Solution by separation of variables

Consider the heat equation without any source ($i.e.$ $q = 0$):

$$u_t = u_{xx}, \qquad u(0,t) = u(\pi,t) = 0, \qquad u(x,0) = f(x).$$

To solve this problem, we use separation of variables and set

$$u(x,t) = X(x)T(t), \qquad \Longrightarrow \qquad XT' = TX'' \quad \text{or} \quad \frac{T'}{T} = \frac{X''}{X}$$

(prime meaning derivative with respect to argument!). But this last relation demands that a function of t equals a function of x, which can only be true if both equal a constant since x and t are independent variables (one can freeze time and vary x, to establish that the function of x is some constant, or fix spatial position and see what happens in t, to see that the time function must be constant).

We let this "separation constant" be $-\lambda$. Hence

$$T' = -\lambda T \qquad \& \qquad X'' = -\lambda X.$$

In other words, we have turned the PDE into two ODEs. The solution for $T(t)$ is proportional to the exponential $e^{-\lambda t}$, whereas there are two possible solutions for $X(x)$: $\sin\sqrt{\lambda}x$ and $\cos\sqrt{\lambda}x$, (multiplied by arbitrary constants). Thus, we may write

$$u(x,t) = e^{-\lambda t}\left(a\cos\sqrt{\lambda}x + b\sin\sqrt{\lambda}x\right).$$

But $u(0,t) = 0$, or $X(0) = 0$, implies that we must set $a = 0$, and $u(\pi,t) = 0$, or $X(\pi) = 0$ indicates that

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

Obviously, putting $b = 0$ is not helpful, and so we must have that $\lambda = n^2$ where $n = 1, 2, \ldots$ As the PDE is linear, we can take all the solutions with different values of n and formulate a linear superposition to generate a more general solution. Thus, we write

$$u(x,t) = \sum_{n=1}^{\infty} b_n e^{-n^2 t}\sin nx. \tag{1}$$

The only other condition that must be satisfied is the initial condition $u(x,0) = f(x)$, where $f(x)$ is some prescribed function. Hence, we must select the b_n constants so that

$$f(x) = \sum_{n=1}^{\infty} b_n \sin nx. \tag{2}$$

This looks a lot like part of a Fourier series, and we can satisfy the constraint by setting (see later)

$$b_n = \frac{2}{\pi}\int_0^{\pi} f(x)\sin nx\, \mathrm{d}x. \tag{3}$$

Note: we selected the separation constant to be $-\lambda$, not $+\lambda$ for three reasons:

• with $+\lambda$, the space ODE would have been $X'' = \lambda X$, with solutions $X(x) \propto e^{\pm\sqrt{\lambda}x}$. But no combination of these two solutions can be made to vanish at the two points $x = 0$ and $x = \pi$, unless we reverse the sign of λ and turn the exponentials back into sines and cosines (using Euler's formula). In other words, we are forced into the choice $-\lambda$ by the need to satisfy the boundary conditions.

• with $+\lambda$, the time ODE would have solution $T(t) \propto e^{\lambda t}$. But diffusion smooths out spatial structure, and so the temperature should decay with time, not grow exponentially.

• hindsight: had we used $+\lambda$, then we would have run into the problems indicated above (mainly the first), been forced to stop, and reverse the sign of the separation constant to make things work. Thus, the approach would have been self-correcting, but we would have lost time and inefficiently done more algebra than needed.

Simple initial condition:

If the initial condition already has the form of one or more of the solutions in the sum, then we are done.

e.g. if $f(x) = 3\sin 3x$, then we keep only the $n = 3$ term and put $b_n = 3$, leading to

$$u(x,t) = 3e^{-9t}\sin 3x.$$

Or, for $f(x) = \sin^3 x$, we note the helpful trig identity $\sin^3 x = \frac{3}{4}\sin x - \frac{1}{4}\sin 3x$. Thus, $b_1 = \frac{3}{4}$ and $b_3 = -\frac{1}{4}$, and we find

$$u(x,t) = \frac{3}{4}e^{-t}\sin x - \frac{1}{4}e^{-9t}\sin 3x.$$

Fourier Series:

For a periodic function $f(x)$ with period $2L$, the Fourier series is

$$f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty}\left[a_n\cos\left(\frac{n\pi x}{L}\right) + b_n\sin\left(\frac{n\pi x}{L}\right)\right]$$

with

$$a_0 = \frac{1}{L}\int_{-L}^{L} f(x)\,\mathrm{d}x, \quad a_n = \frac{1}{L}\int_{-L}^{L} f(x)\cos\left(\frac{n\pi x}{L}\right)\,\mathrm{d}x, \quad b_n = \frac{1}{L}\int_{-L}^{L} f(x)\sin\left(\frac{n\pi x}{L}\right)\,\mathrm{d}x.$$

The formulae for the cefficients can be established using the **helpful integrals**,

$$\int_{-L}^{L}\cos\left(\frac{n\pi x}{L}\right)\,\mathrm{d}x = \int_{-L}^{L}\sin\left(\frac{n\pi x}{L}\right)\,\mathrm{d}x = \int_{-L}^{L}\cos\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right)\,\mathrm{d}x = 0 \tag{4}$$

$$\int_{-L}^{L}\cos\left(\frac{n\pi x}{L}\right)\cos\left(\frac{m\pi x}{L}\right)\,\mathrm{d}x = \int_{-L}^{L}\sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right)\,\mathrm{d}x = \begin{cases} 0, & \text{if } n \neq m \\ L, & \text{if } n = m \end{cases} \tag{5}$$

which follow for any integers n and m on using the handy trig formulae,

$$\cos(A \pm B) = \cos A\cos B \mp \sin A\sin B \qquad \& \qquad \sin(A \pm B) = \sin A\cos B \pm \cos A\sin B.$$

With these integrals in hand, one can multiply the Fourier series by one of 1, $\cos(m\pi x/L)$ or $\sin(m\pi x/L)$, and then integrate x from $-L$ to L. This operation picks out a particular coefficient from the Fourier series and delivers the preceding formula.

