Fourier Solutions to Heat and Wave equations.

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1 Motivation.

Stanford iTunesU has some Fourier transform lectures by Prof. Brad Osgood. He starts with Fourier series and by Lecture 5 has covered this and the solution of the Heat equation on a ring as an example.

Now, for these lectures I get only sound on my ipod. I can listen along and pick up most of the lectures since this is review material, but here's some notes to firm things up.

Since this heat equation

$$\nabla^2 u = \kappa \partial_t u \tag{1}$$

is also the Schrödinger equation for a free particle in one dimension (once the constant is fixed appropriately), we can also apply the Fourier technique to a particle constrained to a circle. It would be interesting afterwards to contrast this with Susskind's solution of the same problem (where he used the Fourier transform and algebraic techniques instead).

2 Preliminaries.

2.1 Laplacian.

Osgood wrote the heat equation for the ring as

$$\frac{1}{2} u_{xx} = u_t$$

where x represented an angular position on the ring, and where he set the heat diffusion constant to $1/2$ for convienience. To apply this to the Schrödinger equation retaining all the desired units we want to be a bit more careful, so let's start with the Laplacian in polar coordinates.

In polar coordinates our gradient is

$$\nabla = \hat{\boldsymbol{\theta}}\frac{1}{r}\frac{\partial}{\partial\theta} + \hat{\mathbf{r}}\frac{\partial}{\partial r}$$

squaring this we have

$$\begin{aligned}
\nabla^2 = \nabla\cdot\nabla &= \hat{\boldsymbol{\theta}}\frac{1}{r}\frac{\partial}{\partial\theta}\cdot\left(\hat{\boldsymbol{\theta}}\frac{1}{r}\frac{\partial}{\partial\theta}\right) + \hat{\mathbf{r}}\frac{\partial}{\partial r}\cdot\left(\hat{\mathbf{r}}\frac{\partial}{\partial r}\right) \\
&= \frac{-1}{r^3}\frac{\partial r}{\partial\theta}\frac{\partial}{\partial\theta} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{\partial^2}{\partial r^2} \\
&= \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{\partial^2}{\partial r^2}
\end{aligned}$$

So for the circularly constrained where r is constant case we have simply

$$\nabla^2 = \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} \tag{2}$$

and our heat equation to solve becomes

$$\frac{\partial^2 u(\theta,t)}{\partial\theta^2} = (r^2\kappa)\frac{\partial u(\theta,t)}{\partial t} \tag{3}$$

2.2 Fourier series.

Now we also want Fourier series for a given period. Assuming the absence of the "Rigor Police" as Osgood puts it we write for a periodic function $f(x)$ known on the interval $I = [a, a+T]$

$$f(x) = \sum c_k e^{2\pi ikx/T}$$

$$\begin{aligned}
\int_{\partial I} f(x)e^{-2\pi inx/T} &= \sum c_k \int_{\partial I} e^{2\pi i(k-n)x/T} \\
&= c_n T
\end{aligned}$$

So our Fourier coefficient is

$$\hat{f}(n) = c_n = \frac{1}{T}\int_{\partial I} f(x)e^{-2\pi inx/T}$$

3 Solution of heat equation.

3.1 Basic solution.

Now we are ready to solve the radial heat equation

$$u_{\theta\theta} = r^2 \kappa u_t, \tag{4}$$

by assuming a Fourier series solution.
Suppose

$$\begin{aligned} u(\theta, t) &= \sum c_n(t) e^{2\pi i n \theta / T} \\ &= \sum c_n(t) e^{i n \theta} \end{aligned}$$

Taking derivatives of this assumed solution we have

$$\begin{aligned} u_{\theta\theta} &= \sum (in)^2 c_n e^{in\theta} \\ u_t &= \sum c_n' e^{in\theta} \end{aligned}$$

