An alternative viewpoint

If we have a function defined for $0 \le x \le \pi$, the previous example suggests that we can extend this function to render it $2\pi-$periodic and odd, ensuring that it may be represented as a Fourier sine series. In other words, we may use this trick to represent the spatial dependence of the function in terms of a bunch of sines. This is convenient as we have much understanding of the properties of such trig functions, including how to differentiate, integrate and manipulate them in general. Thus, in order to solve the original PDE problem, we might just pose such a series to represent the spatial dependence of the solution at the outset. *i.e.* we could simply extend $u(x,t)$ as a $2\pi-$periodic function and write

$$u(x,t) = \sum_{n=1}^{\infty} B_n \sin nx, \quad B_n = \frac{2}{\pi}\int_0^{\pi} u(x,t)\sin nx \, dx, \tag{1}$$

without bothering with separation of variables. This different strategy is more like using a set of basis vectors to represent any vector in some vector space (but for functions, of course). Importantly, the sines themselves guarantee that the boundary conditions are automatically taken care of (*i.e.* $u(0,t) = u(\pi,t) = 0$).

There is one obvious complication: the $t-$dependence of $u(x,t)$ is necessarily carried through into the coefficients; *i.e.* $B_n = B_n(t)$. Nevertheless, this provides us with a different tool to solve the PDE: we pose (1) and introduce a similar representation of the initial condition,

$$u(x,0) = f(x) = \sum_{n=1}^{\infty} b_n \sin nx, \quad b_n = \frac{2}{\pi}\int_0^{\pi} f(x)\sin nx \, dx, \tag{2}$$

which implies a suitable (*i.e.* odd, $2\pi-$periodic) extension of $f(x)$. This demands that we impose the initial conditions,

$$B_n(0) = b_n,$$

on the coefficients of the Fourier sine series for the solution.

Now, in view of the properties of the sines, we may introduce (1) into the PDE to find

$$u_t = u_{xx} \qquad \longrightarrow \qquad \sum_{n=1}^{\infty} \dot{B}_n \sin nx = -\sum_{n=1}^{\infty} n^2 B_n \sin nx,$$

where the dot means time derivative. To solve this last relation, we simply match up coefficients of all the sines:

$$\dot{B}_n = -n^2 B_n \qquad \longrightarrow \qquad B_n(t) = B_n(0)e^{-n^2 t} = b_n e^{-n^2 t}.$$

We thereby arrive at the same solution as found using separation of variables. It is up to you to decide which method was simpler. This second strategy is sometimes called an eigenfunction expansion, as we are expanding a function, to be determined, in terms of a set of known functions, or "eigenfunctions", a term that is connected to Sturm-Liouville theory (to be discussed in a few lectures).

Separation of variables versus an eigenfunction expansion

Let's try out both separation of variable and an eigenfunction expansion on a different problem: the wave equation on a finite spatial domain,

$$u_{tt} = u_{xx}, \quad 0 \le x \le \pi, \quad u_x(0,t) = u_x(\pi,t) = 0, \quad u(x,0) = 0, \quad u_t(x,0) = g(x).$$

Here, we have again scaled space and time to set the coefficients of the PDE (*i.e.* the wavespeed C) to unity and the domain length to π. If $u(x,t)$ were to correspond to the deflection of a string, the (Neumann) boundary conditions would somehow imply that the ends were "free", and the initial conditions would imply that the string was straight ($u(x,0) = 0$) but provided with an instantaneous velocity ($u_t(x,0) = g(x)$) at the beginning.

Proceeding with separation of variables, we put $u = X(x)T(t)$, plug into the PDE and re-arrange:

$$\frac{X''}{X} = \frac{T''}{T} = -\lambda,$$

using the same argument as before about the two sides of the equation must equalling a separation constant. This time, the two ODEs that we obtain are the same:

$$T'' + \lambda T = X'' + \lambda X = 0,$$

and so the choice of sign for the separation constant delivers the solution pairs, $\sin\sqrt{\lambda}x$ and $\cos\sqrt{\lambda}x$ or $\sin\sqrt{\lambda}t$ and $\cos\sqrt{\lambda}t$.

