

Sample Solution of the Diffusion Equation: Equilibrating Bar

In the next few sections we'll discuss some solutions of the diffusion equation. The first thing to notice is that it's a linear, homogeneous equation. This means that any solution can be multiplied by a constant and this yields another solution. Also, the sum of any two solutions is a solution.

In general, the solution must be determined in conjunction with the *boundary conditions*: specifications of the desired solution at a given time from which the solution can be integrated forward (it's a first time derivative). It is often a good idea to expand the solution as a sum of simple solutions such as plane waves. The plane waves can be evaluated at $t = 0$ and adjusted to fit the boundary conditions. Then the diffusion equation is used to determine the time dependence of each wave.

As an example, suppose we have a bar which has been used to conduct heat between a hot reservoir and a cold reservoir. If the bar has come to a steady state, and if it has a uniform cross section, there will be a linear temperature gradient along the bar. Suppose the reservoirs are removed and the bar is isolated from the rest of the world. What happens? Heat flows from the hot end of the bar to the cold end until the bar reaches a uniform temperature distribution. What happens in detail? To answer that, we have to solve the diffusion equation with the initial condition that there is a uniform temperature gradient in the bar.

We let x , $0 < x < L$, represent the coordinate along the bar, with L being the length of the bar. At $t = 0$, when the reservoirs are removed, we can take the temperature in the bar to be

$$\tau(x, 0) = \frac{1}{2}\Delta\tau(1 - 2x/L),$$

where $\Delta\tau$ is the temperature difference from one end to the next. This makes the mean temperature 0. Actually, we can add a constant to this temperature without affecting the problem, so the mean temperature can be the mean temperature of the two reservoirs. Since this is a one-dimensional problem, $\nabla^2 = d^2/dx^2$ and we have $\nabla^2\tau = 0$ which says $d\tau/dt = 0$ which says that the bar just sits there with the linear temperature gradient. We know this can't be right, but where did we go wrong? In fact, it's right when the bar is between the two reservoirs and a steady state has been reached. But in this situation, heat is entering the bar at the hot end and leaving the bar at the cold end. Once we remove the bar from the reservoirs, we need to look for solutions with $J_x(x = 0) = 0$ and $J_x(x = L) = 0$. Since $\mathbf{J} \propto \nabla\tau$, we need solutions with $d\tau/dx = 0$ at the ends of the bar. Our boundary conditions are that at $t = 0$ the bar has a linear temperature gradient as above, and for all time $t > 0$, $d\tau/dx = 0$ at the ends of the bar.

These may seem like incompatible conditions. The problem is the abrupt change of slope at the ends of the bar. We will see that what happens in our solution is that the heat flow in the bar when it's removed from the reservoirs causes an "infinitely" fast flattening

of the slope at the ends so there is no heat flow into or out of the ends. (In real life, it's not possible to remove the bar from the reservoir abruptly, so it's not necessary to have this infinitely fast change!)

Suppose we consider a solution of the form $\sin(kx)f(t)$, where k is a constant (the wave number) and $f(t)$ is a yet to be determined function of time. If we plug this into the diffusion equation, we have

$$-k^2 \sin(kx)f(t) - \frac{1}{D} \sin(kx) \frac{\partial f(t)}{\partial t} = 0,$$

which has the solution for $f(t)$,

$$f(t) = f_0 e^{-Dk^2 t}.$$

Similarly,

$$\tau(x, t) = \cos(kx) e^{-Dk^2 t},$$

is also a solution of the diffusion equation. An arbitrary sum of these solutions is also a solution. So, our plan is to evaluate the solutions at $t = 0$, find a sum which matches the boundary conditions, and then add the time dependence to the sum to get the solution for times greater than $t > 0$. The solutions above don't necessarily satisfy the boundary condition having to do with the gradient of τ at the ends of the bar. In particular, we can't use the $\sin(kx)$ functions at all, because they give $d\tau/dx \propto \cos(kx)$ which is non-zero at $x = 0$. So we can only use the $\cos(kx)$ functions which automatically satisfy the boundary condition at $x = 0$. At $x = L$, we have $d\tau/dx \propto \sin(kL)$. This will be zero if $kL = n\pi$ where n is an integer.

