Fourier Series, Fourier Transforms, and PDEs

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Week 3: Partial Differential Equations

1.1 Introduction

In this second half of the lecture course we will be working with some important equations, which we will derive from first principles and then use for quite realistic real-world problems. When we tackle those problems, we will find that our knowledge of Fourier series and transforms is crucial.

The two main equations we will be concerned with are the *diffusion equation* and the *wave equation*. We will remind ourselves of the maths we need as we go along.

1.2 Deriving the diffusion equation for heat flow

It turns out that one basic equation, called the *diffusion equation*, governs the flow of heat energy in a solid as well as the flow of one material inside another (such as a gas released into air, or atoms of one metal diffusing through another). But we can't just asset this, we need to prove it. In these notes we will derive the diffusion equation for heat flow.

Mathematically, the equation is the same for heat diffusion as it is for matter diffusion. The version for heat is called

The Heat Diffusion Equation (or just Heat Equation),

and the version for matter is called

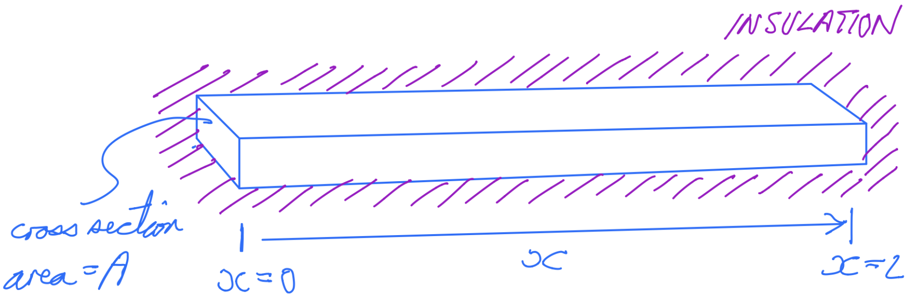
Fick's Second Law.

One of the tasks on Problem Sheet 3 asks you to explore the matter diffusion case by mirroring the heat diffusion example that we are about to do – they are practically line-by-line equivalent except that only the heat diffusion needs to relate temperature (the observable thing) to heat energy (the thing that flows). For the matter case, it's all just density of the matter, so a little easier.

In the following we will talk about *heat energy*, meaning simply energy that is in the form of heat. Sometimes for compactness we will say simply "heat" or simply "energy" – we are always talking about the same thing.

Let's think about heat flow in the context of a long rod of metal. We will assume that the rod is insulated, so that no heat energy can leave the surface. Also, we suppose that there are *no sources or sinks* generating or destroying thermal energy within the material itself. Finally, we will assume that the initial distribution of temperature in the rod is such that there is no variation across the width, only along the length. With these conditions, it will be an excellent approximation to say that the temperature never varies across the rod, only along it. But then, we only need one spatial coordinate, call it x.

Let's sketch the rod:



What will be our starting points for deriving the heat flow equation? We need to be able to capture mathematically the everyday observation that heat flows from hot regions into cold regions. So we need a relationship between the flow of heat energy and a difference in temperature. In fact we want to describe not only the direction that the heat will flow but also the amount of heat that will flow per unit time: our everyday intuition tells us that more heat flows when the difference in temperature is greater. (Put your hand near a red-hot object and you can feel that there's a lot of energy flowing off of it into the environment; put your hand near an object that is only 50°C, say, and you won't feel much.)

The relationship we need between temperature difference and the flow of heat energy is *Fourier's law of heat conduction* (yes, it's Monsieur Joseph Fourier again, he worked on heat flow as well as periodic functions!). His law can be written like this:

$$q = -k\frac{\partial \Theta}{\partial x}.$$

On the left hand side, q is a quantity called the heat flux density, which sounds complicated but it is just the amount of heat energy that is flowing per unit time (so that's power), per unit cross-sectional area. Therefore its SI units are W/m^2.

On the right hand side, Θ is the temperature at some location inside a physical object, and at some time. So for our rod we can write $\Theta(x,t)$. The symbol Θ is a standard alternative to T as a way to denote temperature; we will need to use T for something else later!

The constant k is the material's thermal conductivity; in SI units it is measured in watts per meter kelvin ($W/(m\,K)$).

So what does this equation say? First let's check: if there is no temperature variation at some point along our rod (perhaps one section is all at the same temperature) then we would have

$$\frac{\partial \Theta}{\partial x} = 0$$

and in that case we find $q = 0$ i.e. there is no flow of heat energy. That makes sense. But if

$$\frac{\partial \Theta}{\partial x} = \text{some positive number}$$

then we temperature is increasing in the direction of positive x-axis; in that case Fourier's law says our flow of heat energy will be negative, meaning that it is flowing in the negative direction along the x-axis. That makes sense! Finally we note that the more rapid the variation in temperature along the rod, i.e. the bigger $\frac{\partial \Theta}{\partial x}$ is, the more heat will flow.

So this equation matches our intuition. In fact, it is the simplest equation that could possibly match up with our everyday impressions!

In order to derive an equation for how temperature varies in time and space, we need only one thing besides Fourier's law. That thing is conservation of energy: If more energy is going into a region than is coming out, then the amount of energy within that region must be going up. And conversely, the stored energy must fall when more energy leaving than is entering.

Now we will consider a small 'slice' of the metal rod, and think about how the energy within it varies over a small time. We will write the energy variation as δE. We can express δE by thinking about the change of stored energy (revealed by change in temperature), and then we can separately find the same δE using Fourier's law to track the flow of energy in and out. From conservation of energy, the two expressions must be equal and thus we will obtain the final equation we seek.

