Chapter 4

1D PDE's on infinite Domains: Fourier Transforms

PDE's on **infinite domains** need a new technique.

We've seen that Fourier series naturally arise when representing functions (I.C.'s in PDE's) over finite domains.

Take limit of finite domain as size $\to \infty$.

4.1 Complex Form of the Fourier series

Fourier series can be expressed in a different form using

$$\cos\theta = \frac{e^{i\theta} + e^{-i\theta}}{2}, \qquad \sin\theta = \frac{e^{i\theta} - e^{-i\theta}}{2i}$$

The Fourier series is (see (3.9))

$$\begin{aligned} f(x) &= \sum_{n=0}^{\infty} a_n \cos\left(\frac{n\pi x}{L}\right) + b_n \sin\left(\frac{n\pi x}{L}\right) \\ &= a_0 + \sum_{n=1}^{\infty} a_n \left(\frac{e^{n\pi ix/L} + e^{-n\pi ix/L}}{2}\right) + b_n \left(\frac{e^{n\pi ix/L} - e^{-n\pi ix/L}}{2i}\right) \\ &= a_0 + \sum_{n=1}^{\infty} \tfrac{1}{2}(a_n - ib_n)e^{n\pi ix/L} + \tfrac{1}{2}(a_n + ib_n)e^{-n\pi ix/L} \end{aligned}$$

Let

$$c_n = \tfrac{1}{2}(a_n - ib_n) \text{ for } n > 0, \quad c_0 = a_0, \quad c_{-n} = \tfrac{1}{2}(a_n + ib_n) \text{ for } n > 0$$

Then

$$\begin{aligned} f(x) &= a_0 + \sum_{n=1}^{\infty} c_n e^{n\pi ix/L} + \sum_{n=1}^{\infty} c_{-n} e^{-n\pi ix/L} \\ &= a_0 + \sum_{n=1}^{\infty} c_n e^{n\pi ix/L} + \sum_{n=-\infty}^{-1} c_n e^{n\pi ix/L} \end{aligned}$$

So we have the Fourier Series written in the complex exponential form

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{n\pi i x/L}$$

Now we get a neat formula for the coefficients c_n, For $n > 0$ we have from (3.10,3.12)

$$c_n = \tfrac{1}{2}(a_n - ib_n) = \tfrac{1}{2}\frac{1}{L}\int_{-L}^{L}\left[\cos\left(\frac{\pi n x}{L}\right) - i\sin\left(\frac{\pi n x}{L}\right)\right] f(x)\,dx = \frac{1}{2L}\int_{-L}^{L} f(x)e^{-n\pi i x/L}\,dx$$

It's easy to show that the same formula holds for $n < 0$ and $n = 0$. Summarising our results:

$$\boxed{f(x) = \sum_{-\infty}^{\infty} c_n e^{n\pi i x/L} \quad \text{where} \quad c_n = \frac{1}{2L}\int_{-L}^{L} f(x)e^{-n\pi i x/L}\,dx}$$

If f is real, then this formula for c_n gives $c_{-n} = \overline{c_n}$.

4.1.1 The Spectrum

Oscillation of **period** $2L$ has **frequency** $1/2L$: no. of cycles/unit length.

Defn: Angular frequency = $2\pi\times$ freq, = number of radians/unit length.

Often called k in x-context, and ω in t-context.

Examples: e^{ipx} has angular frequency p, and $\mathrm{e}^{\pi i n x/L}$ has ang. freq. $\pi n/L$.

We often say "frequency" to mean *ang*. freq.

Let's consider a change of variable from n to k: So let $k = n\pi/L$ and $C(k) = 2Lc_n$. Now $k \in \mathbb{R}$, but still takes discrete values of $\ldots, -2\pi/L, -\pi/L, 0, \pi/L, 2\pi/L, \ldots$.

Now our F.S. is:

$$f(x) = \frac{1}{2L}\sum_k C(k)\mathrm{e}^{ikx}$$

where

$$C(k) = \int_{-L}^{L} f(x)\mathrm{e}^{-ikx}\,dx$$

These formulae tell you that a function $f(x)$ is composed of a sum of different "signals" or "modes" each of weight $C(k)/2L$. So $C(k)/2L$ is called the **spectrum** of $f(x)$. At the moment, these are points spaced equally along the k-axis.

E.g.: If $f(x) = \sin(\pi x/L) = \dfrac{1}{2i}\left(e^{i\pi x/L} - e^{-i\pi x/L}\right)$ then it follows that $C(\pi/L)/2L = \dfrac{1}{2i}$ and $C(-\pi/L)/2L = -\dfrac{1}{2i}$ whilst $C(k) = 0$ for all other values of k. So the spectrum has just two components at $k = \pm\pi/L$ of equal and opposite weight.