So, our general solution which satisfies the boundary conditions at the ends of the bar is

$$\tau(x, t) = \sum_{n=1}^{\infty} A_n \cos(k_n x) e^{-Dk_n^2 t}, \quad k_n = \frac{n\pi}{L},$$

where A_n are constants to be adjusted to make the solution have the correct linear dependence at $t = 0$. In other words, we are writing the linear temperature gradient as a Fourier series. To determine the coefficients A_n , we multiply by $\cos(k_m x)$ and integrate from 0 to L . We get 0 for $n \neq m$. For $n = m$, we have

$$\int_0^L A_m \cos(k_m x) \cos(k_m x) dx = A_m L/2.$$

We do the same thing with the desired linear dependence. Note that when n is even the cosine functions are symmetric about the center of the bar. The temperature gradient is

odd about the center of the bar, so there will be no even terms in the sum. For the odd terms, the coefficients are

$$\begin{aligned}
 A_n L/2 &= \int_0^L \frac{1}{2} \Delta\tau (1 - 2x/L) \cos(n\pi x/L) dx, \\
 &= \frac{\Delta\tau L}{2n\pi} (1 - 2x/L) \sin(n\pi x/L) \Big|_0^L + \frac{\Delta\tau L}{2n\pi} \frac{2}{L} \int_0^L \sin(n\pi x/L) dx, \\
 &= 0 - 0 - \frac{\Delta\tau L}{n^2\pi^2} \cos(n\pi x/L) \Big|_0^L, \\
 &= \frac{2\Delta\tau L}{n^2\pi^2}, \quad \text{remember } n \text{ is odd}
 \end{aligned}$$

Which gives

$$A_n = \frac{4\Delta\tau}{n^2\pi^2},$$

and our solution for $t > 0$ is

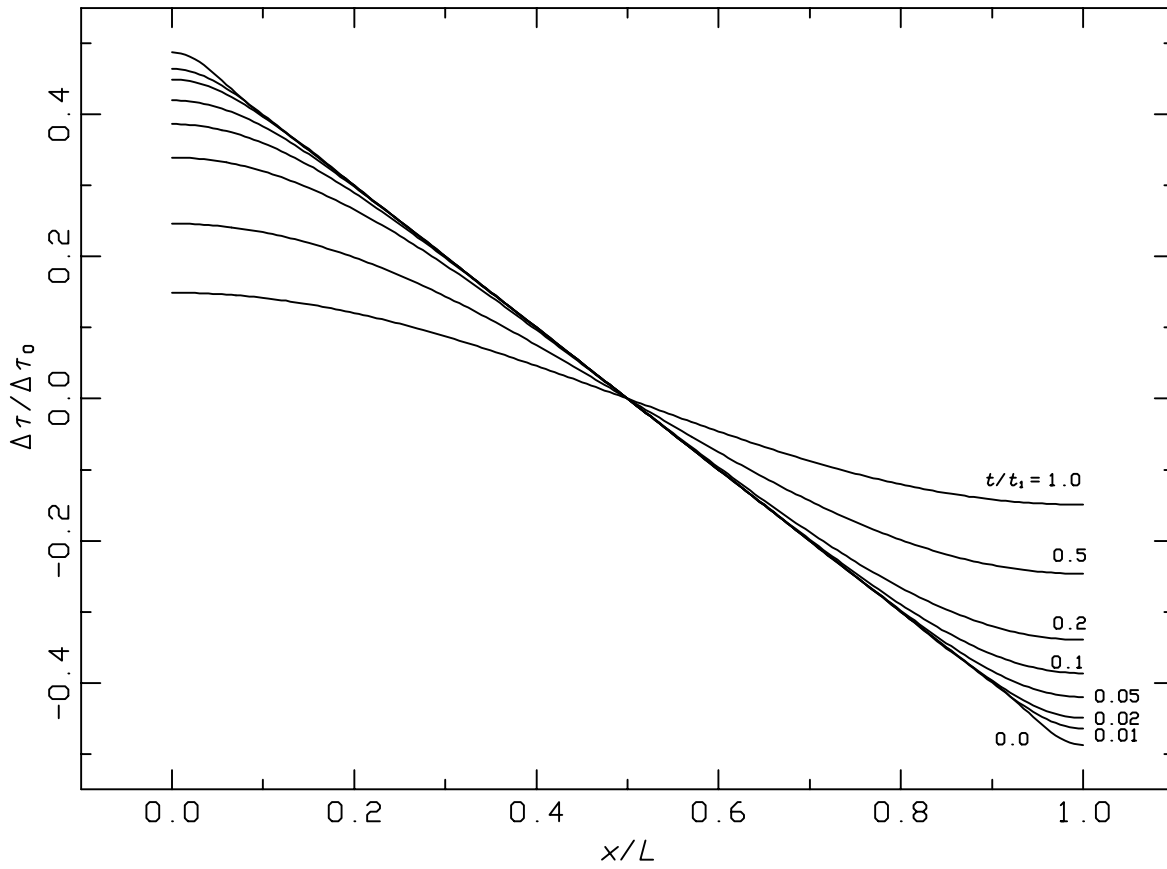
$$\tau(x, t) = \sum_{n=1,3,5,\dots} \frac{4\Delta\tau}{n^2\pi^2} \cos(k_n x) e^{-Dk_n^2 t}, \quad k_n = \frac{n\pi}{L}.$$