Let's sketch the slice we have in mind:

We are thinking about the 'slice' of material between two nearby planes at $x - \delta x$ and $x + \delta x$. In the general case, the slice of material will be gaining or losing heat energy. Our symbol δE will mean the amount of energy gained (it'll be negative if energy is actually lost) by the little slice of width $2\delta x$ during a small period of time δt. We note that δE will be very small indeed since it is the variation of the energy in a small region over a small time!

Let's look at the change in stored energy first. Suppose that the temperature of the slice changes by $\delta\Theta$. The change in stored heat energy in our region is simply the mass of the material, multiplied by its specific heat capacity, multiplied by the temperature change (in Kelvin in SI units). This follows from the definition that *the specific heat capacity is the thermal energy (heat) required to raise the temperature of a body of unit mass by* $1°$*.* We'll use the usual symbol c for the specific heat capacity, and symbol ρ for the density of the material. The mass of our little slice is $2\rho A\delta x$ where A is the cross-sectional area of the rod. So we can say the change in stored energy is

$$\delta E = (2c\rho A\delta x)\delta\Theta$$

and this change $\delta\Theta$ in temperature has occurred over the short time δt. But $\delta\Theta$ is just the rate of change in Θ, multiplied by δt, so

$$\delta E = 2c\rho A\delta x\frac{\partial\Theta}{\partial t}\delta t = \left(2c\rho A\frac{\partial\Theta}{\partial t}\right)\delta x\delta t.$$

As we knew would happen, δE is related to the product of the two small quantities δx and δt.

Now let's think about flow of energy in and out. Consider the imaginary boundary planes at $x-\delta x$ and $x+\delta x$. The trick is to start by saying that the flow of energy at the mid-point in between, at x, is simply the cross-section area A multiplied by some particular flow density q. Then we can write the flow at $x-\delta x$ as

$$A\left(q-\frac{\partial q}{\partial x}\delta x\right)$$

and the flow at $x+\delta x$ as

$$A\left(q+\frac{\partial q}{\partial x}\delta x\right).$$

Remember that positive q means flow in the direction of increasing x, i.e. to the right in our figure. Then the net rate of energy flowing into the slice is

$$(\text{energy in})-(\text{energy out})=A\left(q-\frac{\partial q}{\partial x}\delta x\right)-A\left(q+\frac{\partial q}{\partial x}\delta x\right)=-2A\frac{\partial q}{\partial x}\delta x.$$

But then our quantity δE, which is the change of energy in time δt, is simply this net flow rate multiplied by δt,

$$\delta E=\left(-2A\frac{\partial q}{\partial x}\right)\delta x\delta t=\left(2Ak\frac{\partial^2\Theta}{\partial x^2}\right)\delta x\delta t$$

...where we have used the Fourier law, $q=-k\frac{\partial\Theta}{\partial x}$.

Now we've found δE by two methods. Conservation of energy says they must be equal:

$$\left(2c\rho A\frac{\partial\Theta}{\partial t}\right)\delta x\delta t=\left(2Ak\frac{\partial^2\Theta}{\partial x^2}\right)\delta x\delta t.$$

We see that we can cancel $2A\delta x\delta t$ from both sides. Putting all the remaining constants on one side gives us **the Heat Equation**

$$\frac{\partial\Theta}{\partial t}=\alpha\frac{\partial^2\Theta}{\partial x^2}\qquad\text{where}\qquad\alpha=\frac{k}{c\rho}.\tag{1.1}$$

The new constant α we have introduced is called the *thermal diffusivity.*

One of our initial assumptions was that there are no sources or sinks in energy within the bar. If in fact heat energy is being created at a rate R per unit volume, then our derivation can still work – we would have an extra contribution to δE given by $R\,2\delta xA\,\delta t$, and this would lead to the equation

$$\frac{\partial\Theta}{\partial t}=\alpha\frac{\partial^2\Theta}{\partial x^2}+R(x,t).$$

Aside: How could heat energy be created within a material? How could it be destroyed?

As you will verify in one of the Problem Sheet tasks, the same fundamental equation applies to problems of *matter diffusion*. In that case, instead of temperature we consider the density ϕ of the diffusing species and the constant α will be replaced with the *diffusion coefficient* D of that species. The final expression is one form of **Fick's Second Law** and is

$$\frac{\partial \phi}{\partial t} = D\frac{\partial^2 \phi}{\partial x^2} \tag{1.2}$$

The derivation exactly follows the logic above, except that now we use the conservation of mass rather than energy.

1.3 A side note: Solving using a good guess!

One way to solve any equation is to make a correct guess. The guess may have some flexibility, through constants or even functions that can be pinned down by investigating the guess – if we end up with a solution that satisfies the equation and meets the boundary conditions, then it is correct!

One case where this works is for a distribution of heat that is initially Gaussian: peaked in the middle and smoothly dropping off. It turns out that the future distribution is also a Gaussian, just wider and less tall. Once we've correctly guessed this, we can fill in the details step by step. A full breakdown of this case is shown at the end of this set of notes, for anyone who is curious – it's fairly straightforward, although there is a trick about making the best choice for the time $t = t_0$ when the diffusion process starts; turns out, $t = 0$ isn't the natural choice! But since it is only an example of how to investigate an inspired guess, it can't help us in situations where don't have that guess. So let's move on to more general methods.

1.4 Solving when we can't just guess the answer

Given that we're dealing with a partial differential equation, you might expect things are going to be very tough. But often, it's actually pretty easy. In the following, we'll discuss things in terms of matter diffusion, but remember this is just the same as heat diffusion – the maths is the identical.