As we are dealing with the wave equation, the solutions should somehow be wavy; *i.e.* oscillate in space and time. This is the physical justification for choosing the separation constant $-\lambda$, rather than $+\lambda$. Once more, the mathematical justification comes from the boundary conditions, which will only work for the $-\lambda$ choice (if $\lambda \neq 0$).

For the current problem, the boundary conditions demand $X'(0) = 0$ and $X'(\pi) = 0$. Thus, in order to enforce the first condition, we want $A\cos\sqrt{\lambda}x$ as our space solution, rather than $B\sin\sqrt{\lambda}x$ (for arbitrary constants A and B); the second boundary condition demands that

$$\sqrt{\lambda}A\sin\sqrt{\lambda}\pi = 0.$$

We again avoid the trivial solution with $A = 0$, and conclude once more that $\lambda = n^2$, with $n = 1, 2, \ldots$. However, this time there is a further possibility: $\lambda = 0$, which corresponds to $X(x) = constant$ (the ODE for X is now $X'' = 0$, but the option $X \propto x$ is ruled out by $X'(0) = 0$). This alternative solution is not trivial, so we better keep it too.

Turning now to the time solution, we have $T = C\cos nt$ or $D\sin nt$ if $\lambda = n^2$, with two more arbitrary constants C and D. For $\lambda = 0$, the ODE for $T(t)$ is just $T'' = 0$, and so we have $T = C + Dt$. The initial condition $T(0) = 0$, though, indicates that $C = 0$ for either of these possibilities.

Lumping all the possible solutions back together, we arrive at a general solution

$$u(x,t) = \frac{1}{2}a_0 t + \sum_{n=1}^{\infty} \frac{a_n}{n} \cos nx \sin nt,$$

after compactly rewriting all the combos of arbitrary constants so that

$$g(x) = u_t(x,0) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos nx; \tag{3}$$

i.e. a Fourier cosine series.

Now, if we extend $g(x)$ and $u(x,t)$ beyond $0 \le x \le \pi$ as **even** 2π−periodic functions, then we know that it is justified to represent them in terms of Fourier cosine series. In other words, we expand $g(x)$ as in (3), with

$$a_0 = \frac{2}{\pi}\int_0^\pi g(x)\,\mathrm{d}x \qquad \& \qquad a_n = \frac{2}{\pi}\int_0^\pi g(x)\cos nx\,\mathrm{d}x, \tag{4}$$

and we have solved the PDE.

The eigenfunction expansion follows a parallel route: we first note that the boundary conditions, $u_x(0,t) = u_x(\pi,t) = 0$, are automatically satisfied by the cosines of the Fourier series. Hence we use an even $2\pi-$periodic extension in order to justify the expansion,

$$u(x,t) = \frac{1}{2}A_0(t) + \sum_{n=1}^{\infty} A_n(t)\cos nx,$$

where the coefficients are again all dependent on time. Plugging into the PDE indicates that

$$\frac{1}{2}\ddot{A}_0(t) + \sum_{n=1}^{\infty} \ddot{A}_n(t)\cos nx = -\sum_{n=1}^{\infty} n^2 A_n(t)\cos nx.$$

Matching the coefficients of the constant term and the cosines now furnishes the ODEs

$$\ddot{A}_0 = 0 \qquad \& \qquad \ddot{A}_n = -n^2 A_n.$$

Hence $A_0(t)$ is a linear function of t, whereas $A_n(t)$ is given by $\cos nt$ or $\sin nt$. Demanding the same extension of the initial conditions indicates that we impose

$$A_0(0) = A_n(0) = 0 \qquad \& \qquad \dot{A}_0(0) = a_0,\ \dot{A}_n(0) = a_n,$$

once we expand $g(x)$ as in (3)-(4). We then arrive at

$$A_0(t) = a_0 t \qquad \& \qquad A_n(t) = \frac{a_n}{n}\sin nt,$$

which provides the same solution for $u(x,t)$ as that from separation of variables.

