H2 Topic 18c

Quantum Physics (III):

A Primer of Quantum Mechanics

Content

- Energy of a photon
- The photoelectric effect
- Wave-particle duality
- Energy levels in atoms
- Line spectra
- X-ray spectra
- The uncertainty principle
- Schrodinger model
- Barrier tunnelling

Learning Outcomes

Candidates should be able to:

(a) show an appreciation of the particulate nature of electromagnetic radiation.

(b) recall and use $E = hf$.

(c) show an understanding that the photoelectric effect provides evidence for a particulate nature of electromagnetic radiation while phenomena such as interference and diffraction provide evidence for a wave nature.

(d) recall the significance of threshold frequency.

(e) recall and use the equation $\frac{1}{2}mv_{max}^2 = eV_s$, where V_s is the stopping potential.

(f) explain photoelectric phenomena in terms of photon energy and work function energy.

(g) explain why the maximum photoelectric energy is independent of intensity whereas the photoelectric current is proportional to intensity.

(h) recall, use and explain the significance of $hf = \Phi + \frac{1}{2}mv_{max}^2$.

(i) describe and interpret qualitatively the evidence provided by electron diffraction for the wave nature of particles.

(j) recall and use the relationship for the de Broglie wavelength $\lambda = h/p$.

(k) show an understanding of the existence of discrete electron energy levels in isolated atoms (e.g. atomic hydrogen) and deduce how this leads to spectral lines.

(l) distinguish between emission and absorption line spectra.

(m) recall and solve problems using the relation $hf = E_1 - E_2$.

(n) explain the origins of the features of a typical X-ray spectrum using quantum theory.

(o) show an understanding of and apply the Heisenberg position-momentum and time-energy uncertainty principles in new situations or to solve related problems.

(p) show an understanding that an electron can be described by a wave function Ψ where the square of the amplitude of wave function $|\Psi|^2$ gives the probability of finding the electron at a point. (No mathematical treatment is required.)

(q) show an understanding of the concept of a potential barrier and explain qualitatively the phenomenon of quantum tunnelling of an electron across such a barrier.

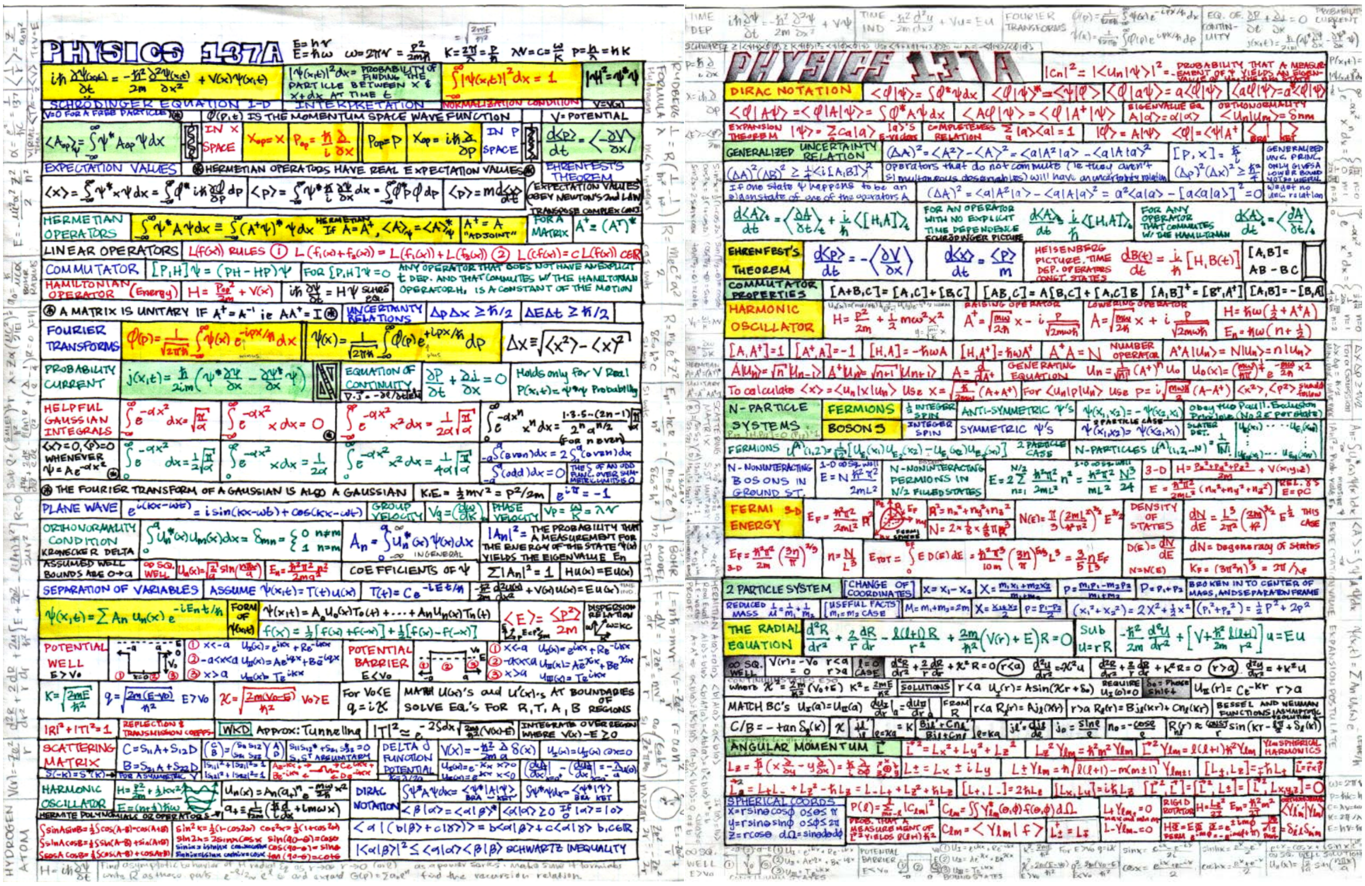
(r) describe the application of quantum tunnelling to the probing tip of a scanning tunnelling microscopy (STM) and how this is used to obtain atomic-scale images of surfaces. (Details of the structure and operation of a scanning tunnelling microscope are not required.)

(s) apply the relationship transmission coefficient $T \propto exp(-2kd)$ for the STM in related situations or to solve problems. (Recall of the equation is not required.)

(t) recall and use the relationship $R + T = 1$, where R is the reflection coefficient and T is the transmission coefficient, in related situations or to solve problems.

18c.0 Introduction

Quantum *mechanics*, as the name implies, is a study on the *behaviour* of quantum objects when subjected to external stimuli. Since the behaviour of quantum objects can be either represented in a wave form or a particle form, one can expect the mathematics involved to be somewhat… *challenging.*



A reasonable "cheatsheet" for introductory Quantum Mechanics at the undergraduate level

Fortunately, we shall aim to achieve a basic understanding of "QM" here without the need for rigorous mathematical treatment.

18c.1 The Heisenberg Uncertainty Principle

Werner Heisenberg was a German theoretical physicist who was awarded the Nobel Prize in Physics in 1932 "for the creation of quantum mechanics". He was best known for his uncertainty principle, which was published in 1927.

His paper puzzled both physicists and historians because of the obscure system of math used. It was later through the combined efforts of other scientists that Heisenberg's findings were transcribed to using matrices. Up to this time, matrices were seldom used by physicists and were considered to belong to the realm of *esoteric* mathematics.

The uncertainty principle asserts a fundamental limit to the degree of precision with which certain pairs of physical properties can be determined at the same time.

It is impossible to simultaneously measure the exact position and exact momentum of an object.