We will try to solve for the density of material $\phi(x,t)$ given the initial concentration at $t=0$, i.e. the function $\phi(x,t=0)$. We'll find that we can get a certain way through the solution and then we'll get stuck: to progress we'll either have to restrict ourselves to silly cases of the initial concentration, or else we'll need to bring in the power of Fourier series!

In what follows, we could be thinking about *any* case where one material is diffusing through some kind of volume – the volume could already be occupied by some 'host' material. So, it could be that we are tracking the progress of some kind of metal 'type A' as its atoms diffuse through a block of another metal 'type B' inside an oven. Or we might think of one gas diffusing into another gas (say, after a partition is removed in the middle of a cylinder). But just for simplicity of our language here we will consider a single gas that is distributed within some enclosed space – it will diffuse until it is of uniform concentration.

Recall that our equation 'Fick's Second Law' mentioned earlier (and which you will derive for yourself in the Problem Sheet tasks) was

$$\frac{\partial\phi}{\partial t} = D\frac{\partial^2\phi}{\partial x^2}$$

where $\phi(x,t)$ is the density of the gas at position x and time t. We'll be assuming a 'long narrow cylinder' scenario where there is no variation across the cylinder, so that the problem has only one spatial dimension.

We know that as time tends to infinity, eventually we'll end up with an even distribution. After that there will be no further changes, so it is the *steady state*. We can work out the steady state density $\phi_{\rm SS}$ just by figuring out total amount of material in the cylinder:

$$\phi_{\rm SS} = \frac{1}{A\,L}\int_0^L \phi(x,t=0)A\,dx = \frac{1}{L}\int_0^L \phi(x,t=0)dx$$

Note that $\phi_{\rm SS}$ is a constant with no x-dependence, however in the more complex problems we'll consider later, the steady state can depend on x. Now let's introduce a new function which we will call the *transient* and we'll define it as the difference between the actual density plus the steady state

$$\phi_{\rm trans}(x,t) \equiv \phi(x,t) - \phi_{\rm SS} \qquad \Leftrightarrow \qquad \phi(x,t) = \phi(x,t)_{\rm trans} + \phi_{\rm SS}.$$

In other words, the actual density at any time is made up of the transient and the steady state.

This is worth doing because we know two things about the transient: its form at $t = 0$ and $t \to \infty$:

$$\begin{aligned}\phi_{\text{trans}}(x, t = 0) &= \phi(x, t = 0) - \phi_{\text{SS}}, \quad \text{and of course we know } \phi(x, t = 0) \\ \phi_{\text{trans}}(x, t \to \infty) &= 0.\end{aligned}$$

It is because ϕ_{trans} must go to zero as time goes to infinity that we call it transient (meaning, temporary).

Moreover, if we substitute $\phi(x,t) = \phi(x,t)_{\text{trans}} + \phi_{\text{SS}}$ into the diffusion equation we obtain just the same equation purely in terms of the transient (because the constant ϕ_{SS} is killed on both sides)

$$\frac{\partial \phi_{\text{trans}}}{\partial t} = D \frac{\partial^2 \phi_{\text{trans}}}{\partial x^2}.$$

So that's all fine, but how can we get any further? What we can do is limit ourselves to a *separable* solution for $\phi_{\text{trans}}(x,t)$. In other words we'll assume

$$\phi_{\text{trans}} = X(x)T(t)$$

where $X(x)$ depends only on x and $T(t)$ only depends on t. This is a **massive assumption**, and would seem to greatly limit us! But let's stick with it and see what we get.

Substituting into the diffusion equation we find

$$X(x)\frac{dT(t)}{dt} = D\frac{d^2X(x)}{dx^2}\,T(t)$$

where now we are deal with *ordinary* differential equations, not partials. And we can rearrange so that

$$\frac{1}{DT(t)}\frac{dT}{dt} = \frac{1}{X(x)}\frac{d^2X}{dx^2}.$$

Let's think about this equation for a bit. The left side depends *only* on t. The right side depends only *only* on x. And yet the expression must be true for all x and t. How can this be so? If we imagine the equation works for some particular values of x and t, and then change only one of the variable, x say, how can the equation remain true? The only solution is that both sides must be equal to a *constant* for all x and all t!

Let's call that constant $-k^2$, anticipating that this will give us the type of solutions (oscillatory in x, decaying in t) that we want.

$$\frac{1}{DT}\frac{dT}{dt} = \frac{1}{X}\frac{d^2X}{dx^2} = -k^2$$

Now we can solve for the two parts separately. Let's do the $T(t)$ part first. It's a well known equation:

$$\frac{d\,T(t)}{dt} = -k^2\ D\,T(t).$$

What function differentiates to just give the same function multiplied by a constant? The exponential function of course. We can quickly confirm that

$$T(t) = C\exp(-k^2\,D\,t)$$

solves the equation for any constant C.

Similarly, we can find the solution to the $X(x)$ part,

$$\frac{d^2X(x)}{dx^2} = -k^2X(x).$$

Again, we should recognise this one right away: sine and cosine have the property that differentiating them twice gives back the original function multiplied by a $(-1)\times(\text{real number})^2$. So we try

$$X(x) = A\cos(kx) + B\sin(kx)$$

and we see that this indeed works for any A and B.

So now we can say that separable solutions have the form:

$$\phi_{\text{trans}}(x,t) = X(x)T(t) = (A\cos(kx) + B\sin(kx))(C\exp(-k^2Dt)).$$

But we may as well omit the constant C since it can just be absorbed into the constants A and B:

$$\phi_{\text{trans}}(x,t) = X(x)T(t) = (A\cos(kx) + B\sin(kx))\exp(-k^2Dt).$$

What physical situations can this separable solution apply to? That's easy to answer, we just set $t = 0$ to see what kind of initial distributions we might have:

$$\begin{aligned}
\phi(x,t=0) &= \phi_{\text{trans}}(x,t=0) + \phi_{\text{SS}} \\
&= A\cos(kx) + B\sin(kx) + K. \\
&= F\,\sin(\theta + kx) + K
\end{aligned}$$

since ϕ_{SS} is just some constant, call it K. We got the last line by remembering that a combination of a sine and a cosine with the same frequency is just a shifted sine, so here constants F and θ replace A and B.

