4 The Heat Equation

Our next equation of study is the heat equation. In the first instance, this acts on functions Φ defined on a domain of the form $\Omega \times [0, \infty)$, where we think of Ω as 'space' and the half–line $[0, \infty)$ as 'time after an initial event'. The equation is

$$\frac{\partial \Phi}{\partial t} = K \nabla^2 \Phi \tag{4.1}$$

where ∇^2 is the Laplacian operator on Ω and K is a real, positive constant known as the *diffusion constant*. For example, in the simplest case of one dimension where $\Omega = [a, b]$ the equation becomes just $\partial\Phi/\partial t = K\, \partial^2\Phi/\partial x^2$ where $x \in [a, b]$.

The heat equation genuinely is one of my favourite equations. It's range of applications is utterly mind–boggling. As the name suggests, it was originally constructed by Fourier in trying to understand how heat flows through a body from a hotter region to a cooler one, but it goes far, far beyond this. It describes the transport of any quantity that diffuses (*i.e.*, spreads out) as a consequence of spatial gradients in its concentration, such as drops of dye in water. The heat equation was used by Black and Scholes to model the behaviour of the stock market, and it underlies Turing's explanation of how the cheetah got its spots and the zebra its stripes. In pure maths, it plays a starring role in the derivation of the Atiyah–Singer index theorem relating topology to geometry, while a modification of the heat equation known as Ricci flow was used by Perelman to affirm the Poincaré conjecture, giving him chance to decline a Fields Medal. And, in the guise of something called *renormalization*, it's the best answer we have to the questions 'why can we understand physics at all?' or 'why is the Universe comprehensible?'[19]. Let's get started!

4.1 The fundamental solution

The first important property of the heat equation is that the total amount of heat is conserved. That is, if Φ solves the heat equation on $\Omega \times [0, \infty)$, then by differentiating under the integral sign

$$\frac{d}{dt}\left(\int_\Omega \Phi \, \mathrm{d}V\right) = \int_\Omega \frac{\partial \Phi}{\partial t} \, \mathrm{d}V = K \int_\Omega \nabla^2 \Phi \, \mathrm{d}V = K \int_{\partial\Omega} \mathbf{n} \cdot \nabla\Phi \, \mathrm{d}S \,, \tag{4.2}$$

where $\mathbf{n}$ is the outward normal to the boundary $\partial\Omega$ of the spatial region. In particular, if $\mathbf{n} \cdot \nabla\Phi|_{\partial\Omega} = 0$, which says that no heat flows out of our region, then

$$\frac{d}{dt}\left(\int_\Omega \Phi \, \mathrm{d}V\right) = 0 \tag{4.3}$$

and the total amount of heat in Ω is conserved. The heat equation moves heat around, but it doesn't just get 'lost'. (Notice that if Ω were non–compact, we'd have to demand that $|\nabla\Phi|$ decays sufficiently quickly as we move out to infinity in the spatial directions for these integrals to be well–defined.)

[19] Sadly, I won't be able to explain this to you in this course. But come to the Part III AQFT course and be amazed...

The second property we'll mention is that if $\Phi(x,t)$ solves the heat equation for (x,t) in $\mathbb{R}^n \times [0,\infty)$, then so too do the translated function

$$\Phi_1(x,t) \equiv \Phi(x - x_0, t - t_0)$$

and the rescaled function

$$\Phi_2(x,t) \equiv A\,\Phi(\lambda x, \lambda^2 t)\,,$$

where A, λ and t_0 are real constants and where $x_0 \in \mathbb{R}^n$. The proof of this is an easy exercise that I'll leave to you. Let's try to choose the constant A so that the total amount of heat in the solution Φ_2 is the same as in our original solution Φ. We have

$$\int_{\mathbb{R}^n} \Phi_2\,\mathrm{d}^n x = A \int_{\mathbb{R}^n} \Phi(\lambda x, \lambda^2 t)\,\mathrm{d}^n x = A\,\lambda^{-n} \int_{\mathbb{R}^n} \Phi(y, \lambda^2 t)\,\mathrm{d}^n y \tag{4.4}$$

where $y = \lambda x$. If we choose $A = \lambda^n$ then the total heat in Φ_2 at time t will be the same as the total heat in Φ at time $\lambda^2 t$. But the total heat is conserved, so they are the same at all times.

The rescaling property is useful because it says there is nothing really new about the time variable t compared to the spatial variables. In other words, although $\Phi(x,t)$ looks as though it depends on n spatial variables and one time variable, we can always rescale so as to eliminate one of these variables. In particular, in 1+1 dimensions the heat equation becomes simply

$$\frac{\partial \Phi}{\partial t} = K \frac{\partial^2 \Phi}{\partial x^2} \tag{4.5}$$

and, choosing $\lambda = 1/\sqrt{Kt}$ nothing is really lost by considering solutions of the form

$$\Phi(x,t) = \frac{1}{\sqrt{Kt}} F(x/\sqrt{Kt}, 1) = \frac{1}{\sqrt{Kt}} F(\eta) \tag{4.6}$$

where we have introduced the *similarity variable*

$$\eta \equiv \frac{x}{\sqrt{Kt}}\,. \tag{4.7}$$

The similarity variable is a dimensionless parameter that is invariant under further rescalings $(x,t) \to (\lambda x, \lambda^2 t)$. We'll see that it characterizes the linear–time spread of heat.

