1 X-ray Spectra

Set-up

The key parts of the x-ray tube are shown in Fig. 1.1. The heated cathode emits electrons which are accelerated by a high voltage of tens to hundreds of kV. A *small* portion (~1%) of the electrons' kinetic energies is converted to x-rays when they collide with the tungsten atoms. The bulk of the kinetic energies become heat that is conducted away by a good conductor or with the use of circulating cooling liquid.

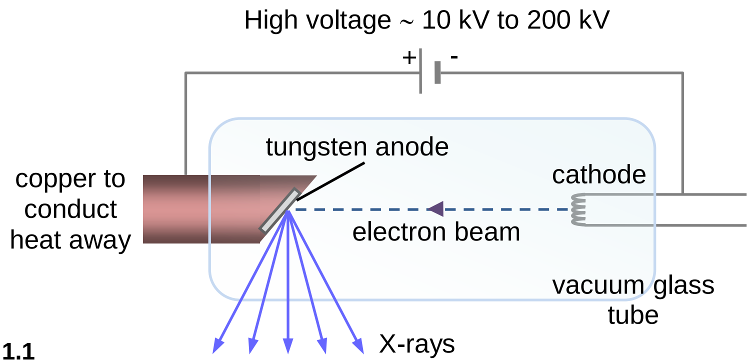

Fig. 1.1

Charged particles are accelerated to high speeds before colliding with target atoms to produce x-rays.

An electron reaching the tungsten target gained KE at the expense of electric PE lost,

$$\boxed{\frac{1}{2}m_e v^2 = eV_a} \quad \text{---- (Eq 1.1)}$$

where V_a is the accelerating p.d, m_e and e are the electron mass and charge respectively.

The KE gained $\frac{1}{2} mv^2 = eV_a$ for electrons of charge e.

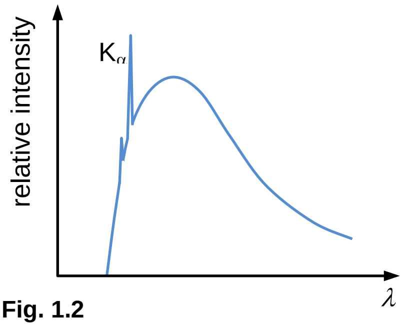

Fig. 1.2

A typical x-ray spectrum can be seen in Fig. 1.2. It is actually a superposition of a *continuous spectrum* and a *line spectrum*. These are produced by two different mechanisms at the atomic level. The spikes from the line spectrum occur at two specific wavelengths that are characteristic of the material used as the target.

The resulting x-ray spectrum is made up of two parts - a continuous spectrum and a discrete spectrum.

Mechanism 1 - Acceleration of Charge

Whenever a charge particle is accelerated or decelerated, it radiates electromagnetic energy.
Also, greater acceleration leads to greater rate of radiation.

The high speeds of the electrons allow them to penetrate the target atoms. The size of an atom is ~ 10^{-10} m while the size of a nucleus is ~ 10^{-15} m and the electron is even smaller. If the nucleus were 1 mm in size, then the atom would be about 100 m across. However, in the vast empty space inside the atom, the electric field of the nucleus attracts an incoming electron and curves it around. The *strong* force and therefore acceleration(centripetal plus linear) results in radiation of an *energetic* x-ray photon, slowing down the electron in the process.

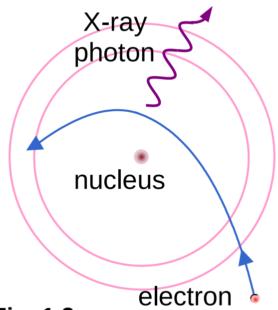

Fig. 1.3

The mechanism for the production of continuous spectrum is based on the fact that accelerated or decelerated charges radiate electromagnetic energy.