4.1.2 Limit as $L \to \infty$

Write $\Delta k = \pi / L =$ distance between the freqs in the spectrum. As $L \to \infty$, $\Delta k \to 0$. By substitution we have

$$f(x) = \frac{1}{2\pi} \sum_k C(k) e^{ikx} \Delta k$$

As $L \to \infty$, $\sum_k \to \int_{-\infty}^{\infty}$ and $\Delta k \to dk$. So

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} C(k) e^{ikx} \, dk$$

where

$$C(k) = \int_{-\infty}^{\infty} f(x) e^{-ikx} \, dx$$

and $f(x)$ is **any** PWC function on $\mathbb{R}$ (i.e. not periodic).

Note: k is a continuous variable and $C(k)$ is the spectrum of the function $f(x)$.

THIS IS NOT RIGOROUS MATHEMATICAL THEORY.

4.2 The Fourier Transform

4.2.1 Definitions

Replace spectrum function $C(k)$ with $\widetilde{f}$ to make the connection with $f(x)$ explicit.

Defn: The **Fourier transform** (F.T.) of $f(x)$ is

$$\widetilde{f}(k) = \int_{-\infty}^{\infty} f(x) e^{-ikx} \, dx$$

Notes:

1. Sometimes, there is a factor of $1/\sqrt{2\pi}$ in the definition; sometimes e^{-ikx} is sometimes e^{ikx}.

   This is OK, as long as *consistent* with the definition of the **inverse**. Also, sometimes $\widetilde{f}$ written as $\overline{f}(k)$ or $F(k)$.

2. Integral only exists if $f(x) \to 0$ "fast enough" as $x \to \pm\infty$.

3. Can think of F.T. as an operation: $\widetilde{f} = \mathscr{F}\{f\}$; $\mathscr{F}$ is a **linear operator**.

Defn: The **inverse F.T.** (from previous section):

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \widetilde{f}(k) e^{ikx} \, dk$$

Can think of this as $f(x) = \mathscr{F}^{-1}\{\widetilde{f}\}$ where $\mathscr{F}^{-1}$ is the inverse operator.

Fourier Integral Theorem. If f is absolutely integrable $\int_{-\infty}^{\infty} |f(x)|\, dx < \infty$ and PWC on $(-\infty, \infty)$ then integral for $\widetilde{f}(k)$ converges. At a point of discontinuity, $x = c$ say, $f(x)$ defined by its inverse F.T. converges to $\frac{1}{2}(f(c-) + f(c+))$ as in F.S.

Proof: too difficult for this course.

Example 1. Take $f(x) = \mathrm{e}^{-a|x|}$, with $a > 0$. Then

$f(x) = \begin{cases} e^{ax} \text{ for } x < 0 \\ e^{-ax} \text{ for } x > 0 \end{cases}$ Taking the F.T.:

$$
\begin{aligned}
\widetilde{f}(k) &= \int_{-\infty}^{0} \mathrm{e}^{(a-ik)x}\, dx + \int_{0}^{\infty} \mathrm{e}^{(-a-ik)x}\, dx \\
&= \left[\frac{1}{a-ik} + \frac{1}{a+ik}\right] \\
&= \left(\frac{2a}{a^2+k^2}\right).
\end{aligned}
$$

Example 2. Inverse F.T. says that

$$
f(x) = \mathrm{e}^{-a|x|} = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{2a}{a^2+k^2} \mathrm{e}^{ikx}\, dk
$$

We don't *need* to confirm this result – the inverse F.T. theorem tells us it must be true. But can we confirm it ? (Useful exercise in integration in the complex plane – sometimes inevitable when considering F.T.'s)

R.H.S. of above is

$$
\frac{a}{\pi} \int_{-\infty}^{\infty} \frac{\mathrm{e}^{ikx}}{a^2+k^2}\, dk
$$

Need complex function theory from Calc 2 here. The integrand can be written as

$$
g(k) = \frac{\mathrm{e}^{ikx}}{(k-ia)(k+ia)}
$$

Treat k as a complex number.

There are **simple poles** (i.e. demoninator vanishes) at $k = ia$ and $k = -ia$.