Substituting this back into 4 we have

$$\sum -n^2 c_n e^{in\theta} = \sum c_n' r^2 \kappa e^{in\theta}$$

equating components we have

$$c_n' = -\frac{n^2}{r^2\kappa} c_n$$

which is also just an exponential.

$$c_n = A_n \exp\left(-\frac{n^2}{r^2\kappa} t\right)$$

Reassembling we have the time variation of the solution now fixed and can write

$$u(\theta, t) = \sum A_n \exp\left(-\frac{n^2}{r^2\kappa} t + in\theta\right) \tag{5}$$

3.2 As initial value problem.

For the heat equation case, we can assume a known initial heat distribution $f(\theta)$. For an initial time $t = 0$ we can then write

$$u(\theta, 0) = \sum A_n e^{in\theta} = f(\theta)$$

This is just another Fourier series, with Fourier coefficients

$$A_n = \frac{1}{2\pi} \int_{\partial I} f(v) e^{-inv} dv$$

Final reassembly of the results gives us

$$u(\theta, t) = \sum \exp\left(-\frac{n^2}{r^2\kappa} t + in\theta\right) \frac{1}{2\pi} \int_{\partial I} f(v) e^{-inv} dv \tag{6}$$

3.3 Convolution.

Osgood's next step, also with the rigor police in hiding, was to exchange orders of integration and summation, to write

$$u(\theta, t) = \int_{\partial I} f(v) dv \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} \exp\left(-\frac{n^2}{r^2\kappa} t - in(v - \theta)\right)$$

Introducing a Green's function $g(v, t)$, we then have the complete solution in terms of convolution

$$g(v, t) = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} \exp\left(-\frac{n^2}{r^2\kappa} t - inv\right) \tag{7}$$

$$u(\theta, t) = \int_{\partial I} f(v) g(v - \theta, t) dv \tag{8}$$

Now, this Green's function is fairly interesting. By summing over paired negative and positive indexes, we have a set of weighted Gaussians.

$$g(v, t) = \frac{1}{2\pi} + \sum_{n=1}^{\infty} \exp\left(-\frac{n^2}{r^2\kappa} t\right) \frac{\cos(nv)}{\pi}$$

Recalling that the delta function can be expressed as a limit of a sinc function, seeing something similar in this Green's function is not entirely unsuprising seeming.

4 Wave equation.

The QM equation for a free particle is

$$-\frac{\hbar^2}{2m}\nabla^2\psi = i\hbar\partial_t\psi \tag{9}$$

This has the same form of the heat equation, so for the free particle on a circle our wave equation is

$$\psi_{\theta\theta} = -\frac{2mir^2}{\hbar}\partial_t\psi \quad \text{ie: } \kappa = -2mi/\hbar$$

So, if the wave equation was known at an initial time $\psi(\theta, 0) = \phi(\theta)$, we therefore have by comparision the time evolution of the particle's wave function is

$$\begin{aligned}
g(w,t) &= \frac{1}{2\pi} + \sum_{n=1}^{\infty} \exp\left(-\frac{i\hbar n^2 t}{2mr^2}\right)\frac{\cos(nw)}{\pi} \\
\psi(\theta,t) &= \int_{\partial I} \phi(v) g(v-\theta,t)dv
\end{aligned}$$

5 Fourier transform solution.

Now, lets try this one dimensional heat problem with a Fourier transform instead to compare. Here we don't try to start with an assumed solution, but instead take the Fourier transform of both sides of the equation directly.

$$\mathcal{F}(u_{xx}) = \kappa\mathcal{F}(u_t)$$

Let's start with the left hand side, where we can evaluate by integrating by parts

$$\begin{aligned}
\mathcal{F}(u_{xx}) &= \int_{-\infty}^{\infty} u_{xx}(x,t)e^{-2\pi isx}dx \\
&= \int_{-\infty}^{\infty} \frac{\partial u_x(x,t)}{\partial x} e^{-2\pi isx}dx \\
&= \left(u_x(x,t)e^{-2\pi isx}\Big|_{x=-\infty}^{\infty} - (-2\pi is)\int_{-\infty}^{\infty} u_x(x,t)e^{-2\pi isx}dx \right)
\end{aligned}$$