Some additional notes

* Had the spatial domain of the PDE been $0 \le x \le L$, rather than 0 to π, we would have had to use the more general version of the Fourier series formulae, but nothing would have otherwise been different.
* Evidently, Dirichlet boundary conditions, $u(0,t) = u(\pi,t) = 0$, lead to a representation of the solution as a Fourier sine series, whereas Neumann conditions, $u_x(0,t) = u_x(\pi,t) = 0$, lead to a Fourier cosine series.
* For different combos of boundary conditions (*e.g.* $u(0,t) = u_x(\pi,t) = 0$), things can get slightly more complicated, obscuring the type of extension that is required to mathematically justify the expansions. However, the simple trick of integrating the initial condition after multiplying by one, a cosine or a sine will always provide the formula for the coefficients of the Fourier series.
* Eigenfunction expansions can be used to solve inhomogeneous PDEs. *e.g.*

$$u_t = u_{xx} + q(x,t), \quad u(0,t) = u(\pi,t) = 0, \quad u(x,0) = 0.$$

We introduce (1) for the solution, along with the expansion

$$q(x,t) = \sum_{n=1}^{\infty} Q_n(t)\sin nx, \qquad Q_n(t) = \frac{2}{\pi}\int_0^{\pi} q(x,t)\sin nx\,\mathrm{d}x,$$

corresponding to the odd $2\pi-$periodic extension of the source term. We then must solve the ODEs,

$$\dot{B}_n = -n^2 B_n + Q_n(t), \qquad B_n(0) = 0.$$

Technical drawbacks:

In some ways, posing the series solution, plugging into the PDE and matching coefficients is simpler and quicker than using separation of variables. However, there are some hidden issues. First, we need to use the best set of eigenfunctions. This is guided by the boundary conditions in the preceding two problems: $u(0,t) = u(\pi,t) = 0$ can be satisfied by the sines of the Fourier series, motivating the odd $2\pi-$periodic extension and the corresponding eigenfunctions; with $u_x(0,t) = u_x(\pi,t) = 0$ it is more natural to employ cosines. Note that, if the eigenfunctions do not automatically satisfy the boundary conditions, those constraints must still be imposed on the series representation of the solution; this corresponds to adding extra algebraic constraints, which complicates the solution procedure terribly, rendering the strategy unworkable except as a numerical technique.

Another mathematical concern comes from the need, in the approach taken above, to differentiate the infinite Fourier series. This is problematic as such series cannot always be differentiated term by term, as the following example illustrates.

Consider $f(x) = x$. The odd $2\pi-$periodic extension of this function gives the sawtooth wave,

$$f(x) = x, \quad -\pi < x < \pi, \quad f(x) = f(x + 2\pi).$$

The even $2\pi-$periodic extension is, however, the triangular waveform

$$f(x) = |x|, \quad -\pi < x < \pi, \quad f(x) = f(x + 2\pi).$$

Both are illustrated in figure 1.