So: any initial condition where the density distribution varies sinusoidally will be OK... but that's a pretty special case! What are the odds that in real life we'll be thinking about an initial distribution which happens to have a sinusoidal variation? It seems that's not much use.

But we've got one more card to play. The diffusion equation is a **linear equation**, and that means that any combination of solutions is also a solution. Thus, while it's true that a separable solution must have the form,

$$\phi_{\text{trans}}(x,t) = X(x)T(t) = (A\cos(kx) + B\sin(kx))\exp(-k^2Dt) \tag{1.3}$$

we could add two different separable solutions and it *will still be* a solution! But it won't be separable anymore, if the two solutions we opt for have different k constants. Let's just confirm that: suppose we have two different constants k_1 and k_2, then

$$\begin{aligned}\phi_{\text{trans}}(x,t) &= (A_1\cos(k_1x) + B_1\sin(k_1x))\exp(-k_1^2Dt)\\ &\quad +(A_2\cos(k_2x) + B_2\sin(k_2x))\exp(-k_2^2Dt)\end{aligned}$$

is a valid solution too. We could verify this by substituting into the diffusion equation – but it must be true simply because the diffusion equation is linear.

However, we need not stop at adding two solutions. We can add any number of solutions together and still obtain a correct solution. So in fact we are free to go for anything of the form

$$\phi_{\text{trans}}(x,t) = \sum_n (A_n\cos(k_nx) + B_n\sin(k_nx))\exp(-k_n^2Dt).$$

What kind of initial conditions will this allow us to have? We need just set $t = 0$ to find out:

$$\begin{aligned}\phi(x,t=0) &= \phi_{\text{SS}} + \phi_{\text{trans}}(x,t=0)\\ &= K + \sum_n A_n\cos(k_nx) + B_n\sin(k_nx).\end{aligned}$$

Of course we recognise this: if we set $k_n = 2n\pi/L$ then this is just a Fourier series with period L. So: if we can describe the initial density distribution with a Fourier series, we can solve the diffusion equation!

This is a huge advance on just being able to have sinusoidally varying initial conditions. Recall that a Fourier series can describe any periodic function *or* any function that is only defined over a finite range (because then we can just make it periodic). But most diffusion problems are likely to have a finite range, such as the length of the cylinder that gas is diffusing into, or the thickness of a metal plate that separates hot and cold fluids. So, since we can now handle any initial distribution that can be described by a Fourier series, actually we can handle *most real problems*. (In the notes for next week, we will however think of the case of diffusion into an infinite space – that's the one situation that can't be solved by Fourier series.)

Before doing a couple of examples, it is interesting to pause at this point and have a think about that time decay term $\exp(-Dk^2t)$. Clearly this term is unity at $t = 0$ and it vanishes as $t \to \infty$. But how would we answer the question *"roughly how fast does the transient vanish"*. Well it only completely vanishes at infinite t, but that's not a very helpful answer.

If we write the term as $\exp(-\frac{t}{t_0})$ using a new constant $t_0 \equiv \frac{1}{Dk^2}$ then this constant provides a measure of how long it takes for the transient to fall to $1/e$ of its original magnitude, a kind of half-life in effect. If a second gas has D that is twice as large, say, then then t_0 will be halved. Also note that the value of our constant k *strongly* effects the rate of diffusion – looking again at our Fourier series for the initial distribution, what does this mean?

1.5 Diffusion example: Pipeline

Let's do a fancy version of the gas diffusion problem. Suppose that we have a long pipeline that is separated into many shorter pipes of equal length. Between the pipes are values that are initially closed. Now we'll assume that at time $t = 0$ the odd-numbered pipes contain gas at a high density ϕ_1 but the even-numbered pipes contain a lower density ϕ_2. Then at $t = 0$ all the valves are completely opened, effectively creating one long pipe (which however is still sealed at the ends). We want to find an equation for the gas density in the pipe at any time t and any place x.

First we'll want to sketch this:

So the initial distribution (which will be our boundary condition) is

$$\begin{aligned}
\phi(x,0) &= \phi_1 \quad \text{for} \quad 0 < x < a \\
\phi(x,0) &= \phi_2 \quad \text{for} \quad a < x < 2a \\
\phi(x,0) &= \phi(x+2a,0)
\end{aligned}$$

and the governing equation is

$$D\frac{\partial^2\phi}{\partial x^2} = \frac{\partial\phi}{\partial t}.$$

As before, we write the general solution for $\phi(x,t)$ as: a part that is the ultimate steady state PLUS a *transient* part that that, we know, eventually vanishes:

$$\phi(x,t) = \phi_{\text{SS}} + \phi_{\text{trans}}(x,t)$$

and since the pipeline is sealed at the far ends, no gas can enter or leave, so

$$\phi_{\text{SS}} = \frac{1}{2a}\int_0^{2a} \phi(x,t=0)dx = (\phi_1+\phi_2)/2.$$

Then for $\phi_{\text{trans}}(x,t) = \phi(x,t) - \phi_{\text{SS}}$ we can write

$$\begin{aligned}
\phi_{\text{trans}}(x,0) &= H \quad \text{for} \quad 0 < x < a \\
\phi_{\text{trans}}(x,0) &= -H \quad \text{for} \quad a < x < 2a \qquad \text{where} \quad H \equiv (\phi_1-\phi_2)/2 \\
\phi_{\text{trans}}(x,0) &= \phi(x+2a,0)
\end{aligned}$$