Plugging the form (4.6) into the heat equation we obtain

$$\begin{aligned} \frac{\partial \Phi}{\partial t} &= -\frac{1}{2}\frac{1}{\sqrt{Kt^3}} F(\eta) + \frac{1}{\sqrt{Kt}}\frac{\partial \eta}{\partial t} F'(\eta) = -\frac{1}{2}\frac{1}{\sqrt{Kt^3}}(F + \eta F') \\ K\frac{\partial^2 \Phi}{\partial x^2} &= \sqrt{\frac{K}{t}}\frac{\partial}{\partial x}\left(\frac{\partial \eta}{\partial x} F'\right) = \frac{1}{t}\frac{\partial \eta}{\partial x} F'' = \frac{1}{\sqrt{Kt^3}} F'' \end{aligned} \tag{4.8}$$

so the heat equation pde reduces to the ode

$$0 = 2F'' + \eta F' + F\,. \tag{4.9}$$

Noting that the *rhs* of this equation is $(2F' + \eta F)'$ we see that $2F' + \eta F = D$ for some constant D. We can set D to zero by requiring that our solution obeys $F'(0) = 0$, and one then finds $F(\eta) = C\mathrm{e}^{-\eta^2/4}$ for some further constant C. It is standard to fix this new constant by normalizing the total amount of heat to be 1. We have[20]

$$1 = \int_{-\infty}^{\infty} \Phi(x,t)\,\mathrm{d}x = \frac{C}{\sqrt{Kt}} \int_{-\infty}^{\infty} \mathrm{e}^{-x^2/4Kt}\,\mathrm{d}x = 2C \int_{-\infty}^{\infty} \mathrm{e}^{-u^2}\,\mathrm{d}u = 2C\sqrt{\pi}\,. \tag{4.10}$$

Therefore our normalized solution is

$$\Phi(x,t) = G(x,t) \equiv \frac{1}{\sqrt{4\pi Kt}} \exp\left(-\frac{x^2}{4Kt}\right) \tag{4.11}$$

It follows from the translation argument above that

$$G(x-x_0, t-t_0) = \frac{1}{\sqrt{4\pi K(t-t_0)}} \exp\left(-\frac{(x-x_0)^2}{4K(t-t_0)}\right) \tag{4.12}$$

also solves the (1+1)–dimensional heat equation. This class of solutions is known as the *heat kernel*, or sometimes as the *fundamental solutions* of the heat equation. It is also straightforward to show (or just to verify) that

$$\Gamma(\mathbf{x}-\mathbf{x}_0, t-t_0) \equiv \frac{1}{(4\pi K(t-t_0))^{n/2}} \exp\left(-\frac{|\mathbf{x}-\mathbf{x}_0|^2}{4K(t-t_0)}\right) \tag{4.13}$$

is the fundamental soluton of the heat equation in $n+1$ dimensions, $\mathbb{R}^n \times (t_0, \infty)$.

The heat kernel is a Gaussian centred on x_0. The rms width (standard deviation) of the Gaussian is $\sqrt{K(t-t_0)}$ while the height of the peak at $x = x_0$ is $1/\sqrt{4\pi K(t-t_0)}$. This means that as $t \to \infty$ this fundamental solution becomes flatter and flatter, with its value at any fixed $x \in \Omega$ approaching zero exponentially rapidly. On the other hand, if we trace the behaviour of the fundamental solution backwards in time then as t approaches the initial time t_0 from above, the Gaussian becomes more and more sharply peaked near its centre x_0, and the height of the curve tends to infinity. The actual limit at $t = t_0$ is known as the *Dirac δ–function*, though it's not really a function at all. We'll meet it again in detail later. Plots of the heat kernel in 1+1 dimensions for various fixed times can be found in figure 4.1.

We have obtained the heat kernel as a solution to the heat equation within the domain $\mathbb{R}^n \times [0, \infty)$ without imposing any particular boundary conditions. However, one use of the heat kernel is as any early time approximation to heat flow problems in an *arbitrary* finite domain Ω near to interior points $x \in \Omega$ where the initial concentration of heat $\Phi(x, 0)$ has a sharp, highly localized spike. Intuitively, this is because it takes some time for this strongly localized interior profile to 'feel the influence' of the boundary conditions. For example, we may be interested in the effect of a sudden blast of heat perhaps coming from a blowtorch that is suddenly turned on, then immediately extinguished. at the centre of a furnace. The spread of heat is constrained by the boundary condition that it cannot penetrate the thick brick walls of the furnace, but at very short times this is irrelevant.

[20]The final integral can be performed by a trick: Let $I = \int_{\mathbb{R}} \mathrm{e}^{-u^2}\,\mathrm{d}u$. Then

$$I^2 = \int_{\mathbb{R}^2} \mathrm{e}^{-(u^2+v^2)}\,\mathrm{d}u\,\mathrm{d}v = 2\pi \int_0^{\infty} \mathrm{e}^{-r^2} r\,\mathrm{d}r = \pi\,[-\mathrm{e}^{-r^2}]_0^{\infty} = \pi\,.$$

Therefore $I = \sqrt{\pi}$, with the positive square root taken because I is the integral of a non–negative function.

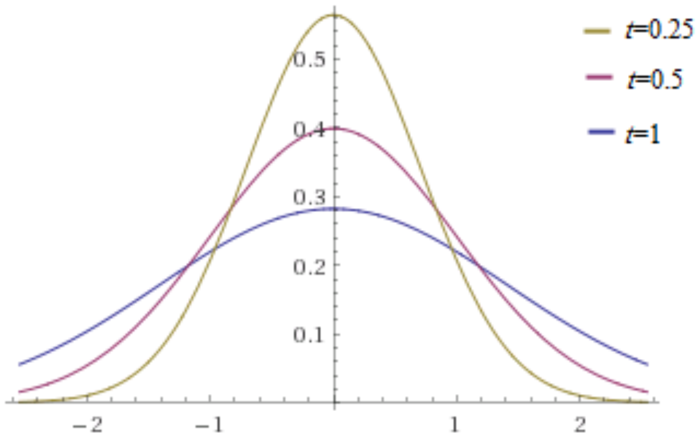

Figure 8. *Plots of the heat kernel* (4.11) *in one space and one time dimension, drawn at successive times $t > t_0 = 0$. For simplicity we have set $K = 1$. The curve is a Gaussian whose height increases without bound as $t \to 0^+$. Since the total heat is conserved, the area under the graph is constant, and equal to 1 by our normalization condition.*

4.2 Heat flow as a smoothing operation

The smoothing we observed in the fundamental solution – moving from a sharp spike to a flat line as $t \to \infty$ – is the generic behaviour of functions under heat flow, and is in accordance with our intuition that heat flows from hotter places to cooler ones. This smoothing property is one of the most important properties of the heat equation. Let's see it more generally.

