9 The heat or diffusion equation

In this lecture I will show how the heat equation

$$u_t = \alpha^2 \Delta u, \quad \alpha^2 \in \mathbf{R}, \tag{9.1}$$

where Δ is the Laplace operator, naturally appears *macroscopically*, as the consequence of the conservation of energy and Fourier's law. Fourier's law also explains the physical meaning of various boundary conditions. I will also give a *microscopic* derivation of the heat equation, as the limit of a simple random walk, thus explaining its second title — the diffusion equation.

9.1 Conservation of energy plus Fourier's law imply the heat equation

In one of the first lectures I deduced the fundamental conservation law in the form $u_t + q_x = 0$ which connects the quantity u and its flux q. Here I first generalize this equality for more than one spatial dimension.

Let $e(t, \boldsymbol{x})$ denote the *thermal energy* at time t at the point $\boldsymbol{x} \in \mathbf{R}^k$, where $k = 1, 2$, or 3 (straight line, plane, or usual three dimensional space). Note that I use bold fond to emphasize that $\boldsymbol{x}$ is a vector. The *law of the conservation of energy* tells me that

> the rate of change of the thermal energy in some domain D is equal to the flux of the energy inside D minus the flux of the energy outside of D and plus the amount of energy generated in D.

So in the following I will use D to denote my domain in $\mathbf{R}^1, \mathbf{R}^2$, or $\mathbf{R}^3$. Can it be an arbitrary domain? Not really, and for the following to hold I assume that D is a domain without holes (this is called *simply connected*) and with a piecewise smooth boundary, which I will denote ∂D. This technical term (*piecewise smooth boundary*) is not simple to define, but for this course it is enough to think that the boundary has either tangent line (in 2D) or tangent plane (in 3D) in almost all of its points; "almost" is necessary to include also such nice domains ar rectangles and cubes, which at their vertices are not smooth.

Mathematically, the law of the conservation of energy can be written as

$$\frac{\mathrm{d}}{\mathrm{d}t} \iiint_D e(t, \boldsymbol{x}) \mathrm{d}\boldsymbol{x} = -\oiint_{\partial D} \boldsymbol{q}(t, \boldsymbol{x}) \cdot \boldsymbol{n} \, \mathrm{d}S + \iiint_D f^*(t, \boldsymbol{x}) \mathrm{d}\boldsymbol{x}.$$

Here $\boldsymbol{q}$ is the flux (note that now it is a vector, naturally, since the notion of the flux assumes a direction), $\boldsymbol{n}$ is the outward normal to the domain D, and the first integral in the right hand side is taken along the boundary of D, the minus sign is necessary because $\boldsymbol{n}$ is the *outward* normal. The dot denotes the usual dot product in $\mathbf{R}^k$. Function f^* specifies the energy generated (or absorbed if it is negative) inside D.

The *divergence* (or *Gauss*) theorem says that

$$\oiint_{\partial D} \boldsymbol{q}(t, \boldsymbol{x}) \cdot \boldsymbol{n} \, \mathrm{d}S = \iiint_D \nabla \cdot \boldsymbol{q}(t, \boldsymbol{x}) \mathrm{d}\boldsymbol{x},$$

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where ∇ is a differential operator, often called "del" or "nabla", in Cartesian coordinates

$$\nabla = (\partial_x, \partial_y, \partial_z).$$

Putting everything together I get

$$\iiint_D \Big(e_t(t,\boldsymbol{x}) + \nabla \cdot \boldsymbol{q}(t,\boldsymbol{x}) - f^*(t,\boldsymbol{x})\Big)\mathrm{d}\boldsymbol{x} = 0,$$

which implies the fundamental conservation law in an arbitrary number of dimensions:

$$e_t + \nabla \cdot \boldsymbol{q} - f^* = 0. \tag{9.2}$$

To proceed, I will use the relation of the temperature u and the thermal energy e as

$$e(t,\boldsymbol{x}) = c(\boldsymbol{x})\rho(\boldsymbol{x})u(t,\boldsymbol{x}),$$

where $c(\boldsymbol{x})$ is the heat or *thermal capacity* (how much energy me must supply to raise the temperature by one degree) at the point $\boldsymbol{x}$, and $\rho(\boldsymbol{x})$ is the density at the point $\boldsymbol{x}$, i.e., the mass per volume unit; for many materials I can assume that both c and ρ are constants (the reality is more complicated, in many cases both c and ρ depend not only the coordinate but also on the current temperature u thus rendering the equations to be nonlinear, but I will avoid such complications in our course). Finally I will use *Fourier's law* that says that