We know that we can handle any initial distribution that can be written as

$$\phi_{\text{trans}}(x,t=0) = \sum_n A_n\cos(k_nx) + B_n\sin(k_nx)$$

but we realise that we already know how to do this, since the $\phi_{\text{trans}}(x,t=0)$ here is simply the square wave, scaled to have height H and period $2a$. We found before that when a square wave has height 1 and period 2π then its Fourier series representation is

$$\frac{4}{\pi}\sum_{n=1,\ n\ odd}^{\infty}\frac{1}{n}\sin(n\,x)$$

so scaling we find

$$\phi_{\text{trans}}(x,t=0) = \frac{2(\phi_1-\phi_2)}{\pi}\sum_{\substack{n=1\\ n\text{ odd}}}^{\infty}\frac{1}{n}\sin\left(\frac{n\pi}{a}x\right).$$

Noticing that we are therefore choosing $k_n = n\pi/a$, we can immediately use Eqn. (1.3) to write down the form of $\phi_{\text{trans}}(x,t)$ for any time t as follows:

$$\phi_{\text{trans}}(x,t) = \frac{2(\phi_1 - \phi_2)}{\pi} \sum_{\substack{n=1 \\ n \text{ odd}}}^{\infty} \frac{1}{n} \sin\left(\frac{n\pi}{a} x\right) \exp\left(-D(\frac{n\pi}{a})^2 t\right).$$

We only need to add on the steady state, $\phi_{\text{SS}} = (\phi_1 - \phi_2)/2$, in order to have the total solution

$$\phi(x,t) = \frac{\phi_1 + \phi_2}{2} + \frac{2(\phi_1 - \phi_2)}{\pi} \sum_{\substack{n=1 \\ n \text{ odd}}}^{\infty} \frac{1}{n} \sin\left(\frac{n\pi}{a} x\right) \exp\left(-D(\frac{n\pi}{a})^2 t\right).$$

Notice that the higher frequency sine terms will decay more quickly. So what will the distribution of material look like as time increases?

Maths software exercise:
Setting $\phi_1 = 1$, $\phi_2 = 0$, $D = 1$ and $a = 20$, use matlab or similar software to confirm this solution and investigate the time evolution. For matlab the code can be,

```
f=0.5;
N=30;
syms x
t=4;
syms pi
for n=1:2:N
    A=2/(pi*n);
    f = f + A*sin(n*pi*x/20)*exp(-(n*pi/20)^2*t);
end
myPlot=fplot(f,[0,50]);
```

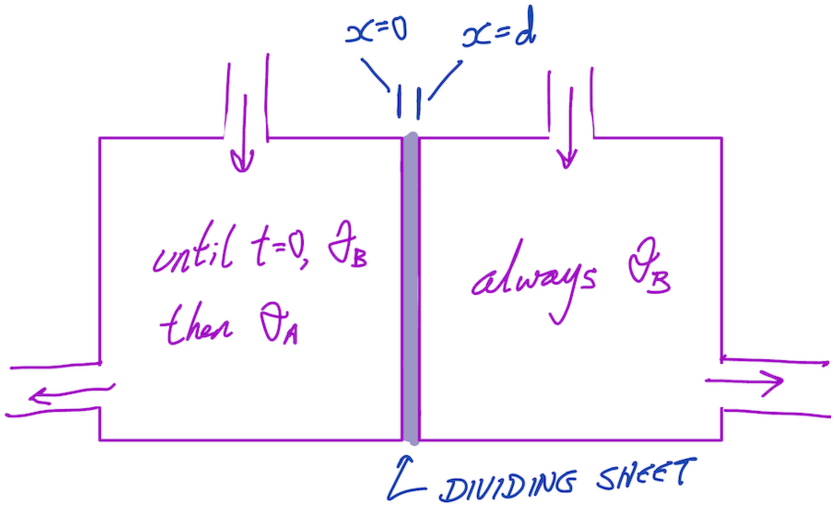
Final thought: Suppose that we had only two sections of pipe, one with initial high pressure ($0 \leq x \leq a$) and one with initial low pressure ($a \leq x \leq 2a$), and a value opens in between at $t = 0$. Then our initial condition $\phi(x,0)$ would be only defined between $0 \leq x \leq 2a$ so we would need to extend it to make it periodic. But it would be a bad choice to simply repeat the function by saying $\phi_(x,0) = \phi(x+2a,0)$ because then we would have an abrupt change at $x = 0$ and $x = 2a$. Instead we should use the following periodic function

$$\begin{aligned} \phi_{\text{trans}}(x,0) &= H \quad \text{for} \quad -a < x \leq a \\ \phi_{\text{trans}}(x,0) &= -H \quad \text{for} \quad a < x \leq 3a \quad \text{where} \quad H \equiv (\phi_1 - \phi_2)/2. \end{aligned}$$

Notice this function has period $4a$, and at the points $x = 0$ and $x = 2a$ nothing changes. Why is this a good choice?

1.6 Heat flow between reservoirs

The previous example took us through a lot of what we need to understand, but there are still three things we haven't tried out: a case where the diffusion is not inside a sealed space, a case where the initial condition isn't periodic, and a case of heat flow (rather than gas flow). Fortunately we can tackle all three at once with a suitable second example!



Consider a large metal tank that is completely divided into two isolated halves by a vertical internal insulating sheet of thickness d. Water at one temperature is continually pumped though the left chamber, while water at another temperature is continually pumped through the right chamber. The flow of water is fast, so that even though some heat flows between the two chambers through the insulating wall, it makes no appreciable difference to the temperatures inside the two chambers (the water is constantly replaced).