First, we note that if $\psi : \Omega \to \mathbb{C}$ is an eigenfunction of the Laplacian (with weight 1) so that $\nabla^2\psi = -\lambda\psi$ for some constant λ, then provided ψ obeys suitable conditions on $\partial\Omega$, the eigenvalue λ is non-negative. This follows because

$$-\lambda \int_\Omega |\psi|^2 \, \mathrm{d}V = \int_\Omega \psi^* \, \nabla^2\psi \, \mathrm{d}V = \int_{\partial\Omega} \psi^* \, \nabla\psi \cdot \mathrm{d}\mathbf{S} - \int_\Omega \nabla\psi^* \cdot \nabla\psi \, \mathrm{d}V \tag{4.14}$$

where $\mathrm{d}V = \mathrm{d}x_1 \, \mathrm{d}x_2 \cdots \mathrm{d}x_d$ is the standard measure on Ω. Since both $\int_\Omega |\psi|^2 \, \mathrm{d}V$ and $\int_\Omega |\nabla\psi|^2 \, \mathrm{d}V$ are the integrals of non-negative functions, we see that provided the boundary term vanishes

$$\lambda = \frac{\int_\Omega |\nabla\psi|^2 \, \mathrm{d}V}{\int_\Omega |\psi|^2 \, \mathrm{d}V} \geq 0 \, . \tag{4.15}$$

In particular all the eigenvalues of a Laplacian on a closed, compact space (so that $\partial\Omega = \emptyset$) are non-negative.

Now, suppose a certain function $\Phi : \Omega \times [0, \infty) \to \mathbb{C}$ evolves in time according to the heat equation $\partial\Phi/\partial t = \nabla^2\Phi$, where ∇^2 is the Laplacian on the closed, compact space Ω and $t \in [0, \infty)$ denotes the time. To reduce clutter, we've also set the diffusion constant to unity. If Φ looks initially like some function $f : \Omega \to \mathbb{C}$, so that $\Phi(\mathbf{x}, 0) = f(\mathbf{x})$, then at finite later times t we have (somewhat formally)

$$\Phi(\mathbf{x}, t) = \exp\left(t\nabla^2\right) \Phi(\mathbf{x}, 0) \, . \tag{4.16}$$

But given a basis $\{\psi_I\}$ of eigenstates of ∇^2 on Ω, we can expand f in this basis as

$$\Phi(\mathbf{x},0) = f(\mathbf{x}) = \sum_I c_I\, \psi_I(\mathbf{x}) \tag{4.17}$$

for some coefficients c_I. (When $\dim\Omega > 1$ the index 'I' really stands for a whole collection of indices, each one of which is being summed over. For example, if $\Omega = T^2 = S^1 \times S^1$ then we will have two indices, each denoting the Fourier components around one of the circles. The sum over I is supposed to indicate a sum over all values of each of these indices, with independent coefficients.) Finally, if $\nabla^2\psi_I = -\lambda_I\psi_I$ then inserting this into equation (4.16) and using the linearity of the Laplacian gives

$$\begin{aligned}\Phi(\mathbf{x},t) &= \exp\left(t\nabla^2\right)\left[\sum_I c_I\,\psi_I\right] = \sum_I c_I\,\mathrm{e}^{-\lambda_I t}\,\psi_I(\mathbf{x}) \\ &\equiv \sum_I c_I(t)\,\psi_I(\mathbf{x})\,.\end{aligned} \tag{4.18}$$

In the final line I've introduced the *time–dependent coefficients* $c_I(t) \equiv \mathrm{e}^{-\lambda_I t}c_I$. Thus, since the eigenvalues are non-negative, the coefficients decay exponentially with time. We saw earlier[21] that the rate at which the coefficients in an eigenfunction expansion decay as one goes out to very high eigenvalues tells us something about the smoothness of the function we're expanding. The important observation is under evolution by the heat equation, that coefficients of eigenfunctions corresponding to the largest values of $|\lambda_I|$ decay most rapidly. Thus, in accordance with our intuition, heat flow *smooths* our function in accordance with our intuition. In fact, the smoothing is so effective that a function that is discontinuous at $t = 0$ becomes continuous for all $t > 0$ if it evolves by the heat equation.

Not only does Φ become smoother, it's also easy to see that the norm of Φ over Ω decreases rapidly. At a fixed time $t \geq 0$ we have

$$\begin{aligned}(\Phi,\Phi) &= \int_\Omega \Phi^*\,\Phi\,\mathrm{d}V = \sum_{I,J}\left[c_I^*(t)\,c_J(t)\int_\Omega \psi_I^*(\mathbf{x})\,\psi_J(\mathbf{x})\,\mathrm{d}V\right] \\ &= \sum_I |c_I(t)|^2 \leq \sum_I |c_I(0)|^2\end{aligned} \tag{4.19}$$

using orthonormality of the eigenfunctions ψ_I.