> The flux of the thermal energy is proportional to the gradient of the temperature, i.e.,

$$\boldsymbol{q}(t,\boldsymbol{x}) = -k\nabla u(t,\boldsymbol{x}),$$

where k is called the *thermal conductivity*. The minus sign describes the intuitively expected fact that the heat energy flows from hotter to cooler regions (think about one dimensional geometry, when $\nabla u = u_x$).

Hence

$$u_t = \frac{1}{c\rho}\nabla \cdot k\nabla u + \frac{f^*}{c\rho}\,,$$

or, using the notations

$$\alpha^2 = \frac{k}{c\rho}\,, \quad f = \frac{f^*}{c\rho}\,, \quad \Delta = \nabla^2 = \nabla \cdot \nabla,$$

the nonhomogeneous heat equation

$$u_t = \alpha^2 \Delta u + f. \tag{9.3}$$

In Cartesian coordinates in 3D I have (assuming for the moment that $f = 0$)

$$u_t = \alpha^2\left(u_{xx} + u_{yy} + u_{zz}\right).$$

If I am dealing with one-dimensional geometry my equation becomes

$$u_t = \alpha^2 u_{xx},$$

which is a particular case of (9.1).

9.2 Initial and boundary conditions for the heat equation

In general, I will need the initial and boundary conditions to guarantee that my problem is *well posed.* The initial condition is given by

$$u(0,\boldsymbol{x})=g(\boldsymbol{x}),\quad \boldsymbol{x}\in D,$$

which physically means that we have an initial temperature at every point of my domain D.

To consider different types of the boundary conditions I will concentrate on the case when I deal with $D\subseteq\mathbf{R}^1$, i.e., my domain is simply the interval $(0,l)\,,l>0$ on the real line. Physically one should imagine a laterally isolated rod of length l, and I am interested in describing the changes in the temperature profile inside this rod.

- *Type I or Dirichlet boundary conditions.* In this case I fix the temperature of the two ends of my rod:

  $$u(t,0)=h_1(t),\quad u(t,l)=h_2(t),\quad t>0.$$

  Please note that h_1 and h_2 specify *not* the temperature of the surrounding medium around the ends of the rod but the exact temperature of the ends themselves, which can be mechanically achieved by using some kind of thermostats fixed at the ends.

- *Type II or Neumann boundary conditions.* In this case I fix the flux at the boundaries:

  $$u_x(t,0)=g_1(t),\quad u_x(t,l)=g_2(t),$$

  where $g_1(t)>0$, $g_2(t)>0$ imply that the heat flows from right to left, and from left to right otherwise. The case $g_1=g_2=0$ is very important and corresponds, clearly, to no flux condition, or, in other words, to the insulated ends of the rod.

- *Type III or Robin boundary conditions.* This means that the temperature of the surrounding medium is specified. I will use Newton's law of cooling, together with Fourier's law, to obtain in this case

  $$u_x(t,0)=\frac{h}{k}\big(u(t,0)-q_1(t)\big),\quad u_x(t,l)=-\frac{h}{k}\big(u(t,l)-q_2(t)\big),$$

  where q_1,q_2 are the temperatured at the left and the right ends respectively. Here k, as before, the thermal conductivity, and h is so-called heat exchange coefficient (which is quite difficult to measure in real systems). Here Newton's law of cooling appears in the form of the difference of two temperatures. Note also that I am careful about signs in my expressions to guarantee that the heat flows from hotter to cooler places, as intuitively expected. Sometimes the same boundary conditions can be written in a more mathematically neutral form as

  $$\alpha_1u(t,0)+\beta_1u_x(t,0)=q_1(t),\quad \alpha_2u(t,l)+\beta_2u_x(t,l)=q_2(t),$$

  for some constants α_i,β_i, $i=1,2$.

