Brownian Motion and the Heat Equation

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1 Thermodynamics and the heat conduction equation of Joseph Fourier

Thermodynamics is a branch of physics and chemistry that studies the effects of changes in temperature, pressure, and volume on physical systems at the macroscopic scale by analyzing the collective motion of their particles using statistics. Roughly, heat means "energy in transit" and dynamics relates to "movement"; thus, in essence thermodynamics studies the movement of energy and how energy instills movement. Historically, thermodynamics developed out of need to increase the efficiency of early steam engines. The starting point for most thermodynamic considerations are the laws of thermodynamics which postulate that energy can be exchanged between physical systems as heat or work. The first established principle of thermodynamics (which eventually became the Second Law) was formulated by Sadi Carnot in 1824. By 1860, as found in the works of those such as Rudolf Clausius and William Thomson, there were two established "principles" of thermodynamics. As the years passed, these principles turned into "laws." By 1873, for example, the theoretical physicist/mathematician Josiah Willard Gibbs clearly stated that there were two absolute laws of thermodynamics.

In the early 19th century, while the study of thermodynamics was still in its infancy, the French scientist Jean Baptiste Joseph Fourier presented a remarkable formula describing the conduction of heat in a solid. In 1807, when Fourier presented this work, opinions were still divided about the nature of heat. However, heat conduction due to temperature differences and heat storage and the associated specific heat of materials had been experimentally established. Nonetheless, it would take many years for Fourier's theories to become widely accepted, and in 1822 he published *Théorie Analytique de la Chaleur* (or the *Analytic Theory of Heat*) introducing his methods to a broad international audience. Over the ensuing century and a half, Fourier's methods began to be applied to analyze problems in many fields such as: heat transfer, electricity, chemical diffusion, fluids in porous media, genetics, and economics. In fact, Fourier's heat conduction equation continues to constitute the conceptual foundation on which rests the analysis of many physical, biological, and social systems.

In its simplest formulation, Fourier's equation in one space variable models heat conduction in a rod. Consider a rod made of a single homogeneous conducting material of length L parallel to the horizontal axis (or x-axis) so that $0 \le x \le L$ describes the position of the rod.

Let κ denote the thermal conductivity of the rod. Recall that thermal conductivity is the ability of a material to conduct heat and is measured in units of Watts per Kelvin-metre. Most good electrical conductors are also good heat conductors; for example, copper, aluminum, gold, iron, silver, lead, tin, platinum, nickel, tungsten.

For $t \geq 0$ and $0 \leq x \leq L$, let $u(x,t)$ denote the temperature of the rod at time t at position x and suppose that $u(x,0) = g(x)$ denotes the initial temperature distribution of the rod. We dictate that the sides of the rod are perfectly insulated so that no heat passes through them. It is most convenient to also assume that the temperature at the ends of the rod is kept constant (and for simplicity we assume this temperature to be 0) which leads to the boundary conditions $u(0,t) = 0$ and $u(L,t) = 0$.

Fourier showed that the function $u(x,t)$ satisfies the partial differential equation

$$\frac{\partial}{\partial t}u(x,t) = \kappa \frac{\partial^2}{\partial x^2}u(x,t)$$

subject to the initial conditions

$$u(x,0) = g(x), \quad u(0,t) = 0, \quad u(L,t) = 0.$$

He also showed how to solve this equation using the technique of *separation of variables.* In fact,

$$u(x,t) = \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi x}{L}\right) \exp\left\{\frac{-n^2\pi^2\kappa t}{L^2}\right\} \tag{1}$$

where

$$c_n = \frac{2}{L}\int_0^L g(x) \sin\left(\frac{n\pi x}{L}\right) \mathrm{d}x.$$

This method of solution (and its generalizations) is now considered standard undergraduate material and is taught in a first course on differential equations such as MATH 217. It should also be noted that this solution is not as "obvious" as it might seem since there is no *a priori* guarantee that the sum on the right side of (1) converges. It took over 50 more years of research to establish the theoretical foundations of these so-called *Fourier series.*

2 Robert Brown's erratic motion of pollen

In the summer of 1827, the Scottish botanist Robert Brown observed that microscopic pollen grains suspended in water move in an erratic, highly irregular, zigzag pattern. Following Brown's initial report, other scientists verified the strange phenomenon. Brownian motion was apparent whenever very small particles were suspended in a fluid medium, for example smoke particles in air. It was eventually determined that finer particles move more rapidly, that their motion is stimulated by heat, and that the movement is more active when the fluid viscosity is reduced.