Incidentally, I hope you now see the reason I've emphasized that the time variable t in the heat equation takes values on the half–line $[0,\infty)$ rather than $t \in \mathbb{R}$. If we try to follow heat flow backwards in time, then the convergence of our series becomes exponentially *worse*, with the eigenfunctions having greater and greater $|\lambda_I|$ rapidly becoming more and more important. In fact, if we start from a generic smooth function and trace its evolution back in time, then it's a theorem that we'll arrive at an arbitrarily badly singular function in finite time. Setting the diffusion constant to 1 for simplicity, we sometimes say that

[21] We saw this just in the special case of Fourier series in one dimension, but something similar is true quite generally.

the operators $e^{t\nabla^2}$ form a *semigroup*, because for t_1 and t_2 both ≥ 0 we have the group multiplication law

$$e^{(t_1+t_2)\nabla^2} = e^{t_1\nabla^2}\, e^{t_2\nabla^2}$$

while setting $t = 0$ gives the identity operator. However, we're not allowed to consider heat flow for negative times because we'd meet too singular functions, so the inverse operators do not exist and heat flow is a one–way street.

The fact that evolution via the heat equation smears out sharp features can be both a blessing and a curse, as the following two examples illustrate:

4.2.1 The transatlantic cable

In 1858 the first telegraph cable was laid under the Atlantic, with Great Britain and the United States both looking forward to the benefits this new form of communication could bring to trade and governance. The first message to be sent was a 98 word greeting from Queen Victoria to President Buchanan. The British telegraph operators dutifully tapped out the message in Morse code and sent it on its way. But by the time the signal made landfall in Newfoundland, it had degraded so as to be barely detectable, let alone readable. What went wrong? Because seawater is a much better conductor than air, the signal traveling along the submerged cable obeyed the heat equation, not the wave equation[22] as it would for an overland telegraph wire. The form of the fundamental solution of equation (4.11) shows that an initially sharp spike traveling along a (one–dimensional!) cable of length L in accordance with the heat equation will emerge as a broad pulse spread over a time $T \sim L^2$. The precise dots and dashes of Morse code had been smeared out so much that it took the American engineers 16 hours to decipher the message.

Desperate to please his employers, the chief engineer tried to make the signal more distinct by increasing the voltage to 2000V. This promptly fried the cable's protective cover somewhere in the mid Atlantic, destroying the cable. The chief engineer was sacked. Following the advice of his replacement, a further cable was laid with thicker insulation and higher quality copper wire (thus increasing the conductivity K). It was driven at low voltage with a sensitive 'mirror galvanometer' used to detect the incoming signal. The new cable was a resounding success.

The first engineer's name was Wildman Whitehouse − you've never heard of him. His replacement William Thomson was rewarded with the title of Lord Kelvin, grew an impressive beard and became very wealthy.

4.2.2 The Atiyah–Singer index theorem

The index theorem of Atiyah & Singer provides a fundamental link between topological information about a (closed, compact) space Ω to local information, such as how curved the space is near some point. A beautiful proof of this theorem was provided by Atiyah & Bott. Their proof uses properties we know about the heat equation.

The point is that under heat flow, a function spreads out and ultimately smears itself all over the compact space Ω, giving us access to global information about the topology

[22] We'll see in the next chapter that signals propagating via the wave equation preserves their integrity.

of Ω. More specifically, if we follow the behaviour of some $\Phi(\mathbf{x},t)$ under heat flow right through to arbitarily late times, then from equation (4.18) we find

$$\lim_{t\to\infty}\Phi(\mathbf{x},t)=\lim_{t\to\infty}\sum_I c_I\,\mathrm{e}^{-t\lambda_I}\,\psi_I(\mathbf{x})=\sum_{I\,:\,\lambda_I=0}c_I\,\psi_I(\mathbf{x})\,, \tag{4.20}$$

where the final sum is over only those eigenfunctions of the Laplacian whose eigenvalues are zero. This always includes the constant function, but on a manifold with interesting topology there may be non–trivial functions that nonetheless have zero eigenvalue[23]. However, if at $t=0$ we choose Φ to have support just inside some small compact region $R\subset\Omega$, then for early times Φ remains exponentially small outside R.

Heat flow from $t=0$ to $t\to\infty$ thus provides a natural link between local and global properties of Ω. The idea of Atiyah & Bott was to find a quantity – known as the "index of a Dirac operator" – that can be proved to be *independent* of time and track it during heat flow. At early times one finds the index can be computed in terms of local, geometric information while at late times it depends only on topological properties of Ω.

4.3 Brownian motion and the existence of atoms

The fact that heat always flows from a hotter to a cooler body – just the smoothing property we examined above – posed a challenge to the Newtonian, mechanical view of the world. According to the hypothesis that matter is fundamentally made up of atoms (dating back in some form to the ancient Greeks), heat is simply the kinetic energy of these atoms as they jiggle around. The problem is that at the microscopic level, Newton's laws of motion are time reversible: for forces such as electromagnetism, gravity, or collisions between hard particles, $\mathbf{F}=m\mathbf{a}$ is invariant under the replacement $t\mapsto -t$. Philosophers such as Mach and chemists such as Ostwald thought that this microscopic time reversibility was incompatible with the macroscopic arrow of time inherent in heat flow, and concluded that atoms did not exist.

Einstein realized that the apparently random motion of small dust particles observed by the botanist Robert Brown must be due to their random collisions with water molecules. To construct a one–dimensional model of this problem, assume that our dust particle is jostled at regular time intervals Δt. We let $p(y)$ be the probability that the dust particle moves through a displacement y at each time step, with $\int_{-\infty}^{\infty}p(y)\,\mathrm{d}y=1$. The key assumption is that $p(y)$ is *independent of which time step we're considering*. That is, the process is memoryless – the probability $p(y)$ does not depend on the previous motion of the particle. This is also known as a *Markov process*. We further assume that $p(y)$ is homogeneous, so that it does not depend on the actual location of the dust particle. Finally, we'll assume that $p(y)$ is an even function of y so that the mean value $\langle y\rangle$ is zero. This just means that there is no preference for the particle to drift either to the left or right; it's easy to drop this final assumption.

