1. More on Fourier transform

In the preceding section we showed that the solution of the Heat equation on the real line

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad -\infty < x < \infty, \quad t > 0$$
$$u(x,0) = f(x) \in L^2(\mathbb{R})$$

can be expressed in terms of the Fourier transform as follows:

$$u(x,t) = \left(e^{-\xi^2 t}\,\widehat{f}\right)^{\vee}.$$

In this section we will find an explicit formula for $u(x,t)$ which involves the so-called Heat kernel.

First we recall that the "hat" symbol is used for the direct Fourier transform while the "check" denotes the inverse Fourier transform:

$$\begin{aligned}\widehat{f}(\xi) &= \int_{-\infty}^{\infty} e^{-i\,\xi\,x}\, f(x)\, dx \\ g^{\vee}(x) &= \frac{1}{2\,\pi}\int_{-\infty}^{\infty} e^{i\,\xi\,x}\, g(\xi)\, d\xi\end{aligned}$$

In "hat-check" notation the Fourier inversion theorem is, simply:

$$f = (\widehat{f})^{\vee}.$$

This, by the way, is far from obvious. We deduced the Fourier inversion theorem by applying a limiting process to the series solution of the Heat equation on a finite interval. As an exercise, try to prove the Fourier inversion formula directly. You will gain renewed appreciation of Fourier series and will likely run into some interesting questions. Meanwhile, we give one more reminder—that about the meaning of the symbol $L^2(\mathbb{R})$. It stands for the space of "square integrable functions" on the real line. A function f belongs to that space if its L^2 norm is finite:

$$\int_{-\infty}^{\infty} f^2(x)\, dx < \infty.$$

For example, $y = (1 + x^2)^{-1/2}$ is a member of $L^2(\mathbb{R})$ while $y = (1 + x^2)^{-1/4}$ is not (confirm that). Henceforth L^2 will be the default space for initial conditions whenever we work with Fourier transforms of any kind.

1.1. **L^p spaces.** It may seem like a mathematical formality that we specify initial conditions in L^2 and, in this course, it largely is: our computational procedures do not depend on that fact. Still, it is important to bear in mind that Fourier transform cannot be defined for arbitrary functions and therefore its domain must be restricted. Actually, a more natural restriction would be to L^1—a space we have not encountered yet. We therefore interrupt the discussion of the Heat Equation with a brief foray into functional analysis.

The spaces $L^1(\mathbb{R})$ and $L^2(\mathbb{R})$ are both instances of L^p spaces which, in general, are defined by the condition:

$$\int_{-\infty}^{\infty} |f(x)|^p \, dx < \infty.$$

The parameter p must be greater or equal to 1 and can be set to infinity. The nonnegative number

$$\|f\|_p = \left\{ \int_{-\infty}^{\infty} |f(x)|^p \, dx \right\}^{\frac{1}{p}}$$

is called the p-norm of f and can be regarded as a synonym of "length". For $p = \infty$ it turns out that

$$\|f\|_\infty = \lim_{p \to \infty} \|f\|_p = \max_{x \in \mathbb{R}} |f(x)|.$$

Actually, it is more appropriate to use the so-called *supremum* sup instead of max but we will sweep this subtlety under the rug.

By now we have learned to associate the 2-norm with the L^2 inner product:

$$\|f\|_2 = \sqrt{\langle f, f \rangle}.$$

This may suggest that the p-norm should be associated with L^p-inner product. Unfortunately, there is no such thing: the p-norms in general do not come from inner products. Therefore, unless $p = 2$, in L^p one can only measure lengths of vectors but not the angles between them. This explains the prominence of L^2 among L^p spaces and our preference for it.

Let us return to the Fourier transform which prompted this diversion. It is easy to show that the Fourier transform is well-defined on L^1. Indeed, for $f \in L^1(\mathbb{R})$:

$$\left| \int_{-\infty}^{\infty} e^{-i\xi x} f(x) \, dx \right| \le \int_{-\infty}^{\infty} \left| e^{-i\xi x} f(x) \right| \, dx = \int_{-\infty}^{\infty} |f(x)| \, dx < \infty.$$

(Study this simple argument—do not take it for granted!) However, L^1 lacks an inner product and is often far removed from the physical reality. We therefore need to define the Fourier transform on L^2 which is frequently called for by the physics itself (e.g., the 2-norm may have the meaning of energy which must be finite).

