

Classical waves

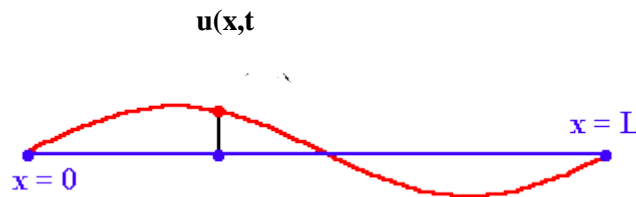


Figure 2.1: A vibrating string

A linear partial differential equation

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

Boundary conditions

$$u(0,t) = 0 \quad \text{and} \quad u(L,t) = 0 \quad \text{at all times}$$

Separation of variables: A technique used when the two variables are independent

$$u(x,t) = X(x)T(t)$$

which gives

$$\frac{1}{X(x)} \frac{d^2 X(x)}{dx^2} = \frac{1}{v^2 T(t)} \frac{d^2 T(t)}{dt^2}$$

Since LHS is only dependent on the position and RHS on time they must be equal to a constant, K

$$\frac{d^2 X(x)}{dx^2} - KX(x) = 0 \quad \text{and} \quad \frac{d^2 T(t)}{dt^2} - Kv^2 T(t) = 0$$

These are linear differential equations with constant coefficients.

Solutions $K = 0, K < 0, K > 0$

For $K = 0$, the solution are trivial – no use

For $K > 0$, its a subset of the solution for $K < 0$

For $K < 0$

Lets rewrite the equation in this form $\frac{d^2 y}{dx^2} + k^2 y = 0$ where $K = -\beta^2$

We need a solution that when differentiated twice gives back the same function. Lets try $y = e^{\alpha x}$

This gives, $(\alpha^2 + \beta^2) y(x) = 0$

i.e. $\alpha = \pm i \beta$

The general solution is then

$$y(x) = c_1 e^{i\beta x} + c_2 e^{-i\beta x}$$

Using Euler's formula,

$$e^{\pm i\theta} = \cos\theta \pm i \sin\theta$$

we get

$$y(x) = A \cos \beta x + B \sin \beta x$$

See for yourself that the case of $K > 0$ is a special case of the solutions for $K < 0$.

Boundary conditions: See the two equations for $X(x)$ and $T(t)$

$$X(0) = 0 \text{ implies } A = 0$$

$$X(l) = 0 \text{ implies } X(l) = B \sin \beta l = 0 \quad B = 0 \text{ is trivial. So, } \sin \beta l = 0 \text{ gives}$$

$$\beta l = n\pi \quad n = 1, 2, 3 \dots$$

$n = 0$ is not a solution because the wave does not exist.

$$X(x) = B \sin \frac{n\pi x}{l}$$

Also, for $T(t)$

$$\frac{d^2 T(t)}{dt^2} + \beta^2 v^2 T(t) = 0$$

The general solution (remember $\beta = n\pi/l$) is

$$T(t) = D \cos \omega_n t + E \sin \omega_n t$$

So the amplitude of the wave u is given by (it now depends on n)

$$\begin{aligned} u_n(x, t) &= X(x)T(t) = \left(B_n \sin \frac{n\pi x}{l} \right) (D_n \cos \omega_n t + E_n \sin \omega_n t) \\ &= (F_n \cos \omega_n t + G_n \sin \omega_n t) \sin \frac{n\pi x}{l} \end{aligned}$$

Superposition

As each $u_n(x, t)$ is a solution to the linear differential equation, so is any sum of the $u_n(x, t)$'s.

A most general solution is

$$u(x, t) = \sum_{n=1}^{\infty} (F_n \cos \omega_n t + G_n \sin \omega_n t) \sin \frac{n\pi x}{l}$$

or

$$u(x, t) = \sum_{n=1}^{\infty} A_n \cos(\omega_n t + \phi_n) \sin \frac{n\pi x}{l}$$

where A is the amplitude and ϕ the phase angle. No matter how the string is plucked its shape will evolve according to the above equations.