[23] To come clean, I'll admit that Φ should really be something more general than a 'function' here, and we need to be careful about what we mean by the Laplacian in this more general context. Believe it or not, the case relevant to the Atiyah–Singer index theorem is where Φ is the quantum mechanical wavefunction describing a type of relativistic electron.

If we now let $P(x,t)$ be the probability density that the dust particle is located at some position $x \in \mathbb{R}$ at time t, then we have

$$P(x;t+\Delta t) = \int_{-\infty}^{\infty} p(y)\, P(x-y;t)\, \mathrm{d}y\,. \tag{4.21}$$

This equation says that the probability the particle is located at x at time $t + \Delta t$ is the product of the probability it was some amount y away at the previous time interval, times the probability it stepped through exactly y, for any choice of y. Expanding $P(x-y;t)$ as a Taylor series in y we have

$$\begin{aligned} P(x;t+\Delta t) &= \int_{-\infty}^{\infty} p(y) \left(P(x;t) - y\frac{\partial P}{\partial x}(x;t) + \frac{1}{2}y^2\frac{\partial^2 P}{\partial x^2}(x;t) + \cdots \right) \mathrm{d}y \\ &= \sum_{r=0}^{\infty} \frac{\langle y^r \rangle}{r!} \frac{\partial^r P}{\partial x^r}(x;t) \end{aligned} \tag{4.22}$$

where by $\langle y^r \rangle$ we mean simply the average value $\int_{-\infty}^{\infty} y^r\, p(y)\, \mathrm{d}y$ of y^r. By our assumption, $\langle y \rangle = 0$. Furthermore, if the motion of the particle is small so that $p(y)$ is concentrated near $y = 0$, then $\langle y^r \rangle$ will drop rapidly as r increases. Keeping only the leading non–trivial term we have

$$P(x;t+\Delta t) - P(x;t) = \frac{1}{2}\langle y^2 \rangle \frac{\partial^2 P}{\partial x^2}(x;t)\,. \tag{4.23}$$

In the limit of small time steps $\Delta t \to 0$ we find that $P(x,t)$ satisfies the heat equation

$$\frac{\partial P}{\partial t} = K\frac{\partial^2 P}{\partial x^2} \tag{4.24}$$

where the diffusion constant K can be identified as $\langle y^2 \rangle / 2\Delta t$.

THIS SECTION NEEDS MORE WORK!! NOT YET RELATED TO EXISTENCE OF ATOMS

4.4 Boundary conditions and uniqueness

Let $M \equiv \Omega \times [0,T]$ where $\Omega \subset \mathbb{R}^n$ is a compact domain with boundary $\partial\Omega$, and where $[0,T)$ is the time direction. We'd now like to check whether there is a unique solution to the heat equation $\partial\psi/\partial t = K\nabla^2\psi$ in the interior of M that obeys the Dirichlet conditions

$$\begin{aligned} \psi|_{\Omega\times\{0\}} &= f(x) \qquad &\text{(initial condition)} \\ \psi|_{\partial\Omega\times[0,T]} &= g(x,t) \qquad &\text{(boundary condition)} \end{aligned} \tag{4.25}$$

for some given functions $f : \Omega \to \mathbb{R}$ and $g : \partial\Omega \times [0,T] \to \mathbb{R}$.

As in the case of Laplace's equation, suppose on the contrary that ψ_1 and ψ_2 are two such solutions, each obeying the boundary conditions (4.25). Then if $\delta\psi \equiv \psi_1 - \psi_2$ we have

$$0 = \int_{\Omega} \delta\psi \left(\frac{\partial \delta\psi}{\partial t} - K\nabla^2\delta\psi \right) \mathrm{d}V \tag{4.26}$$

where the integral is over the spatial region Ω at some arbitrary fixed time t. Hence differentiating the integral with respect to time we have

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\int_\Omega \delta\psi^2\,\mathrm{d}V &= \int_\Omega \delta\psi\,\frac{\partial\delta\psi}{\partial t} = K\int_\Omega \delta\psi\,\nabla^2\delta\psi \\ &= -K\int_\Omega (\nabla\delta\psi)\cdot(\nabla\delta\psi)\,\mathrm{d}V + K\int_{\partial\Omega}\delta\psi\,\nabla\delta\psi\,\cdot\mathrm{d}\mathbf{S}\end{aligned} \tag{4.27}$$

The boundary term vanishes since ψ_1 and ψ_2 agree on $\partial\Omega$ at all times, and the remaining term is $-K$ times the integral of a non–negative function. Therefore

$$\frac{d}{dt}\left(\int_\Omega \delta\psi^2\,\mathrm{d}V\right) \le 0\,. \tag{4.28}$$

The quantity $E(t) \equiv \int_\Omega \delta\psi^2\,\mathrm{d}V$ is the integral of a non–negative function, which by (4.28) can never increase. Since $E(0) = 0$ by our initial conditions, we must have $E(t) = 0$ at all times t for which the heat equation holds. This is only possible if $\delta\psi = 0$ everywhere in Ω and at all times $t \in [0, T]$, so that the solutions ψ_1 and ψ_2 agree everywhere in M.