Defining the Fourier transform on L^2 is neither obvious nor trivial. In fact, there are functions in L^2 for which the Fourier integral diverges! For example, take

$$f(x) = \frac{1}{\sqrt{1+x^2}}$$

which, as we indicated earlier, is a member of $L^2(\mathbb{R})$. The Fourier transform of f is:

$$\widehat{f}(\xi) = \int_{-\infty}^{\infty} \frac{e^{-i\,\xi\,x}}{\sqrt{1+x^2}}\,dx$$

This Fourier transform does not exist at zero:

$$\widehat{f}(0) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{1+x^2}}\,dx = \infty.$$

Nevertheless, in this example $\widehat{f}$ exists for all other frequencies ξ and can be used to solve problems, such as the Heat Equation. This happens to be the general situation. Thus even though the Fourier integral of $f \in L^2$ may diverge for some frequencies, these "bad" frequencies can be ignored and $\widehat{f}$ may be considered well-defined.

We conclude this section with a definition of another useful functional space. Let $\mathscr{S}$ (this is a scripted 'S') denote the space of *smooth rapidly decreasing functions* which is also called *Schwartz space*. These functions are characterized by the condition

$$\lim_{|x|\to\infty} |x^n\, f^{(m)}(x)| = 0$$

which must hold for all integers n and m. In words, the functions are smooth—have derivatives of all orders—and, furthermore, the derivatives must decrease rapidly at infinity—fast enough to counteract any polynomial growth. A prototypical example of a smooth rapidly decreasing function is a Gaussian e^{-x^2}.

It should be clear that $\mathscr{S}$ is a subset L^2. What is not immediately clear is how large a subset it is. It turns out that *any* function in L^2 can be approximated with a sequence of smooth rapidly decreasing functions which are therefore *dense* in L^2. The situation is analogous to approximation of real numbers by sequences of rational numbers. Every real number can be regarded as a limit of a sequence of rational numbers: the rationals are dense in the set of reals. Likewise any square integrable function can be approximated by a smooth rapidly decreasing one.

Density allows us to effectively replace L^2 with $\mathscr{S}$. For instance, in order to define $\widehat{f}$ for some $f \in L^2$ we can take a sequence $\{f_n\}_{n=1}^\infty$ of smooth rapidly decreasing functions which converge to f. Then we can set

$$\widehat{f} = \lim_{n\to\infty} \widehat{f}_n.$$

All Fourier transforms on the right are well-defined and the limit is guaranteed to exist because of continuity of the Fourier transform. This definition of the Fourier transform on L^2 is commonly adopted in advanced texts.

1.2. **Fourier transform of a Gaussian.** We now return to the task of rewriting the solution of the Heat equation without the Fourier transform. First, after interchanging orders of integration, we can write:

$$u(x,t) = \left(e^{-\xi^2\,t}\,\widehat{f}\right)^{\vee} = \int_{-\infty}^{\infty} \left[\frac{1}{2\,\pi} \int_{-\infty}^{\infty} e^{-\xi^2\,t}\, e^{i\,\xi\,(x-y)}\, d\xi\right] f(y)\, dy.$$

This shows that

$$u(x,t) = \int_{-\infty}^{\infty} K_t(x-y)\, f(y)\, dy.$$

where

$$K_t(x) = \frac{1}{2\,\pi} \int_{-\infty}^{\infty} e^{-\xi^2\,t}\, e^{i\,\xi\,x}\, d\xi$$

is the Heat Kernel. Incidentally, if f and g are two functions in L^2 the integral

$$(f \star g)(x) = \int_{-\infty}^{\infty} f(x-y)\, g(y)\, dy$$

is another function in L^2 which is called *convolution* of f and g. Convolution is a commutative and associative operation. Moreover, the Fourier transform of a convolution is a product of Fourier transforms:

$$\widehat{f \star g} = \widehat{f}\,\widehat{g}.$$

The solution of the Heat Equation is thus given by convolution of the initial temperature with the Heat Kernel: $u(x,t) = K_t(x) \star f(x)$. To derive an explicit formula for K_t we are going to use some general properties of the Fourier transform and a Calculus III trick.

