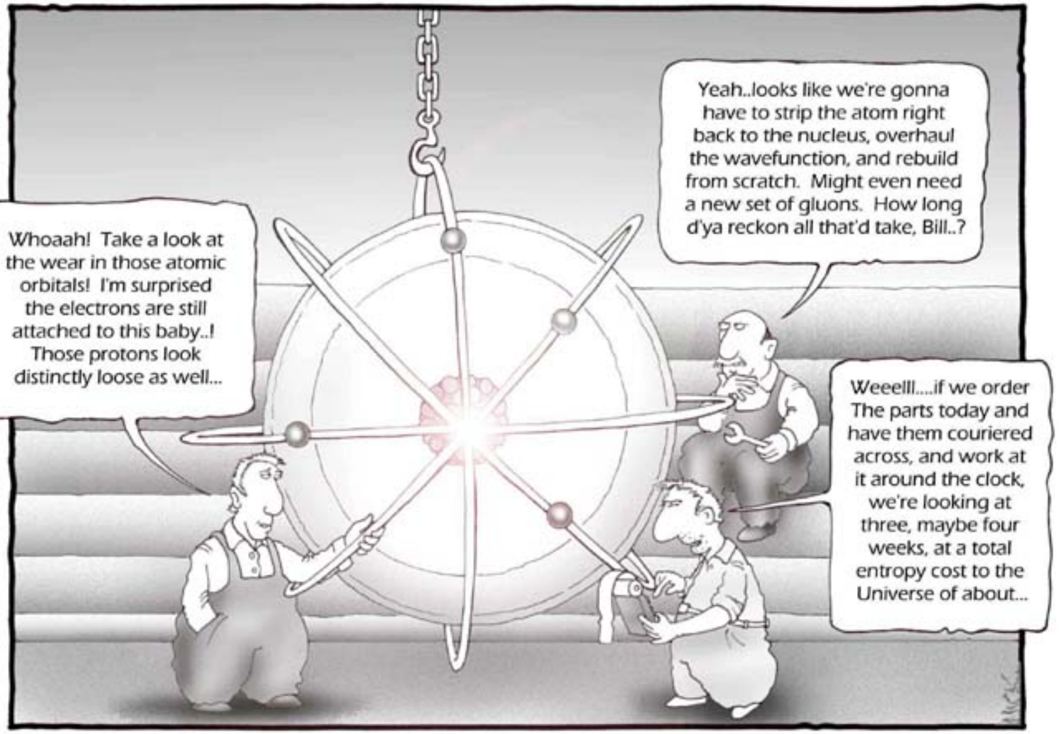
Reminder: http://www.star.le.ac.uk/nrt3/QM/

Lecture 4: extending the ideas

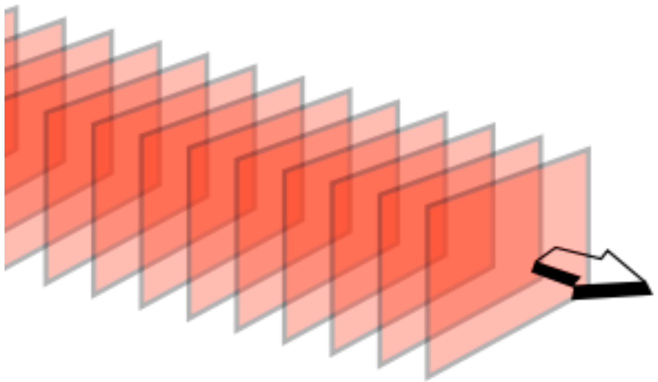
In this lecture we introduce quantum mechanics applied to free particles and time varying situation. We also meet further examples of how QM can explain phenomena which are observed in nature, but are not allowed by classical physics.



Quantum mechanics.