Similarly the boundary conditions for two or three dimensional spatial domains can be defined. Sometimes some part of the boundary has Type I condition and another part has Type II condition. In this case it is said that *mixed boundary conditions* are set. If h_i,g_i,q_i are identically zero then it is said that the boundary conditions are *homogeneous.*

Example 9.1. Suppose we have a copper rod 200 cm long that is laterally insulated and has an initial temperature $0°C$. Suppose that the top of the rod ($x = 0$) is insulated, while the bottom ($x = 200$) is immersed into moving water that has the constant temperature of $q_2(t) = 20°C$.

The mathematical model for this problem will be

$$\begin{aligned}
&\text{PDE} \quad && u_t = \alpha^2 u_{xx}, \quad 0 < x < 200, \quad t > 0,\\
&\text{BC} \quad && \begin{cases} u_x(t, 0) = 0, \\ u_x(t, 200) = -\dfrac{h}{k}\big(u(t, 200) - 20\big), \end{cases}\\
&\text{IC} \quad && u(0, x) = 0, \quad 0 \leq x \leq 200.
\end{aligned}$$

Exercise 1. Can you guess what happens with the solution to the previous problem when $t \to \infty$? Can you prove your expectations mathematically?

9.3 A microscopic derivation of the diffusion equation

Consider a one dimensional *simple random walk*. This means that I have, e.g., a particle that moves h (note that this h has nothing to do with the h from the previous section!) units up with probability p and h units down with probability q, $p + q = 1$, starting from the origin, one step every τ units of time (see Figs. 1 and 2 for some inspiration). My goal in this problem is to determine the probability, which I denote $u_{k,N}$, that after N steps (i.e., at the time $t = N\tau$) I will find this particle at the position kh, $-N \leq k \leq N$. The usual notation is

$$u_{k,N} = \mathrm{P}\left(X = kh\right),$$

for the position X of the particle, which is an example of a *random variable*.

Exercise 2. Let $p = q = \frac{1}{2}$, $N = 3$, $h = 1$, what are $u_{k,3}$, $-3 \leq k \leq 3$? What is $\sum_{k=-3}^{3} u_{k,3}$?

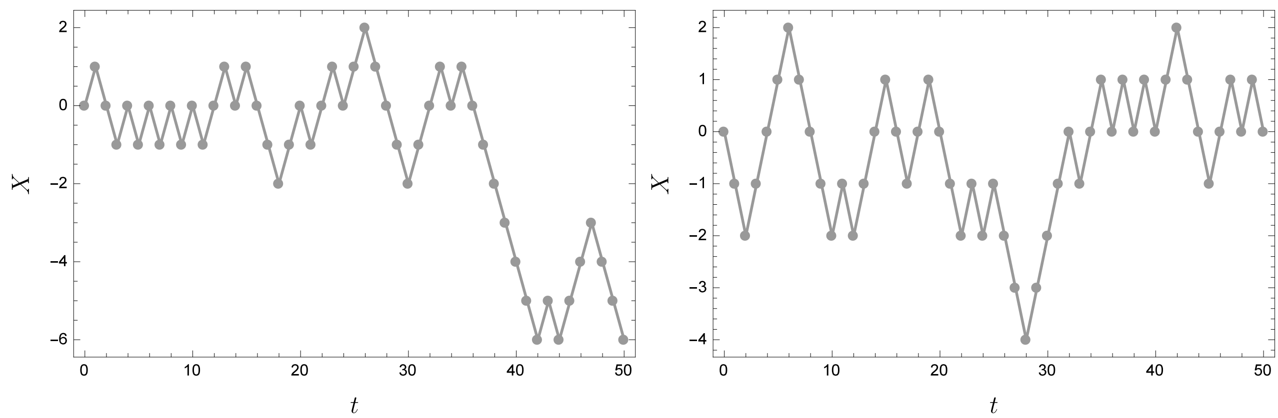

Figure 1: Two examples of a symmetric ($p = q = 1/2$) random walk with $h = \tau = 1$, $N = 50$.

Actually, the previous exercise can be solved exactly for arbitrary k and N. I am, however, is more interested in understanding what happens if $h, \tau \to 0$ and hence my simple random walk becomes *continuous* in both time and space. I will use, taking into account my limiting procedure, the notation

$$u_{k,N} = u(t, x).$$

To obtain the desired result I write down the *fundamental relation*

$$u(t+\tau,x)=pu(t,x-h)+qu(t,x+h),$$

which literally says that the probability to find the particle at the position x at time $t+\tau$ can be found as the sum of the probability to be at the position $x-h$ at time t times the probability move up (which is equal to p) and the probability to be at the position $x+h$ at time t times the probability move down (which is q). (In probability theory this is called the law of total probability, but do not worry if you did not see this before).

