PARTIAL DIFFERENTIAL EQUATIONS

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It's important to know how to solve separable first-order ODEs and second-order ODEs with constant coefficients (these are covered in CHE1215).

1. Separable PDEs

A PDE involving a function $f(x, y)$ is said to be *separable* if its solution can be written in the form $f(x) = X(x)Y(y)$, i.e., a function in x alone multiplied by a function in y alone.

Example 1. For example, consider the PDE

$$\frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} = 0. \tag{1}$$

Assuming that its solution is of the form $f(x, y) = X(x)Y(y)$, then using the product rule,

$$\frac{\partial f}{\partial x} = \frac{\partial}{\partial x}\big(X(x)Y(y)\big) = \frac{\partial X}{\partial x}Y + X\frac{\partial Y}{\partial x} = \frac{dX}{dx}Y,$$

where $\frac{\partial Y}{\partial x} = 0$ since Y is a function of y alone. Similarly, we get that

$$\frac{\partial f}{\partial y} = \frac{dY}{dy}X.$$

Therefore, plugging this back into (1), we have

$$\frac{dX}{dx}Y + \frac{dY}{dy}X = 0,$$

and dividing throughout by XY,

$$\frac{1}{X}\frac{dX}{dx} + \frac{1}{Y}\frac{dY}{dy} = 0.$$

Notice that the expression $\frac{1}{X}\frac{dX}{dx}$ depends solely on x, and similarly $\frac{1}{Y}\frac{dY}{dy}$ depends solely on y. Thus, since x and y are independent from each other, and these expressions should always add up to 0, this can only happen if $\frac{1}{X}\frac{dX}{dx} = C$ and $\frac{1}{Y}\frac{dY}{dy} = -C$ for some fixed constant C.

Thus, we've reduced the PDE in (1) to two separate ordinary first-order differential equations,

$$\frac{1}{X}\frac{dX}{dx} = C \qquad \text{and} \qquad \frac{1}{Y}\frac{dY}{dy} = -C.$$

Integrating both sides, we get

$$\log X = Cx + \log A \qquad \text{and} \qquad \log Y = -Cy + \log B,$$

thus

$$X = Ae^{Cx} \qquad \text{and} \qquad Y = Be^{-Cy},$$

and therefore, since $f(x, y) = XY$, we get the general solution

$$f(x, y) = De^{C(x-y)},$$

where C, D are arbitrary constants.

Exercise 2. Determine general solutions for the following PDEs, assuming that they are separable.

(1) $2\frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} = 0$

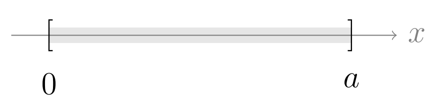
(2) $y\frac{\partial f}{\partial x} - x^2\frac{\partial f}{\partial y} = 0$

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

(4) $y\frac{\partial^2 f}{\partial x^2} - x\frac{\partial^2 f}{\partial y^2} = f(x, y)$

2. The Schrödinger Equation: the one-dimensional case

In CHE1215, we saw the solution of the Schrödinger equation in a "one dimensional box", i.e., the wave function $\Psi(x)$ we are solving for assigns a probability to a particle which lives in an interval $[0, a]$ of real numbers:



Let's review the solution in the one-dimensional case. The Schrödinger equation for a particle of mass m moving along the x axis is

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + V\Psi = E\Psi,$$

where $V(x)$ is the potential energy of the particle at position x, E is the (constant) total energy, and Ψ is the wave function.

The way we model the box is by taking the potential energy function

$$V(x) = \begin{cases} 0 & \text{if } 0 < x < a \\ \infty & \text{otherwise.} \end{cases}$$

The constant value of V inside the box ensures that no force acts on the particle in this region; setting $V = 0$ means that the energy E is the (positive) kinetic energy of the particle. The infinite value of V at the "walls" and outside the box ensures that the particle cannot leave the box; in quantum mechanics this means that the wave function is zero at the walls and outside the box.

For the particle within the box, we therefore have the boundary value problem

$$-\frac{\hbar}{2m}\frac{d\Psi}{dx^2} = E\Psi,$$

with boundary conditions $\Psi(0) = \Psi(a) = 0$. If we let $\omega^2 = 2mE/\hbar^2$, then this is

$$\frac{d^2\Psi}{dx^2} + \omega^2\Psi = 0,$$

which has auxiliary equation

$$k^2 + \omega^2 = 0 \implies k = \pm\omega i,$$

and so we have the general solution

$$\Psi(x) = A\cos(\omega x) + B\sin(\omega x).$$

applying the boundary conditions, we see that

$$\Psi(0) = 0 \implies A\cos(0) + B\sin(0) \implies A = 0,$$

and

$$\Psi(a) = 0 \implies B\sin(\omega a) = 0 \implies \omega a = n\pi$$

for $n = 0, \pm1, \pm2, \ldots$, since the sine function is zero precisely at integer multiples of π. In other words, the solutions of the problem are

$$\Psi_n(x) = B\sin\left(\frac{n\pi x}{a}\right), \qquad n = 1, 2, 3, \ldots$$

where the permitted solutions are labelled with the **quantum number** n. The value $n = 0$ is excluded since the trivial solution $\Psi_0(x) = 0$ has no physical meaning, and the negative values are excluded since $\Psi_{-n} = -\Psi_n(x)$ is simply Ψ_n with a change of sign.