Travelling waves hitting a step

Plane waves of fixed momentum are described by wavefunctions $\psi\,(x,t) = Ae^{i(kx\,-\omega t)}$ where $k = 2\pi\,/\lambda$ is the **wavenumber** and $\omega = 2\pi f$ is the **angular frequency**. If potential fixed, can apply the time-independent form of the Schrodinger equation even in problems involving travelling waves:



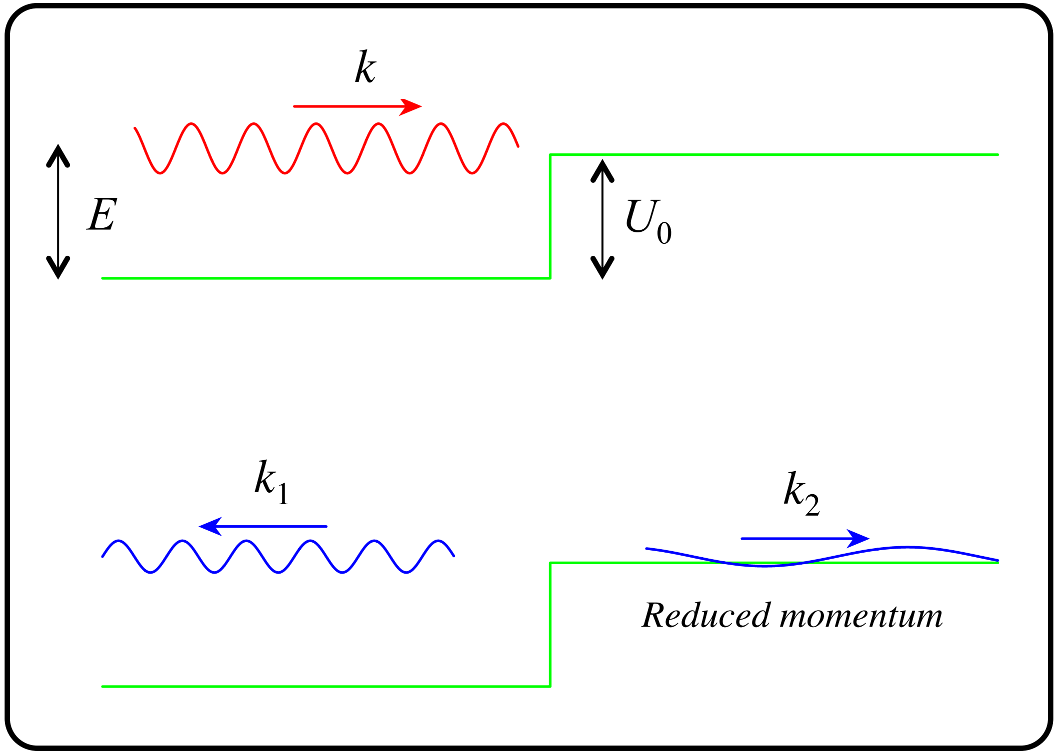
*Aside: in general wave-functions are **complex** and the probabilities really come from evaluating the **square modulus** $|\psi\,|^2 = \psi\psi^*$, where ψ^* is the complex conjugate.*

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

$$\Rightarrow \quad k = \sqrt{\frac{2m(E-V)}{\hbar^2}}$$

Travelling waves hitting a step

For example, consider such a wave hitting a potential step where $E > U_0$. We are interested in the properties of the reflected and transmitted waves.



$$k = -k_1 = \sqrt{\frac{2mE}{\hbar^2}}\ ;\ k_2 = \sqrt{\frac{2m(E-U_0)}{\hbar^2}}$$

Travelling waves hitting a step

Combined wavefunction left of step (at fixed time): $\psi = A\exp(ik_1 x) + B\exp(-ik_1 x)$

And right of step: $\psi = C\exp(ik_2 x)$

Consider $A=1$ (since dealing with relative flux before and after hitting step), and apply continuity and differentiability requirement at the step ($x=0$):