However, it was only in 1905 that Albert Einstein, using a probabilistic model, could provide a satisfactory explanation of the Brownian motion. He asserted that the Brownian motion originates in the continual bombardment of the pollen grains by the molecules of the surrounding water, with successive molecular impacts coming from different directions and contributing different impulses to the particles. As a result of the continual collisions, the particles themselves had the same average kinetic energy as the molecules. Thus, he showed that Brownian motion provided a solution (in a certain sense) to Fourier's famous heat equation

$$\frac{\partial}{\partial t}u(x,t) = \kappa\frac{\partial^2}{\partial x^2}u(x,t).$$

Note that in 1905, belief in atoms and molecules was far from universal. In fact, Einstein's "proof" of Brownian motion helped provide convincing evidence of atomic existence. Einstein had a busy 1905, also publishing seminal papers on the special theory of relativity and the photoelectric effect. In fact, his work on the photoelectric effect won him a Nobel prize. Curiously, though, history has shown that the photoelectric effect is the *least* monumental of his three 1905 triumphs. The world at that time simply could not accept special relativity!

Since Brownian motion described the physical trajectories of pollen grains suspended in water, Brownian paths must be continuous. But they were seen to be so irregular that the French physicist Jean Perrin believed them to be non-differentiable. (The German mathematician Karl Weierstrass had recently discovered such pathological functions do exist. Indeed the continuous function

$$h(x) = \sum_{n=1}^{\infty} b^n \cos(a^n \pi x)$$

where a is odd, $b \in (0,1)$, and $ab > 1 + 3\pi/2$ is nowhere differentiable.) Perrin himself worked to show that colliding particles obey the gas laws, calculated Avogadro's number, and won the 1926 Nobel prize.

Finally, in 1923, the mathematician Norbert Wiener established the mathematical existence of Brownian motion by verifying the existence of a stochastic process with the required properties.

3 Albert Einstein's proof of the existence of Brownian motion

We now summarize Einstein's original 1905 argument. Suppose there are K particles suspended in a liquid. In a short time interval T, the x-coordinate of a single particle will increase by ε where ε has a different value for each particle. For the value of ε, a certain probability law will hold.

In the time interval T, the number $\mathrm{d}K$ of particles which experience a displacement between ε and $\varepsilon + \Delta\varepsilon$ can be expressed by the equation

$$\mathrm{d}K = K\varphi(\varepsilon)\,\mathrm{d}\varepsilon$$

where φ only differs from 0 for very small values of ε and satisfies

$$\int_{-\infty}^{\infty} \varphi(\varepsilon)\,\mathrm{d}\varepsilon = 1, \quad \varphi(\varepsilon) = \varphi(-\varepsilon).$$

Since φ is an even function, we see that

$$\int_{-\infty}^{\infty} \varepsilon\, \varphi(\varepsilon)\, \mathrm{d}\varepsilon = 0.$$

We will now investigate how the coefficient of diffusion depends on φ restricted to the case where the number of particles per unit volume depends on x and t only. Let $f(x,t)$ denote the number of particles per unit volume at location x at time t so that

$$\int_{-\infty}^{\infty} f(x,t)\, \mathrm{d}x = K$$

and define α^2 by

$$\alpha^2 := \frac{1}{2T} \int_{-\infty}^{\infty} \varepsilon^2\, \varphi(\varepsilon)\, \mathrm{d}\varepsilon.$$

Our goal is to now calculate the distribution of particles a short time later. By the definition of $\varphi(\varepsilon)$, we have

$$f(x, t+T) = \int_{-\infty}^{\infty} f(x+\varepsilon, t)\, \varphi(\varepsilon)\, \mathrm{d}\varepsilon. \tag{2}$$

By Taylor's theorem (ignoring higher infinitesmals), we have in one case

$$f(x,t+T) = f(x,t) + \frac{\partial f}{\partial t} T \tag{3}$$

and in the other case

$$f(x+\varepsilon, t) = f(x,t) + \frac{\partial f}{\partial x}\varepsilon + \frac{1}{2}\frac{\partial^2 f}{\partial x^2}\varepsilon^2. \tag{4}$$

Substituting (4) into (2) yields

$$\begin{aligned} f(x,t+T) &= \int_{-\infty}^{\infty} f(x+\varepsilon, t)\, \varphi(\varepsilon)\, \mathrm{d}\varepsilon \\ &= \int_{-\infty}^{\infty} \left[f(x,t) + \frac{\partial f}{\partial x}\varepsilon + \frac{1}{2}\frac{\partial^2 f}{\partial x^2}\varepsilon^2 \right] \varphi(\varepsilon)\, \mathrm{d}\varepsilon \\ &= f(x,t) + \alpha^2 \frac{\partial^2 f}{\partial x^2} T \end{aligned} \tag{5}$$

using the properties of $\varphi(\varepsilon)$ above.

By equating the two approximations, one with respect to time (3), and the other with respect to (random) displacements (5), we obtain the partial differential equation

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

which is the well-known differential equation for diffusion (i.e., the heat equation) where α^2 is the coefficient of diffusion (i.e., thermal conductivity). From this it may be concluded that

$$f(x,t) = \frac{K}{\alpha\sqrt{4\pi t}} \exp\left\{ -\frac{x^2}{4\alpha^2 t} \right\}.$$

Einstein followed the standard assumption in statistical mechanics that the "movements of the single particles are mutually independent," and that the "movements executed by a particle in consecutive time intervals are independent." Naturally, the path of the particle is continuous. Notice that the formula for $f(x,t)$ is K times a $\mathcal{N}(0, 2\alpha^2 t)$ density function.