Some comments are in order. Each mode decays like $\exp(-t/t_n)$ where the decay time is

$$t_n = \frac{L^2}{Dn^2\pi^2},$$

so short wavelength (large k_n) modes decay very fast compared to the $n = 1$ mode. The decay time is inversely proportional to the **square** of the wavenumber. It is the very short wavelengths that are necessary to produce the discontinuity in slope at the ends of the bar. The discontinuity decays very rapidly (infinitely rapidly if we go all the way to $n = \infty!$).

The figure shows the temperature as a function of position in the bar for several



times including $t = 0$, and $t = (0.01, 0.02, 0.05, 0.1, 0.2, 0.5, 1)t_1$ where $t_1 = L^2/D\pi^2$ is the decay time of the longest mode. The plotted functions include the Fourier terms $n = 1, 3, 5, 7, 9, 11, 13, 15$. The function for $t = 0$ has some small wiggles at the ends. This is because it's missing the high frequency ($n > 15$) components. By the time the $n = 1$ component has experienced one decay time, the next slowest decaying term, $n = 3$, has experienced 9 decay times. In other words the temperature profile becomes indistinguishable from a half cycle of a cosine very quickly!

The Dispersion Relation

When considering the diffusion equation, we found that an expansion in cosine components was quite useful. One might also ask under what conditions is a plane wave a solution of the diffusion equation? Suppose

$$\tau(\mathbf{r}, t) = \tau_0 e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)} .$$

Plug into the diffusion equation and get

$$-k^2 \tau_0 e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)} + \frac{i\omega}{D} \tau_0 e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)} = 0 ,$$

or

$$Dk^2 = i\omega .$$

A relation between k and ω is called a *dispersion relation*. This comes from the fact that if k and ω are not proportional then a wave pulse disperses (or spreads out).

In the example of the equilibrating bar, the spatial parts of the solutions are composed of pure oscillations. This means k is real and k^2 is positive. The dispersion relation tells us that ω is pure imaginary,

$$\omega = -iDk^2 .$$

When plugged back into the plane wave solution, the negative i in ω times the negative i in the plane wave exponent gives -1 , so we get an exponential decay in time.

We'll consider some other consequences of the dispersion relation later.