$$1 + B = C \quad ; \quad k_1 - Bk_1 = Ck_2$$

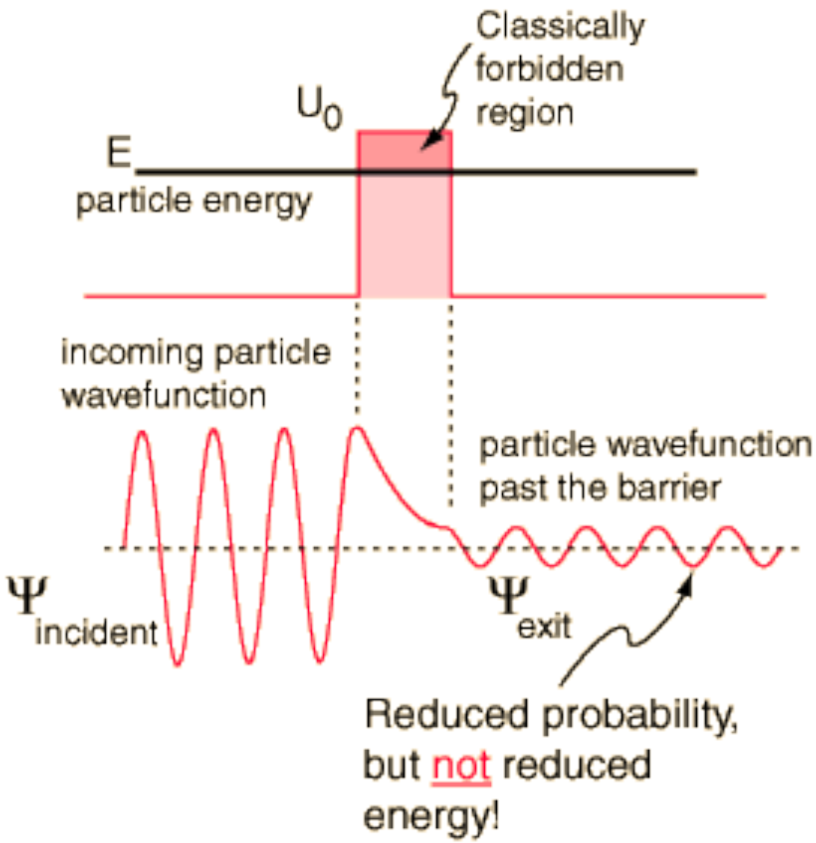
$$\Rightarrow \quad k_2(1+B) = k_1(1-B) \quad \Rightarrow B(k_2 + k_1) = k_1 - k_2$$

The probability of reflection P_R and transmission P_T of an individual photon can be obtained by squaring:

$$P_R = B^2 = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} \quad , \quad P_T = 1 - P_R = \frac{4k_1 k_2}{(k_1 + k_2)^2}$$

Travelling waves hitting a barrier

Another application we can analyse is that of quantum waves hitting a potential barrier. Of particular interest is when the incoming particle(s) have lower energy than the barrier.



Travelling waves hitting a barrier

If barrier has height U_0, then within the barrier solution to SE is:

$$\psi = A\exp(-\alpha x)\,; \quad \alpha = \sqrt{\frac{2m}{\hbar^2}(U_0 - E)}$$

Hence for barrier of width L the amplitude of the wavefunction after the barrier is given by:

$$B = A\exp(-\alpha L)$$

Unlike classical particles, even when a quantum wave impinges on a barrier which is higher than the energy of the particle, there is some small probability that the particle "**tunnels**" through and is found at the other side:

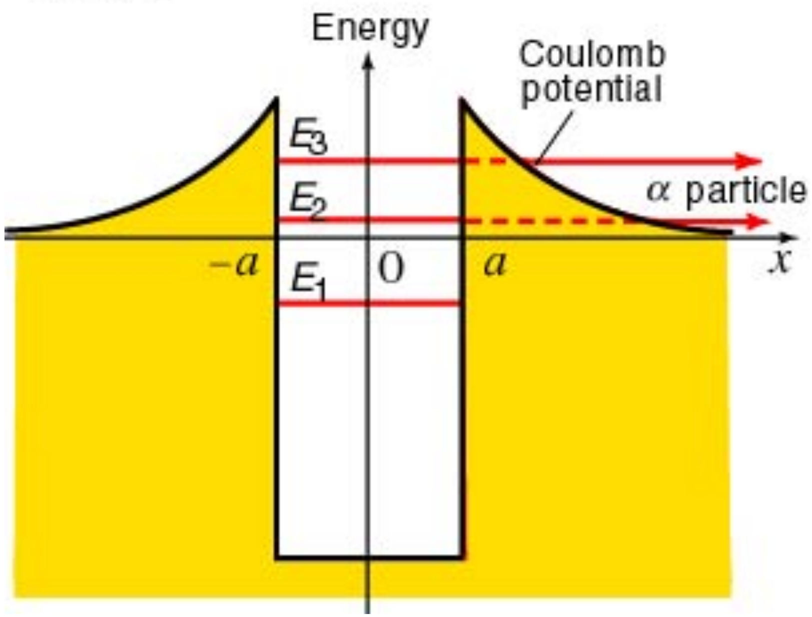
$$P_T = \frac{B^2}{A^2} = \exp(-2\alpha L)$$