4 Mathematical definition of Brownian motion and the solution to the heat equation

We can formalize the standard statistical mechanics assumptions given above and define Brownian motion in a rigorous, mathematical way. A one-dimensional real-valued stochastic process $\{W_t, t \geq 0\}$ is a *Brownian motion* (with variance parameter σ^2) if

- $W_0 = 0$ and the function $t \mapsto W_t$ is continuous (with probability one),
- for any $t_0 < t_1 < \ldots < t_n$ the increments $W_{t_0}, W_{t_1} - W_{t_0}, \ldots, W_{t_{n-1}} - W_{t_n}$ are independent, and
- for any s, $t \geq 0$, the increment $W_{t+s} - W_s \sim \mathcal{N}(0, \sigma^2 t)$ is normally distributed.

We will be interested in the case where the variance parameter is $\sigma^2 = 1$ in which case we have $W_t \sim \mathcal{N}(0, t)$ for each $t > 0$. We can also define Brownian motion starting at $x \in \mathbb{R}$ by setting $B_t = W_t + x$ for each $t \geq 0$.

Suppose that $\{B_t, t \geq 0\}$ is a Brownian motion starting at x. Since $B_t \sim \mathcal{N}(x, t)$, we define the *transition density* by

$$p(t; x, y) = \frac{1}{\sqrt{2\pi t}} \exp\left\{-\frac{1}{2t}(y-x)^2\right\}, \quad -\infty < y < \infty.$$

Informally, $p(t; x, y)$ represents the probability that Brownian motion starting at x will be at position y at time t. Of course, $p(t; x, y)$ is a density function for a continuous random variable and so we must interpret it to mean

$$P\{B_t \in V \mid B_0 = x\} = \int_V p(t; x, y)\, \mathrm{d}y$$

for any set $V \subset \mathbb{R}$.

Exercise. Consider Brownian motion starting at 0. The transition density for B_t can therefore be written as

$$p(t; 0, x) = \frac{1}{\sqrt{2\pi t}} \exp\left\{-\frac{x^2}{2t}\right\}, \quad -\infty < x < \infty.$$

Compute

$$\frac{\partial}{\partial t} p(t; 0, x) \quad \text{and} \quad \frac{1}{2}\frac{\partial^2}{\partial x^2} p(t; 0, x).$$

Notice that they are the same!

Thus, we see that the transition density for Brownian motion satisfies the heat equation, and so motivated by Einstein's argument, it seems natural to guess that Brownian motion should solve the heat equation.

Theorem. The unique bounded solution to the heat equation

$$\frac{\partial}{\partial t}u(x,t) = \frac{1}{2}\frac{\partial^2}{\partial x^2}u(x,t)$$

subject to the initial conditions

$$u(x,0) = g(x), \quad u(0,t) = 0, \quad u(L,t) = 0.$$

is given by

$$\boxed{u(x,t) = \mathbb{E}\left[g(B_t) \cdot I(t,\tau) \,|\, B_0 = x\right]}$$

where

$$I(t,\tau) = \begin{cases} 1, & t < \tau, \\ 0, & \text{otherwise}, \end{cases}$$

and τ is the (random) first time that BM hits either end of the rod.

Note that using the transition density we can write (for $t < \tau$)

$$\mathbb{E}\left[g(B_t) \,|\, B_0 = x\right] = \int_{-\infty}^{\infty} g(y)P\{B_t = y \,|\, B_0 = x\}\,\mathrm{d}y = \int_{-\infty}^{\infty} g(y)p(t;x,y)\,\mathrm{d}y.$$

5 Further Reading

For an introduction to partial differential equations and techniques for solving a variety of diffusion-type problems, the book by Farlow [1] is recommended. He uses a lot of pictures and intuition to motivate the derivations. Einstein's famous 1905 papers have been reprinted numerous times. A revision of [4] released in 2005 to commemorate the centenary of Einstein's *annus mirabilis* includes commentary and a new introduction. The probabilistic connections between Brownian motion and the heat equation are developed in detail by Lawler in [2], and a nice historical account of Fourier's work and related developments in thermodynamics at the start of the 19th century is given by Narasimhan [3] (whose paper is freely available online).

References

[1] S. J. Farlow. *Partial Differential Equations for Scientists and Engineers.* Dover, Mineola, NY, 1993.

[2] G. F. Lawler. *Introduction to Stochastic Processes, Second Edition.* Chapman & Hall/CRC, Boca Raton, FL, 2006.

[3] T. N. Narasimhan. Fourier's heat conduction equation: History, influence, and connections. *Reviews of Geophysics*, 37:151–172, 1999.

[4] J. Stachel. *Einstein's Miraculous Year.* Princeton University Press, Princeton, NJ, 2005.