To compute the $\int_{-\infty}^{\infty} \ldots dk$, form a closed contour in the complex k-plane which includes the real k-axis. Why ? Because **Cauchy's residue theorem** (CRT) tells us that *the integral round a closed contour is equal to* $2\pi i$ *times the sum of the residues at the poles inside the contour.*

Residue at $k = ia$ is $\lim_{k \to ia} (k - ia) g(k) = \dfrac{\mathrm{e}^{ix(ia)}}{2ia}$.

Residue at $k = -ia$ is $\lim_{k \to -ia} (k + ia) g(k) = \dfrac{\mathrm{e}^{ix(-ia)}}{-2ia}$.

How to close the contour ?

Two (sensible) possibilities: Either close contour with a large semi-circle in the upper-half complex k-plane or in the lower-half plane. Which way to go ?

Large semi-circle is $k = Re^{i\theta}$ as $R \to \infty$. Then

$$\exp\{ikx\} = \exp\{ixRe^{i\theta}\} = \exp\{iRx\cos\theta\}\exp\{-Rx\sin\theta\}$$

- If $x > 0$ then if $0 < \theta < \pi$ above tends to zero as $R \to \infty$. I.e. go into **upper** half plane.
- If $x < 0$ then if $0 > \theta > -\pi$ above tends to zero as $R \to \infty$. I.e. go into **lower** half plane.

I.e. if $x > 0$,

$$\frac{a}{\pi}\int_{-\infty}^{\infty} \frac{e^{ikx}}{a^2+k^2}\,dk = 2\pi i\left(\frac{a}{\pi}\right)\frac{e^{-ax}}{2ia} = e^{-ax}$$

by CRT, picking up pole at $k = ia$.

If $x < 0$ then pick up residue from pole at $k = -ia$

$$\frac{a}{\pi}\int_{-\infty}^{\infty} \frac{e^{ikx}}{a^2+k^2}\,dk = -2\pi i\left(\frac{a}{\pi}\right)\frac{e^{ax}}{-2ia} = e^{ax}$$

where the minus sign out front is because the contour being closed is now *clockwise* (CRT is usually stated for anticlockwise contours).

This confirms the result !

Example 3: Take $f(x) = e^x$. F.T. does not exist because the integral not convergent. Same for e^{-x}.

Example 4: Take $f_{th}(x) = \begin{cases} 1/2a \text{ for } |x| < a \\ 0 \text{ for } |x| > a \end{cases}$.

This is called a "**top-hat**" function. Then

$$\widetilde{f}_{th}(k) = \int_{-a}^{a} \frac{1}{2a}.e^{-ikx}\,dx = \left[\frac{e^{ika} - e^{-ika}}{2ika}\right] = \frac{\sin ka}{ka}$$

Example 5:

Take $f(x) = \dfrac{e^{-x^2/a^2}}{a\sqrt{\pi}}$.

This is a "Gaussian" with a peak of $\frac{1}{2}$-width a.

Note: $\boxed{\dfrac{1}{a\sqrt{\pi}}\displaystyle\int_{-\infty}^{\infty} e^{-x^2/a^2}\,dx = 1}$ is a standard integral (from probability).

Then (see problem sheet)

$\widetilde{f} = \mathrm{e}^{-a^2k^2/4}$.

So transform of a Gaussian of half-width a is a Gaussian of half-width $2/a$.

Note: Last two examples have shown how "narrow signals" give "wide transforms".

4.2.2 Simple Properties

1. $\mathscr{F}$ is a linear operator: For fns f, g and consts a, b we have
$\mathscr{F}\{af + bg\} = a\mathscr{F}\{f\} + b\mathscr{F}\{g\}$

2. If $f(x)$ is even in x, then $\widetilde{f}(k)$ is even in k.
Proof:

$$\begin{aligned} \widetilde{f}(k) = \int_{-\infty}^{\infty} f(x)\mathrm{e}^{-ikx}\,dx &= \int_{-\infty}^{\infty} f(-x)\mathrm{e}^{ikx}\,dx \\ &= \int_{-\infty}^{\infty} f(x)\mathrm{e}^{-i(-k)x}\,dx \\ &= \widetilde{f}(-k) \end{aligned}$$

where $f(x) = f(-x)$ and a change of variables $x \to -x$ have been used.
Similarly, if $f(x)$ is odd then $\widetilde{f}(k)$ is odd also.

3. Furthermore, if f is real & even, then $\widetilde{f}$ is real.
Proof:

$$\begin{aligned} \widetilde{f}(k) &= \int_{-\infty}^{0} f(-x)\mathrm{e}^{-ikx} + \int_{0}^{\infty} f(x)\mathrm{e}^{-ikx}\,dx \\ &= 2\int_{0}^{\infty} f(x)\cos(kx)\,dx \end{aligned}$$

Similarly, if $f(x)$ is real & odd, then $\widetilde{f}(k)$ is imaginary.

