H^2$, Publ. Math., Inst. Hautes Etud. Sci. **81** (1995), 207–237.

[Mal95] P. Malliavin, *Integration and probability*, Springer-Verlag, New York, 1995, With the collaboration of Hélène Airault, Leslie Kay and Gérard Letac, Edited and translated from the French by Kay, With a foreword by Mark Pinsky.

[Mas72] V. P. Maslov, *Theórie des perturbations et méthodes asymptotiques*, Dunod, Paris, 1972, russian original 1965.

[Mei92] E. Meinrenken, *Semiclassical principal sympols and Gutzwillers trace formula*, Rep. on Math. Phys. **31** (1992), 271–294.

[Mei94] E. Meinrenken, *Trace formulas and the Conley-Zehnder index*, J. of Geom. and Phys. **13** (1994), 1–15.

[MF81] V. P. Maslov and M. V. Fedoriuk, *Semi-classical approximation in quantum mechanics*, Reidel, Dordrecht, 1981.

[Moy49] J. E. Moyal, *Quantum mechanics as a statistical theory*, Proc. Camb. Philos. Soc. **45** (1949), 99–124.

[MP49] S. Minakshisundaram and A. Pleijel, *Some properties of the eigenfunctions of the Laplace operator on Riemannian manifolds*, Canad. J. Math. **1** (1949), 242–256.

[MS73] V. P. Maslov and B. Ju. Sternin, *The canonical operator (the complex case)*, pp. 169–195, 199, Akad. Nauk SSSR Vsesojuz. Inst. Naučn. i Tehn. Informacii, Moscow, 1973.

[MS75] A. Melin and J. Sjöstrand, *Fourier integral operators with complex-valued phase functions*, pp. 120–223. Lecture Notes in Math., Vol. 459, Springer, Berlin, 1975.

[MS98] D. McDuff and D. Salamon, *Introduction to symplectic topology*, Oxford University Press, Oxford, 1998.

[MSS90] A. S. Mishchenko, V. E. Shatalov, and B. Yu. Sternin, *Lagrangian manifolds and the Maslov operator*, Springer, Berlin, 1990, russian original 1978.

[Omn94] R. Omnès, *The interpretation of quantum mechanics*, Princeton University Press, Princeton, 1994.

[Omn97] R. Omnès, *Quantum-classical correspondence using projection operators*, J. Math. Phys. **38** (1997), no. 2, 697–707.

[Pau97] T. Paul, *Semi-classical methods with emphasis on coherent states*, In Rauch and Simon [RS97], pp. 51–88.

[Per73] I. C. Percival, *Regular and irregular spectra*, J. Phys. B. **6** (1973), L229–232.

[Per86] A. Perelomov, *Generalized coherent states and their applications*, Springer-Verlag, Berlin, 1986.

[PR85] V. Petkov and D. Robert, *Asymptotique semi-classique du spectre d'hamiltoniens quantiques et trajectoires classiques périodiques*, Comm. Partial Differential Equations **10** (1985), no. 4, 365–390.

[PU91] T. Paul and A. Uribe, *Sur la formule semiclassique des traces*, C.R. Acad. Sci. Paris **313 I** (1991), 217–222.

[PU93] T. Paul and A. Uribe, *A construction of quasi-modes using coherent states*, Ann. Inst. H. Poincaré Phys. Théor. **59** (1993), no. 4, 357–381.

[PU98a] T. Paul and A. Uribe, *Weighted trace formula near a hyperbolic trajectory and complex orbits*, J. Math. Phys. **39** (1998), no. 8, 4009–4015.

[PU98b] T. Paul and A. Uribe, *Weighted Weyl estimates near an elliptic trajectory*, Rev. Mat. Iberoamericana **14** (1998), no. 1, 145–165.

[Ral76] J. V. Ralston, *On the construction of quasimodes associated with stable periodic orbits*, Comm. Math. Phys. **51** (1976), no. 3, 219–242.

[Ral79] J. V. Ralston, *Erratum: "On the construction of quasimodes associated with stable periodic orbits" (Comm. Math. Phys.* **51** *(1976), no. 3, 219–242)*, Comm. Math. Phys. **67** (1979), no. 1, 91.