Now I assume that if $h,\tau\to 0$ then u becomes a sufficiently smooth function of x and t, such that I can use Taylor's series similar to what I did when I deduced the wave equation. I have

$$\begin{aligned} u(t+\tau,x)&=u(t,x)+u_t(t,x)\tau+o(\tau),\\ u(t,x\pm h)&=u(t,x)\pm u_x(t,x)h+\frac{1}{2}u_{xx}(t,x)h^2+o(h^2), \end{aligned}$$

where $g(x)=o(f(x))$ means the terms such that $\lim_{x\to 0}\frac{g(x)}{f(x)}\to 0$. For example, $\tau^2=o(\tau)$, $h^3=o(h^2)$; $o(1)$ means any expression tending to 0 as $x\to 0$. I plug these series into the fundamental relation, cancel the terms that can be canceled and find that

$$u_t\tau+o(\tau)=(q-p)hu_x+\frac{h^2}{2}u_{xx}+o(h^2).$$

Dividing by τ yields

$$u_t+o(1)=\frac{(q-p)h}{\tau}u_x+\frac{h^2}{2\tau}u_{xx}+o\left(\frac{h^2}{\tau}\right).$$

Now to get a meaningful result, I must consider a special way when both h and τ tend to zero. First, I assume that

$$\lim_{h,\tau\to 0}\frac{h^2}{2\tau}=\alpha^2>0.$$

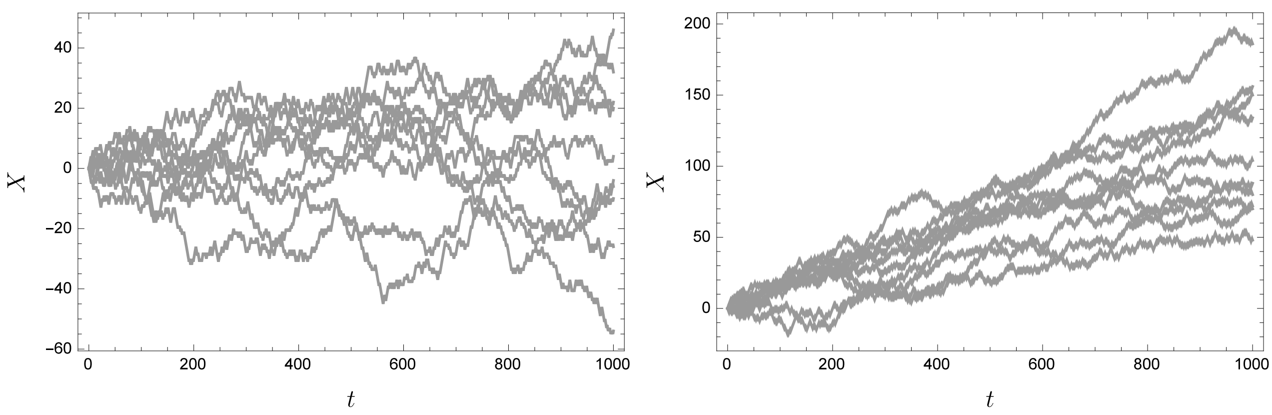

Figure 2: Left: ten realizations of a symmetric ($p=q=1/2$) random walk with $h=\tau=1$ and $N=1000$. Right: ten realizations of a random walk with drift ($p=0.56$, $q=0.44$).

Second,

$$\lim_{h,\tau\to 0}\frac{(q-p)h}{\tau}=\lim_{h,\tau\to 0}\frac{(q-p)h^2}{h\tau}=\beta 2\alpha^2=:c$$

for a constant β, this can be always achieved by taking

$$q=\frac{1}{2}+\frac{\beta}{2}h+o(h),\quad p=\frac{1}{2}-\frac{\beta}{2}h+o(h),$$

i.e., when the random walk is microscopically symmetric.