4. (V. Important) $\widetilde{f'}(k) \equiv \mathscr{F}\left\{\frac{df}{dx}\right\} = ik\widetilde{f}(k)$. This is key result for application of F.T.'s to PDEs.
Proof:

$$\begin{aligned} \widetilde{f'}(k) &= \int_{-\infty}^{\infty} \frac{df}{dx}\mathrm{e}^{-ikx} \\ &= \left[f(x)\mathrm{e}^{-ikx}\right]_{-\infty}^{\infty} + ik\int_{-\infty}^{\infty} f(x)\mathrm{e}^{-ikx}\,dx \\ &= ik\widetilde{f}(k) \end{aligned}$$

by integration by parts and using $f(x) \to 0$ as $x \to \pm\infty$.

5. (Shift Property) If $g(x) = f(x+a)$, then $\widetilde{g}(k) = \mathrm{e}^{ika}\widetilde{f}(k)$.
Proof:

$$\widetilde{g}(k) = \int_{-\infty}^{\infty} f(x+a)\mathrm{e}^{-ikx}\,dx = \int_{-\infty}^{\infty} f(x')\mathrm{e}^{ika}\mathrm{e}^{-ikx'}\,dx' = \mathrm{e}^{ika}\widetilde{f}(k)$$

After using $x' = x + a$.

4.2.3 Products and Convolutions

$\mathscr{F}\{fg\} \neq \mathscr{F}\{f\}\mathscr{F}\{g\}$, it's more complicated.

Defn: The **convolution** of fns f, g is the fn $f * g$ defined by

$$(f * g)(x) = \int_{-\infty}^{\infty} f(\xi)g(x-\xi)\,d\xi$$

Then $f * g = g * f$.

Proof: Easy.

$$(g * f)(x) = \int_{-\infty}^{\infty} g(\xi)f(x-\xi)\,d\xi = \int_{-\infty}^{\infty} g(x-\xi')f(\xi')\,d\xi'$$

after a change of variables $\xi' = x - \xi$.

Transforms of Products and Convolutions

$\mathscr{F}\{f * g\} \equiv \widetilde{f * g} = \widetilde{f}\widetilde{g}$

Proof: Start with the L.H.S. of above:

$$\begin{aligned}
\int_{-\infty}^{\infty} e^{-ikx}\left[\int_{-\infty}^{\infty} f(\xi)g(x-\xi)\,d\xi\right]dx &= \int_{-\infty}^{\infty} f(\xi)e^{-ik\xi}\left[\int_{-\infty}^{\infty} g(x-\xi)e^{-ik(x-\xi)}\,dx\right]d\xi \\
&= \int_{-\infty}^{\infty} f(\xi)e^{-ik\xi}\left[\int_{-\infty}^{\infty} g(\xi')e^{-ik\xi'}\,d\xi'\right]d\xi \\
&= \widetilde{f}(k)\widetilde{g}(k)
\end{aligned}$$

after switching order of integration and using a change of variable $\xi' = x - \xi$, get

4.3 The Delta "Function"

4.3.1 Introduction

From e.g. 5 in §4.2.1 we showed that if $f(x) = \dfrac{e^{-x^2/a^2}}{a\sqrt{\pi}}$ then (i) $\int_{-\infty}^{\infty} f(x)\,dx = 1$ and (ii) $\widetilde{f}(k) = e^{-a^2k^2/4}$

As $a \to 0$ the peak becomes narrower and higher; area under the curve is always equal to 1.

Also $\widetilde{f}(k) \to 1$ as $a \to 0$.

We can think of $f(x)$ as representing a **distribution of density** s.t. the total mass, $\int_{-\infty}^{\infty} f(x)\,dx = 1$ is always the same.

Suppose all the mass is concentrated at $x = 0$, s.t. $f(x) = 0$ for $x \neq 0$, and yet $\int_{-\infty}^{\infty} f(x)\,dx = 1$ remains.

This is impossible for "ordinary functions" but can define such as function as a "**generalised function**" or "distribution". Equations involving distributions can be made rigorous by first multiplying by a suitable arbitrary test function (with sufficient smoothness and rapid decay at infinity) and then integrating, but this is well beyond the scope of this unit.

Define

$$\delta(x) = \lim_{a\to 0} f(x) = \lim_{a\to 0} \frac{e^{-x^2/a^2}}{a\sqrt{\pi}}.$$

Then

Defn: The Dirac delta function, $\delta(x)$, is defined by

- $\delta(x) = 0$ for $x \neq 0$
- $\int_a^b \delta(x)\,dx = 1$ for any $a < 0 < b$.