The x-rays produced in this way are called 'Brehmsstrahlung' in German for 'braking radiation'. Each incoming electron can potentially produce a few such x-ray photons of different energies by interacting with a series of different atoms. Also, an incoming electron can approach nuclei with different proximity and thus experience different forces and emit photons of different energies. A beam of incoming electrons will thus produce photons with a continuous range of energies or frequencies resulting in a spectrum as shown in Fig. 1.4

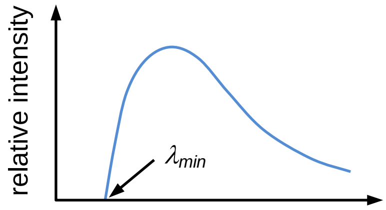

Fig. 1.4

There is a shortest wavelength for the continuous spectrum because the greatest frequency or energy of a photon occurs when all the KE of an incoming electron is given to that photon.

The maximum photon energy E_p is equal to the maximum amount of KE(Eq. 1.1) an electron can lose at one go. Hence

$$E_p = eV_a \quad \text{but} \quad E_p = hf_{max} = hc/\lambda_{min}$$
$$hc/\lambda_{min} = eV_a$$
$$\lambda_{min} = hc/eV_a$$

where the minimum wavelength of the continuous spectrum gets smaller as the accelerating p.d. gets larger. In other words, the spectrum extends more to the left as v_a increases as shown in Fig. 1.5.

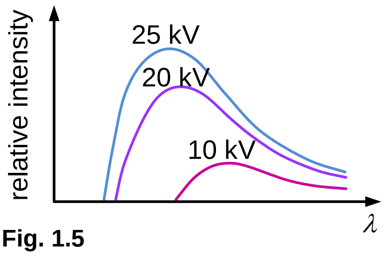

Fig. 1.5

Mechanism 2 - Dislodging Innermost Electron

An incoming electron can also knock out an electron from the inner orbits of a target atom. The vacancy will be quickly filled by an electron from one of the outer orbits with higher energy levels, thus emitting an x-ray photon.

The second mechanism for x-ray production is due to the knocking out of an electron from the innermost orbits. X-ray photons of discrete energies are then produced due to electrons from outer orbits jumping to fill up the vacancy.

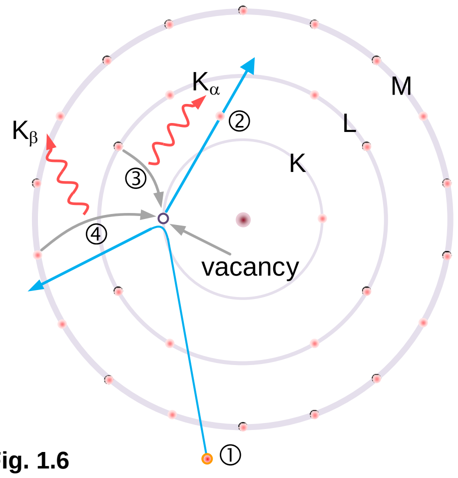

Fig. 1.6

① incoming electron knocks out an innermost electron.

② dislodged electron.

③ L shell electron may jump in to fill the vacancy (give K_α spectral line) or

④ M shell or other outer shell electron may jump in to fill the vacancy.

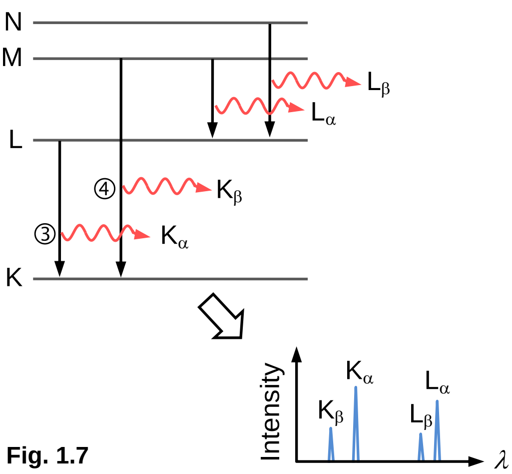

Fig. 1.7

Recall from Quantum I that jumping of valence (outermost) electron from higher to lower energy levels give rise to discrete emission spectrum. Similarly, here the finite number of possible transitions leads to a discrete number of spectral lines as in Fig. 1.7

Energy gaps between inner orbits are greater than between outer orbits, thus accounting for higher photon energies.