[Ran78] B. Randol, *The Riemann hypothesis for Selberg's zeta-function and the asymptotic behavior of eigenvalues of the Laplace operator*, Trans. Amer. Math. Soc. **236** (1978), 209–223.

[Rob83] M. Robnik, *Classical dynamics of a family of billiards with analytic boundaries*, J. Phys. A **16** (1983), 3971–3986.

[Rob84] M. Robnik, *Quantising a generic family of billiards with analytic boundaries*, J. Phys. A **17** (1984), 1049–1074.

[Rob87] D. Robert, *Autour de l'approximation semi-classique*, Birkhäuser, Boston, 1987.

[RS80] M. Reed and B. Simon (eds.), *Methods of modern mathematical physics*, vol. 1, Academic Press, Boston, 1980.

[RS97] J. Rauch and B. Simon (eds.), *Quasiclassical methods*, The IMA volumes in Mathematics and its Applications, vol. 95, Springer, New York, 1997.

[RZ84] W. Rouhuai and C. Zhiyong, *Generalized Leray formula on positive complex Lagrange-Grassmann manifolds*, Chin. Ann. of Math. **5** (1984), 215–235.

[Sar95] P. Sarnak, *Arithmetic quantum chaos*, Isr. Math. Conf. Proc. **8** (1995), 183–236.

[Sch26] E. Schödinger, *Der stetige Übergang von der Mikro- zur Makromechanik*, Naturwissenschaften **14** (1926), 664–666.

[Sch95] R. Schubert, *The trace formula and the distribution of eigenvalues for Schrödinger operators on manifolds all of whose geodesics are closed*, DESY-report, no. 95-090, 1995.

[See67] R. T. Seeley, *Complex powers of an elliptic operator*, Proc. Sympos. Pure Math. **10** (1967), 288–307.

[Seg47] I. E. Segal, *Postulates for general quantum mechanics*, Ann. Math. **48** (1947), no. 4, 930–948.

[Sel56] A. Selberg, *Harmonic analysis and discontinous groups in weakly symmetric Riemannian spaces with applications to Dirichlet series*, J. Indian Math. Soc. **20** (1956), 47–87.

[Shn] A. I. Shnirelman, *On the asymptotic properties of eigenfunctions in the regions of chaotic motion*, in V. F. Lazutkin: *KAM Theory and Semiclassical Approximations to Eigenfunctions*, Springer, Berlin (1993).

[Shn74] A. I. Shnirelman, *Ergodic properties of eigenfunctions* (russian), Usp. Math. Nauk **29** (1974), 181–182.

[Shu87] M. A. Shubin, *Pseudodifferential operators and spectral theory*, Springer, Berlin, 1987.

[Sim80] B. Simon, *The classical limit of quantum partition functions*, Comm. Math. Phys. **71** (1980), no. 3, 247–276.

[Sim85] B. Simon, *Semiclassical analysis of low lying eigenvalues. IV. The flea on the elephant*, J. Funct. Anal. **63** (1985), no. 1, 123–136.

[Ste94] F. Steiner, *Quantum chaos*, Universität Hamburg 1994: Schlaglichter der Forschung zum 75. Jahrestag (R. Ansorge, ed.), Dietrich Reimer Verlag, 1994, p. 543.

[Sun97] T. Sunada, *Quantum ergodicity*, Progress in inverse spectral geometry (S. Andersson, ed.), Trends in Mathematics, Birkhäuser, Basel, 1997, pp. 175–196.

[Tay81] M. Taylor, *Pseudodifferential operators*, Princeton Univ. Press, Princeton, 1981.

[Tay96] M. Taylor, *Partial differential equations I*, Springer, New York, 1996.

[Thi79] W. Thirring, *Quantenmechanik von Atomen und Molekülen*, Lehrbuch der Mathematischen Physik, vol. 3, Springer, New York, 1979.

[Thi88] W. Thirring, *Klassische dynamische Systeme*, 2 ed., Lehrbuch der Mathematischen Physik, vol. 1, Springer, New York, 1988.

[Tre80] F. Treves, *Introduction to pseudodifferential and Fourier integral operators*, vol. 1,2, Plenum Press, New York, 1980.

[TS73] V. N. Tulovskii and M. A. Shubin, *On the asymptotic distribution of eigenvalues of pseudodifferential operators in* $\mathbb{R}^n$, Math. USSR Sbornik **21** (1973), 565–583.

