3.

Notes on the heat equation, the Jacobi theta function, and sums of two squares.

3.1.

Heat is kinetic energy Q in a state of transfer between two systems. Temperature is a measure T of the average kinetic energy of a physical system. Over an infinitesimal distance dz, in an instant dt, heat transfer is proportional to the change in temperature:

$$Q\,dt \;\propto\; dT\,dz.$$

Now imagine a perfectly conductive solid cylinder of infinitesimal thickness. We write z for the position coordinate. Temperature then becomes a function $T(z,t)$. Fix z and imagine the infinitesimal cross-section from z to $z + dz$. In terms of T, how much heat is transferred to the cross-section over an instant dt?

Experiments suggest that it is proportional to the difference in $\frac{\partial T}{\partial z}$ between z and $z + dz$:

$$Q\,dt \;\propto\; \left(\frac{\partial T}{\partial z}(z+dz,t) - \frac{\partial T}{\partial z}(z,t)\right) dt.$$

Combining the two equations above and rearranging,

$$\frac{\partial T}{\partial t}(z,t) \;\propto\; \frac{1}{dz}\left(\frac{\partial T}{\partial z}(z+dz,t) - \frac{\partial T}{\partial z}(z,t)\right).$$

But the right-hand side is just $\frac{\partial^2 T}{\partial z^2}(z,t)$. Writing $\alpha > 0$ for the proportionality constant, we arrive at the heat equation for the cylinder:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial z^2}.$$

3.2.

Suppose that the cylinder is the interval $0 \le z \le 1$, and that at time $t = 0$, both ends start at absolute zero. Here, Fourier solved the heat equation as follows.

First he guessed that the general solution $T(z,t)$ could be written as an (infinite) superposition of separable solutions, meaning those of the form $A(z)B(t)$ for some functions A and B. In the simplest case where $T(z,t) = A(z)B(t)$, we get

$$\frac{B'(t)}{B(t)} = \alpha \frac{A''(z)}{A(z)}.$$

Since z and t are independent variables, there must be a constant λ such that

$$A'' = \lambda A \quad \text{and} \quad B' = \alpha\lambda B.$$

If $\lambda > 0$, then A has the general solution $c_1 e^{\lambda^{1/2} z} + c_2 e^{-\lambda^{1/2} z}$. But then our boundary conditions force $c_1 + c_2 = 0$ and $c_1 e^{\lambda^{1/2}} + c_2 e^{-\lambda^{1/2}} = 0$. Together these imply $c_1 = c_2 = 0$. If instead $\lambda = 0$, then A has the general solution $c_1 z + c_2$, so our boundary condition again force $c_1 = c_2 = 0$.

The only interesting case is $\lambda < 0$. Here A and B have the general solutions

$$\begin{aligned} A &= c_1 \cos(|\lambda|^{1/2} z) + c_2 \sin(|\lambda|^{1/2} z), \\ B &= c_3 e^{\alpha \lambda t}. \end{aligned}$$

Our boundary conditions force $c_1 = 0$ and $|\lambda|^{1/2} = \pi n$ for some positive integer n. Altogether:

Theorem 3.1 (Fourier)**.** *On a perfectly conductive cylinder from $z = 0$ to $z = 1$ of infinitesimal thickness, any separable solution to the heat equation looks like*

$$T(z,t) = \sin(\pi n z) e^{-\alpha(\pi n)^2 t}$$

for some $n > 0$.

Remember that Fourier expected the general solution to be a superposition of separable solutions: say,

$$T(z,t) = \sum_{n=1}^{\infty} a_n \sin(\pi n z) e^{-\alpha(\pi n)^2 t}$$

for some coefficients a_n. He observed a very beautiful inversion formula for the a_n, which explains why we now call them Fourier coefficients.

Theorem 3.2 (Fourier)**.** *If $T(z,t)$ is sufficiently "nice", then for all n, we have*

$$a_n = 2 \int_0^1 T(z,0) \sin(\pi n z)\, dz.$$

3.3.

Now suppose that at time $t = 0$, there is a temperature spike at $z = 1/2$ and the temperature everywhere else is absolute zero. More precisely suppose that $T(z,0)$ is the Dirac delta given by:

$$\int_0^1 T(z,0)\varphi(z)\, dz = \varphi(\tfrac{1}{2}) \quad \text{for any smooth } \varphi \text{ integrable on } [0,1].$$

For such T, we have

$$a_n = 2\sin(\tfrac{\pi n}{2}) = \begin{cases} 0 & n \equiv 0 \pmod 4 \\ \pm 2 & n \equiv \pm 1 \pmod 4 \end{cases}$$

which in turn gives

$$\begin{aligned}
T(z,t) &= 2\left(\sin(\pi z)e^{-\alpha\pi^2 t} - \sin(3\pi z)e^{-\alpha(3\pi)^2 t} + \sin(5\pi z)e^{-\alpha(5\pi)^2 t} - \cdots\right) \\
&= \sum_{n\in\mathbf{Z}} e^{2\pi i(n+1/2)(z-1/2)} e^{-\alpha(4\pi^2)(n+1/2)^2 t}
\end{aligned}$$

via de Moivre's formula. Above, the last sum converges because of the fast decay of $e^{-\alpha(4\pi^2)(n+1/2)^2 t}$ with respect to n.