Funks with Jumps

If $f(x)$ has a discontinuity at $x = x_*$, the Fourier series converges to $\frac{1}{2}f^- + \frac{1}{2}f^+$, where f^- is the limit of $f(x)$ as x approaches x_* from the left, and f^+ is the limit of $f(x)$ as x approaches x_* from the right. Thus, if $f(x)$ is defined to be anything other than $\frac{1}{2}f^- + \frac{1}{2}f^+$ at the jump, the Fourier series will not converge to $f(x)$ at $x = x_*$. At any jumps of $f(x)$, the Fourier series can display persistent "ringing" if truncated at a finite number of terms because smooth functions (*i.e.* sines and cosines) are being used to represent something that is discontinuous. This is "Gibbs phenomenon".

Even and odd functions

A function is *even* if $f(x) = f(-x)$; it is *odd* if $f(x) = -f(-x)$. In view of these properties

$$\int_{-L}^{L}(\text{Even Funk})\mathrm{d}x = 2\int_{0}^{L}(\text{Even Funk})\mathrm{d}x \qquad \& \qquad \int_{-L}^{L}(\text{Odd Funk})\mathrm{d}x = 0.$$

Cosine is even ($\cos(-\kappa x) = \cos\kappa x$, for constant κ); sine is odd ($-\sin(-\kappa x) = \sin\kappa x$).
• Products of even functions remain even; *i.e.* if $f(x)$ and $g(x)$ are both even, then $f(x)g(x)$ is even.
• Products of odd functions are also even: if $f(x)$ and $g(x)$ are both odd, then $f(x)g(x)$ is even.
• If $f(x)$ is even and $g(x)$ is odd, then $f(x)g(x)$ is odd.
It follows that

$$\int_{-L}^{L}(\text{Even Funk})\cos\kappa x\,\mathrm{d}x = 2\int_{0}^{L}(\text{Even Funk})\cos\kappa x\,\mathrm{d}x \qquad \& \qquad \int_{-L}^{L}(\text{Even Funk})\sin\kappa x\,\mathrm{d}x = 0,$$

$$\int_{-L}^{L}(\text{Odd Funk})\cos\kappa x\,\mathrm{d}x = 0 \qquad \& \qquad \int_{-L}^{L}(\text{Odd Funk})\sin\kappa x\,\mathrm{d}x = 2\int_{0}^{L}(\text{Odd Funk})\sin\kappa x\,\mathrm{d}x.$$

This means that for an even function, the coefficients of the sine terms of the Fourier series must vanish ($b_n = 0$), and we arrive at the "Fourier cosine series",

$$f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos\left(\frac{n\pi x}{L}\right), \quad a_0 = \frac{2}{L}\int_0^L f(x)\mathrm{d}x, \quad a_n = \frac{2}{L}\int_0^L f(x)\cos\left(\frac{n\pi x}{L}\right)\,\mathrm{d}x \quad (f \text{ EVEN}).$$

Similarly, an odd function has $a_0 = a_n = 0$ and the "Fourier sine series",

$$f(x) = \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi x}{L}\right), \quad b_n = \frac{2}{L}\int_0^L f(x)\sin\left(\frac{n\pi x}{L}\right)\,dx \quad (f \text{ ODD}). \tag{6}$$

Periodic extensions

If $f(x)$ or $u(x,t)$ is defined only for $0 \le x \le \pi$ and satisfies $f(0) = f(\pi) = u(0,t) = u(\pi,t) = 0$ then we can use the fact there is no information for $x < 0$ and $x > \pi$ to extend both functions however we want. In particular, we can **demand** that the two functions are **odd** over $-\pi \le x \le \pi$, and then periodically extend them by insisting that $f(x) = f(x+2\pi)$ and $u(x,t) = u(x+2\pi,t)$. This makes $f(x)$ and $u(x,t)$ into odd periodic functions with period 2π. Both therefore can be represented by an odd Fourier series like that in (6) (with $L = \pi$). This strategy can be referred to as "making the odd $2\pi-$periodic extension" of the functions, and establishes (from Fourier series theory) that it is mathematically justifiable to represent both the initial condition and the solution to our PDE in the manner of (1)–(3).

The issue is: "how do we know that any old function defined on $0 < x < \pi$ can be represented as an infinite series of sine functions?" Could a finite number suffice? Do sine functions have the right or enough properties? The answers are "Because Fourier series theory tells us that this is so", "No" and "Yes", once we make the odd periodic extension.

All that said, however, the only purpose of the extension is to mathematically justify (1)–(3), which follow immediately from using separation of variables and the helpful integrals in (4)-(5) (along that path, we write down the general solution (1) and the constraint imposed by the initial condition (2), then integrate that constraint after multiplying by $\sin mx$ to arrive at (3); the Fourier series formulae, though, and in particular (6), allow us to skip the final step).

An example

If $f(x) = x(\pi - x)$, introducing the odd $2\pi-$periodic extension of this function we arrive at

$$x(\pi - x) = \sum_{n=1}^{\infty} b_n \sin nx, \quad b_n = \frac{2}{\pi}\int_0^{\pi} x(\pi - x)\sin nx\,\mathrm{d}x = \frac{4}{n^3\pi}[1 - (-1)^n],$$

after integrating by parts twice. The PDE solution is then (1), with this set of b_n's. It works because $u(x,t)$ can be extended as an odd $2\pi-$periodic function.