[Uhl72] K. Uhlenbeck, *Eigenfunctions of Laplace operators*, Bull. Amer. Math. Soc. **78** (1972), 1073–1076.

[Uhl76] K. Uhlenbeck, *Generic properties of eigenfunctions*, Amer. J. Math. **98** (1976), no. 4, 1059–1078.

[vNW29] J. von Neumann and E. Wigner, *Über das Verhalten von Eigenwerten bei adiabatischen Prozessen*, Z. Physik **30** (1929), 553–556.

[Vor76] A. Voros, *Semi–classical approximations*, Annales de l'Institut Henri Poincaré A **24** (1976), 31–90.

[Vor77] A. Voros, *Asymptotic* $\hbar$*–expansions of stationary quantum states*, Annales de l'Institut Henri Poincaré A **26** (1977), 343–403.

[Wal82] P. Walters, *An introduction to ergodic theory*, Springer-Verlag, Berlin, 1982.

[Wei77] A. Weinstein, *Lectures on symplectic manifolds*, Regional conference series in mathematics, vol. 29, Amer. Math. Soc., Providence, 1977.

[Wey28] H. Weyl, *Quantenmechanik und Gruppentheorie*, Z. Physik **46** (1928), 1–46.

[Wie32] N. Wiener, *Tauberian theorems*, Ann. of Math. **33** (1932), 1–100.

[Wig32] E. P. Wigner, *On the quantum correction for thermodynamic equilibrium*, Phys. Rev. **40** (1932), 749–759.

[Wil87] M. Wilkinson, *A semiclassical sum rule for matrix elements of classically chaotic systems*, J. Phys. A **20** (1987), no. 9, 2415–2423.

[Wod82] M. Wodzicki, *Spectral asymmetry and zeta functions*, Inv. Math. **66** (1982), 115–135.

[Wun99] J. Wunsch, *The trace of the generalized harmonic oscillator*, Ann. Inst. Fourier (Grenoble) **49** (1999), no. 1, viii, xi–xii, 351–373.

[Zas81] G. M. Zaslavski, *Stochasticity in quantum systems*, Phys. Reports **80** (1981), 157–250.

[Zel87] S. Zelditch, *Uniform distribution of eigenfunctions on compact hyperbolic surfaces*, Duke. Math. J. **55** (1987), 919–941.

[Zel90] S. Zelditch, *Quantum transition amplitudes for ergodic and for completely integrable systems*, J. Func. An. **94** (1990), 415–436.

[Zel97] S. Zelditch, *Wave invariants at elliptic closed geodesics*, Geom. Funct. Anal. **7** (1997), no. 1, 145–213.

[Zel98] S. Zelditch, *Wave invariants for non-degenerate closed geodesics*, Geom. Funct. Anal. **8** (1998), no. 1, 179–217.

[ZZ96] S. Zelditch and M. Zworski, *Ergodicity of eigenfunctions for ergodic billiards*, Commun. Math. Phys. **175** (1996), 673–682.

Zusammenfassung

Die vorliegende Dissertation ist dem Studium der Eigenschaften von quantenmechanischen Systemen im semiklassischen Grenzfall gewidmet. Insbesondere der Einfluß des klassischen Systems auf die Eigenschaften des quantenmechanischen Systems, vor allem auf die Struktur der Eigenfunktionen, steht im Zentrum des Interesses. Das breite Spektrum der möglichen Eigenschaften des klassischen Systems kann sich in vielfältiger Weise im korrespondierendem quantenmechanschen System widerspiegeln. Ein Leitmotiv dieser Arbeit ist die Frage, wie sich die Existenz von invarianten Gebieten, oder allgemeiner von invarianten Maßen, im Phasenraum auf das quantenmechanische System auswirkt. Ein klassisches System, dessen Phasenraum ein invariantes Gebiet enthält, läßt sich zerlegen in die Einschränkung des Systems auf dieses Gebiet und in die Einschränkung des Systems auf das Komplement des Gebietes. Damit erhält man eine Zerlegung des klassischen Systems in zwei Teilsysteme, die nicht miteinander wechselwirken. Die Frage ist nun, ob sich das quantenmechanische System, zumindest näherungsweise, ähnlich verhält, nämlich wie zwei Teilsysteme, die nicht oder nur schwach miteinander wechselwirken. So erwartet man dann z.B., daß die Eigenfunktionen bzw. ihre Wignertransformierten, im semiklassischen Limes auf den jeweiligen invarianten Gebieten im Phasenraum konzentriert sind. Weiterhin möchte man natürlich wissen, wie sich weitere Charakteristika der klassischen Dynamik, wie Ergodizität oder Integrabilität, auf die Struktur der Eigenfunktionen auswirken.