Until $t = 0$ the system has been operating with temperature θ_B in both chambers. Consequently, the metal in the dividing wall is also at this temperature. But at $t = 0$ suddenly the temperature in the left chamber drops to a new, colder fixed value θ_A. We can assume that the entire left side of the tank fills with this new cooler fluid instantaneously. We want to find the temperature within the metal wall as a function of time.

This is a problem involving *thermal reservoirs* i.e. regions that stay at the same temperature regardless of how much heat they supply or absorb. It's easy to imagine a thermal reservoir is so large, compared to other parameters in the problem, that it will not change perceptively (imagine the hot engine of a speedboat supplying heat to a lake). But in our case the temperature of the reservoirs is maintained because they are constantly replenished by some external source.

Now we are interested in the temperature as a function of x, where $x = 0$ is the left side of the dividing wall, and $x = d$ is the right side. Assume that the wall is so large in the $y - z$ plane that is it effectively infinite.

- At all times the right surface of the wall ($x = d$) is held at temperature θ_B, since it is in physical contact with water at that temp.
- All times $t \geq 0$ the left surface of our wall (defined by $x = 0$) is held at temperature θ_A as it is in physical contact with water at that temp.
- At $t = 0$, for $x > 0$ the material of the whole wall is at temperature θ_B.

The heat diffusion equation is the usual one, where we'll use α as the constant

$$\frac{\partial \Theta}{\partial t} = \alpha \frac{\partial^2 \Theta}{\partial x^2}.$$

Let's write those conditions compactly:

$$\begin{aligned} \Theta(x = 0, t) &= \theta_A \quad \text{for all } t \geq 0 \\ \Theta(x = d, t) &= \theta_B \quad \text{for all } t \geq 0 \\ \Theta(x, t = 0) &= \theta_B \quad \text{for } 0 < x \leq d \end{aligned}$$

Notice we've been careful to use $0 < x$ in the third condition to avoid conflicting with the first one! We can sketch a graph of $\Theta(x, t = 0)$ as defined by the boundary conditions. We note the abrupt jump at $x = 0$.

Let's work out the ultimate steady state $\Theta_{\rm SS}(x) \equiv \Theta(x, t \to \infty)$, i.e. the temperature variation with x in the long time limit. We know that in the long time limit, we will have reached a steady state where the temperature is not changing with time (even though heat will still be flowing). So then

$$\frac{\partial \Theta}{\partial t} = 0 \qquad \text{therefore} \qquad \frac{\partial^2 \Theta}{\partial x^2} = 0,$$

in other words, the gradient of our temperature function $\Theta_{\rm SS}(x)$ with respect to x must be constant.

$$\Theta_{\rm SS}(x) = Ax + B$$

but $\Theta_{\rm SS}(0) = \theta_A$ and $\Theta_{\rm SS}(d) = \theta_B$ and so

$$\Theta_{\rm SS}(x) = \theta_A + \frac{\theta_B - \theta_A}{d} x.$$

Let's add this to the figure:

Even though this steady state function is more complex than in the previous example (since it isn't a constant), still we see that when we apply the diffusion equation

$$\frac{\partial \Theta}{\partial t} = \alpha \frac{\partial^2 \Theta}{\partial x^2}$$

to the sum of the steady state and transient parts

$$\Theta(x, t) = \Theta_{\rm SS}(x) + \Theta_{\rm trans}(x, t)$$

we will find that the differentials 'kill' the steady state on both sides, so as usual we just have the differential equation for the transient

$$\frac{\partial \Theta_{\rm trans}(x, t)}{\partial t} = \alpha \frac{\partial^2 \Theta_{\rm trans}(x, t)}{\partial x^2}.$$

But we already know the form that the solution to this can take, i.e.

$$\Theta_{\text{trans}}(x,t) = \sum_n (A_n \cos(k_n x) + B_n \sin(k_n x)) \exp(-k_n^2 \alpha t). \tag{1.4}$$

So the challenge, as before, is to set $t = 0$ and match the initial transient. Now since $\Theta_{\text{trans}}(x,t) = \Theta(x,t) - \Theta_{\text{SS}}(x)$ we can see that

$$\begin{aligned}
\Theta_{\text{trans}}(x, t=0) &= 0 && \text{for } x = 0 \text{ and } x = d \\
\Theta_{\text{trans}}(x, t=0) &= (\theta_B - \theta_A)\left(1 - \frac{x}{d}\right) && \text{for } 0 < x \leq d
\end{aligned}$$

To get a Fourier series for this function we will need to extend it beyond the limits where its defined, thus making it a periodic function. How should we extend? Let's try the rule that

$$\Theta_{\text{trans}}(x,0) = \Theta_{\text{trans}}(x+d,0).$$

Sketch what this periodic function looks like

This has a hidden problem: the Fourier series would have a constant term (how can we see this must be so?) which we can think of as $C\cos(0x)$. But then if we use our rule Eqn. (1.4) for making that term into a solution to the diffusion equation, we see we have $k = 0$ and thus the function of time we multiply by is $\exp(0t) = 1$. But then it would never vanish – and we need our transient to vanish! Therefore we try the next most simple extension:

We can write this as

$$\begin{aligned}
\Theta_{\text{trans}}(x,0) &= 0 && \text{for } x = 0 \text{ and } x = 2d \\
\Theta_{\text{trans}}(x,0) &= (\theta_B - \theta_A)\left(1 - \frac{x}{d}\right) && \text{for } 0 < x < 2d \\
\Theta_{\text{trans}}(x+2d,0) &= \Theta_{\text{trans}}(x,0)
\end{aligned}$$