There's an important caveat to the above argument: Compactness of Ω in all spatial directions is important. If, for example, we replaced the compact region Ω by the semi–infinite bar $\{(x, y, z) \in \mathbb{R}^3\ :\ 0 \le x \le a\,,\ 0 \le y \le b\,,\ z \ge 0\}$ then our argument above might be invalid, because it could be that the integrals over the spatial region now *diverge*. This is not just a technical nicety: it's really true that, when Ω has non–compact directions, solutions to the heat equation are *not* unique unless we impose a limit of the rate of growth of ψ as we head out towards infinity in Ω. In the case of the semi–infinite bar, the correct limit turns out to be $|\psi| \le A\mathrm{e}^{\lambda|z|^2}$ as $z \to \infty$, for some constants A and λ, although I won't prove that here.

4.5 Heat conduction in a plane medium

After the above, rather formal, considerations, in the next few sections we'll return to actually solving the heat equation in the presence of boundary and initial conditions.

One of Fourier's original motivations for introducing his series was to study the problem of heat flow through a plane medium. In particular, he wanted to study how the temperature Θ of the soil at a depth $x \ge 0$ beneath the surface was affected by the regular heating and cooling of the daily cycle. For simplicity, we'll assume that the earth is flat and that ground level may be represented by the plane $x = 0$. If the sun's rays strike the earth evenly, then the problem may be modeled by the heat equation

$$\frac{\partial\Theta}{\partial t}(x, t) = K\frac{\partial^2\Theta}{\partial x^2}(x, t) \tag{4.29}$$

in 1+1 dimensions, where K is the thermal diffusivity of the soil. The boundary conditions are that the temperature decays to a constant as $x \to +\infty$ (deep under the surface of the earth) and that at $x = 0$ the temperature oscillates both daily and annually as

$$\Theta(0, t) = \Theta_0 + A\cos(2\pi t/t_{\mathrm{D}}) + B\cos(2\pi t/t_{\mathrm{Y}}) \tag{4.30}$$

where $t_{\rm D}$ is the length of one day, and $t_{\rm Y}$ the length of one year in whatever units we're using to measure time. The constants A and B govern the size of the daily and annual variation around the average temperature Θ_0.

We again separate variables, writing $\Theta = T(t)X(x)$, and discover that the heat equation (4.29) becomes

$$T' = \lambda T\,, \qquad\qquad X'' = \frac{\lambda}{K}X \tag{4.31}$$

for some constant λ. Noting that we want oscillatory behaviour in time, with an eye on the boundary condition at $x=0$ we set $\lambda = {\rm i}\omega$ with $\omega\in\mathbb{R}$. The heat equation is then solved by

$$\Theta = \Theta_\omega \equiv {\rm e}^{{\rm i}\omega t}\left(a_\omega\,{\rm e}^{-x\sqrt{{\rm i}\omega/K}} + b_\omega\,{\rm e}^{x\sqrt{{\rm i}\omega/K}}\right) \tag{4.32}$$

for some choice of ω and constants a_ω, b_ω. By linearity, we can add solutions with different values of the separation constant ω. Since $\sqrt{{\rm i}\omega} = (1+{\rm i})\sqrt{|\omega|/2}$ for $\omega>0$ and $\sqrt{{\rm i}\omega} = ({\rm i}-1)\sqrt{|\omega|/2}$ for $\omega<0$, the boundary condition that Θ decays to a constant as $x\to+\infty$ shows that we must take $b_\omega = 0$ when $\omega>0$ and $a_\omega=0$ when $\omega<0$. Writing the boundary condition at $x=0$ as

$$\Theta(0,t) = \Theta_0 + \frac{A}{2}\left({\rm e}^{{\rm i}\omega_{\rm D}t} + {\rm e}^{-{\rm i}\omega_{\rm D}t}\right) + \frac{B}{2}\left({\rm e}^{{\rm i}\omega_{\rm Y}t} + {\rm e}^{-{\rm i}\omega_{\rm Y}t}\right) \tag{4.33}$$

we see that we should choose $a_\omega = b_\omega = 0$ for all ω except

$$\omega = \pm\omega_{\rm D} \equiv \pm 2\pi/t_{\rm D}\,, \qquad \omega = \pm\omega_{\rm Y}\equiv \pm2\pi/t_{\rm Y}\,, \qquad \text{and} \qquad \omega = 0\,.$$

The case $\omega=0$ just gives the constant Θ_0. For the remaining cases we have

$$a_{\omega_{\rm D}} = b_{-\omega_{\rm D}} = \frac{A}{2}\,, \qquad a_{\omega_{\rm Y}} = b_{-\omega_{\rm Y}} = \frac{B}{2} \tag{4.34}$$

so that the general solution obeying the boundary condition becomes

$$\begin{aligned}\Theta(x,t) \;&=\; \Theta_0 \;+\; A\exp\left(-\sqrt{\frac{\omega_{\rm D}}{2K}}\,x\right)\,\cos\left(\omega_{\rm D}t - \sqrt{\frac{\omega_{\rm D}}{2K}}\,x\right)\\ &\qquad\;+\; B\exp\left(-\sqrt{\frac{\omega_{\rm Y}}{2K}}\,x\right)\,\cos\left(\omega_{\rm D}t - \sqrt{\frac{\omega_{\rm Y}}{2K}}\,x\right)\,.\end{aligned} \tag{4.35}$$

It is a worthwhile exercise to check that this does indeed obey the heat equation (4.29).

The solution we've found tells us how the temperature of the soil at a depth x and time t responds to the sun's warmth. Examining it, we see that both temperature variations decay exponentially rapidly with increasing depth, so that the diurnal and annual cycles have little effect on the temperature Θ_0 deep underground. Note however that the fall–off of the higher frequency, daily variation is far more rapid than that of the annual variation.