The limiting form of the Gaussian is not the only definition – there are many – of $\delta(x)$.

E.g. Take "top-hat" e.g. 4 in §4.2.1: $f_{th}(x) = \begin{cases} 0, & |x| > a \\ 1/2a, & |x| < a \end{cases}$. Then $\int_{-\infty}^{\infty} f_{th}(x)\,dx = 1$ and clearly then the definition above is satisfied by writing

$$\delta(x) = \lim_{a\to 0} f_{th}(x)$$

4.3.2 Properties of the Delta Function

1. $\delta(x)$ is an even function.
   Proof: $\delta(-x) = 0$ for $x \neq 0$ and
   $$\int_a^b \delta(-x)\,dx = \int_{-b}^{-a} \delta(x)\,dx = 1, \qquad a < 0 < b$$
2. Shifted δ-Function. (obvious) $\delta(x-c) = 0$ for $x \neq c$ and $\int_a^b \delta(x-c)\,dx = 1$ provided $a < c < b$. Otherwise integral is zero.
3. Sampling Property (V. Important). For any sufficiently smooth function $f(x)$ (i.e. f and all derivatives are continous) then
   $$\int_{-\infty}^{\infty} \delta(x-c) f(x)\,dx = f(c)$$
   I.e. it "picks out" value of $f(x)$ at $x = c$.
   Justification: Use $\delta(x) = \lim_{a\to 0} f_{th}(x)$.

Then

$$\begin{aligned}
\int_{-\infty}^{\infty} \delta(x-c) f(x)\, dx &= \lim_{a\to 0} \int_{c-a}^{c+a} \left(\frac{1}{2a}\right) f(x)\, dx \\
&= \lim_{a\to 0} \frac{1}{2a} \int_{c-a}^{c+a} [f(c) + (x-c)f'(c) + \tfrac{1}{2}(x-c)^2 f''(c) + \ldots]\, dx \\
&= \lim_{a\to 0} \left[f(c) + \frac{1}{6}a^2 f''(c) \ldots \right] = f(c)
\end{aligned}$$

NOTE: need $f(x)$ to be suff. smooth.

4.3.3 Relationship to discontinuous functions

Defn: The **Heaviside function** $H(x)$ is defined by

$$H(x) = \begin{cases} 0 & \text{for } x < 0 \\ \frac{1}{2} & \text{for } x = 0 \\ 1 & \text{for } x > 0 \end{cases}$$

$H'(x) = 0$ for $x \neq 0$, but $H'(x)$ not defined for $x = 0$, whilst

$$\int_a^b H'(x)\, dx = H(b) - H(a) = 1, \qquad \text{if } a < 0 < b$$

Suggests $H'(x) = \delta(x)$...

Justification: Let $H(x) = \lim_{a\to 0} h(x)$ where

$$h(x) = \begin{cases} 0 & \text{for } x < -a \\ \dfrac{x+a}{2a} & \text{for } |x| < a \\ 1 & \text{for } x > a \end{cases}$$

And so $h'(x) = f_{th}(x)$ (top-hat function). So limit as $a \to 0$ gives

$$H'(x) = \delta(x)$$

Notes:

1. $\mathrm{sgn}(x) = \begin{cases} -1 & \text{for } x < 0 \\ 0 & \text{for } x = 0 \\ 1 & \text{for } x > 0 \end{cases}$ (the signum function). Then

$$H(x) = \frac{1}{2}(1 + \mathrm{sgn}(x)), \quad \text{and} \quad \frac{d}{dx}[\mathrm{sgn}(x)] = 2H'(x) = 2\delta(x)$$

2. Can we differentiate $\delta(x)$? Yes - but not needed here.

4.3.4 Fourier Transforms

$$\mathscr{F}\{\delta(x)\} = \int_{-\infty}^{\infty} \delta(x)\mathrm{e}^{-ikx}\,dx = 1$$

So F.T. of $\delta(x)$ is unity !

Fourier inversion formula gives

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{ikx}\,dk = \frac{1}{\pi}\int_{0}^{\infty} \cos kx\,dk \qquad !!$$

since $\sin kx$ is odd in k and integrates to zero.

Transform of Shifted Delta Function

$$\mathscr{F}\{\delta(x-a)\} = \int_{-\infty}^{\infty} \delta(x-a)\mathrm{e}^{-ikx}\,dx = \mathrm{e}^{-ika}$$

(Consistent with the general property of FTs that if $g(x) = f(x+a)$ then $\widetilde{g} = e^{ika}\widetilde{f}$.)