Now here the Fourier series will *not* have a constant term (why?). Any function with this shape is called a 'saw tooth' and it's easy to derive the Fourier series. For the basic saw tooth $f(x)$ with period 2π and limits of $f(0) = +1$ at $f(2\pi) = -1$, the solutions is as follows (the derivation is an exercise for the reader)

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

Then we need only scale its amplitude and period to match our function (which has period $2d$), so our solution is

$$\Theta_{\text{trans}}(x, t=0) = \frac{2(\theta_B - \theta_A)}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\sin(\frac{n\pi}{d}x).$$

Noting that we have set $k_n = \frac{n\pi}{d}$ we can now put back the exponential terms for the general, $t > 0$ case by using Eqn. (1.3):

$$\Theta_{\text{trans}}(x,t) = \frac{2(\theta_B - \theta_A)}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\sin(\frac{n\pi}{d}x)\exp\left(-\alpha(\frac{n\pi}{d})^2 t\right).$$

Our full solution is thus obtained just by adding in $\Theta_{\text{SS}}(x)$:

$$\Theta(x,t) = \theta_A + \frac{\theta_B - \theta_A}{d}x + \Theta_{\text{trans}}(x,t).$$

We can write it all out as:

$$\Theta(x,t) = \theta_A + (\theta_B - \theta_A)\left(\frac{x}{d} + \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\sin(\frac{n\pi}{d}x)\exp\left(-\alpha(\frac{n\pi}{d})^2 t\right)\right).$$

Does this match the guess we made earlier for how Θ would vary with time?

Maths software exercise:
Setting $d = 1$ and $\alpha = 1$, and use matlab or similar software to confirm this solution and investigate the time evolution. The matlab code given in the previous blue box can be modified for this present case.

1.7 Summary: Tackling Diffusion Problems with Fourier Series

Check you understand what the basic quantity you are modelling is - e.g. the temperature, the concentration of "Substance S" or whatever. In the following steps I'll suppose that the quantity is temperature $\Theta(x,t)$.

Write the out the boundary conditions, including the initial condition, imposed on $\Theta(x,t)$. Sketch it.

Now write $\Theta(x,t) = \Theta_{\mathrm{SS}}(x) + \Theta_{\mathrm{trans}}(x,t)$. Here $\Theta_{\mathrm{SS}}(x)$ is the steady-state part and $\Theta_{\mathrm{trans}}(x,t)$ is the transient part.

Work out the steady state-part: it is either just a constant, or depends linearly on x. So generally $\Theta_{\mathrm{SS}}(x) = A + Bx$. It can't be more complicated since

$$\frac{\partial \Theta_{\mathrm{SS}}}{\partial t} = 0$$

(i.e. it doesn't depend on time of since it is the steady-state!) and therefore

$$\frac{\partial^2 \Theta_{\mathrm{SS}}}{\partial x^2} = 0.$$

In a problem with a fixed amount of heat energy (or a fixed amount of diffusing material) it will just be a constant equal to initial distribution averaged out. In a problem where there is *flow* of heat (or matter) in the steady-state, the x term will be there. Think about boundary conditions to get A and B.

Now tackle the transient term $\Theta_{\mathrm{trans}}(x,t)$.

(a) By putting the whole function $\Theta(x,t) = \Theta_{\mathrm{SS}}(x) + \Theta_{\mathrm{trans}}(x,t)$ into the governing diffusion equation, show that the equation only really involves the transient part.

$$\frac{\partial \Theta}{\partial t} = \alpha \frac{\partial^2 \Theta}{\partial x^2} \quad \Rightarrow \quad \frac{\partial \Theta_{\mathrm{trans}}}{\partial t} = \alpha \frac{\partial^2 \Theta_{\mathrm{trans}}}{\partial x^2}$$

(b) By assuming a *separable* form $\Theta_{\text{trans}} = X(x)T(t)$ show that a solution is $\Theta_{\text{trans}} = (A\cos(kx) + B\sin(kx))\exp(-k^2\alpha t)$ for any A, B, k.

(c) Now write down the form the transient $\Theta_{\text{trans}}(x,t)$ must have at $t = 0$, using the boundary conditions you were given and remembering that the transient is the difference between the steady-state and the actual distribution. Then use Fourier series techniques to find the particular sum of sine and/or cosine terms that can make your $t = 0$ transient function.

This works if either the original situation is periodic (like our pipeline example) or if it is involves a fixed region $0 \le x \le d$ in which case we can (carefully!) extend it into a periodic function.

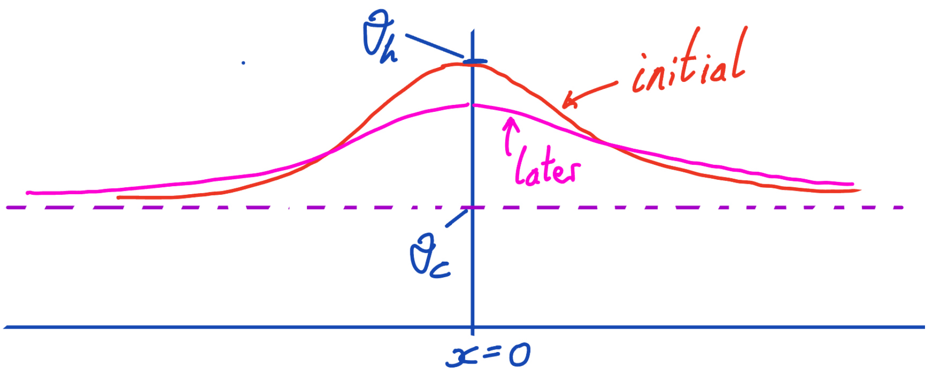
(d) Finally write out the solution as the steady-state part plus that Fourier series, remembering that for time $t > 0$ each of those Fourier terms has its own $\exp(-k^2\alpha t)$ multiplier.