We also see there is a depth–dependent phase delay of $(\omega_{\rm D}/K)^{1/2}\,x$ for the daily, and $(\omega_{\rm Y}/K)^{1/2}\,x$ for the annual temperature variation. Thus, at some depths beneath the surface of the earth the temperature can be completely out of step with that on the surface. The depth at which this occurs depends on the heat conductivity K of the soil, but for reasonable soil types one finds that at a depth of around 2 to 3 metres, the ground is warmer in winter and cooler in summer. That's why it's a good idea to store food and wine in cellars.

4.6 Steady heat conduction in a finite rod

As a small variation of this problem, suppose we have a bar of length $2L$. We'll look for a function ψ that solves the heat equation $\partial\psi/\partial t = K\partial^2\psi/\partial x^2$ everywhere inside the domain $[-L, L] \times [0, \infty)$ and subject to the initial condition

$$\psi(x,0) = \Theta(x) \equiv \begin{cases} 1 & 0 < x \leq L \\ 0 & -L \leq x < 0\,, \end{cases} \tag{4.36}$$

as well as the boundary condition

$$\psi(L,t) = 1\,, \qquad \psi(-L,t) = 0 \tag{4.37}$$

so that each end of the bar is kept at a (different) fixed temperature for all time.

The most important thing to note about this example is that *neither the initial nor the boundary condition is homogeneous*. Thus if we try to seperate variables immediately, we'll find there are no homogeneous boundary conditions to impose, and we will not find any constraint on the allowed separation constants. To get around this, we first look for *any particular* solution ψ_s of the wave equation that obeys the boundary condition (4.37), but not necessarily the initial condition (4.36). Any other solution obeying the same boundary conditions will differ from this one by a solution ϕ obeying the homogeneous boundary conditions

$$\phi(-L,t) = 0\,, \qquad \phi(L,t) = 0 \tag{4.38}$$

and so may be found via separation of variables.

To keep our lives simple, we can look for a particular solution $\phi_s(x)$ that is independent of time – known as a *steady state* solution. Since the time–independent heat equation becomes $\phi_s''(x) = 0$ we have $\phi_s(x) = ax + b$ and to satisfy the boundary condition (4.37) we must choose the constants so that

$$\phi_s(x) = \frac{x+L}{2L}\,. \tag{4.39}$$

We now look for a function $\phi(x,t) = \psi(x,t) - \phi_s(x)$ obeying the heat equation subject to the conditions

$$\begin{aligned} \phi(\pm L,t) &= 0 && (\textit{homogeneous} \text{ boundary condition}) \\ \phi(x,0) &= \Theta(x) - \frac{x+L}{2L} && (\text{adjusted initial condition}) \end{aligned} \tag{4.40}$$

that reflect the effect of our particular solution.

We now proceed as usual. Write $\phi(x,t) = X(x)T(t)$ and find

$$T' = -K\lambda T\,, \qquad X'' = -\lambda X \tag{4.41}$$

for some separation constant $\lambda \in \mathbb{R}$. We can solve these as

$$X(x)T(t) = \left[a\,\sin(\sqrt{\lambda}x) + b\,\cos(\sqrt{\lambda}x)\right] \mathrm{e}^{-K\lambda t}\,.$$

The initial condition $\phi(x,0) = \Theta(x) - (x+L)/2L$ is an *odd* function, so we anticipate that we can set $b = 0$. The homogeneous boundary conditions $\phi(\pm L, 0) = 0$ shows that the general solution is then

$$\psi(x,t) = \sum_{n=1}^{\infty} a_n \sin\left(\frac{n\pi x}{L}\right) \mathrm{e}^{-Kt\sqrt{n\pi/L}} . \tag{4.42}$$

The last step is to choose the coefficients a_n so as to obey the inhomogeneous initial condition. This will be achieved if we set

$$a_n = \frac{1}{L}\int_{-L}^{L} \sin\frac{n\pi x}{L}\left[\Theta(x) - \frac{x+L}{2L}\right] \mathrm{d}x = \frac{1}{n\pi} , \tag{4.43}$$

where the last equality requires a short calculation (*please check!*). Finally therefore, the solution to the heat equation obeying the original boundary conditions (4.36)-(4.37) is

$$\psi(x,t) = \frac{x+L}{2L} + \frac{1}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\sin\frac{n\pi x}{L}\,\mathrm{e}^{-Kt\sqrt{n\pi/L}} . \tag{4.44}$$

Note once more that the convergence of this infinite sum improves rapidly as t increases, and that

$$\lim_{t\to+\infty} \psi(x,t) = \phi_s(x) \tag{4.45}$$

so that $\phi_s(x)$ does indeed emerge as the late time equilibrium solution of our problem.

4.7 Cooling of a uniform sphere

At the end of the nineteenth century, one of the most apparently serious problems faced by Darwinian evolution was that the evolutionary process was so slow that the Earth had not been around for long enough for the observed diversity of life to have arisen. The main proponent of this argument was Kelvin (again) whose argument was as follows.

Kelvin knew the temperature at which rock melts (typically in the range $1000 \pm 300°$C for most types of rock) and it seemed reasonable to assume that life could not have been present at the time when the whole surface of the earth was molten magma. He also knew from Fourier's results of section 4.5 that, while the temperature of the surface of the Earth undergoes wide daily and annual variations, the sun's influence diminishes rapidly once one heads more than a few hundred metres down into the ground. He thus felt justified in ignoring the sun's influence and took as a boundary condition that the temperature at the surface of the Earth was zero, appropriate for outer space.

The stage was set. If Kelvin could determine how long it would take a sphere, initially heated uniformly to around 1000°C, to cool into outer space so as to form a temperature gradient near its surface of the size then observed, then this time would set an upper limit on the time available for evolution.