So if we assume (or require) that the derivative of our unknown function u is zero at infinity, and then similarily require the function itself to be zero there, we have

$$
\begin{aligned}
\mathcal{F}(u_{xx}) &= (2\pi is)\int_{-\infty}^{\infty}\frac{\partial u_x(x,t)}{\partial x}e^{-2\pi isx}dx \\
&= (2\pi is)^2\int_{-\infty}^{\infty}u(x,t)e^{-2\pi isx}dx \\
&= (2\pi is)^2\mathcal{F}(u)
\end{aligned}
$$

Now, for the time derivative. We want

$$
\mathcal{F}(u_t) = \int_{-\infty}^{\infty}u_t(x,t)e^{-2\pi isx}dx
$$

But can pull the derivative out of the integral for

$$
\begin{aligned}
\mathcal{F}(u_t) &= \frac{\partial}{\partial t}\left(\int_{-\infty}^{\infty}u(x,t)e^{-2\pi isx}dx\right) \\
&= \frac{\partial\mathcal{F}(u)}{\partial t}
\end{aligned}
$$

So, now we have an equation relating time derivatives only of the Fourier transformed solution.

Writing $\mathcal{F}(u) = \hat{u}$ this is

$$
(2\pi is)^2\hat{u} = \kappa\frac{\partial\hat{u}}{\partial t} \tag{10}
$$

With a solution of

$$
\hat{u} = A(s)e^{-4\pi^2s^2t/\kappa}
$$

Here $A(s)$ is an arbitrary constant in time integration constant, which may depend on s since it is a solution of our simpler frequency domain partial differential equation 10.

Performing an inverse transform to recover $u(x,t)$ we thus have

$$
\begin{aligned}
u(x,t) &= \int_{-\infty}^{\infty}\hat{u}e^{2\pi ixs}ds \\
&= \int_{-\infty}^{\infty}A(s)e^{-4\pi^2s^2t/\kappa}e^{2\pi ixs}ds
\end{aligned}
$$

Now, how about initial conditions. Suppose we have $u(x,0) = f(x)$, then

$$f(x) = \int_{-\infty}^{\infty} A(s) e^{2\pi i x s} ds$$

Which is just an inverse Fourier transform in terms of the integration "constant" $A(s)$. We can therefore write the $A(s)$ in terms of the initial time domain conditions.

$$\begin{aligned} A(s) &= \int_{-\infty}^{\infty} f(x) e^{-2\pi i s x} dx \\ &= \hat{f}(s) \end{aligned}$$

and finally have a complete solution of the one dimensional Heat equation. That is

$$u(x,t) = \int_{-\infty}^{\infty} \hat{f}(s) e^{-4\pi^2 s^2 t/\kappa} e^{2\pi i x s} ds$$

5.1 With Green's function?

If we put in the integral for $\hat{f}(s)$ explicitly and switch the order as was done with the Fourier series will we get a similar result? Let's try

$$\begin{aligned} u(x,t) &= \int_{-\infty}^{\infty} \left(\int_{-\infty}^{\infty} f(u) e^{-2\pi i s u} du \right) e^{-4\pi^2 s^2 t/\kappa} e^{2\pi i x s} ds \\ &= \int_{-\infty}^{\infty} du f(u) \int_{-\infty}^{\infty} e^{-4\pi^2 s^2 t/\kappa} e^{2\pi i (x-u) s} ds \end{aligned}$$

Cool. So, with the introduction of a Green's function $g(w,t)$ for the fundamental solution of the heat equation, we therefore have our solution in terms of convolution with the initial conditions. It doesn't get any more general than this!

$$g(w,t) = \int_{-\infty}^{\infty} \exp\left(-\frac{4\pi^2 s^2 t}{\kappa} + 2\pi i w s \right) ds \tag{11}$$

$$u(x,t) = \int_{-\infty}^{\infty} f(u) g(x-u,t) du \tag{12}$$

Compare this to 7, the solution in terms of Fourier series. The form is almost identical, but the requirement for periodicity has been removed by switch to the continuous frequency domain!