Random Walks and Diffusion

A simple one-dimensional *random walk* consists of N steps. Each step is of length ℓ but may be to the left or right. The probability for either direction is the same, $1/2$. The question is, after N steps, how far from the origin (where you started) have you randomly walked? The probability of n steps to the right and $(N - n)$ steps to the left is just the binomial distribution (see lecture 3)

$$P(n) = \binom{N}{n} \frac{1}{2^N} .$$

The distance from the origin is the number of positive steps minus the number of negative steps times the length per step

$$d = [n - (N - n)]\ell = (2n - N)\ell .$$

The average distance is 0. What's the root mean square distance?

$$\sqrt{\langle d^2 \rangle} = \sqrt{4\langle (n - N/2)^2 \rangle \ell^2} = \sqrt{4(Np(1-p))\ell^2} = \ell\sqrt{N} .$$

In other words, the mean position is still the origin, but the spread around the mean position grows as the square root of the number of steps. Now suppose each step is accomplished at speed \bar{c} . Since each step is of length ℓ , the time per step is ℓ/\bar{c} . If the random walk lasts for time t , the number of steps is $N = t/(\ell/\bar{c}) = t\bar{c}/\ell$ and

$$\sqrt{\langle d^2 \rangle} = \sqrt{t\bar{c}\ell} .$$

Notice that what's multiplying t inside the square root is basically the diffusivity! So, our simple random walk satisfies

$$\langle d^2 \rangle = Dt ,$$

The variance in position is proportional to the time and the proportionality constant is D .

What does this have to do with transport and the diffusion equation, you ask? Recall, our picture for transport is that a molecule travels (on the average) at speed \bar{c} for about one mean free path ℓ . At that point (on the average), it has a randomizing collision and goes off in a random direction. This is three dimensional, but other than that it's the random walk we've been discussing.

Let's consider again the example of the equilibrating bar. This time, we'll think of it as energy that must randomly walk until equilibrium is achieved. That is, until the energy is sufficiently spread out (sufficiently large variance) that it appears uniform on the scale of interest. Consider a mode with wave number $k_n = n\pi/L$. The characteristic distance for this mode is k_n^{-1} . Our random walk model says that the energy will random walk to this rms distance in time t_n given by

$$t_n = \frac{1}{D} d_n^2 = \frac{L^2}{Dn^2\pi^2} ,$$

and sure enough, t_n is the decay time for mode n . This is a characteristic property of diffusion processes and random walks: doubling the length scale quadruples the time scale.

Sample Solution: A Temperature Oscillation

Suppose we consider a slab of material which has a boundary at $x = 0$. The material extends to $x > 0$. We suppose everything is uniform in the y and z directions. Suppose that the $x = 0$ boundary is forced (by some external agent) to undergo a sinusoidal temperature oscillation,

$$\tau(0, t) = \tau_0 \operatorname{Re} \left(e^{-i\omega t} \right) .$$

Since the diffusion equation is linear, the real part of a complex solution is a solution, so we'll usually drop the indication that we're considering the real part and take it to be implied.

We want to know the temperature distribution, $\tau(x, t)$ in the slab. We'll have a plane wave propagating in the x direction. The wave number is determined by the dispersion relation,

$$k^2 = \frac{i\omega}{D} .$$

We can take the square root,

$$k = \pm \sqrt{i} \sqrt{\frac{\omega}{D}} = \pm \sqrt{\frac{\omega}{2D}} (1 + i) = \pm k_1 (1 + i) ,$$

where $k_1 = \sqrt{\omega/2D}$ is a handy abbreviation. So the solution is

$$\tau(x, t) = \tau_0 e^{\pm ik_1 x \mp k_1 x - i\omega t} = \tau_0 \left(e^{\mp k_1 x} \right) \left(e^{\pm ik_1 x - i\omega t} \right) .$$

So the solution is a plane wave (the last factor above) times an exponential decay (or growth) in the x -direction (the middle factor above).

The exponential growth of the wave into the material is unphysical, and we must take the upper sign to be sure the wave decays as we go into the slab. We have a wave, but it is damped with a damping length comparable to its wavelength. This means that the wave “doesn't get very far” (in terms of wavelengths). K&K give some numerical examples showing that not much dirt is needed to insulate underground pipes from the day-night cycle or the summer-winter cycle!