Each $u_n(x, t)$ is called a normal mode. The time dependence of each normal mode represents harmonic motion of frequency $\nu_n = \omega_n/2\pi = vn/2l$ (since $\omega_n = n\pi v/l$)

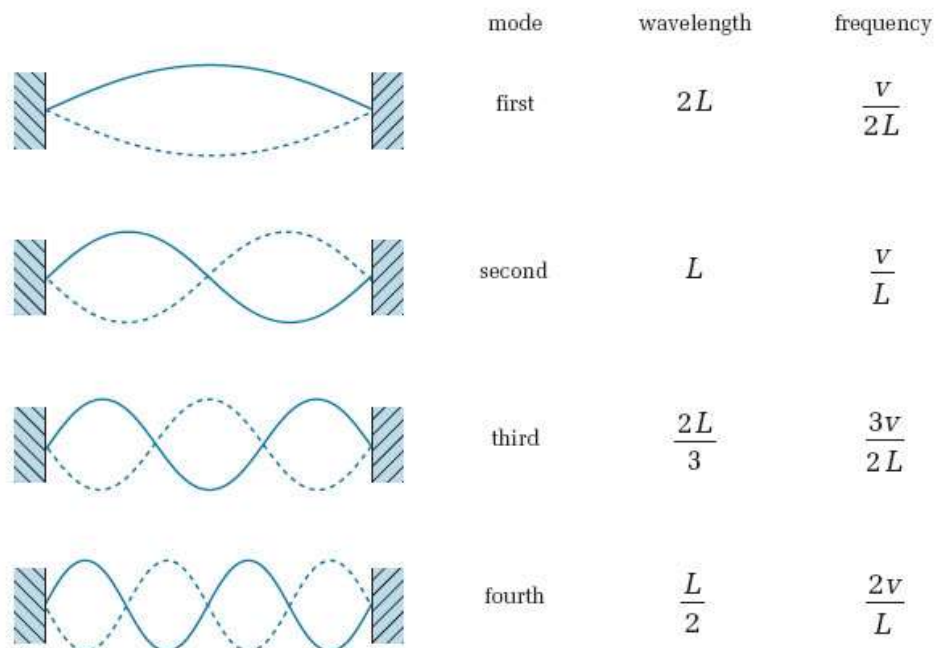


Figure 1.2: The first few modes of vibration

First harmonic = fundamental mode, frequency $v/2l$

Second harmonic = first overtone, frequency v/l

Mid-point of the second harmonic does not change with time. Its fixed at zero. This is a **node** which you will also encounter in quantum mechanics. $x = 0$ and $x = l$ are not nodes – they are boundary conditions.

These are standing waves.

Add up the first two harmonics, phase shifted by 90°

$$u(x, t) = \cos \omega_1 t \sin \frac{\pi x}{l} + \frac{1}{2} \cos \left(\omega_2 t + \frac{\pi}{2} \right) \sin \frac{2\pi x}{l}$$

Some work: sketch the travelling wave.

Schrödinger Equation

Lets start with the classical wave equation

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 u}{\partial t^2}$$

which as we have seen above can be solved to give

$$u(x, t) = \psi(x) \cos \omega t$$

$\psi(x)$ is called the spatial amplitude of the wave. This gives,

$$\frac{d^2 \psi}{dx^2} + \frac{\omega^2}{v^2} \psi(x) = 0$$

Since $\omega = 2\pi\nu$ and $\nu\lambda = v$,

$$\frac{d^2 \psi}{dx^2} + \frac{4\pi^2}{\lambda^2} \psi(x) = 0$$

Now the total energy

$$E = KE + PE = \frac{p^2}{2m} + V(x)$$

and so

$$p = \{2m[E - V(x)]\}^{1/2}$$

Use de Broglie relation $\lambda = h/p$. This is where quantum mechanics comes in

$$\lambda = \frac{h}{p} = \frac{h}{\{2m[E - V(x)]\}^{1/2}}$$

and we get,

$$\frac{d^2 \psi}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)] \psi(x) = 0$$

or

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V(x)\psi(x) = E \psi(x)$$

This is the time-independent Schrödinger equation

In this course we will not worry about the time-dependent Schrödinger equation

Operators

An operator operates – it does something. For example, an “turn 90° left” is an operator that tells us to turn left by 90°. Another example could be “walk five paces ahead”.