5.2 Wave equation.

With only a change of variables, setting $\kappa = -2mi/\hbar$ we have the general solution to the one dimensional zero potential wave equation 9 in terms of an initial wave function. However, we've a form of the Fourier transform that obscures the physics has been picked here unfortunately. Let's start over in super speed mode directly from the wave equation, using the form of the Fourier transform that substituites $2\pi s \rightarrow k$ for wave number.

We want to solve

$$-\frac{\hbar^2}{2m}\psi_{xx} = i\hbar\psi_t$$

Now calculate

$$\begin{aligned}
\mathcal{F}(\psi_{xx}) &= \frac{1}{2\pi}\int_{-\infty}^{\infty}\psi_{xx}(x,t)e^{-ikx}dx \\
&= \frac{1}{2\pi}\psi_x(x,t)e^{-ikx}\Big|_{-\infty}^{\infty} - (-ik)\frac{1}{2\pi}\int_{-\infty}^{\infty}\psi_x(x,t)e^{-ikx}dx \\
&= \cdots \\
&= \frac{1}{2\pi}(ik)^2\hat{\psi}(k)
\end{aligned}$$

So we have

$$-\frac{\hbar^2}{2m}(ik)^2\hat{\psi}(k,t) = i\hbar\frac{\partial\hat{\psi}(k,t)}{\partial t}$$

This provides us the fundamental solutions to the wave function in the wave number domain

$$\begin{aligned}
\hat{\psi}(k,t) &= A(k)\exp\left(-\frac{i\hbar k^2}{2m}t\right) \\
\psi(x,t) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}A(k)\exp\left(-\frac{i\hbar k^2}{2m}t\right)\exp(ikx)dk
\end{aligned}$$

In particular, as before, with an initial time wave function $\psi(x,0) = \phi(x)$ we have

$$\begin{aligned}
\phi(x) = \psi(x,0) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}A(k)\exp(ikx)dk \\
&= \mathcal{F}^{-1}(A(k))
\end{aligned}$$

So, $A(k) = \hat{\phi}$, and we have

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{\phi}(k) \exp\left(-\frac{i\hbar k^2}{2m} t\right) \exp(ikx) dk$$

So, ending the story we have finally, the general solution for the time evolution of our one dimensional wave function given initial conditions

$$\psi(x,t) = \mathcal{F}^{-1} \left(\hat{\phi}(k) \exp\left(-\frac{i\hbar k^2}{2m} t\right) \right) \tag{13}$$

or, alternatively, in terms of momentum via $k = p/\hbar$ we have

$$\psi(x,t) = \mathcal{F}^{-1} \left(\hat{\phi}(p) \exp\left(-\frac{ip^2}{2m\hbar} t\right) \right) \tag{14}$$

Pretty cool! Observe that in the wave number or momentum domain the time evolution of the wave function is just a continual phase shift relative to the initial conditions.

5.3 Wave function solutions by Fourier transform for a particle on a circle.

Now, thinking about how to translate this Fourier transform method to the wave equation for a particle on a circle (as done by Susskind in his online lectures) makes me realize that one is free to use any sort of integral transform method appropriate for the problem (Fourier, Laplace, ...). It doesn't have to be the Fourier transform. Now, if we happen to pick an integral transform with $\theta \in [0, \pi]$ bounds, what do we have? This is nothing more than the inner product for the Fourier series, and we come full circle!

Now, the next thing to work out in detail is how to translate from the transform methods to the algebraic bra ket notation. This looks like it will follow immediately if one calls out the inner product in use explicitly, but that's an exploration for a different day.