Inverse F.T.

$$\delta(x-a) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{ik(x-a)}\,dk$$

Transform of Complex Exponential

$$\mathscr{F}\{\mathrm{e}^{iax}\} = \int_{-\infty}^{\infty} \mathrm{e}^{-i(k-a)x}\,dx = 2\pi\delta(k-a)$$

using formula above (and interchanging the variables, k and x, and conjugating).

4.4 Diffusion Equation on an ∞-Domain

Consider

$$u_t = Du_{xx} \qquad \text{for} \qquad -\infty < x < \infty$$

with an I.C. of

$$u(x,0) = \phi(x), \qquad \phi(x) \text{ a given function}$$

Let $\widetilde{u}(k,t) = \int_{-\infty}^{\infty} u(x,t)\mathrm{e}^{-ikx}\,dx$ (i.e. $\widetilde{u}(k,t)$ is the F.T. of $u(x,t)$ w.r.t. x).

Take the F.T. of P.D.E. (i.e. multiply $u_t = Du_{xx}$ by e^{-ikx} and integrate over $-\infty < x < \infty$). Then

$$\mathscr{F}\{u_t\} = D\mathscr{F}\{u_{xx}\}$$

or

$$\int_{-\infty}^{\infty} \frac{\partial u}{\partial t} e^{-ikx} dx = D \int_{-\infty}^{\infty} \frac{\partial^2 u}{\partial x^2} e^{-ikx} dx$$

and so

$$\frac{\partial}{\partial t} \int_{-\infty}^{\infty} u e^{-ikx} dx = D(ik)\mathscr{F}\{u_x\} = D(ik)^2 \mathscr{F}\{u\}$$

which gives

$$\widetilde{u}_t = -Dk^2 \widetilde{u}$$

because $\partial/\partial t$ does not interfere with the F.T. in x and using the property of F.T.'s of derivatives.

This is just a 1st order O.D.E. in t.

Solution: $\widetilde{u}(k,t) = C\mathrm{e}^{-k^2 Dt}$

for the "integration constant", $C \equiv C(k)$ but independent of t.

To determine $C(k)$ need extra info... the I.C. is what we need (there are no 'boundaries' in this problem, although $\pm\infty$ may be regarded as boundaries. In some problems – not this one – boundedness of solutions at infinity is required to determine unique solutions.

Taking the F.T. of the I.C. gives

$$\widetilde{u}(k,0) = \widetilde{\phi}(k)$$

as before, trivial O.D.E. in t with I.C. fixing the integration "constant".

I.e. Solution in **Transform space** is:

$$\widetilde{u}(k,t) = \widetilde{\phi}(k) e^{-Dk^2 t}.$$

Inversion ? For specific $\phi(x)$, will know $\widetilde{\phi}(k)$ and may be able to invert directly.

Here we don't have a specific $\widetilde{\phi}(k)$... Can use **convolution** because $\widetilde{u}$ is in the form of a **product** of two transform functions of k. All that's needed for convolution to work is that we know the functions that give the two F.T.'s in the product.

Well $\mathscr{F}\{\phi(x)\} = \widetilde{\phi}(k)$, so that's easy.

Example 5 from §4.2.1 says $\mathscr{F}\{\mathrm{e}^{-x^2/a^2}/(a\sqrt{\pi}\} = \mathrm{e}^{-a^2k^2/4}$. To fit in with what we have, choose $a^2 = 4Dt$ and then we have

$$\mathscr{F}\left\{ \frac{\mathrm{e}^{-x^2/4Dt}}{\sqrt{4\pi Dt}} \right\} = \mathrm{e}^{-k^2 Dt}$$

So the **convolution theorem** gives

$$\boxed{u(x,t) = \mathscr{F}^{-1}\{\widetilde{\phi}(k) e^{-k^2 Dt}\} = \frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{\infty} \phi(\xi) \mathrm{e}^{-\frac{(x-\xi)^2}{4Dt}} \, d\xi}$$

We can check by direct substitution that this satisfies the PDE and IC. For the IC, note that

$$\lim_{t\to 0} = \frac{e^{-\frac{(x-\xi)^2}{4Dt}}}{\sqrt{4\pi Dt}} = \delta(x-\xi)$$

and use the sampling property of the delta function (4.3.2, part 3).