One property of the Fourier transform is its interaction with the derivative:

$$\widehat{\frac{df}{dx}} = (i\,\xi)\,\widehat{f}.$$

(We used this property to convert the Heat Equation into an ODE; if you forgot it, derive it using integration by parts.) This property has a dual:

$$\widehat{(-i\,x)\,f} = \frac{d\widehat{f}}{d\xi}.$$

To see this, simply differentiate the Fourier integral $\widehat{f}$ with respect to frequency under the integral sign.

Now let $\widehat{\phi} = e^{-t\,\xi^2}$. Then

$$\frac{d\widehat{\phi}}{d\xi} = -\frac{2\,t}{i}\,(i\,\xi)\,\widehat{\phi}.$$

We can interpret the left-hand side as $\widehat{(-i\,x)\,\phi}$. Meanwhile, the right-hand side is a multiple of the Fourier transform of the derivative:

$$\widehat{(-i\,x)\,\phi} = -\widehat{\frac{2\,t}{i}\,\frac{d\phi}{dx}}.$$

Since two Fourier transforms are equal only if the functions are equal, we must have

$$(-i\,x)\,\phi = -\frac{2\,t}{i}\,\frac{d\phi}{dx},$$

which is equivalent to:

$$\frac{d\phi}{dx} = -\frac{x}{2\,t}\,\phi.$$

We conclude that

$$\phi = K_t(x) = \phi(0)\,e^{-\frac{x^2}{4\,t}}$$

where $\phi(0)$ does not depend on x and is given by:

$$\phi(0) = \frac{1}{2\,\pi}\int_{-\infty}^{\infty} e^{-t\,\xi^2}\,d\xi.$$

In order to compute this integral, we first substitute $\xi = \frac{u}{\sqrt{t}}$. Then

$$\phi(0) = \frac{1}{2\,\pi\sqrt{t}}\int_{-\infty}^{\infty} e^{-u^2}\,du.$$

Consequently,

$$K_t(x) = \frac{C}{2\,\pi\sqrt{t}}\,e^{-\frac{x^2}{4\,t}}, \quad C = \int_{-\infty}^{\infty} e^{-u^2}\,du.$$

Finally, to find the constant C, we use the following Calculus III trick:

$$\begin{aligned} C^2 &= \int_{-\infty}^{\infty} e^{-x^2}\,dx \int_{-\infty}^{\infty} e^{-y^2}\,dy = \iint_{\mathbb{R}^2} e^{-x^2-y^2}\,dx\,dy \\ &= \int_0^{2\pi}\int_0^{\infty} e^{-r^2}\,r\,dr\,d\theta = \pi. \end{aligned}$$

Hence $C = \sqrt{\pi}$ which results in

$$K_t(x) = \frac{1}{2\sqrt{\pi\, t}}\, e^{-\frac{x^2}{4\,t}}$$

and the following final formula for the solution of the Heat Equation:

$$u(x,t) = \int_{-\infty}^{\infty} \frac{1}{2\sqrt{\pi\, t}}\, e^{-\frac{(x-y)^2}{4\,t}}\, f(y)\, dy$$

Let

$$\Phi(x,y,t) = \frac{1}{2\sqrt{\pi\, t}}\, e^{-\frac{(x-y)^2}{4\,t}}.$$

It is straightforward to check that Φ satisfies the Heat Equation for all y. Therefore $u(x,t) = \int_{-\infty}^{\infty} \Phi(x,y,t)\, f(y)\, dy$ satisfies the Heat Equation. Checking the initial condition is, however, much more difficult.