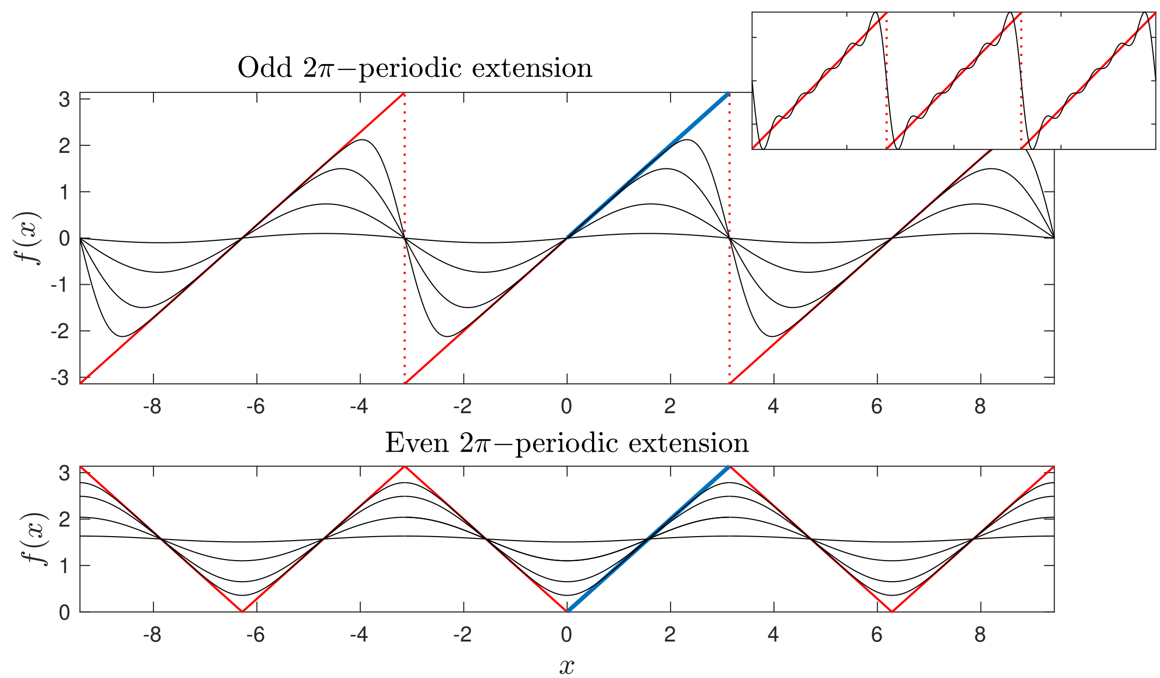

Figure 1: Periodic extensions of $f(x) = x$. The blue line is the original function; the red lines are the extensions. The black lines show snapshots of the solution of the heat equation using these extensions as initial conditions. In the first case, the overlaid plot shows the Gibbs phenomenon associated with the representation of the discontinuous initial condition by the truncated Fourier series.

The first of these extensions has jumps at $x = \pm\pi$, where the Fourier series converges to the mean value of $f(\pm\pi) = 0$ (which ensures that the boundary conditions are satisfied if this was the initial condition for a PDE with $u(0,t) = u(\pi,t) = 0$). The representation as a Fourier sine series is

$$f(x) = \sum_{n=1}^{\infty} b_n \sin nx, \quad b_n = \frac{2}{\pi}\int_0^{\pi} x \sin nx \, \mathrm{d}x = \frac{2}{n}(-1)^{n+1}.$$

More explicitly,

$$f(x) = 2\left(\sin x - \tfrac{1}{2}\sin 2x + \tfrac{1}{3}\sin 3x - ...\right) \qquad \& \qquad f'(x) = 2\left(\cos x - \cos 2x + \cos 3x - ...\right).$$

If we put $x = 0$, the series for $f'(x) = 2(1 - 1 + 1 - ...)$ is undefined, but should provide $f'(0) = 1$. In fact, we should find $f'(x) = 1$, except at the jumps, where the derivative cannot be defined. In other words, differentiating the series, which was originally convergent, can turn it into a divergent one.

The reason that this happens is precisely because of the jumps in the function. Awkwardly, our methodology for solving PDEs involves introducing various periodic extensions outside the original domain of the PDE, which usually introduces jumps into the extended functions or their derivatives, as the example above demonstrates.

Despite this, as long as $f(x)$ is not singular somewhere and does have a Fourier cosine or sine series (as with the example), there is nothing wrong with using this function as our initial condition for the heat equation: for the Neumann conditions $u_x(0,t) = u_x(\pi,t) = 0$, the situation corresponds to the even extension shown at the bottom of figure 1. Given that

$$a_0 = \frac{2}{\pi}\int_0^{\pi} x \, \mathrm{d}x = \pi \qquad \& \qquad a_n = \frac{2}{\pi}\int_0^{\pi} x \cos nx \, \mathrm{d}x = \frac{2}{\pi n^2}[(-1)^n - 1]$$

for this extension, the PDE solution is

$$u(x,t) = \tfrac{1}{2}\pi - \tfrac{4}{\pi}\left(e^{-t}\cos x + \tfrac{1}{9}e^{-9t}\cos 3x + \tfrac{1}{25}e^{-25t}\cos 5x + ...\right).$$

This solution, truncated to the three terms shown, is also plotted in figure 1 by the thinner black lines, for the times $t = \frac{1}{10}$, $\frac{1}{3}$, 1 and 3.