Mathematical operators tell us to perform a mathematical operation on a function $f(x)$ to give another function $g(x)$.

Some examples of mathematical operators

$$\text{INTEGRATE: } \int_0^1 f(x) = g(x)$$

$$\text{SQR: } (f(x))^2 = g(x)$$

$$\text{DIFFERENTIATE: } \frac{d}{dx} f(x) = g(x)$$

In general we can denote an operator using a hat on it,

$$\hat{A} f(x) = g(x)$$

Operators and quantum mechanics

In quantum mechanics, we encounter only linear operators. This is one of the postulates of QM which we will discuss later.

$$\hat{A} [c_1 f_1(x) + c_2 f_2(x)] = c_1 \hat{A}(f_1(x)) + c_2 \hat{A}(f_2(x))$$

Here c_1 and c_2 can be complex numbers.

Differentiate and integrate are linear. Squaring is non-linear.

Operators may not commute like numbers, i.e. $\hat{A} \hat{B} f(x)$ is not necessarily equal to $\hat{B} \hat{A} f(x)$. As an example consider the case of a person walking five paces and turning 90°.

Eigenfunctions and Eigenvalues

A function that gets operated and results in the same function apart from a multiplicative factor is an eigenfunction of the operator

$$\hat{A} f(x) = a f(x)$$

Finding the eigenfunction of the operator and the eigenvalue is called an eigenvalue problem.

The Schrödinger equation can be written as

$$\left[-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V(x) \right] \psi(x) = E \psi(x)$$

or

$$\hat{H} \psi(x) = E \psi(x)$$

where \hat{H} is called the Hamiltonian operator and the eigenvalue is the energy. So there is a correspondence between the operator and a measurable. Such correspondences between operators and classical-mechanical variables are fundamental to the formalism of QM.

Since the energy is KE + PE, and $\widehat{PE} = V(x) \therefore \widehat{KE} = -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2}$

$$KE = \frac{p^2}{2m} \Rightarrow \hat{p}^2 = -\hbar^2 \frac{d^2\psi}{dx^2}$$

$$\therefore \hat{p} \cdot \hat{p} = -\hbar^2 \frac{d^2\psi}{dx^2} \text{ or } \hat{p} = -i\hbar \frac{d}{dx} \text{ (the minus sign is needed for the correct direction)}$$

Probability

Discrete Events

An experiment has n possible outcomes, each with probability p_j . We perform the experiment a large number of times (ideally infinite number of times)

$$p_j = \lim_{n \rightarrow \infty} \frac{N_j}{N} \quad j = 1, 2, 3 \dots n$$

$$0 \leq p_j \leq 1 \quad \text{and} \quad \sum p_j = 1 \quad (\text{normalization})$$

Suppose we get a value x_j at the j^{th} experiment, then the average is defined as

$$\langle x \rangle = \sum x_j p_j = \sum x_j p(x_j)$$

Second moment

$$\langle x^2 \rangle = \sum_{j=1}^n x_j^2 p_j$$

Second central moment or variance

$$\sigma_x^2 = \langle (x - \langle x \rangle)^2 \rangle = \sum_{j=1}^n (x_j - \langle x \rangle)^2 p_j = \langle x^2 \rangle - \langle x \rangle^2$$

σ_x is called the standard deviation.

Continuous distributions

$$\text{prob}(x, x + dx) = p(x)dx$$

$$\text{prob}(a \leq x \leq b) = \int_a^b p(x)d(x)$$

Normalization condition

$$\int_{-\infty}^{\infty} p(x) d(x) = 1$$

Average and standard deviation

$$\langle x \rangle = \int_{-\infty}^{\infty} x p(x) d(x)$$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 p(x) d(x)$$

$$\sigma_x^2 = \int_{-\infty}^{\infty} (x - \langle x \rangle)^2 p(x) d(x)$$

Quantum mechanics and probability

If we restrict the particle in a certain region, then the probability of finding the particle in this region is one. Outside this region the particle does not exist. Since the intensity of a wave is the square of the magnitude of the amplitude, mathematically we say $\psi^*(x)\psi(x)dx$ is the probability that the particle is located between x and $x + dx$.