Sometimes the L_α & L_β lines may not be present because those transitions do not correspond to x-rays but other lower frequency part of the EM spectrum.

Combined Discrete and Continuous Spectrum

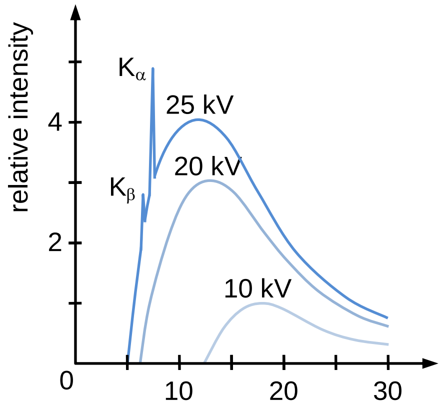

Fig. 1.8

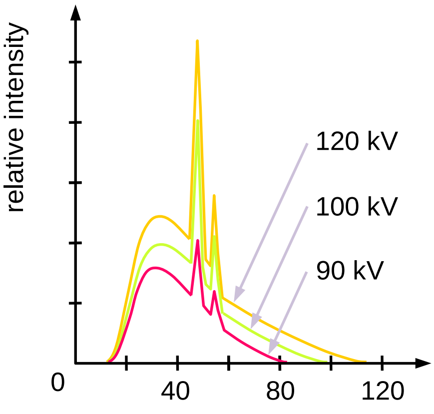

Fig. 1.9

Fig. 1.8 shows that when accelerating p.d. is too low, the incoming electrons do not have enough energy to knock out the innermost electrons and so the spectrum only has the continuous part without the discrete contribution known as the *characteristic* x-rays. At a high enough p.d. of 25 kV, the characteristic spikes are present. The *characteristic* radiation is so called because the exact wavelengths and spacing of the lines or spikes are characteristic of the specific kind of target atoms.

The key difference between Fig. 1.8 and Fig. 1.9 is that the horizontal axis is photon *wavelength* and *energy* respectively. Fig. 1.9 is similar to a plot against frequency ($E = hf$).

The discrete spectrum is also known as *characteristic* spectrum because the exact wavelengths and spacing of the spikes are characteristic of the kind of target atoms.

2 Potential Wells and Barriers

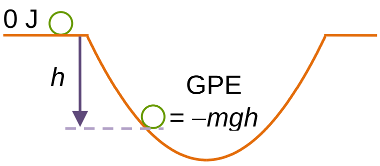

Fig. 2.1

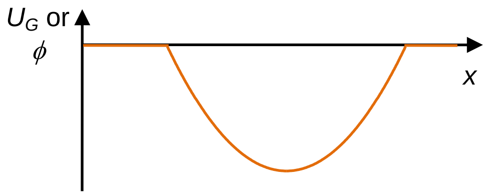

Fig. 2.2

Consider a depression in the ground (Fig. 2.1). If we take gravitational PE, U_G, to be zero at ground level, then at any depth h, $U_G = -mgh$. Gravitational potential $\phi = U_G/m$, $\therefore$ ϕ at each h is equal to $-gh$. If we plot U_G or ϕ versus horizontal position x, the result is shown in Fig. 2.2. The plot is called a gravitational *potential energy well* or just *potential well*.

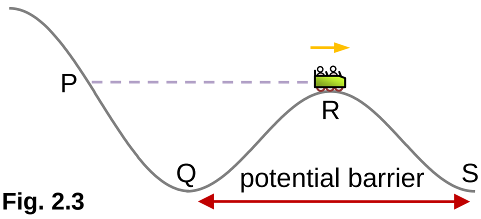

Fig. 2.3

Consider a roller coaster ride as shown in Fig. 2.3. If the car were to start at *rest* below point P instead of above, it would not be able to reach S. We call the section QRS a gravitational *potential barrier*. For the car to cross the potential barrier from the left side, it must have total energy (GPE + KE) greater than its GPE at R.