Appendix: Solving using a good guess!

Suppose I have a very long metal bar (call it infinitely long), and initially the whole bar is at some cold temperature Θ_c. But I heat a specific region in the middle with a blow torch for a while, which raises the temperature in the middle of that region to Θ_h. At the moment the torch is turned off, the initial temperature distribution is a Gaussian centred on $x = 0$.

$$\text{Initially:} \quad \Theta(x) = \Theta_c + \Delta_{\text{init}} \exp\left(-\frac{x^2}{L_{\text{init}}^2}\right) \quad \text{for all} \quad -\infty < x < \infty$$

Here Δ_{init} is a constant and we can see by putting in $x = 0$ that we want $\Delta_{\text{init}} = \Theta_h - \Theta_c$. This is actually pretty simple! Let's sketch it. Notice how the hot zone doesn't have sharp end points, but the width is roughly characterised by the value of L_{init}.



Now a sneaky trick: it will turn out that it's helpful to allow our start time, the time our stopwatch is showing at instant the blow torch is turned off, to be a certain non-zero number. For now we'll call it t_{init}. We could insist on defining the first instant as $t = 0$ but then we'd end up having a less neat solution, so we'll permit this non-zero start time since we don't really care how it's labelled.

So how would we *guess* that this heat distribution will evolve as the clock runs forward, $t > t_{\text{init}}$? We'll assume that no heat can escape the bar, it just flows along the bar. We might speculate that perhaps, as time passes the temperature distribution will just get *wider* but with a *lower maximum*. See the sketch of a possible later time curve on the graph above. So our idea is that the temperature distribution is *always* Gaussian, but with a width that is a function of time.

$$\text{We are guessing that:} \quad \Theta(x,t) = \Theta_c + \Delta(t)\ \exp\left(-\frac{x^2}{L(t)^2}\right)$$

Notice that now, both Δ and L have become functions of time. At our start time $t = t_{\text{init}}$ they are just equal to our constants Δ_{init} and L_{init} above. Before we try this on the Heat Equation, we can see how we should relate $L(t)$ and $\Delta(t)$ by using conservation of heat: The total heat energy in the bar (after the blow torch is off!) is conserved. So at *any* time $t \geq t_{\text{init}}$

$$\int_{-\infty}^{\infty} C\ \Theta(x,t)\,dx = (\text{some constant})$$

Here C is just the heat capacity of our bar (per unit length); we don't need to know it. By sketching a couple of Gaussians with different L and Δ we can quickly see that, if the integral is going to be independent of t then we will need $\Delta(t) \propto 1/L(t)$, i.e. "as the distribution gets wider, we will need the max temp to get lower, to maintain the area under the curve". So then our guess becomes

$$\Theta(x,t) = \Theta_c + \frac{K}{L(t)}\ \exp\left(\frac{-x^2}{L(t)^2}\right)$$

where $K = \Delta_{\text{init}}\,L_{\text{init}}$. Finally, we'll just have to put this into the Heat Equation (1.1) and ask "What function $L(t)$, if any, can make this work?". The differentials will remove the Θ_c constant, and K factors will cancel, so

$$\frac{\partial}{\partial t}\Big(\frac{1}{L(t)}\ \exp\left(-x^2/L(t)^2\right)\Big) = \alpha\frac{\partial^2}{\partial x^2}\Big(\frac{1}{L(t)}\ \exp\left(-x^2/L(t)^2\right)\Big)$$

Performing the partial differentials and simplifying, we will find

$$-L'(t)\ \exp\left(x^2/L(t)^2\right) = \frac{-2\alpha}{L(t)}\ \exp\left(x^2/L(t)^2\right)$$

So this works if $L'(t) = \dfrac{2\alpha}{L(t)}$ which is solved by $L(t) = 2\sqrt{\alpha t}$.

Here's where it helps that we were willing to be flexible about the clock time that we assigned to the moment the torch is turned off; we've been writing it as t_{init} and we now see that we should use

$$t_{\text{init}} = L_{\text{init}}^2/(4\alpha) \quad \text{so as to ensure that} \quad L(t_{\text{init}}) = L_{\text{init}}$$

So then this proves our intuition was correct. And we've found that the Gaussian spreads out such that its width increases with the square root of time: so it spreads more and more slowly, which makes sense as the temperature gradient is less and less dramatic. Our overall solution is

$$\Theta(x,t) = \Theta_c + \frac{\big(\Theta_h - \Theta_c\big)\,L_{\text{init}}}{2\sqrt{\alpha t}}\ \exp\left(-\frac{x^2}{4\alpha t}\right)$$

which is pretty complicated looking, and that's only if we are willing to set the initial clock time as $t_{\text{init}} = L_{\text{init}}^2/(4\alpha)$. If we insist on using $t = 0$ as the first instant of the story, then we'd have to rewrite this solution by replacing t with $t + L_{\text{init}}^2/(4\alpha)$ making it far worse!

Here's a nice observation: In solving the case above, we have actually solved a quite different scenario as well. Suppose that I heat one end of a bar that starts at $x = 0$ and goes off to infinity in the positive x direction. If the initial heat distribution is

$$\Theta(x) = \Theta_c + \Delta_{\text{init}} \exp\left(-\frac{x^2}{L_{\text{init}}^2}\right) \qquad \text{for all} \quad x > 0$$

then the solution is the same as the one above (just with the $x \geq 0$ constraint). The reason is the powerful principle of symmetry. Have a think about it! It may help to sketch.