Similarly, with the Dirichlet conditions $u(0,t) = u(\pi,t) = 0$, the odd $2\pi-$periodic extension gives

$$u(x,t) = 2\left(e^{-t}\sin x - \tfrac{1}{2}e^{-4t}\sin 2x + \tfrac{1}{3}e^{-9t}\sin 3x - \tfrac{1}{4}e^{-16t}\sin 4x + \tfrac{1}{5}e^{-25t}\sin 5x...\right),$$

which is again plotted in figure 1. Also included in the figure is the representation of the initial condition by the series truncated to the five terms given in the equation; this truncation shows the persistent ringing of the Gibbs phenomenon, and signifies that five terms provides a poor approximation.

The snapshots of the PDE solutions shown in figure 1 display an important property of the diffusion equation: the solutions have discontinuities in either the initial condition or its derivative, as a result of the conflict between the boundary and initial conditions. *i.e.* $f(x) = x$ cannot satisfy $f(\pi) = 0$ without introducing a jump discontinuity (for the first case); nor can this function satisfy $f'(0) = f'(\pi) = 0$ without adding jumps in derivative (in the second case). However, the PDE solution $u(x,t)$ for any finite time $t > 0$ is different: the additional exponential factors, $e^{-n^2 t} < 1$ for $t > 0$, in the Fourier series solution for $u(x,t)$ or $u_x(x,t)$ accelerate the convergence and ensure that these series are never divergent. The consequence can be seen in figure 1: the solution or its space derivative immediately become continuous after the initial moment. This is the impact of diffusion, which smooths any jump structure over an infinitely short time. It also means that we can accept conflicts between the initial and boundary conditions, but still find a nice solution. However, this is a feature of the diffusion equation and not always true; in the theory of PDEs, people consider carefully when the PDE, initial and boundary conditions all lead to a sensible solution. Especially for nonlinear PDEs, sensible solutions cannot always be found, as we shall see at the end of Math400 when solving problems with the method of characteristics. In other problems (such as with the wave equation, which simply propagates spatial structure around without any smoothing), the solution can be sensible, but the discontinuities present in the initial condition may remain for all time.

Projection

The discussion above suggests that jump discontinuities in the initial condition or its derivative are not necessarily problematic for solving the heat equation. However, the worry remains that we needed to differentiate term-by-term when using the eigenfunction expansion, which is a dangerous operation for an infinite series. However, term-by-term differentiation is not, in fact, necessary to arrive at the ODEs for the coefficients. An alternative, but more longwinded, approach is to use **projection**.

Consider $u_t = u_{xx}$ with $u(0,t) = u(\pi,t) = 0$. The eigenfunction expansion is (1). Instead of plugging and chugging with the series and PDE, let's instead take the PDE, mutiply by $\sin nx$ and integrate:

$$\int_0^\pi u_t \sin nx \, \mathrm{d}x = \int_0^\pi u_{xx} \sin nx \, \mathrm{d}x.$$

The partial time derivative can be slipped outside the integral, at which point it is equivalent to an ordinary derivative. Then, because both the $\sin nx$ and $u(x,t)$ vanish at the endpoints of the integral, two integration by parts on the other term gives

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_0^\pi u \sin nx \, \mathrm{d}x = -n^2 \int_0^\pi u \sin nx \, \mathrm{d}x.$$

But this is just equivalent to $\dot{B}_n = -n^2 B_n$ in view of the definition of $B_n(t)$ from the Fourier series formulae. *i.e.* we can arrive at the ODEs for the coefficients by projecting the PDE onto each eigenfunction (by which we mean the operation of multiplying by that eigenfunction and integrating in x). Thus, the projection avoids any term-by-term differentiation but eventually gives the same result as doing that whilst plugging, chugging and matching. All that is needed is that a Fourier series exist for $u(x,t)$.

For those wanting to see more about all this, Haberman's book has a chapter on Fourier series, including a detailed discussion of when one can differentiate term-by-term.