Jacobi got very interested in this function, but in a generalization to complex variables. Namely, for any $z, \tau \in \mathbf{C}$ with $\mathrm{Im}(\tau) > 0$, let

$$\Theta(z,\tau) = \sum_{n\in\mathbf{Z}} e^{2\pi i n z} e^{\pi i n^2 \tau}.$$

For fixed z, the formula for Θ defines an analytic function on the upper half-plane of $\mathbf{C}$. When $\alpha = \frac{1}{4\pi}$, we get $T(z,t) = e^{\pi i(z-1/2)} e^{-t/4} \Theta(z + \frac{it}{2} - \frac{1}{2}, it)$.

3.4.

Set $\theta(\tau) = \Theta(0,\tau)$. It turns out that θ satisfies many nice symmetry properties: notably,

(1) $\theta(\tau+1) = \theta(\tau)$.
(2) $\theta(-\frac{1}{\tau}) = \sqrt{-i\tau}\,\theta(\tau)$, where $\sqrt{-i\tau}$ is the square root in the upper half-plane.

The hard one is item (2), which uses a theorem from Fourier analysis called Poisson summation.

Now set $q^{\pi i \tau}$. We notice that $\theta(\tau) = \sum_{n\in\mathbf{Z}} q^{n^2}$, and therefore,

$$\theta(\tau)^2 = \sum_{m\geq 0} r_2(m) q^m, \quad \text{where } r_2(m) = |\{(a,b) \in \mathbf{Z}^2 \mid m = a^2 + b^2\}|.$$

The function r_2 has been studied since antiquity. Brahmagupta noticed that

$$\text{if } m = a^2 + b^2 \text{ and } n = c^2 + d^2, \quad \text{then } mn = (ac+bd)^2 + (ad-bc)^2,$$

which shows that if $r_2(m), r_2(n) > 0$, then $r_2(mn) > 0$. Motivated by the same observation, Fermat focused attention on $r_2(m)$ for prime values of m:

$$r_2(2) = 4, \quad r_2(3) = 0, \quad r_2(5) = 8, \quad r_2(7) = 0, \quad r_2(11) = 0, \quad r_2(13) = 8, \quad \ldots$$

In general, let

$$\xi(\tau) = 1 + 4\sum_{m\geq 1}(d_1(m) - d_3(m))q^m, \quad \text{where } d_k(m) = \left|\left\{\begin{array}{c}\text{divisors of } m \\ \equiv k \bmod 4\end{array}\right\}\right|.$$

It turns out that:

Theorem 3.3 (Jacobi)**.** *We have $\theta^2 = \xi$ as functions of τ, or of q. Equivalently,*

$$r_2(m) = 4(d_1(m) - d_3(m))$$

for any integer $m \geq 1$.

Most courses in number theory prove this theorem through pure algebra, and starting from the simpler case due to Fermat where m is prime. Following Stein–Shakarchi, we sketch an analytic proof of the full theorem. First, via some combinatorics,

$$\xi(\tau) = 1 + 4\sum_{m\geq 1} \frac{q^m}{1+q^{2m}} = \sum_{n\in\mathbf{Z}} \frac{2}{q^n + q^{-n}} = \sum_{n\in\mathbf{Z}} \frac{1}{\cos(\pi n\tau)}.$$

Using the last formula, one shows:

Theorem 3.4. *The functions θ^2 and ξ are both examples of functions $f(\tau)$ such that*

(1) $f(\tau + 2) = f(\tau)$.
(2) $f(-\frac{1}{\tau}) = -i\tau f(\tau)$.
(3) *f is analytic on the upper half-plane such that $f(\tau) \to 1$ and $f(1 - \frac{1}{\tau}) \sim -4i\tau e^{\pi i\tau/2}$ as $\mathrm{Im}(\tau) \to \infty$. Moreover, f is nonvanishing.*

Corollary 3.5. *The ratio of functions $F = \xi/\theta^2$ satisfies*

(1) $F(\tau + 2) = F(\tau)$.
(2) $F(-\frac{1}{\tau}) = F(\tau)$.
(3) *F is analytic and uniformly bounded on the upper half-plane.*

You may have seen a famous theorem of complex analysis called Liouville's theorem, stating that if a uniformly bounded function is analytic over all of $\mathbf{C}$, then it must be constant. The same conclusion holds for functions F satisfying the properties above. Indeed, the properties of F are summarized by saying that it is a "holomorphic modular form of weight 0 for the theta congruence subgroup". The only such modular forms are constant. Therefore, θ^2 and ξ are scalar multiples of each other. But they both have constant term 1 in their q-expansions. Therefore $\theta^2 = \xi$.