REAL AND IMAGINARY DIFFUSIONS

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Abstract. We will consider the Schrödinger and heat equations in a box and on the line and compare their solutions with the same boundary/initial conditions.

1. The PDEs

The Schrödinger equation for a particle of mass m in a potential V reads

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x,t)+V(x)\psi(x,t)=-i\frac{\partial}{\partial t}\psi(x,t) \qquad (x\in\mathbb{R}^n,\ t\in\mathbb{R}) \tag{1}$$

and the heat equation is

$$\nabla^2 u(x,t)=\kappa\frac{\partial}{\partial t}u(x,t) \qquad (x\in\mathbb{R}^n,\ t\in\mathbb{R}) \tag{2}$$

where $\hbar$ is a constant of nature and κ depends on the heat-conducting material. The Schrödinger equation's solution function $\psi(x,t)$, when one takes the absolute square, gives the probability density of finding the particle in question at position x at time t. Similarly, the heat equation's solution $u(x,t)$ gives the temperature at x at t.

1.1. **Initial/boundary conditions.** We will pose similar initial/boundary conditions on these two PDEs so that we can compare them. First, take the space dimension, $n=1$ so that we are talking about the particle confined to a thin tube and the heat conduction taking place in a fine wire.

For equation (1), take

$$V(x)=\begin{cases} 0 & x\in[0,\pi] \\ \infty & x\notin[0,\pi] \end{cases}.$$

It is true that doing so confines the wave function ψ to the interval $[0,\pi]$, meaning that $\psi(x,t)=0$ for all $x\notin[0,\pi]$ and all $t\in\mathbb{R}$. Let us do the same for u, demanding that $u(x,t)=0$ in the same set.

Further, let us assume that the two equations have similar initial conditions. We let

$$\psi(x,0) = u(x,0) = \phi(x) = \begin{cases} 1 & x \in [0.9, 1.1] \\ 0 & x \notin [0.9, 1.1] \end{cases}.$$

General theorems on the existence of solutions to PDEs give that the problems set so far are *well-posed*, meaning (among other things) that they have unique solutions. I will describe a method of solving them.

First, simplify equation (1). Taking $n = 1$ and V as given above, we obtain

$$\frac{\partial^2}{\partial x^2}\psi(x,t) = \frac{2mi}{\hbar}\frac{\partial}{\partial t}\psi(x,t) \qquad (x \in [0,\pi],\ t \in \mathbb{R}). \tag{3}$$

Let us abbreviate the notation and change time units so that the combination $2m/\hbar = 1$. We are left with

$$\psi_{xx}(x,t) = i\psi_t(x,t) \qquad (x \in [0,\pi],\ t \in \mathbb{R}).$$

Similarly, changing units so that $\kappa = 1$, the heat equation becomes

$$u_{xx}(x,t) = u_t(x,t) \qquad (x \in [0,\pi],\ t \in \mathbb{R}).$$

It is a pun of nature that these two differ only by the factor of i in the time-derivatives and tempts us to compare and contrast the behaviors of these these two functions. Let us handle these in a unified way, writing

$$u_{xx}(x,t) = (i)\ u_t(x,t) \qquad (x \in [0,\pi],\ t \in \mathbb{R}) \tag{4}$$

to mean that I include the factor of i when thinking about Schrödinger and don't when thinking of heat.

2. Separation of Variables

The standard way to solve both problems is called *separation of variables.* First, one considers a factorization of u into simple functions, each of one variable:

$$u(x,t) = X(x)T(t). \tag{5}$$

Of course, general functions of two variables do not necessarily factor this way, ($e.g.$ $u(x,t) = x+t$) but we will handle that later. Substituting equation (5) into (4),

$$(XT)_{xx} = (i)\ (XT)_t \rightsquigarrow X''T = (i)\ XT'.$$

Restrict now to the heat equation. Dividing both sides of this last expression by XT, we get

$$\frac{X''T}{XT} = \frac{XT'}{XT} \rightsquigarrow \frac{X''}{X} = \frac{T'}{T}. \tag{6}$$

The last expression asserts the equality of a function of x alone $(X''(x)/X(x))$ and a function of t alone, $(T'(t)/T(t))$. The only way this can happen is for each of them to be constant:

$$\frac{X''}{X} = \frac{T'}{T} = C.$$

For the heat equation, the equation $T' = CT$ implies an exponential factor in XT. Since the boundary conditions force $u = 0$ there and this is about conduction, we take $C < 0$ and write, for convenience,

$$\frac{X''}{X} = \frac{T'}{T} = -\lambda^2, \qquad \lambda \in \mathbb{R}.$$

This yields two ordinary differential equations:

$$X''(x) + \lambda^2 X(x) = 0 \qquad T'(t) + \lambda^2 T(t) = 0$$

with solutions

$$X''(x) = A_\lambda \cos(\lambda x) + B_\lambda \sin(\lambda x), \qquad T(t) = C_\lambda e^{-\lambda^2 t}.$$

Reassembling u, we get

$$u_\lambda(x,t) = e^{-\lambda^2 t}[A_\lambda \cos(\lambda x) + B_\lambda \sin(\lambda x)]$$

where we have absorbed the constant C_λ into A_λ and B_λ.