The Heisenberg Uncertainty Principle (Position and Momentum)

If a measurement of the position of a particle is made with precision Δx,
and a simultaneous measurement of its momentum is measured in the x-direction
with precision Δp,
the product of these two uncertainties can never be smaller than $\frac{\hbar}{2}$.

$$\Delta x \, \Delta p \geq \frac{\hbar}{2}$$

where $\hbar$ (h-bar) is the reduced Planck's constant, $\hbar = \frac{h}{2\pi}$.

Loosely speaking, if we restrict the length in which a quantum particle is allowed to move around, it starts to move all around violently.

Example 1

The size of a nucleus in an atom is about 1.0×10^{-15} m (or 1 *femto*-metre). If an electron of mass $m_e = 9.11 \times 10^{-31}$ kg is confined within the nucleus, estimate the uncertainty in the velocity of the electron.

Solution:

By Heisenberg Uncertainty Principle:

$$\Delta x\, \Delta p \geq \frac{\hbar}{2}$$

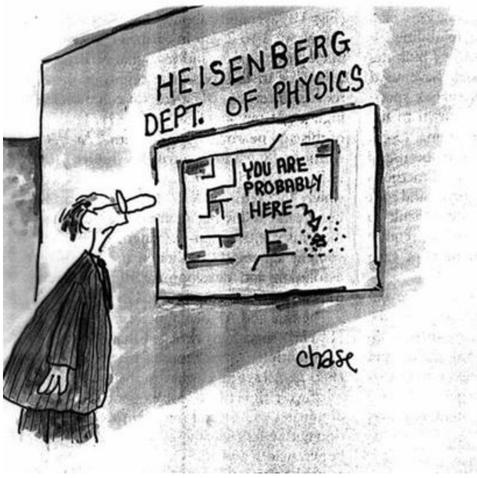
$$\Delta x\, [m_e(\Delta v)] \geq \frac{h}{4\pi}$$

$$\Delta v \geq \frac{h}{4\pi m_e \Delta x}$$

$$\geq \frac{6.63 \times 10^{-34}}{4\pi(9.11 \times 10^{-31})(1.0 \times 10^{-15})}$$

$$\Delta v \geq 5.7 \times 10^{10} \text{ m s}^{-1}$$

NB: The uncertainty "allows" the electron to be possibly faster than the speed of light. Hence, it is not physically possible for an electron to be confined within an atomic nucleus



Example 2

The Bohr's model of a hydrogen atom assumes that the lone electron revolves around the 1-proton nucleus in a circular path with a fixed, well-defined radius. The tangential velocity of the electron is estimated to be 2.2×10^6 ms^{-1}.

Estimate the uncertainty in the position of the electron if the uncertainty in the momentum is half the momentum of the electron ($\Delta p = \frac{1}{2}p$).

Solution:

By Heisenberg Uncertainty Principle:

$$\Delta x \, \Delta p \geq \frac{\hbar}{2}$$

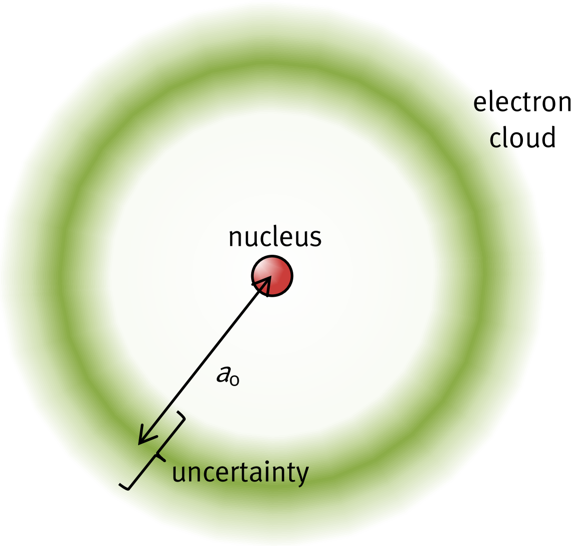
$$\Delta x \geq \frac{\hbar}{2\Delta p}$$

$$\geq \frac{h}{4\pi\left(\frac{1}{2}mv\right)}$$

$$\geq \frac{h}{2\pi m_e v}$$

$$\geq \frac{6.63 \times 10^{-34}}{2\pi(9.11 \times 10^{-31})(2.2 \times 10^6)}$$

$$\Delta x \geq 0.0526 \text{ nm}$$



NB: The "average" distance the electron is from the nucleus, denoted as a_0, is 0.529 nm, which makes the uncertainty to be at 10%.

This is where the concept of an "electron cloud" and the "orbital" being "a region of space around the nucleus with the highest probability of locating electrons" comes about; we can never really exactly pinpoint where the electron is.

The Heisenberg Uncertainty Principle (Energy and Time)

There is another form of the uncertainty principle which sets a limit to the change in energy of a system ΔE, over a finite time internal Δt.

$$\Delta E \, \Delta t \geq \frac{\hbar}{2}$$

Example 3

Lasers ideally output light of a fixed wavelength. However, there is a slight margin of error in the wavelength due to the Heisenberg Uncertainty Principle. Given that the lifetimes of atomic de-excitations occur in the order of 3 ns, find the range of output wavelengths for a laser designed to provide laser of wavelength 590 nm.

Solution:

Photon energy of laser:

$$E = hf = \frac{hc}{\lambda}$$

By Heisenberg Uncertainty Principle:

$$\Delta E \, \Delta t \geq \frac{\hbar}{2}$$

$$\Delta E \approx \frac{h}{4\pi\Delta t}$$

Wavelength limits:

$$E_{limits} = E \pm \Delta E = \frac{hc}{\lambda_{limits}}$$

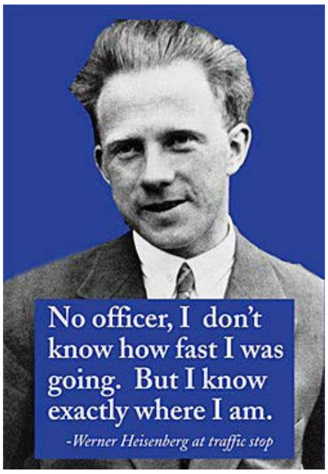
$$\lambda_{limits} = \frac{hc}{E \pm \Delta E}$$

$$= \frac{hc}{\frac{hc}{\lambda} \pm \frac{h}{4\pi\Delta t}}$$

$$= \frac{1}{\frac{1}{\lambda} \pm \frac{1}{4\pi c\Delta t}}$$

$$= \frac{1}{\frac{1}{590 \times 10^{-9}} \pm \frac{1}{4\pi(3 \times 10^{8})(3 \times 10^{-9})}}$$

$$= [589, 590] \text{ nm}$$



Example Quattro

The force which holds the protons and neutrons together in an atomic nucleus is known as the *nuclear strong force*. It has to be far stronger than the forces of electromagnetism, in order to overcome the electrostatic repulsion between protons.

The *strong force* is facilitated by the nucleons (either protons or neutrons) exchanging elementary particles called **gluons,** which travel at light speed. Given that the *rest* mass of the gluon is 265 m_e, estimate the (i) range of the nuclear strong force and (ii) the life-time over which the exchange takes place.

Solution:

(i)By Heisenberg Uncertainty Principle:

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

$$(mc^2)\Delta t \geq \frac{h}{4\pi}$$

$$\text{Range} \approx c\Delta t \approx \frac{h}{4\pi mc}$$

$$\approx \frac{6.63\times10^{-34}}{4\pi(265)(9.11\times10^{-31})(3\times10^{8})}$$

$$\approx 0.73\text{ fm }(0.73\times10^{-15}\text{ m})$$

(ii)

$$\Delta t \approx \frac{\text{range}}{c}$$

$$\approx 2.4\times10^{-24}\text{ s}$$

NB: the range of the nuclear strong force, going by this estimation, is about 0.6 times the radius of a proton.