4.5 Particular Initial Conditions

4.5.1 Delta Function

If $u(x,0) = \delta(x)$ (e.g. all the heat/chemical initially dumped at the origin – a decent mathematical model), then $\phi(x) = \delta(x)$

and

$$u(x,t) = \frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{\infty} \delta(\xi) \mathrm{e}^{-\frac{(x-\xi)^2}{4Dt}} \, d\xi = \frac{\mathrm{e}^{-\frac{x^2}{4Dt}}}{\sqrt{4\pi Dt}}$$

Defn: This is the **fundamental solution** of the diffusion equation.

Properties of this solution

- Initially $u(x,0) = \delta(x)$ and so $\int_{-\infty}^{\infty} u dx = 1$. This is the total amount of "stuff" in the system at $t = 0$.
- For each fixed t, $u(x,t)$ is a Guassian in x, but spreads out with increasing t.
- For $t > 0$ we have $\displaystyle\int_{-\infty}^{\infty} u \, dx = \frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{\infty} e^{-x^2/4Dt} \, dx = \frac{1}{\sqrt{4\pi Dt}} \sqrt{4\pi Dt} = 1$ (from e.g.5 in §4.2.1). I.e. the amount of stuff in the system remains constant. Expected.
- For the I.C. to $u(x,0) = \delta(x-a)$, easy to see solution is $u(x,t) = \dfrac{\mathrm{e}^{-\frac{(x-a)^2}{4Dt}}}{\sqrt{4\pi Dt}}$

4.5.2 Heaviside Function

Assume $u(x,0) = H(x) = \begin{cases} 1 & \text{for } x > 0 \\ 0 & \text{for } x < 0 \end{cases}$.

Note: Appears not to be valid, as one can't take the F.T. of the I.C. (it doesn't tend to zero at infinity), but can be made rigorous by taking limits (see problem sheet).

From the General Solution,

$$u(x,t) = \frac{1}{\sqrt{4\pi Dt}} \int_{0}^{\infty} \mathrm{e}^{-(x-\xi)^2/4Dt} d\xi$$

Change of variable: $s = (\xi - x)/\sqrt{4Dt}$. Then

$$u(x,t) = \frac{1}{\sqrt{\pi}} \int_{-x/\sqrt{4Dt}}^{\infty} \mathrm{e}^{-s^2} ds = \frac{1}{2}\mathrm{erfc}(-x/\sqrt{4Dt})$$

where

$$\mathrm{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_{z}^{\infty} \mathrm{e}^{-s^2} ds$$

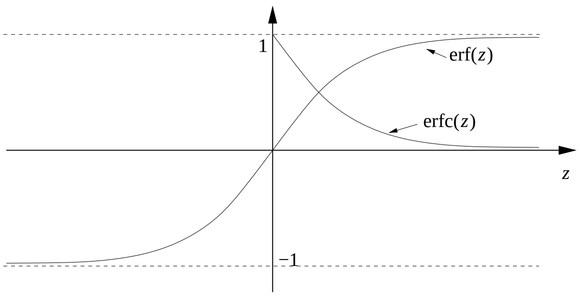
is a special function called the **Complementary Error Function**. Also, define

$$\mathrm{erf(z)} = 1 - \mathrm{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_{0}^{z} \mathrm{e}^{-s^2} ds$$

as the **Error Function**. This relationship follows since

$$\mathrm{erf}(\infty) = \frac{2}{\sqrt{\pi}} \int_{0}^{\infty} \mathrm{e}^{-s^2} ds = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-s^2} ds = 1$$

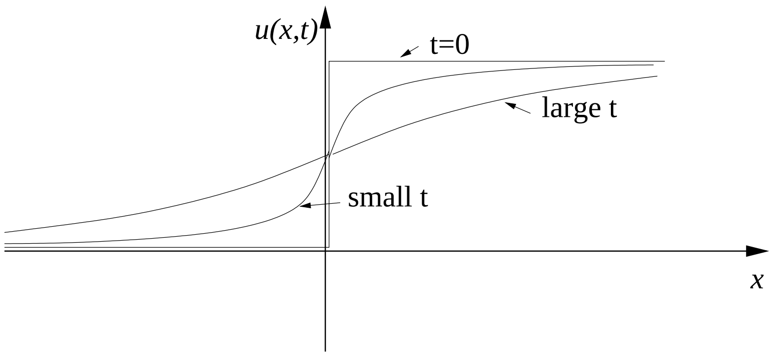
using e.g. 5 in §4.2.1. Note also that $\mathrm{erf}(z) = -\mathrm{erf}(-z)$ is an odd function whilst $\mathrm{erf}(0) = 0$.