Linearity of the heat equation (and of Schrödinger) imply that we may add functions of the form u_λ, obtaining general solutions:

$$u(x,t) = \sum_{\lambda \in S} e^{-\lambda^2 t}[A_\lambda \cos(\lambda x) + B_\lambda \sin(\lambda x)] \tag{7}$$

where S is some set of real numbers.

2.1. **Satisfying boundary conditions.** We have required that $u(0,t) = u(\pi,t) = 0$ for all $t \in \mathbb{R}$. Substituting into (7), these conditions read

$$u(0,t) = 0 = \sum_{\lambda \in S} e^{-\lambda^2 t}[A_\lambda \cos(\lambda 0) + B_\lambda \sin(\lambda 0)] = \sum_{\lambda \in S} e^{-\lambda^2 t} A_\lambda$$

suggesting that we take $A_\lambda = 0$ for all $\lambda \in S$. Not so similarly, the other boundary condition,

$$u(\pi,t) = 0 = \sum_{\lambda \in S} e^{-\lambda^2 t}[B_\lambda \sin(\lambda \pi)]$$

suggests either that we take $B_\lambda = 0$ also (implying $u(x,t) = 0$ identically) or we adjust the set S so that the term $\sin(\lambda\pi) = 0$ for all $\lambda \in S$. We'll do the latter, thus $S = \{1, 2, 3, \dots\}$.

The solution (so far) of the heat equation is thus of the form

$$u(x,t) = \sum_{k=1}^{\infty} B_k e^{-k^2 t} \sin(k\pi). \tag{8}$$

2.2. **Initial condition.** In order to get our unique solution, we must determine the constants B_k. For this we use the initial condition:

$$u(x,0) = \phi(x) = \sum_{k=1}^{\infty} B_k e^{-k^2 0} \sin(k\pi) = \sum_{k=1}^{\infty} B_k \sin(k\pi).$$

So we must find a way to expand the functions $\sin(kx)$, $k = 1, 2, 3, \dots$ in order that the linear combination be ϕ *in some sense*.

3. Fourier Series

In Calculus III we all learned that a vector had a decomposition in an orthonormal basis in terms of a the dot product:

$$\mathbf{v} = \sum_{k=1}^{3} (\mathbf{v} \cdot \mathbf{e}_k)\mathbf{e}_k. \tag{9}$$

We see that the family of functions $\sin kx$, $k = 1, 2, 3, \ldots$ is orthogonal. we will rescale it, defining

$$e_k(x) = \sqrt{\frac{2}{\pi}} \sin(kx), \qquad (k = 1, 2, 3, \ldots). \tag{10}$$

We will postpone discussion of completeness (i.e. that "any" function ϕ can be expanded in the $\sin(kx)$) till later–much later.

Assuming all this, an expansion of the form in equation (9) makes sense as soon as we understand how to generalize the dot product. It turns out that

$$\mathbf{u} \cdot \mathbf{v} = \sum_{k=1}^{3} \mathbf{u}_k \mathbf{v}_k$$

is a good start as it suggests

$$\langle u, v \rangle = \int_0^\pi u(x)v(x)dx. \tag{11}$$

Strictly speaking, we should take the complex conjugate of the second function v when we deal with complex-valued functions.

In analogy now to the formula (9), and using the "basis" in (10) and the inner product in (11), we are led to the expression

$$\phi(x) = \sum_{k=1}^{\infty} \langle \phi, e_k \rangle e_k(x).$$

This we will experimentally "verify" with *Mathematica*.

4. Solution to the Heat Equation

Putting this all together, we obtain the following:

Suppose $u = u(x,t)$, and we are given ϕ, a function that is not too bad on $[0,\pi]$, then the initial/boundary value problem

$$u_{xx} = u_t$$

$$u(0,t) = u(\pi,t) = 0$$

$$u(x,0) = \phi(x)$$

has solution

$$u(x,t) = \sqrt{\frac{2}{\pi}}\ \sum_{k=1}^{\infty} \langle \phi, e_k \rangle e^{-k^2 t} \sin(k\pi).$$

The relevant calculation is

$$\phi(x) = \sum_{k=1}^{\infty} B_k \sin(kx) = \sum_{k=1}^{\infty} B_k \sqrt{\frac{\pi}{2}} e_k(x) = \sum_{k=1}^{\infty} \langle \phi, e_k \rangle e_k(x),$$

thus $B_k = \sqrt{2/\pi}\langle \phi, e_k \rangle$. Now substitute in equation (8).