18c.2 The Wave Function

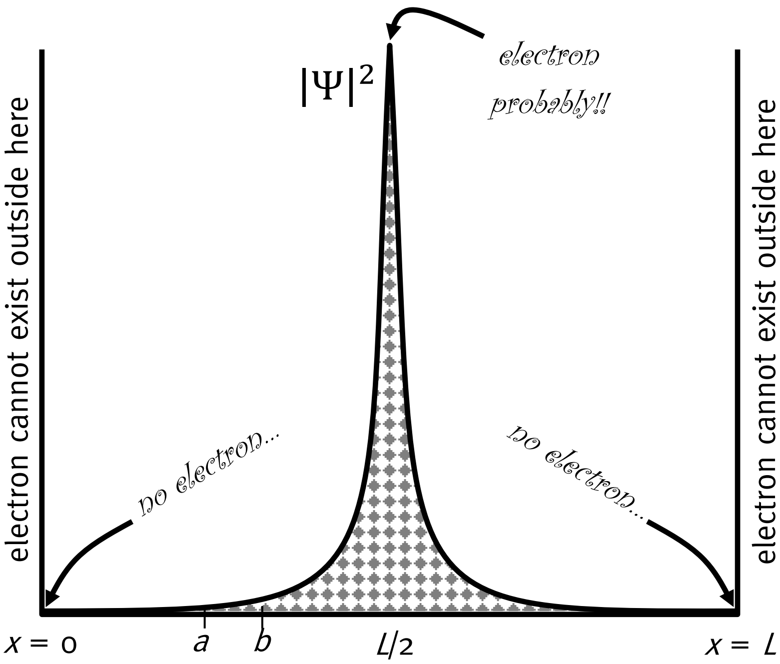
Erwin Schrödinger was an Austrian physicist who was awarded the Nobel Prize for Physics in 1933 for the formulation of the Schrödinger equation.

Since a quantum particle can behave both as a particle and as a wave, the equation completely describes all the various properties of the quantum particle.

Here, we deal with a wave function representing an electron, confined along a 1-dimensional length.

The Wave Function Ψ

The square of the amplitude of wave function $|\Psi|^2$ gives the probability of finding the electron at a point.



When we graph out the square of the wave function along the x-axis, we obtain the probability distribution function. This *PDF* is for the probability of locating the quantum particle. It follows that

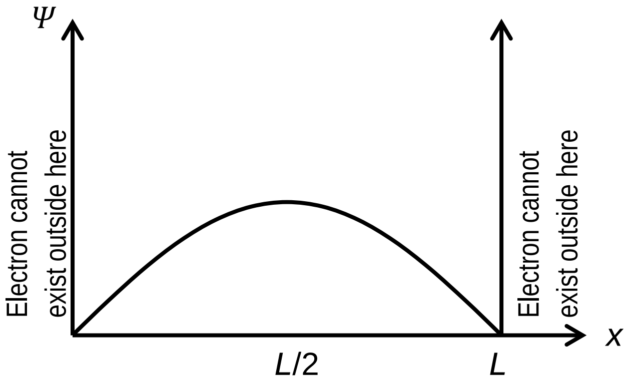
(i) the total area marked by the diagonal checks is 1

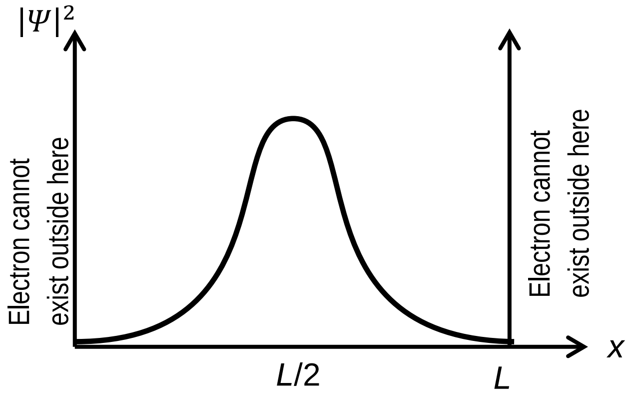
(ii) to find the probability of finding the electron between a and b, we find the area under graph (mathematically, $\int_a^b |\Psi|^2 \, dx$)

Example 5

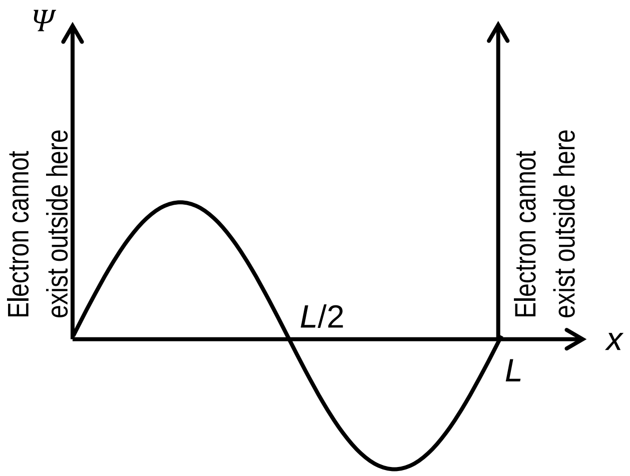
The wave-functions for individual electrons are given on the left-hand columns. Sketch the probability function for the corresponding electron on the right.

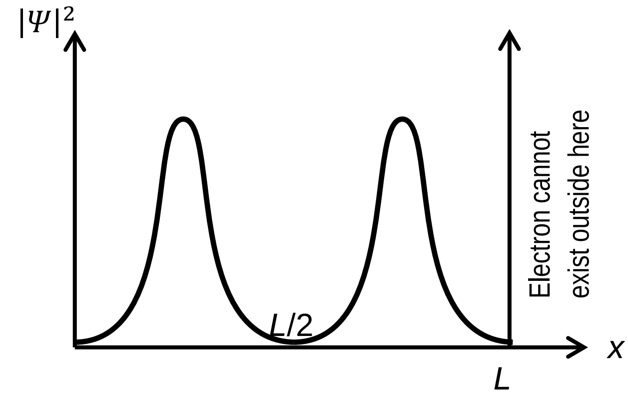
Solutions:



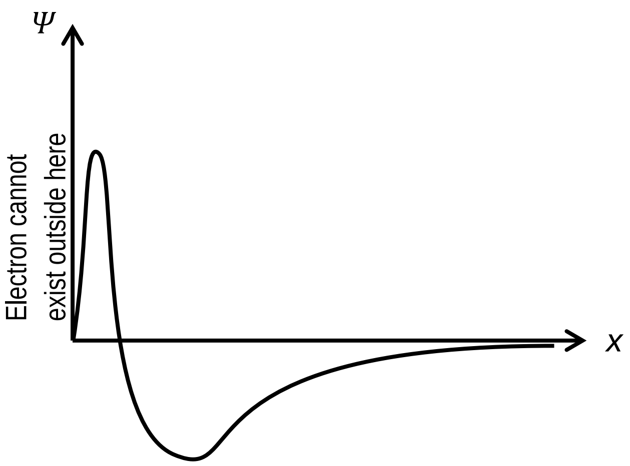


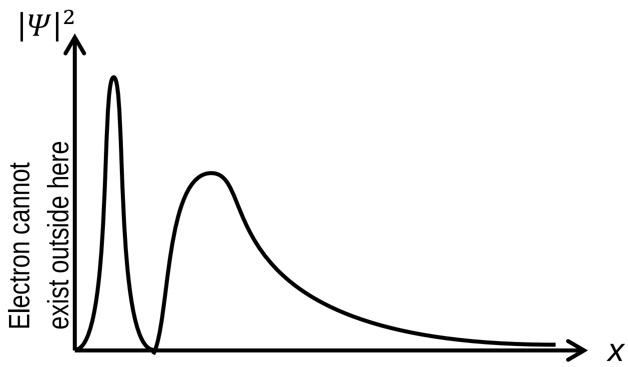
Electron is most likely to be at $L/2$. Total area under graph is 1.