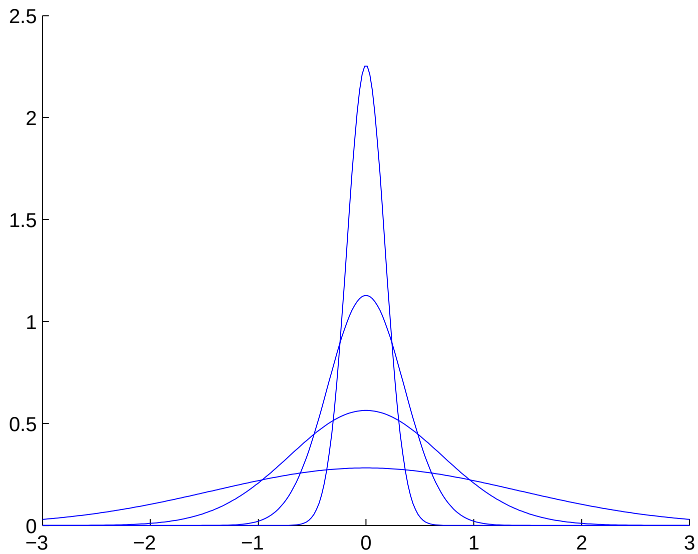

FIGURE 1. Heat kernel $K_t(x)$ for $t = 1/4^k$, $k = 0, 1, 2, 3$. As time goes to zero, the plot becomes a sharp peak centered at the origin.

Figure 1 shows four plots of $K_t(x)$ for $t = 1/4^k$, $k = 0, 1, 2, 3$. It is evident from the plots that, as time goes to zero, the Heat Kernel becomes more and more of a peak centered at the origin. The height of the peak goes to infinity as it becomes more and more narrow. However it can be shown (exercise) that the area of the peak is 1 for all t. This is an example of a *summability* (or delta) kernel. More generally, we will say that $K_t(x)$ is a summability kernel if:

(1) $K_t(x) \geq 0$ for all x and t.
(2) $\int_{-\infty}^{\infty} K_t(x)\, dx = 1$ for all t.
(3) Given any $\epsilon > 0$ one can make $K_t(x)$ arbitrarily small outside of $[-\epsilon, \epsilon]$ by shrinking t.

If $K_t(x)$ is a summability kernel such as the Heat Kernel then it can be shown that

$$\lim_{t \to \infty} \int_{-\infty}^{\infty} K_t(x)\, f(x)\, dx = f(0)$$

and

$$\lim_{t \to \infty} \int_{-\infty}^{\infty} K_t(x-y)\, f(y)\, dy = f(x).$$

The argument, however, is not elementary and will be omitted for now.

1.3. **Exercises.**

(1) Use `quadgk` to confirm numerically that

$$\left(e^{-t\,\xi^2}\right)^{\vee} = \frac{1}{2\sqrt{\pi\, t}}\, e^{-\frac{x^2}{4\,t}}$$

for $t = .1$ and $x \in [-2, 2]$.

(2) Compute the Fourier transforms of the following functions:

$$\begin{aligned} y &= \begin{cases} 1, & \text{if } -a < x < a \\ 0, & \text{otherwise.} \end{cases} \\ y &= e^{-|x|} \\ y &= \begin{cases} e^{-a\,x} \cos b\, x, & \text{if } x > 0 \\ 0, & \text{otherwise.} \end{cases} \end{aligned}$$

In each case, confirm your symbolic result with numerical computation, as in the previous problem.

(3) Use Fourier transform to solve the Wave Equation:

$$\begin{aligned} &\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}, \quad -\infty < x < \infty, \quad t > 0 \\ &u(x,0) = f(x) \in L^2(\mathbb{R}), \quad \frac{\partial u}{\partial t}(x,0) = 0. \end{aligned}$$

Hint: Use the translational property to compute the inverse Fourier transform.

(4) Consider the following ODE:

$$\frac{d^2u}{dt^2} + \frac{du}{dt} + u = f(t)$$

where

$$f = \begin{cases} e^{-2t}\cos 6\,t, & \text{if } t \geq 0 \\ 0, & \text{otherwise.} \end{cases}$$

(There are no initial conditions.) Find an explicit formula for $\widehat{u}$ where the Fourier transform is taken with respect to time. Attempt to compute u for $t \in [0, 1]$ using numerical inversion. List your observations.