5. the Schrödinger Equation

Going back to equation (6) and reinstating the i, we get the pair of ordinary differential equations:

$$X''(x) + \lambda^2 X(x) = 0 \qquad T'(t) + i\lambda^2 T(t) = 0$$

with solutions

$$X''(x) = A_\lambda \cos(\lambda x) + B_\lambda \sin(\lambda x), \qquad T(t) = C_\lambda e^{-i\lambda^2 t},$$

where we interpret $e^{is} = \cos(s) + i\sin(s)$. Reassembling u, we get

$$u_\lambda(x,t) = e^{-i\lambda^2 t}[A_\lambda \cos(\lambda x) + B_\lambda \sin(\lambda x)].$$

The same arguments as before yield that the problem for $u = u(x,t)$

$$u_{xx} = iu_t$$

$$u(0,t) = u(\pi,t) = 0$$

$$u(x,0) = \phi(x)$$

has solution

$$\psi(x,t) = \sqrt{\frac{2}{\pi}} \sum_{k=1}^{\infty} \langle \phi, e_k \rangle e^{-ik^2 t} \sin(k\pi).$$

As it is only the real function $|\psi|^2$ that is physically meaningful, it is that which we graph.

6. The Fourier Transform

When the physical situation is not confined to an interval, the methods change somewhat. For that, rather than Fourier series, Fourier integrals are used. For $f : \mathbb{R} \to \mathbb{C}$, define

$$(\mathcal{F}f)(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\xi x} f(x)dx \quad \text{and} \quad (\mathcal{F}^{-1}f)(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\xi x} f(\xi)d\xi$$

when the integrals exist (*e.g.* when $f \in L^1(\mathbb{R})$). The transformations satisfy the following properties. (1) The two are inverses; (2) $\mathcal{F}(f * g)(\xi) = (\mathcal{F}f)(\xi)(\mathcal{F}g)(\xi)$, where the *convolution* $f * g$ is defined by

$$(f * g)(x) = \int_{-\infty}^{\infty} f(y)g(x-y)dx.$$

Furthermore, an integration by parts shows that (3),

$$(\mathcal{F}f')(\xi) = i\xi(\mathcal{F}f)(\xi).$$

We saw above that the introduction of the boundary conditions $u(0,t) = u(\pi,t) = 0$ forced us to restrict the set S from an arbitrary collection of real numbers to the integers. In the present case, where we solve heat and Schrödinger on the whole real line, we will get no restriction.

We may proceed as follows (or modify equation (7)). Take the Fourier transform in the x variable of the equation $u_{xx} = (i)u_t$. Use the tilde to denote the new function. One obtains

$$-\xi^2 \tilde{u}(\xi,t) = (i)\tilde{u}_t(\xi,t).$$

This is a family of ordinary differential equations (in t) having solutions

$$\tilde{u}(\xi,t) = A_\xi e^{-(-i)\xi^2 t}.$$

As usual we drop the term in the parentheses for the heat equation.

The initial value, $u(x,0) = \phi(x)$ now can be used obtaining

$$\tilde{u}(\xi,0) = (\mathcal{F}\phi)(\xi) = A_\xi.$$

Putting these together, we get

$$\tilde{u}(\xi,t) = (\mathcal{F}\phi)(\xi)e^{-(-i)\xi^2 t}.$$

With the inverse transform, we have

$$u(x,t) = \mathcal{F}^{-1}((\mathcal{F}\phi)(\xi)e^{-(-i)\xi^2 t}) = \phi * [\mathcal{F}^{-1}e^{-(-i)\xi^2 t}](x,t) \tag{12}$$

where all the inverse transforms are taken in the ξ variable.

A couple calculations in *Mathematica* or by hand identify the functions

$$[\mathcal{F}^{-1}e^{-\xi^2 t}](x,t) = \frac{e^{-x^2/4t}}{2\sqrt{\pi t}}$$

and

$$[\mathcal{F}^{-1}e^{-(-i)\xi^2 t}](x,t) = \frac{e^{-ix^2/4t}}{2\sqrt{-i\pi t}},$$

which, together with equation (12), solves the problem completely on the line:

$$u(x,t) = \phi * \frac{e^{-x^2/4t}}{2\sqrt{\pi t}}$$

for the heat equation, and similarly

$$u(x,t) = \phi * \frac{e^{-ix^2/4t}}{2\sqrt{-i\pi t}}$$

for the Schrödinger equation, the convolutions of course being taken in the x variable.