The electron is half as probable to be in [0, $L/2$] as [$L/2$, L]. Total area under graph is 1.





There is still a remote possibility of finding an electron as $x \rightarrow \infty$. Total area under graph is 1.

Example 6

The probability density function for the location of the lone electron in a hydrogen atom can be described by the equation

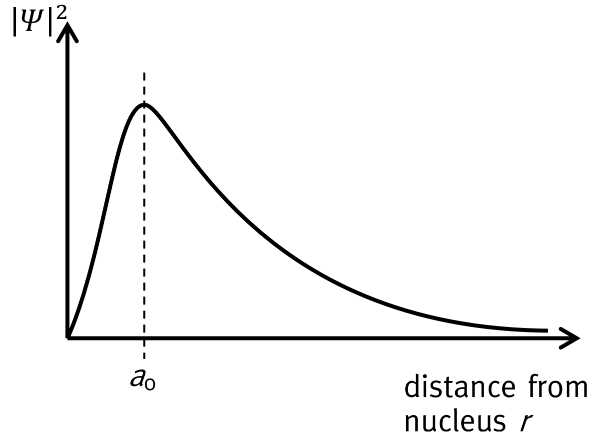
$$|\Psi|^2 = \frac{4r^2}{a_0^3} e^{-\frac{2r}{a_0}}$$

where a_0 is the Bohr radius, a constant defined by $a_0 = \frac{\hbar^2}{me^2} = 0.0529$ nm.

Sketch (i) the probability density function of the location of the electron and hence (ii) state the distance away from the nucleus at which the electron is most probably located.

Solution:

(i)



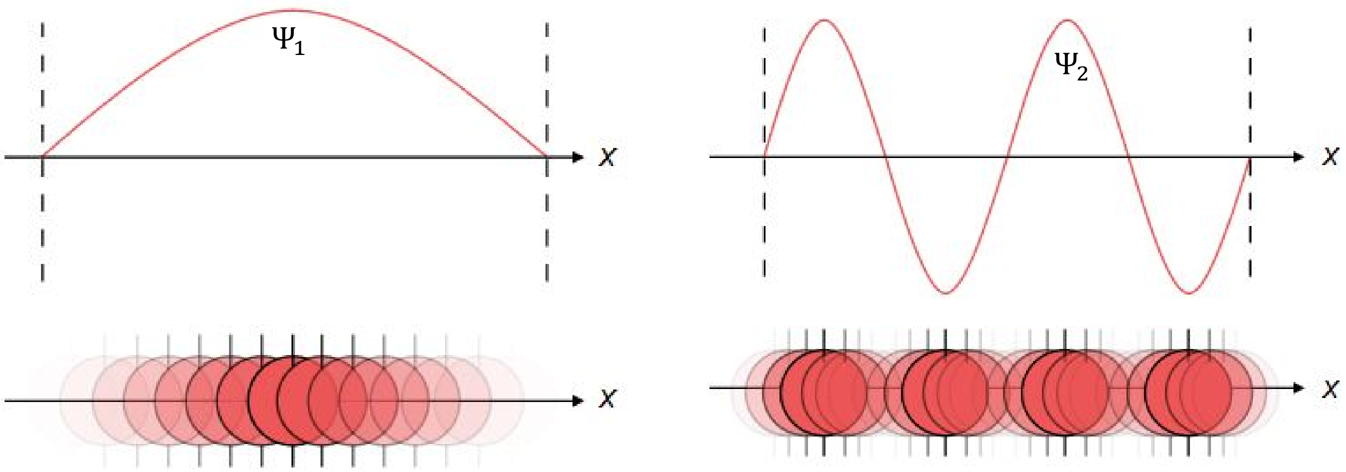
(ii)

The electron has the highest probability of being found 0.0529 nm away from the centre of the nucleus.

NB: It should be within your H2 mathematical ability to show that

$$\int_0^\infty |\Psi|^2 \, dr = 1$$

Hint: by parts… twice

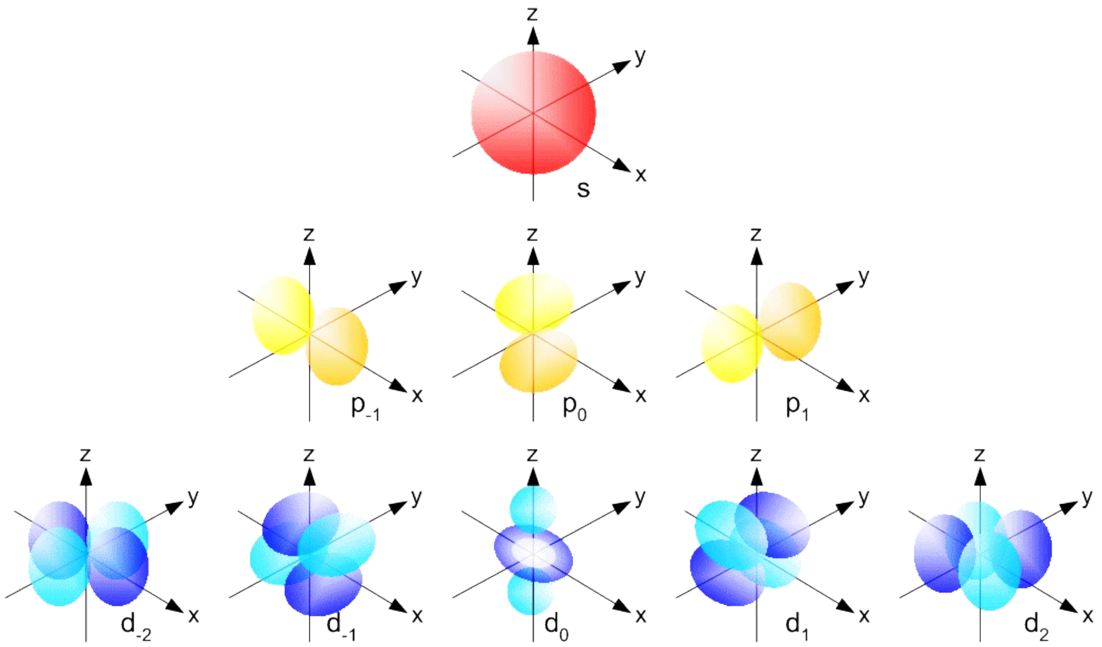


We can only say how probable it is to find the lone electron along x.

For the Chemistry students…

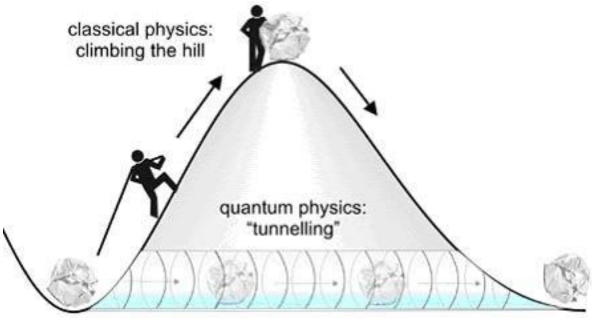
It was through solving the Schrödinger's wave equation for the hydrogen atom that we obtain the *spdf* orbitals. The hydrogen atom was chosen because it is the simplest atom; having only 1 electron "orbiting" a lone proton for nucleus.