The Diffusion of a One Dimensional Bump

When we looked at a one dimensional random walk, we found that the variance in position grows in proportion to the time. We've also argued that microscopically, diffusion is just a random walk. So, we might expect that if we start with an excess of energy concentrated at $x = 0$, it will diffuse away from the origin in such a way that the mean position of the energy remains at the origin, but the variance of the location of the energy grows with time. Furthermore, since the macroscopic energy distribution is determined by many small events, we might expect the distribution to be Gaussian. So, we guess that the one-dimensional temperature distribution

$$\tau(x, t) = \frac{1}{\sqrt{2\pi at}} e^{-\frac{x^2}{2at}},$$

might be a solution of the diffusion equation. Here, a is a constant that must have the same dimensions as a diffusion constant. This distribution is a Gaussian, centered at 0, with variance at . To find out if this is a solution, we must plug into the diffusion equation for the temperature. We find

$$\begin{aligned} \frac{\partial^2 \tau}{\partial x^2} &= \frac{1}{\sqrt{2\pi at}} e^{-x^2/2at} \left[-\frac{1}{at} + \frac{x^2}{a^2 t^2} \right], \\ \frac{\partial \tau}{\partial t} &= \frac{1}{\sqrt{2\pi at}} e^{-x^2/2at} \left[-\frac{1}{2t} + \frac{x^2}{2at^2} \right], \end{aligned}$$

The one-dimensional diffusion equation for the temperature is

$$\frac{\partial^2 \tau}{\partial x^2} - \frac{1}{D} \frac{\partial \tau}{\partial t} = 0,$$

which is solved by our distribution provided $a = 2D$.

This result reinforces the interpretation of diffusion as a random walk. It also has another application. The solution we've just constructed has the following interesting properties. First of all,

$$\int_{-\infty}^{+\infty} \tau(x, t) dx = 1.$$

In other words, the solution is normalized to unit "total temperature" for all $t > 0$. As $t \rightarrow 0$, the distribution gets infinitely narrow and infinitely high—but it still integrates to 1. Therefore if $g(x)$ is any reasonably well behaved function, it must be that

$$\lim_{t \rightarrow 0} \int_{-\infty}^{+\infty} g(x) \tau(x, t) dx \rightarrow g(0) \lim_{t \rightarrow 0} \int_{-\infty}^{+\infty} \tau(x, t) dx \rightarrow g(0).$$

If you know about δ -functions, what we've just shown is that as $t \rightarrow 0$, our temperature distribution behaves like $\delta(x)$. We can shift the origin to x' simply by subtracting x' in the argument of the exponential. We can shift the origin of time to t' by subtracting t' from t in both places where t occurs. We can also call this function $G(x, x', t, t')$ rather than $\tau(x, t)$. Now we have

$$G(x, x', t, t') = \frac{1}{\sqrt{4\pi D(t-t')}} e^{-\frac{(x-x')^2}{4D(t-t')}}.$$

This is a solution to the thermal diffusion equation in x and $t > t'$ and it corresponds to a "point source" of unit temperature at $x = x'$ and $t = t'$. The point source diffuses away from where it starts as time goes on.

Now suppose that at t' we have an arbitrary distribution of temperature $\tau(x, t')$. Note that

$$\tau(x, t) = \lim_{t \rightarrow t'} \int_{-\infty}^{+\infty} \tau(x', t') G(x, x', t, t') dx'.$$

In other words, if we multiply our temperature distribution by G , integrate over x' and take the limit $t \rightarrow t'$, we get back the temperature distribution we put in. What we've done is to treat the temperature distribution at t' as an infinite number of point sources located at x' . The strength of each point source is $\tau(x', t') dx'$. Remember, the diffusion equation is linear and homogeneous so any sum of solutions is a solution. We know how a point source diffuses; the diffusion of a sum of point sources is just the sum of the diffusion of the individual point sources. In other words, if the temperature distribution at time t' is $\tau(x, t')$, the distribution at a later time t is

$$\tau(x, t) = \int_{-\infty}^{+\infty} \tau(x', t') G(x, x', t, t') dx'.$$

If you look at what's going on, you see that we are convolving the original temperature distribution with the Gaussian G to get the later temperature distribution. Convolving with a Gaussian is a smoothing operation. In fact, it's often called a low pass filter. As time goes on, the filter gets wider in proportion to the square root of the time.