Using this information, gives

$$u(x,t) = \tfrac{1}{2}(1 + \mathrm{erf}(x/\sqrt{4Dt}))$$

as the solution with the Heaviside function as the I.C.



Final note: $\dfrac{d}{dx}(\mathrm{erf}(x/\sqrt{4Dt})) = \dfrac{\mathrm{e}^{-x^2/4Dt}}{\sqrt{4Dt}}$.

4.5.3 Use of Superposition

The P.D.E. is *linear*, so can apply the principle of superposition. E.g. infinite domain with mass Q_a at $x = a$ and mass Q_b at $x = b$. Then solution is the sum of the solutions of the two parts separately:

$$u(x,t) = \frac{Q_a e^{-(x-a)^2/4Dt} + Q_b e^{-(x-b)^2/4Dt}}{\sqrt{4\pi Dt}}$$

4.6 Diffusion Equation on Semi-Infinite Domain

Problem:

$$u_t = Du_{xx} \text{ and } u(x,0) = \phi(x) \text{ for } x > 0$$

Need BC at $x = 0$.

4.6.1 Zero BC at $x = 0$

Let $u(0,t) = 0$ for $t > 0$.

Now $\phi(x)$ is given for $x > 0$. Let Φ be its *odd* extension.

I.e. let $\Phi(x) = \phi(x)$ for $x > 0$ and let $\Phi(x) = -\phi(-x)$ for $x < 0$.

Now consider P.D.E. for $x \in \mathbb{R}$ with I.C. $u(x,0) = \Phi(x)$. Solution is from before

$$\begin{aligned} u(x,t) &= \frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{\infty} \Phi(\xi) e^{-\frac{(x-\xi)^2}{4Dt}}\, d\xi \\ &= \frac{1}{\sqrt{4\pi Dt}} \left[\int_{-\infty}^{0} + \int_{0}^{\infty} \right] \\ &= \frac{1}{\sqrt{4\pi Dt}} \int_{0}^{\infty} \phi(\xi) \left[e^{-\frac{(x-\xi)^2}{4Dt}} - e^{-\frac{(x+\xi)^2}{4Dt}} \right] d\xi \end{aligned}$$

where in the negative integral, a change of vars, $\xi \to -\xi$, has been applied, and oddness, $\Phi(-\xi) = -\phi(\xi)$ used.

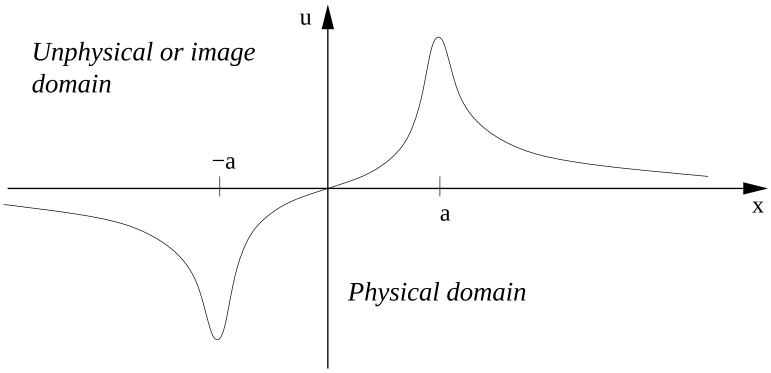
Clearly $u(0,t) = 0$ (as required)

So this integral, for $x > 0$, gives solution of diffusion eqn. for $x > 0$ with $u(0,t) = 0$ for all $t > 0$.

Example: $\phi(x) = \delta(x-a)$.

$$u(x,t) = \frac{e^{-\frac{(x-a)^2}{4Dt}} - e^{-\frac{(x+a)^2}{4Dt}}}{\sqrt{4\pi Dt}}.$$

This is fundamental solution for diffusion eqn. on half-line with zero B.C.



4.6.2 No-Flux Condition at $x = 0$

Similar argument using *even* extension of ϕ gives soln of diffusn eqn for $x > 0$ with $u_x(0,t) = 0$:

$$u(x,t) = \frac{1}{\sqrt{4\pi D t}} \int_0^\infty \phi(\xi) \left[e^{-\frac{(x-\xi)^2}{4Dt}} + e^{-\frac{(x+\xi)^2}{4Dt}} \right] d\xi$$

Easy to check the B.C. holds.

Example: $\phi(x) = \delta(x - a)$.

$$u(x,t) = \frac{e^{-\frac{(x-a)^2}{4Dt}} + e^{-\frac{(x+a)^2}{4Dt}}}{\sqrt{4\pi D t}}.$$