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Conjugate pairing in the three-dimensional periodic Lorentz gas

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We numerically evaluate the Lyapunov exponents for the three-dimensional periodic Lorentz gas in an electric field, with a Gaussian thermostat. For small values of the field, the dynamics appears to be ergodic. For larger fields there are chaotic and periodic windows. The Lyapunov exponents are found to obey the conjugate pairing rule in both chaotic and stable regions, indicating that conjugate pairing can occur for small systems, and is not restricted to the large N limit.

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Hamiltonian systems have the well known property that the Lyapunov exponents occur in pairs, that is, if λ is one exponent, then so is $-\lambda$. This property follows from the symplectic eigenvalue theorem [1], and is well understood. Recently it has been found that systems with a constant damping factor [2] or a thermostat [3,4] exhibit a generalized pairing rule: For each ergodic trajectory there is a single constant C so that if λ_i is one exponent, then so is $C-\lambda_i$ for all i. We call this the conjugate pairing rule. The case of a constant damping factor is similar to the Hamiltonian case, and has been proven using similar methods. For thermostated systems, there is only numerical evidence, together with an argument valid in the limit of a large number of particles [5]. We demonstrate here that a system with the smallest possible number of pairs of exponents (two) for which a test may be performed exhibits conjugate pairing to a high degree of accuracy, and suggest that a more general result should exist, independent of the number of degrees of freedom.

The Lorentz gas is a system which has enjoyed much popularity since it was first propounded by Lorentz [6] in 1905 as a model for the motion of electrons in solids. It is one of the few nontrivial chaotic systems about which rigorous mathematical statements may be made [7]. It may be extended to include an external electric field and Gaussian thermostat [8], and as such, has provided much understanding about the relation of microscopic nonlinear dynamics to nonequilibrium statistical mechanics. In particular it exhibits a steady macroscopic current in the direction of the field while retaining reversible equations of motion.

The Lyapunov exponents of a thermostated system are important, not only in distinguishing between chaotic and regular regimes, but also because the sum of all the exponents is related to a macroscopic transport coefficient [8]. For example, in the nonequilibrium Lorentz gas, the sum of the exponents is directly related to the current, which is the product of the field and the conductivity. If the conjugate pairing rule is valid generally for these systems, at least for the statistically significant ergodic trajectories, it is necessary to compute only the largest and smallest exponents in order to make this connection. The largest exponent is the easiest to evaluate numerically, while the smallest exponent may be easily computed using time reversed trajectories. Calculating all of the exponents, especially for a large system, may be very difficult.

The three-dimensional periodic Lorentz gas consists of a particle wandering in a hexagonal close packed lattice of spheres, with which it undergoes hard collisions. The particle is also subject to a force which has two components, a constant electric field f in the negative z direction, and a thermostating force in the direction of motion, which keeps the kinetic energy constant. The equations of motion for a free flight are

$$\dot{\mathbf{x}}=\frac{\mathbf{p}}{m}, \tag{1}$$

$$\dot{\mathbf{p}}=-f\mathbf{e}_z+\alpha\mathbf{p}, \tag{2}$$

where $\alpha=-p_zf/p^2=-\epsilon\cos\theta$. Here, as in previous studies, $\epsilon=f/p$. Expressing the momentum variables in terms of angles

$$p_x=p\,\sin\theta\,\cos\phi, \tag{3}$$

$$p_y=p\,\sin\theta\,\sin\phi, \tag{4}$$

$$p_z=p\,\cos\theta, \tag{5}$$

and scaling the variables so that p, m and the radius of the spheres are all equal to 1, these equations may be integrated analytically to obtain

$$\phi=\phi_0, \tag{6}$$

$$\tan\frac{\theta}{2}=\tan\frac{\theta_0}{2}\,\exp\frac{t-t_0}{\epsilon}, \tag{7}$$

$$x=x_0+\frac{\theta-\theta_0}{\epsilon}\cos\phi_0, \tag{8}$$

$$y=y_0+\frac{\theta-\theta_0}{\epsilon}\sin\phi_0, \tag{9}$$

$$z=z_0+\frac{1}{\epsilon}\ln\frac{\sin\theta}{\sin\theta_0}, \tag{10}$$

where a subscript 0 indicates the initial value.