The experimental results were in good agreement, and the Chemists took over the subsequent studies for other atoms, introducing correction factors as needed, and using the theory to further explain aspects of atomic structure and chemical bonding.

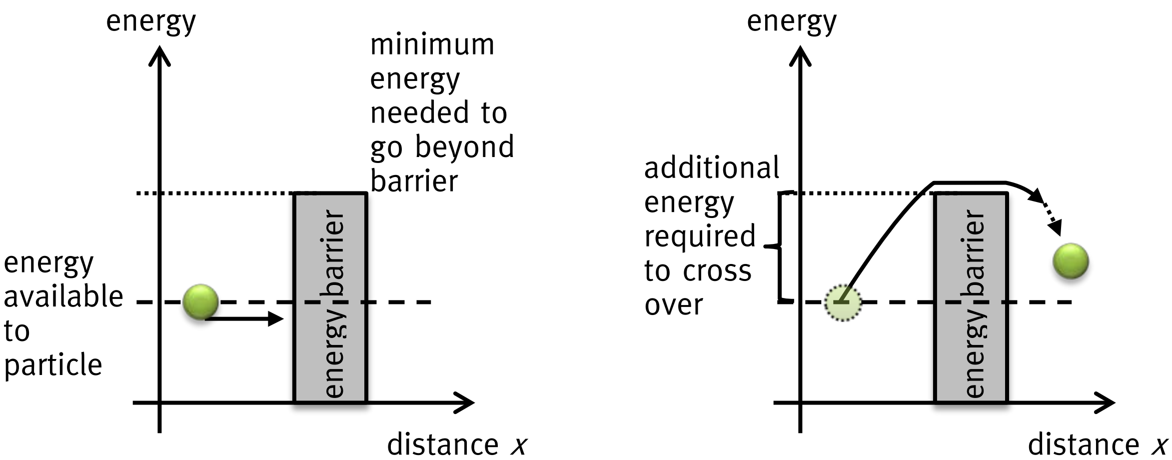


18c.3 Quantum Tunnelling

When we think of "tunnelling", we often picture the burrowing of a passage way under and through a tall obstacle, instead of going over the top.



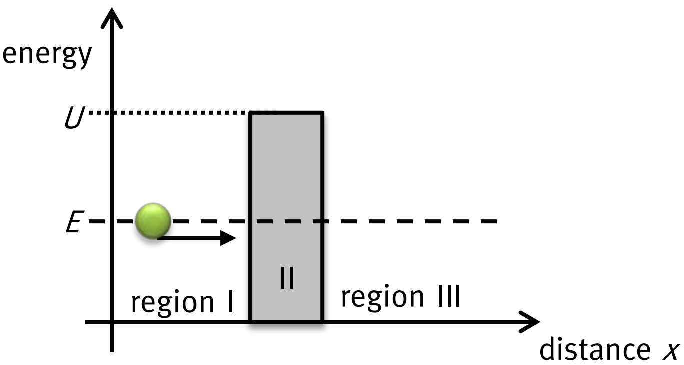
For a classical particle, it can pass over an impenetrable *barrier* only if supplied extra energy to overcome it:



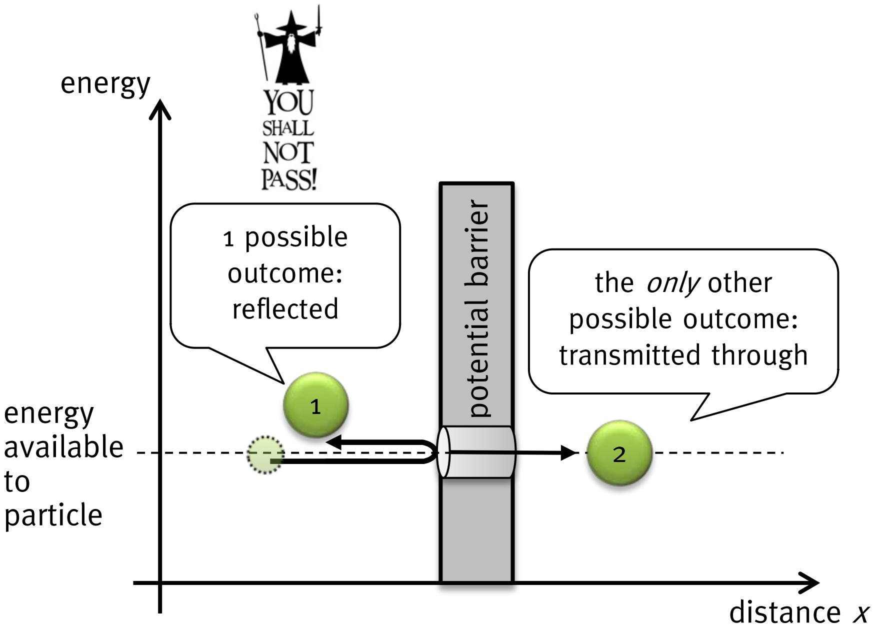
Potential Barrier

A region of higher potential energy which tends to prevent a particle from passing from one side of the barrier to another.

Classically, the particle will be reflected when it hits the barrier. Hence, region II and region III are forbidden to the particle.

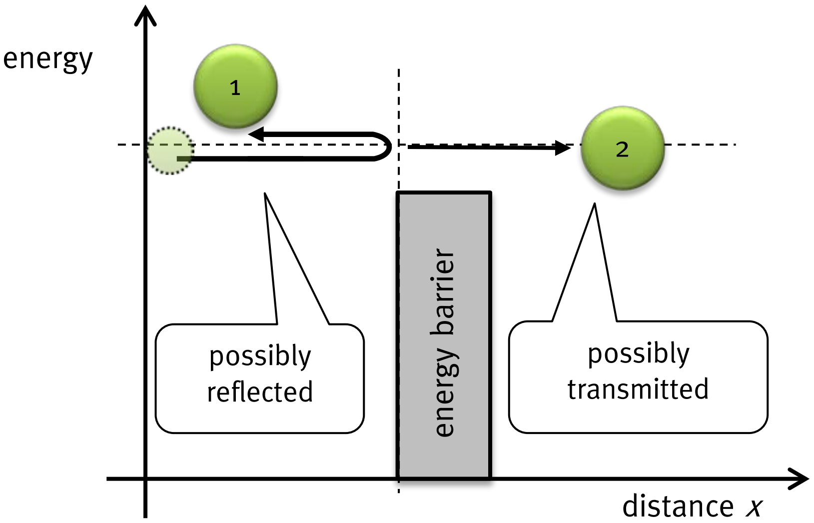


In quantum tunnelling, the particle can pass through the barrier without any loss of energy. The particle "tunnels" through and penetrates a *classically-forbidden* region.



NB: In fact, in the quantum realm, even if the particle has more energy than the barrier, there is still a chance of being reflected.

(But don't worry too much about this phenomena in our context.)



Transmission Coefficient

The transmission coefficient ***T*** is the probability of a particle tunnelling through a potential barrier and appearing on the other side.