Die mathematischen Methoden, mit denen man solche Fragen studieren kann, stammen hauptsächlich aus dem Gebiet der mikrolokalen Analysis. Wir geben einen ausführlichen Überblick über dieses Gebiet, von einer semiklassischen Perspektive aus. Die Methoden aus der mikrolokalen Analysis geben einen rigorosen Rahmen, in dem man sehr schön verstehen kann, wie die Strukturen der klassischen Mechanik im Hochenergie-Limes aus der Quantenmechanik hervorgehen. Wir zeigen insbesondere, wie man den üblichen Formalismus so modifizieren kann, daß der semiklassische Limes in einer formal befriedigenden Weise ausgeführt werden kann.

Eine häufig auftauchende Klasse von quantenmechanischen Zuständen bilden die sogenannten Lagrange Zustände. Diese sind im semiklassischen Limes auf einer Lagrange Untermannigfaltigkeit des Phasenraumes konzentriert. Wir studieren eine allgemeinere Klasse von Lagrangeschen Zuständen, bei denen die Lagrange Untermannigfaltigkeit komplex werden kann; in dieser allgemeineren Klasse sind auch die kohärenten Zustände enthalten. Die Ehrenfest Zeit, die angibt, wie lange die quantenmechanische Zeitentwicklung der klassischen folgt, wird in Abhängigkeit von der Chaotizität des klassischen Systems

untersucht.

Kohärente Zustände werden dann zur Einführung der Anti-Wick Quantisierung benutzt. Dieses Quantisierungsverfahren erlaubt die Quantisierung von nicht-glatten Distributionen. Wir studieren insbesondere die Anti-Wick Quantisierung von Maßen und zeigen, daß die Norm dieser Operatoren durch die Hausdorff Dimension der Maße bestimmt ist. Im Weiteren wird die Anti-Wick Quantisierung dann benutzt um approximative Projektionsoperatoren als Quantisierung von charakteristischen Funktionen von offenen Teilmengen des Phasenraumes einzuführen.

Die Konstruktion der approximativen Projektionsoperatoren assoziiert mit invarianten Gebieten des Phasenraumes, und das Studium ihrer Eigenschaften gehört zu den zentralen Resultaten der Arbeit. Wenn das invariante Gebiet im klassischen System stabil ist unter kleinen Störungen des klassischen Systems, dann gelingt die Konstruktion von approximativen Projektionsoperatoren, deren Kommutator mit dem Hamiltonoperator kleiner ist als jede Potenz des semiklassischen Parameters. Dieses zunächst vielleicht recht technisch anmutende Resultat hat ein Reihe von wichtigen Konsequenzen. Zum einen ergibt sich damit eine approximative Zerlegung des quantenmechanischen System in zwei Teilsysteme, die fast invariant sind unter der Zeitentwicklung. Die Zeitskala, über die die Teilsysteme invariant bleiben, ist dabei polynomial im semiklassischen Parameter und damit deutlich größer als die Ehrenfest Zeit. Weiterhin lässt sich zum einen die Existenz von approximativen Lösungen der stationären Schrödingergleichung, sogenannter Quasimoden, in den einzelnen Teilsystemen folgern, und zum anderen folgt ein lokales Quantenergodizitätstheorem, welches eine Verallgemeinerung des bekannten Theorems auf den Fall ergodischer Komponenten darstellt.

Im letzten Kapitel diskutiere ich dann allgemeine Eigenschaften von Quasimoden und einige konkrete Konstruktionen. Dabei steht das Studium der Stabilität von Quasimoden unter kleinen Störungen im Vordergrund, welches zu zwei Vermutungen über generische Zusammenhänge zwischen Quasimoden und Eigenfunktionen führt. An konkreten Beispielen wird dann diskutiert, daß die Stabilitätsbedingung nicht redundant ist, d.h. es gibt Quasimoden, die nicht stabil sind.