In this paper the distance between the centers of the spheres is always $R=2.3$. The other parameters which may

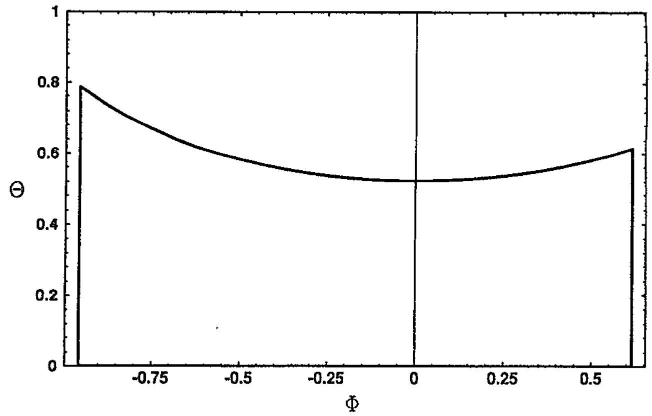

FIG. 1. The minimal domain of Θ and Φ, which determine the orientation of the field relative to the lattice. The region is determined by the conditions $-\arctan\sqrt{2}\leqslant\Phi\leqslant\arctan(1/\sqrt{2})$, $0\leqslant\Theta\leqslant\arctan(\sqrt{3}\cos\Phi)^{-1}$.

be varied are (apart from the field) the angles which give the orientation of the lattice and the field. We must define the direction of the field with respect to the lattice, and not the other way round, as the field does not contain enough directional information to define a coordinate system. We define a coordinate system x', y', z' aligned with the lattice, so the lattice vectors are $R\mathbf{e}'_z$, $R(\sqrt{3}\mathbf{e}'_x/2+\mathbf{e}'_z/2)$ and $R(\sqrt{3}\mathbf{e}'_x/6+\sqrt{6}\mathbf{e}'_y/3+\mathbf{e}'_z/2)$. Then, the field is at spherical coordinates (Θ,Φ), that is,

$$f'_x=f\ \sin\Theta\ \cos\Phi, \tag{11}$$

$$f'_y=f\ \sin\Theta\ \sin\Phi, \tag{12}$$

$$f'_z=f\ \cos\Theta. \tag{13}$$

The lattice symmetries may be used to restrict the domain of Θ and Φ. The minimal domain which is equivalent to the whole solid angle and has values of Θ and Φ closest to zero is shown in Fig. 1. For the numerical calculations it is much simpler to work in the original coordinate system, which is aligned to the field. Specifically, the lattice vectors are rotated by an angle $-\Phi$ around the z' axis, then rotated by an angle $-\Theta$ around the new y' axis, which then becomes the y axis.

There is one orientation which is qualitatively different from the others, which in our coordinate system corresponds to $\Theta=0$. Unlike the two-dimensional case, the three-dimensional Lorentz gas with periodically spaced spherical scatterers has an infinite horizon, even when the spheres are touching $(R=2)$. That is, there is a set of straight line trajectories (in the zero field case) of zero Liouville measure which never hit a scatterer. They are parallel to lines of scatterers. This means that rigorous proofs are more difficult (see, for example, Ref. [7]), and the zero field case is qualitatively different. If a nonzero field is aligned to one of these directions, that is, $\Theta=0$, most trajectories end up in one of these regions of phase space and remain there. For other field orientations, the behavior is similar to the two-dimensional case with finite horizon [9].

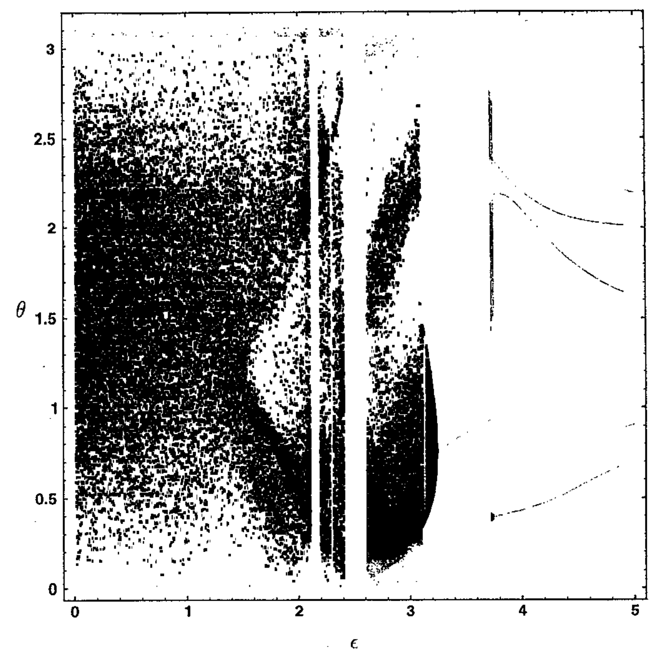

FIG. 2. The bifurcation diagram for the case $\Theta=\Phi=\arctan(1/\sqrt{2})$.

Numerical simulation of this system is difficult, since the equations determining the collisions are transcendental. Standard integration techniques fail because there is no guarantee that the trajectory has not passed through a sphere between successive points. We approximate the path by a circle to obtain a lower bound on the time before the next collision. After several such steps, when the distance to the surface of a sphere is less than 10^{-14}, a collision takes place. Lyapunov exponents are estimated numerically by considering neighboring trajectories, using a Gram-Schmidt renormalization at every collision. This is similar in spirit to one of the standard algorithms [10], except that the equations are not linearized explicitly. The collisions make it prohibitively complicated to write down the linearized equations in this way, so we have resorted to small (10^{-7}) rather than infinitesimal perturbations. Note that the scale of these perturbations is much greater than the errors associated with the collisions.

