

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 and u(l,t) = 0 at all times

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

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

which gives

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

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

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

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  $\frac{d^2y}{dx^2} + k^2y = 0$  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 implies A = 0

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

$$\beta l = n\pi$$
  $n = 1,2,3...$ 

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)

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

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)

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

#### **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  $\phi$  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  $v_n = \omega_n/2\pi = vn/2l$  (since  $\omega_n = n\pi v/l$ )

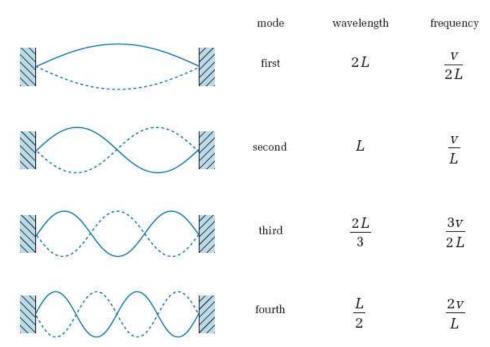


Figure 1.2: The first few modes of vibration

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

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

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

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

and we get,

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

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

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

 $SQR: (f(x))^2 = g(x)$ 

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

$$\widehat{H}\,\psi(x)=\,E\,\psi(x)$$

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  $\widehat{PE} = V(x)$   $\therefore$   $\widehat{KE} = -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2}$ 

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

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

### **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)

$$p_j = \lim_{n \to \infty} \frac{N_j}{N} \qquad \qquad j = 1, 2, 3 \dots n$$
$$0 \le p_j \le 1 \quad \text{and} \quad \Sigma p_j = 1 \quad (\text{normalization})$$

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

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

Second momemt

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

Second central moment or variance

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

 $\sigma_{\chi}$  is called the standard deviation.

**Continuous distributions** 

$$prob(x, x + dx) = p(x)dx$$

$$prob \ (a \le x \le b) = \int_{a}^{b} p(x)d(x)$$

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.