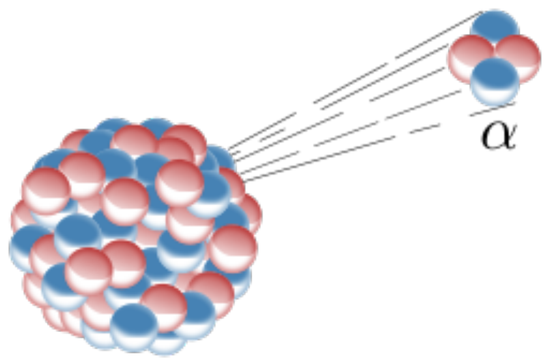
Logically, the probability of reflection: $P_R = 1 - P_T$

Tunnelling

Tunnelling of this sort can also allow particles to escape from a potential well when the seemingly have insufficient energy. The best known example is that of **alpha decay**, in which a He nucleus is ejected from a heavier nucleus, despite the strong nuclear forces acting on it.

Fig. (B)





Time-dependent Schrodinger equation

So far we have considered systems which are analogous to static potential problems in classical mechanics, but frequently systems evolve with time. The Schrodinger equation, discovered in 1926, which incorporates time evolution of the potential is somewhat more complicated.

It replaces Newton's classical laws of motion (of course, Newton's laws are a consequence of quantum mechanical rules when applied to large systems). The left hand side now represents the **energy operator,** which applied to the wave-function tells us the energy. Other properties can be determined by applying other **differential operators**.

$$\boxed{i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}.\frac{\partial^2\psi}{\partial x^2} + V(x,t)\psi(x,t)}$$

Note: historically, the equivalent (but often less practical) method of **matrix mechanics** was developed by Heisenberg in 1925 (and both were subsumed into an even more general mathematical scheme by Dirac in 1927, who also went on to develop the relativistic version of quantum theory).

Operator formalism

The time derivative in the Schrodinger equation is known as the energy operator. To find the expectation for energy we actually evaluate:

$$\langle E \rangle = \int_{-\infty}^{\infty} \psi^{*} \, i\hbar \frac{\partial}{\partial t} \psi \, dx$$

Other properties can be found with different operators, e.g. momentum operator is:

$$\hat{p} = -i\hbar \frac{\partial}{\partial x}$$

Higher dimensions

Most problems in the real world are 3-dimensional, and the mathematics is easily extended.

The 3D version of the time-dependent Schrodinger wave equation is:

$$\boxed{i\hbar\frac{\partial}{\partial t}\psi(\mathbf{x},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{x},t) + V(\mathbf{x},t)\psi(\mathbf{x},t)}$$

Where ∇^2 is the Laplacian operator:

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$$

The uncertainty principle revisited

In addition to Heisenberg's original position-momentum uncertainty principle, quantum mechanics limits the accuracy of other pairs of observable properties. Of particular importance is the energy-time uncertainty principle:

$$\Delta E \Delta t > \frac{\hbar}{2}$$

It is better to understand this as limiting the precision we can measure the energy of a quantum state if we observe a system over a limited interval of time Δt. This has the implication that it is possible to create energy from nothing for a short period. The startling consequence is that even in a vacuum particles (called **virtual particles**) can be appear spontaneously, as long as they annihilate and disappear on a time scale that doesn't contravene the uncertainty relation. In modern quantum field theory, the fundamental forces of nature are understood to be transmitted by particular virtual particles!