Figure 2 shows the bifurcation diagram for the case $\Theta=\Phi=\arctan(1/\sqrt{2})$ as a function of the field strength. The variable plotted is the value of θ after a collision. For $\epsilon<2$ the trajectory appears to fill the whole of phase space. This is an artifact of using only a single variable θ, as the attractor has a dimension less than that of phase space. It shows that for small values of the field, the trajectory does not approach a stable periodic orbit, and may be ergodic within the attractor. At larger values of the field windows of stable periodic orbits with 2, 3, 6, and 9 collisions appear. "Periodic" in this case means up to lattice translations. The symmetry of the lattice relative to the direction of the field results in degeneracy, where collisions in these orbits may have equal values of θ. Ergodicity is broken, as in the two-dimensional case [9], since differing initial conditions lead to different stable orbits. Choosing less special directions of field breaks the degeneracy, but the overall structure is similar.

The Lyapunov exponents for this case (Fig. 3) show a

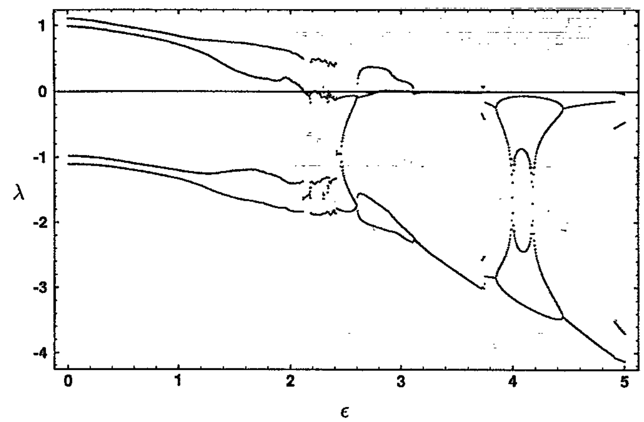

FIG. 3. The four Lyapunov exponents for the case $\Theta=\Phi=\arctan(1/\sqrt{2})$.

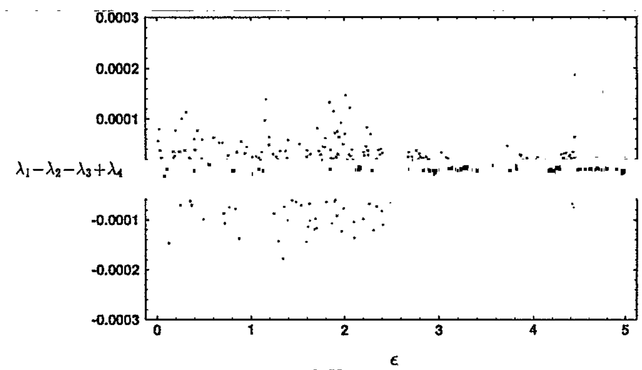

FIG. 4. The combination $\lambda_1-\lambda_2-\lambda_3+\lambda_4$ which is equal to zero if the conjugate pairing rule holds. Note the scale on the axes.

very rich structure. Near $\epsilon=2.15$ the first two exponents are almost equal. Near $\epsilon=2.45$ the second and third exponents are equal. Near $\epsilon=3.2$ the first two exponents are nearly equal and close to zero. In all of these cases, as well as the ergodic region for small field, the conjugate pairing rule, $\lambda_1+\lambda_4=\lambda_2+\lambda_3$, is very nearly valid. To illustrate this point we have plotted $\lambda_1-\lambda_2-\lambda_3+\lambda_4$ as a function of field in Fig. 4. The result is (almost) random scatter with a maximum amplitude of about 2×10^{-4}. The exponents presented here were calculated using 10^5 collisions and are accurate to about 3 significant figures. The conjugate pairing improves as the number of collisions, n, increases, with an error approximately proportional to $1/n$, and holds for all the other field directions we have tried. Note that the accuracy with which the conjugate pairing rule is obeyed is greater than the accuracy of the individual exponents themselves, which is roughly proportional to $1/\sqrt{n}$, and that the rule is obeyed regardless of the nature of the trajectories (either chaotic or stable).

What is clear from this work is that the requirement for a large number of particles in the original result [5] is not a necessary condition for the conjugate pairing rule. This suggests that the present argument, based upon the symplectic properties of the dynamics, uses overly restrictive preconditions and that it may be possible to obtain an exact proof, valid for small systems such as this three-dimensional Lorentz gas. Another system in which conjugate pairing is observed numerically is SLLOD dynamics, used to simulate planar Couette flow [4].

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