It decreases exponentially with the barrier thickness *d*.

$$T \propto e^{-2kd}$$

Transmission and Reflection Coefficient

The reflection coefficient ***R*** is the probability of a particle failing to tunnel through the potential barrier and getting reflected by a potential barrier.

$$T + R = 1$$

For $T \propto e^{-2kd}$,

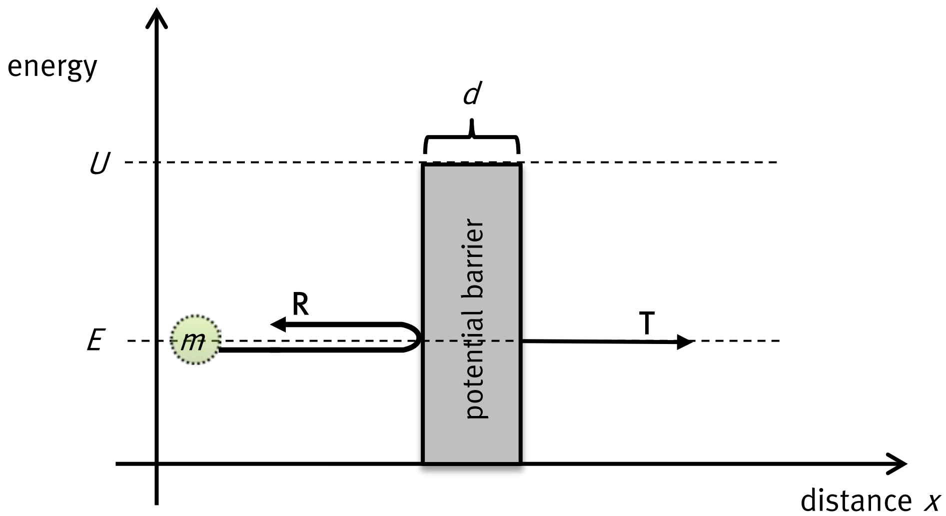
$$k = \sqrt{\frac{8\pi^2 m(U-E)}{h^2}}$$

d: the thickness of the barrier in metres

m: mass of the particle in kilogrammes

U: the "height" of the potential barrier in joules (i.e. the energy needed to overcome the barrier)

E: the total energy of the particle in joules (both KE and PE)

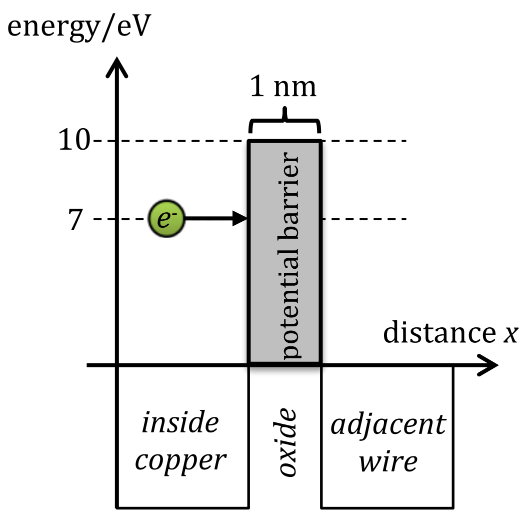


Example 7

Two copper conducting wires are separated by an insulating oxide layer. Modelling the oxide layer as square barrier of height 10.0 eV, estimate the transmission coefficient and the reflection coefficient for penetration by electrons with energy of 7.00 eV if the thickness of the layer is 1.00 nm.

Given: $T \approx A\,e^{-2kd}$ where $A = 16\frac{E}{U}\left(1-\frac{E}{U}\right)$

Solutions:



$T \approx Ae^{-2kd}$

$\approx \frac{16E}{U}\left(1-\frac{E}{U}\right)e^{-2\sqrt{\frac{8\pi^2 m_e(U-E)}{h^2}}d}$

$\approx$

$16\left(\frac{7}{10}\right)\left(1-\frac{7}{10}\right)e^{-2\sqrt{\frac{8\pi^2(9.11\times10^{-31})(10-7)(1.6\times10^{-19})}{(6.63\times10^{-34})^2}}(10^{-9})}$

$\approx 6.74\times10^{-8}$

$R + T = 1$

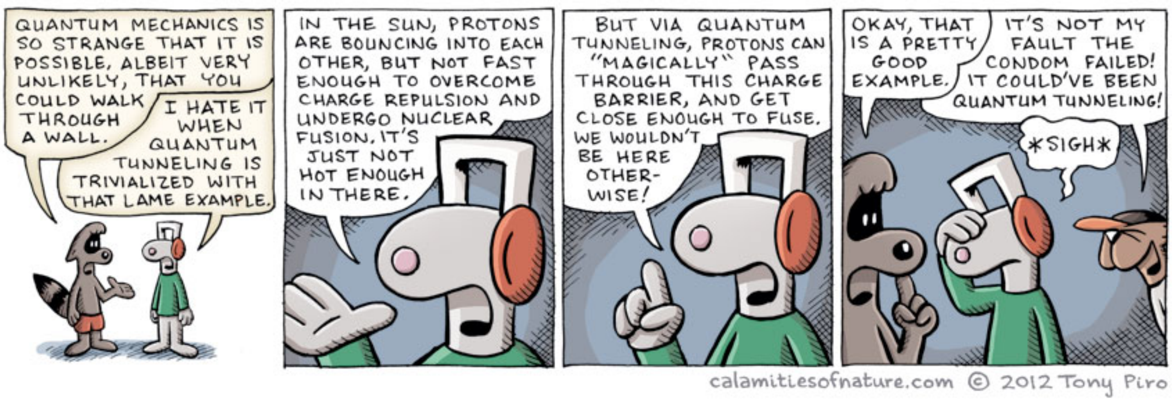
$R = 1 - T$

$= 1 - 6.74\times10^{-8}$

≈ 0.999999932

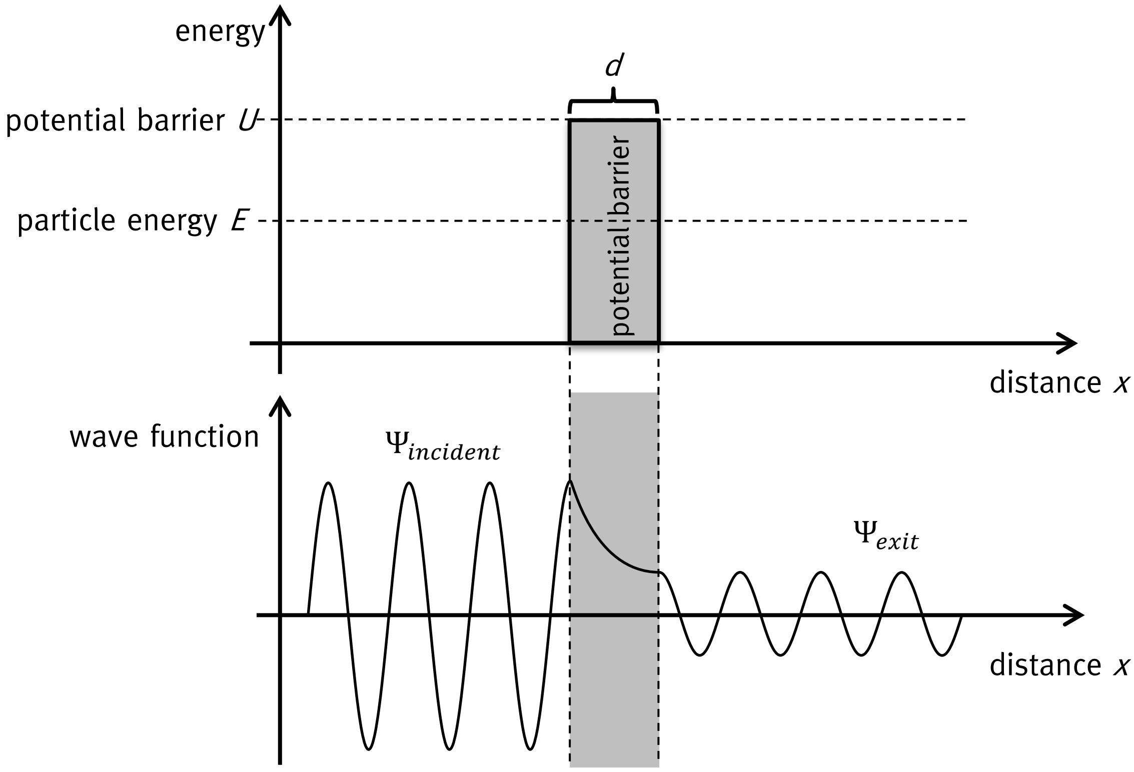
NB: Tunnelling is highly unlikely. Most of the electrons reaching the barrier will be reflected.