Interesting point: suppose you have a temperature distribution at time t_1 . To propagate the temperature distribution to time t_2 , you can use $G(x, x', t_2, t_1)$. To propagate from t_1 to $t_3 > t_2$ you can use $G(x, x', t_3, t_1)$. OR, you can propagate to t_2 and then regard the temperature distribution at t_2 as the initial distribution and propagate that to t_3 with

$G(x, x', t_3, t_2)$. In other words

$$\begin{aligned}\tau(x, t_3) &= \int_{-\infty}^{+\infty} \tau(x', t_1) G(x, x', t_3, t_1) dx' , \\ &= \int_{-\infty}^{+\infty} \tau(x', t_2) G(x, x', t_3, t_2) dx' , \\ &= \int_{-\infty}^{+\infty} \left[\int_{-\infty}^{+\infty} \tau(x'', t_1) G(x', x'', t_2, t_1) dx'' \right] G(x, x', t_3, t_2) dx' , \\ &= \int_{-\infty}^{+\infty} \tau(x'', t_1) \left[\int_{-\infty}^{+\infty} G(x, x', t_3, t_2) G(x', x'', t_2, t_1) dx' \right] dx'' .\end{aligned}$$

Or,

$$G(x, x'', t_3, t_1) = \int_{-\infty}^{+\infty} G(x, x', t_3, t_2) G(x', x'', t_2, t_1) dx' .$$

To get the filter for time $t_1 \rightarrow t_3$, we convolve (or filter) the filter for $t_1 \rightarrow t_2$ with the filter for $t_2 \rightarrow t_3$. A mathematical property of Gaussians is that when Gaussians are convolved, the variances add. This is just what we need for diffusion as the variance is proportional to the time.

Mathematical note: $G(x, x', t, t')$ is called a Green's function. It is the response of the system at x, t to a unit point source located at x', t' . You've used Green's functions before, you just didn't know it. For example, a unit point charge located at \mathbf{r}' produces an electric potential at \mathbf{r}

$$G(\mathbf{r}, \mathbf{r}') = \frac{1}{|\mathbf{r} - \mathbf{r}'|} .$$

Then to find the electric potential from a distribution of charge, you convolve the charge distribution with the Green's function

$$\Phi(\mathbf{r}) = \int \rho(\mathbf{r}') G(\mathbf{r}, \mathbf{r}') d^3\mathbf{r}' = \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3\mathbf{r}' .$$

There's no time dependence in this electrostatics problem, but the basic idea of convolution and a Green's function is the same.

Mathematical note 2: We've worked out the one dimensional Green's function for the diffusion problem. In K&K chapter 15, problem 2, the two and three dimensional pulse response functions are worked out.

Mathematical note 3: The Green's function depends on the geometry of the system. We've assumed a one-dimension system that's infinite in both directions. Temperature (or internal energy) can diffuse away to infinity. If we had a finite medium which did not permit heat flow past its boundaries, the Green's function would be different. If we had a non-uniform medium, the Green's function would be different, etc.

Mathematical note 4: Given a uniform, one-dimensional, infinite medium. we've completely "solved" the initial value problem. Given the temperature distribution at one time, we can find it at all later times just by doing an integral. (Well, actually an integral for each point and time!)

Physics(!) note: The key idea is that in the absence of heat sources, sinks, or reservoirs, etc., temperature non-uniformities just diffuse away with time. Any non-uniformity spreads to a size $\sqrt{2Dt}$ after time t and has its amplitude reduced by the same factor. (This assumes of course, that its initial size was much smaller than $\sqrt{2Dt}$.) In three dimensions, the size grows at the same rate, but the amplitude decreases as the cube since it's spreading out in three dimensions rather than just one.