Each solution Ψ_n has corresponding energy value

$$E_n = \frac{\hbar^2\omega^2}{2m} = \frac{h^2\left(\frac{n\pi}{a}\right)^2}{8\pi^2m^2} = \frac{n^2h^2}{8ma^2},$$

since Planck's constant is $h = \hbar/2\pi$.

Finally, since this is a probability function, we require that the "total probability" is 1, i.e., $\int_{-\infty}^{\infty} \Psi(x)^2 \, dx = 1$. The integral is $\frac{a}{2}B^2$, which forces $B = \sqrt{\frac{2}{a}}$.

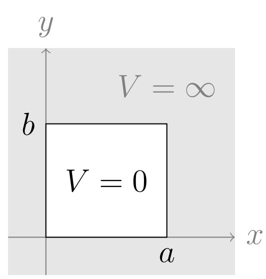
Thus, the solution is

$$\Psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right), \qquad n = 1, 2, 3, \ldots$$

3. The Schrödinger Equation: the two-dimensional case

Now here is the new part which we do not cover in CHE1215: a box which is two dimensional. This time, the "box" is a rectangle in the xy-plane, which we model with the potential energy function

$$V(x, y) = \begin{cases} 0 & \text{if } 0 < x < a \text{ and } 0 < y < b, \\ \infty & \text{otherwise.} \end{cases}$$



This time, the Schrödinger equation is

$$-\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi = E\Psi,$$

where ∇^2 denotes the *Laplacian operator*, defined by

$$\nabla^2 \Psi = \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2}.$$

This is the two-dimensional generalisation of the second derivative.

For particles inside the box, we therefore have the boundary value problem

$$-\frac{\hbar^2}{2m} \nabla^2 \Psi = E\psi,$$

with the boundary conditions $\Psi(x, 0) = \Psi(x, b) = 0$ for all x and $\Psi(0, y) = \Psi(a, y)$ for all y.

assuming $\Psi(x,y)$ is separable, i.e., we can express $\Psi(x,y) = X(x)Y(y)$, then the equation becomes

$$\frac{d^2X}{dx^2}Y + X\frac{d^2Y}{dy^2} = -\frac{2mE}{\hbar^2}\Psi,$$

and dividing through by $\Psi = XY$, we get

$$\frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\frac{d^2Y}{dy^2} = -\frac{2mE}{\hbar^2}.$$

Thus we have

$$\frac{1}{X}\frac{d^2X}{dx^2} = -C_1 \qquad \text{and} \qquad \frac{1}{Y}\frac{d^2Y}{dy^2} = -C_2$$

where $C_1 + C_2 = 2mE/\hbar^2$. In other words,

$$X'' + C_1X = 0 \qquad \text{and} \qquad Y'' + C_2Y = 0.$$

These are both separate instances of the one-dimensional box case, which have general solutions

$$X = A\sin(\sqrt{C_1}x) \qquad \text{and} \qquad Y = B\sin(\sqrt{C_2}y)$$

respectively (notice the boundary conditions $X(0) = Y(0) = 0$ give the forms above).

Moreover, since $X(a) = 0$, we have $\sin(\sqrt{C_1}a) = 0$, so we must have $\sqrt{C_1}a = m\pi$ for some m, i.e., $\sqrt{C_1} = m\pi/a$. Similarly, since $Y(b) = 0$, we get that $\sqrt{C_2} = n\pi/b$ for some integer n.

Thus, relabelling AB with C, we get

$$\Psi_{m,n}(x) = XY = C\sin\left(\frac{m\pi}{a}x\right)\sin\left(\frac{n\pi}{b}y\right).$$

Similarly to before, we want $\iint_{\mathbb{R}^2}\Psi(x,y)^2\,dx\,dy = 1$, which forces the constant $C = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{b}} = \sqrt{\frac{4}{ab}}$. Thus the solutions are

$$\Psi_{m,n}(x) = \sqrt{\frac{4}{ab}}\sin\left(\frac{m\pi}{a}x\right)\sin\left(\frac{n\pi}{b}y\right),$$

and the corresponding energy values are

$$E_{m,n} = \frac{h^2}{8m}\left(\frac{m^2}{a^2} + \frac{n^2}{b^2}\right).$$

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