Electrons inside the copper exist as part of a sea of freely-moving mobile electrons; and hence can move around without loss in total energy. The oxide is an insulator and doesn't permit conduction, and hence poses as a barrier.



At this point, it is important to take note of how we represent the wave nature of the matter wave:

Representing Wave Function in Tunnelling



Important features:

(i) We typically represent a *moving* particle with a sinusoidal wave function.

In discussing the probability of locating the particle earlier, the particle is confined to that length along the x-axis.

(ii) A quantum particle has a wave nature which is completely described by a wave function.

(iii) The square of the amplitude of the wave function gives the probability of locating the quantum particle.

(iv) The amplitude of Ψ_{exit} is **not** zero.

There is a finite probability of finding the particle to the right of the barrier.

(v) The amplitude of Ψ_{exit} is reduced compared to $\Psi_{incident}$.

*The probability of finding the particle on the right hand side of the barrier (**T**) is lower. The wave function of the reflected wave (**R**) is not shown.*

(vi) The amplitude of the wave function decays <u>exponentially</u> inside the barrier.

*The transmission coefficient **T** decays exponentially with barrier width.*

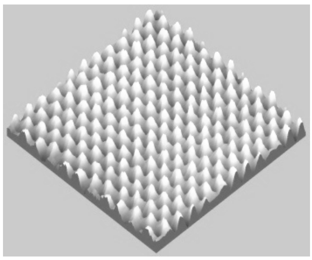
(vii) The total energy of the particle is **not** reduced.

This is shown by the wavelength remaining constant. Recall how the energy of a particle is related to the de Broglie wavelength: $E = \frac{p^2}{2m} = \frac{\left(\frac{h}{\lambda}\right)^2}{2m}$

18c.4 Scanning Tunnelling Microscope (STM)

***M*icroscopy**

The STM allows us to visualize an electrically-conductive surface at the atomic level.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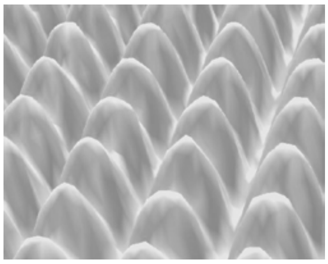
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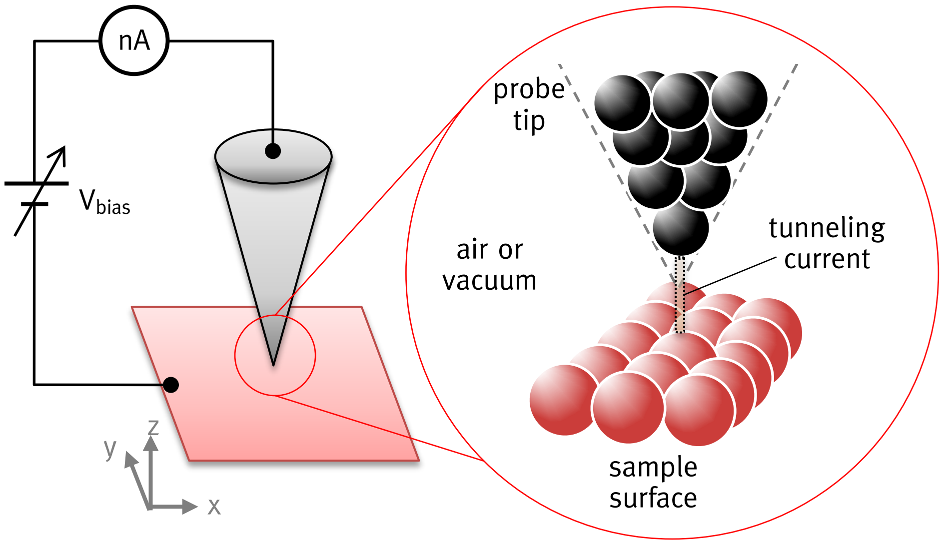
***T*unnelling**

The STM is a practical application of the quantum tunnelling effect.

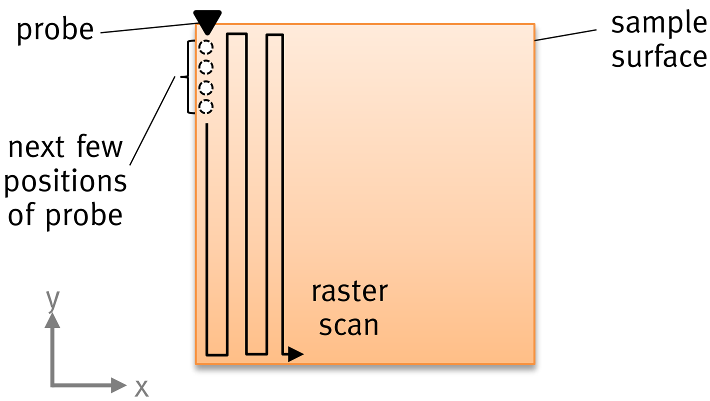
A sharp conducting metal tip (only a few atoms at the tip) is placed very close to the surface of the electrically-conductive sample. The vacuum or air in between the tip and surface serves as the potential barrier.



There is a small potential difference applied between the tip and the sample. A weak *tunnelling current* occurs and it decays exponentially with the distance between the probe and surface.

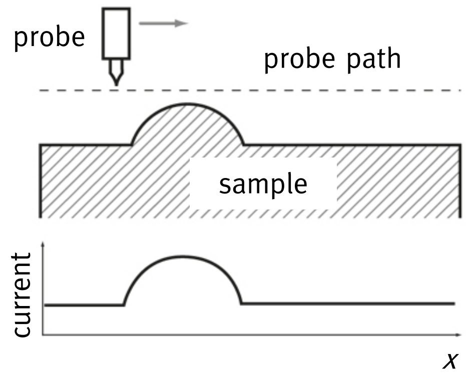
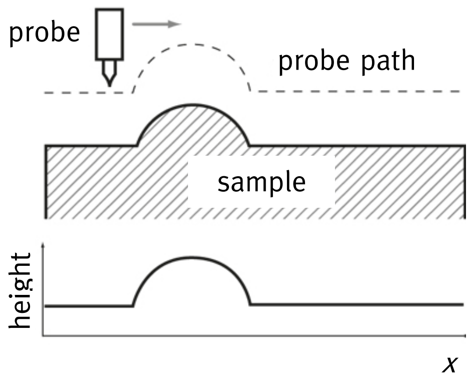
***S*canning**

The tip is moved across the surface in a *raster scan* fashion in order to build the image one point at the time.