Let's make the rough assumption that the Earth is a homogeneous ball of radius R formed from rock with thermal diffusivity K. Under our homogeneity assumptions we expect the solution to be spherically symmetric, so we let $\Theta(r,t)$ denote the temperature at a radius r from the centre of the Earth, at time t. The behaviour of Θ will be governed by the heat equation

$$\frac{\partial \Theta}{\partial t} = K\nabla^2\phi = K\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial \Theta}{\partial r}\right) . \tag{4.46}$$

We want to solve this equation inside the Earth, subject to the initial condition and boundary condition

$$\begin{aligned} \Theta(r,0) &= \Theta_0 \qquad && \text{for all } r < R \\ \Theta(R,t) &= 0 && \text{for all } t > 0\,, \end{aligned} \tag{4.47}$$

where Θ_0 is the temperature of molten rock.

We can solve this using our standard method of separation of variables. Making the usual ansatz $\Theta(r,t) = R(r)T(t)$ the heat equation reduces to the two o.d.e.s

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) = -\lambda^2 r^2 R\,, \qquad\qquad \frac{dT}{dt} = -\lambda^2 KT \tag{4.48}$$

for some separation constant λ. The second equation is uniquely solved by $T = A_\lambda\,\mathrm{e}^{-\lambda^2 Kt}$ for some constant A_λ, whereas the radial equation is solved by

$$R(r) = B_\lambda\frac{\sin(\lambda r)}{r} + C_\lambda\frac{\cos(\lambda r)}{r} . \tag{4.49}$$

(One way to convince yourself of this is to substitute in $S(r) \equiv r\,R(r)$ whereupon the radial equation reduces to $S'' = -\lambda^2 S$.) We insist that our solution remains regular at $r = 0$ and so we set $C_\lambda = 0$. The boundary condition that $\Theta(R,t) = 0$ then forces

$$\lambda = \frac{n\pi}{R}\,, \qquad n \in \mathbb{Z} \tag{4.50}$$

so our general solution obeying this boundary condition is

$$\Theta(r,t) = \frac{1}{r}\sum_{n\in\mathbb{Z}} A_n \sin\left(\frac{n\pi r}{R}\right)\exp\left(-\frac{n^2\pi^2}{r^2}Kt\right) . \tag{4.51}$$

We must now choose the separation constants A_n to enforce the inhomogeneous initial condition $\Theta(r,0) = \Theta_0$. Setting $t = 0$ and multiplying through by r we have

$$r\Theta_0 = \sum_{n\in\mathbb{Z}} A_n \sin\left(\frac{n\pi r}{R}\right) \tag{4.52}$$

and therefore

$$A_n = \Theta_0\int_0^R \sin\left(\frac{n\pi r}{R}\right) r\,\mathrm{d}r = (-1)^{n+1}\frac{\Theta_0 R}{n\pi} \tag{4.53}$$

as follows from integration by parts. Thus our solution at all times is

$$\Theta(r,t) = \frac{\Theta_0 R}{\pi r}\sum_{n\in\mathbb{Z}}(-1)^{n+1}\frac{1}{n}\sin\left(\frac{n\pi r}{R}\right)\exp\left(-\frac{n^2\pi^2}{r^2}Kt\right) \qquad \text{for } r \leq R. \tag{4.54}$$

Incidentally, this solution would be valid for arbitrarily large values of r in some fictitious problem where the Earth extends forever, but with $r = R$ held fixed at zero temperature.

In the real situation, the thermal diffusivity K abruptly changes at the surface of the Earth from its value for rock to its value for air, then empty space (where $K = 0$). Thus we do not believe our solution for $r > R$. However, within the Earth's surface the solution (4.54) is good: we have found *a* solution that satisfies both the boundary and initial conditions and our uniqueness theorem guarantees it is the only one.

Miners had long reported the presence of the geothermal gradient – a temperature increase of around 25°C/km as one moves deeper underground – and Kelvin used this information to fix a timescale. From the solution (4.54) we find

$$\left.\frac{\partial \Theta}{\partial r}\right|_{r=R} = -\frac{\Theta_0}{R}\sum_{n\in\mathbb{Z}} \exp\left(-\frac{n^2\pi^2}{R^2}Kt\right) \tag{4.55}$$

where the minus sign indicates the fact that Θ increases as we head towards the centre of the Earth. To go further, notice that the very fact that the rocks do indeed get considerably hotter as one goes deeper – we still have volcano eruptions! – suggests that the Earth's age is not so very great that the exponential term has yet had much effect, since if it had then $\Theta(r,t)$ would itself be vanishingly small. But if $Kt/R^2 \ll 1$ (actually true in our case) then we may approximate

$$\sum_{n\in\mathbb{Z}} \exp\left(-\frac{n^2\pi^2}{R^2}Kt\right) \approx \int_{-\infty}^{\infty} \exp\left(-\frac{x^2\pi^2}{R^2}Kt\right)\,\mathrm{d}x = \sqrt{\frac{R^2}{\pi K t}}$$

Combining all the pieces we find that there will be a geothermal gradient of order G at a time of order

$$t_0 \sim \frac{\Theta_0^2}{G^2}\frac{1}{\pi K}\,. \tag{4.56}$$

Plugging in his numbers, Kelvin found that it would have taken the Earth not more than 100 million years to cool from its molten beginnings to the present temperature. This, Darwin knew, was not nearly enough time for the current diversity of species to have evolved by natural selection.

Darwin was tremendously worried by Kelvin's conclusions, more than by any other argument proposed against his Theory of Evolution. Kelvin's mathematics was impeccable, so what's going on? We now know that radioactivity – a source of energy unknown to Kelvin – primarily from Uranium deposits deep under the Earth's mantle is responsible for heating the Earth from within. This extra source of heat generation was unaccounted for in the calculation above, and has kept our planet warm for $4\frac{1}{2}$ billion years. Evolution reigns triumphant.