Now taking the limits $\tau, h\to 0$ yields the diffusion equation with drift (this is the term cu_x below)

$$u_t=\alpha^2u_{xx}+cu_x.$$

If I do not have the drift, i.e., $p=q=0.5$, then I recover the familiar homogeneous one dimensional heat equation

$$u_t=\alpha^2u_{xx}.$$

Now it should be clear why α^2 is often called the *diffusivity or diffusion coefficient*.

As a side remark I note that if $\alpha^2=0$ then I end up with the familiar linear transport equation

$$u_t-cu_x=0,$$

which has the general solution

$$u(t,x)=F(x+ct),$$

which is geometrically a linear traveling wave moving in the negative direction if $c>0$ (i.e., if $q>p$, note this corresponds to the movement from top to bottom in terms I described it) or in the positive direction if $c<0$ (i.e, if $q<p$, from bottom to the top), as expected.

As I a final remark I note that when $h,\tau\to 0$ then $u_{k,N}$ ceases to be the actual probability and becomes, in the language of probability theory, the *probability density function* such that the probability to find a particle in the interval $[x_1,x_2]$ at time t becomes

$$\mathrm{P}\left(x_1\leq X\leq x_2\right)=\int_{x_1}^{x_2}u(t,x)\mathrm{d}x.$$

I can similarly consider a simple random walk on a plane, when each particle has four different directions to move at each time moment, or in the space, when now my particle has six directions to choose from. Assuming that the probabilities to move in each direction are the same I, after similar analysis, can conclude that u must satisfy in the continuous limit to the equations

$$u_t=\alpha^2\left(u_{xx}+u_{yy}\right)$$

and

$$u_t=\alpha^2\left(u_{xx}+u_{yy}+u_{zz}\right)$$

respectively.

9.4 Test yourself

9.1. What is the definition of ∇?

9.2. Formulate Fourier's law.

9.3. Formulate Newton's cooling law.

9.4. Formulate Gauss (or divergence) theorem.

9.5. Use the definition of ∇ to write ∇u and $\nabla \cdot \nabla u$ in Cartesian coordinates for a function u of three independent variables. The same question for $\nabla \cdot \boldsymbol{q}$ for the vector $\boldsymbol{q} \in \mathbf{R}^3$. What are the names for the obtained results?

9.6. What physical system is described by the following problem:

$$u_t = \alpha^2 u_{xx}, \quad u(0, x) = g(x), \quad u(t, 0) = u(t, 1) = 1?$$

9.7. What physical system is described by the following problem:

$$u_t = \alpha^2 u_{xx}, \quad u(0, x) = g(x), \quad u_x(t, 0) = u_x(t, 1) = 1?$$

9.8. What physical system is described by the following problem:

$$u_t = \alpha^2 (u_{xx} + u_{yy}), \quad u(0, x, y) = g(x, y), \quad x^2 + y^2 < 1, \quad u(t, x, y) = 1, \quad x^2 + y^2 = 1?$$

9.5 Solutions to the exercises

Exercise 1. For this exercise I must assume that as time proceeds the temperature distribution settles and (almost) does not change with time. Such temperature distribution is called *stationary*. If the stationary distribution does exist, it means that the temperature does not depend on t and hence satisfies the ODE $u'' = 0$, which has the general solution $u(x) = Ax + B$, for some constants A, B. First boundary condition yields $A = 0$, the second one — $0 = -\frac{h}{k}(B - 20)$, whence $B = 20$. Therefore the stationary distribution (as should be expected intuitively) is simply the constant $u(x) = 20$. ■

Exercise 2. There is only one way to get to the position $k = -3$ or $k = 3$. In the former case I need to jump 3 times to the right, the event of probability q^3, in the letter case, there will be three jumps to the left, the event of probability p^3. It is impossible to find itself in either $k = 2$ or $k = -2$ for 3 steps (as well as in $k = 0$), therefore, $u_{2,3} = u_{-2,3} = u_{0,3} = 0$. Finally, there are three different ways to reach both $k = 1, k = -1$. In the first case there will be 2 jumps to the left and one to the right, in the second — 2 jumps to the right and one to the left, hence $u_{1,3} = 3p^2 q, u_{-1,3} = 3pq^2$. Clearly, the answer for the second questions in this exercise is 1, in detail

$$\sum_{k=-3}^{3} u_{k,3} = p^3 + 3p^2 q + 3q^2 p + q^3 = (p + q)^3 = 1.$$

■