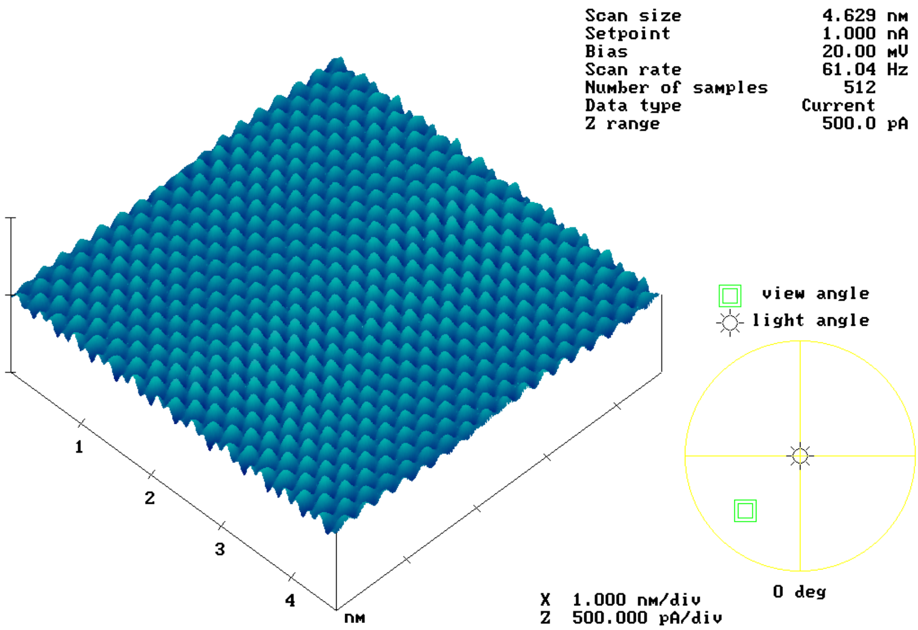


Operation Modes

The tip of the STM can be made to move in 2 ways.

Mode	Advantage	Disadvantage	
Constant Height Tip is moved across the surface at constant height. Tunnelling current is recorded at each (*x*,*y*) point.	Faster	Danger of tip crash. Only good for relatively smooth surfaces.	
Constant Current Tunnelling current is maintained by constantly adjusting vertical distance (*z*) between sample surface and probe tip. Change in vertical distance is recorded at each (*x*,*y*) point.	Can measure surfaces with larger irregular features	Slower	

After the data is recorded at each (*x*,*y*) point, a computer can display the information as a 3D image.

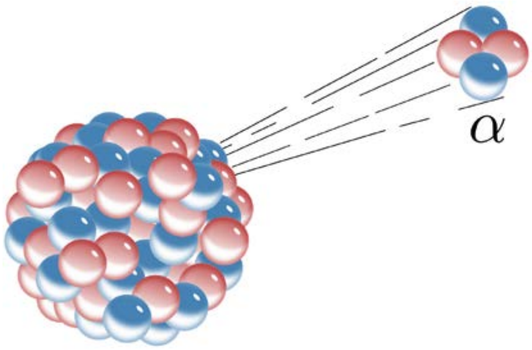


The inventors of the STM, Gerd Binning and Heinrich Rohrer of IBM, shared the Nobel Prize in Physics in 1986 for the development of the instrument.

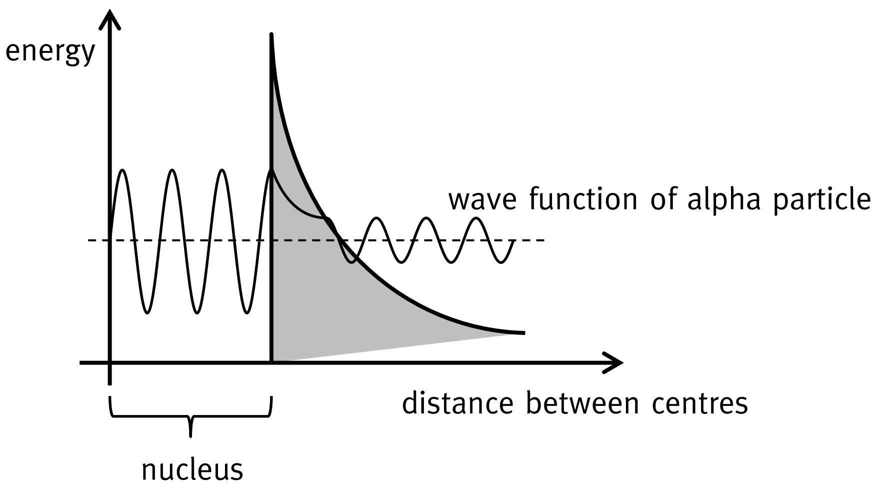
18c.5.1 Other Applications of Quantum Tunnelling: Alpha Decay

One form of radioactive decay is the emission of alpha particle(s) (nuclei of Helium atoms) from an unstable, massive nucleus.

$$^{A}_{Z}X \rightarrow \, ^{A-2}_{Z-2}Y + \, ^{4}_{2}He$$



The nucleus is originally held intact by an attractive nuclear strong force, one which is able to overcome the electrostatic static repulsion of positively-charged protons in close proximity.



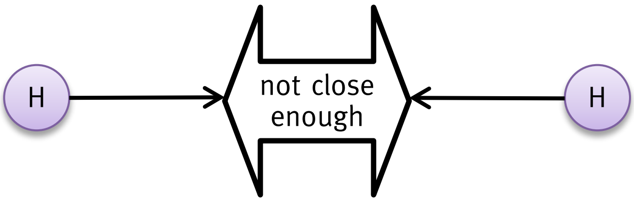
The wave function of the alpha particle is superimposed on the energy profile of the potential barrier. (c.f. page 17)

The electrostatic (Coulombic) force poses as a potential barrier. There is a finite probability that an alpha particle can tunnel through the barrier and leave the nucleus.

18c.5.2 Other Applications of Quantum Tunnelling: Nuclear Fusion in Sun

The source of energy for the Sun is the nuclear fusion of hydrogen atoms. The atoms have kinetic energy due to the temperature of the sun.

However, the energy is not enough to allow the hydrogen atoms to be close enough for nuclear fusion; the proton nuclei repel each other due to electrostatic repulsion.



The electrostatic force of repulsion is the potential barrier. For nuclear fusion to successfully take place, quantum tunnelling must occur.

18c.6 Tutorial Questions

T1 Suppose that the x-component of the velocity of a 2 x 10^{-4} kg mass is measured to an accuracy of $\pm 10^{-6}$ m s^{-1}. Determine the limit of the accuracy with which we can locate the particle along the x-axis.

T2 (a) A pulse of radio wave lasts for 1.0×10^{-5} s. A photon of the radio wave may be considered to be at a point anywhere within this pulse, although the location of the point is not known. Calculate

(i) the length of the pulse, [1]

(ii) the uncertainty in the position of the photon, [1]

(iii) the uncertainty in the momentum of the photon. [3]

(b) Show, with the aid of a diagram, what is meant by a potential barrier. Discuss how the wave nature of particles allows particles to tunnel through such a barrier. [3]

(c) The process in (b) is used in a scanning tunneling microscope, where it is possible to see individual atoms. Outline how these atomic-scale images may be obtained. [3]

T3 An electron with a total energy E of 5.1 e V approaches a barrier of height 6.8 e V and thickness 750×10^{-12} m. Given: $T \approx A\, e^{-2kd}$ where $A = 16\frac{E}{U}\left(1-\frac{E}{U}\right)$

(a) Estimate the probability that the electron will be transmitted through the barrier. [3]

(b) A proton with the same energy as the electron approaches the barrier.

Compare (without calculations) the probability of this proton being transmitted through the barrier, with the probability calculated in (a).

Explain your comparison. [2]