Potential wells and barriers can also be electromagnetic instead of gravitational. It all depends on the type of force or field involved. In general, a potential barrier is

> a *region*, in a force field, with *higher potential than its surrounding* such that an object requires energy to pass through it.

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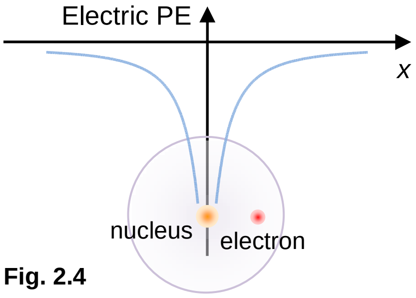


Fig. 2.4

A potential well or barrier need not be concrete and visible. For example, Fig. 2.4 shows the potential energy between a nucleus and an electron in an isolated atom for variable electron position x. An electron with negative total energy is thus trapped in a potential energy well of the same shape as the plotted graph.

Potential wells and barriers are very common. In photoelectric effect, the electrons are trapped in a potential well so are the electrons in an atom. There is also a gravitational potential barrier between Earth and moon.

Fig. 2.5 shows the invisible potential barrier between Earth and moon such that a spacecraft from Earth that wishes to land on moon must have enough energy to pass through the potential barrier region.

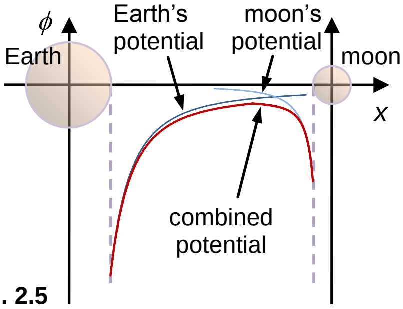


Fig. 2.5

3 Wave and Probability Density Functions

Recall that de Broglie came up with the relation $\lambda = h/p$ for the wavelength of particles. The waves of particles with mass are called *matter waves*. In 1926, Schrödinger developed an equation($i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + U(x)\Psi$) for these matter waves. Ψ is a mathematical function which describes how the values of Ψ vary with spatial coordinates and time just like those displacement-time and displacement-distance equations or functions in the topic Waves. Thus Ψ is called a *wave function* as it represents a waveform which may progress in time. If we want to highlight its spatial(3D) and time dependence we would write it as $\Psi(x,y,z,t)$.

De Broglie's equation $\lambda = h/p$ where $p = mv$ gives the wavelength of *matter waves*.

Just as a quadratic equation has solutions which are some *numbers*, the Schrödinger equation has solutions but they are mathematical *functions*. For example, $x^2 - x - 2 = 0$ is $(x + 1)(x - 2) = 0$ and has solutions $x = -1, 2$ while the solutions of the 1D Schrödinger equation looks like $\Psi(x,t) = C[\cos(kx - \omega t) + i\sin(kx - \omega t)]$ where C, k & ω are constants & $i = \sqrt{-1}$.

Matter waves are described by *wave functions* Ψ which do not correspond to any physically measurable quantities. However, they contain information like an object's momentum & energy.

The last two paragraphs are not needed for exams but just to provide some sense of how the wave function comes about. The important thing is regarding the interpretation of the wave function. In the same year that Schrödinger published his equation, Max Born provided the *probability interpretation* of the wave function Ψ:

> The square of the absolute value of the wave function gives the *probability density function* $P(x,t) = |\Psi(x,t)|^2$. For 1-dimensional case, $P(x,t)$ tells us the probability per unit length for finding a particle at x at time t.

The square of the absolute value of the wave function gives the *probability density function* $P(x,t) = |\Psi(x,t)|^2$. For 1D case, $P(x,t)$ tells us the probability per unit length for finding a particle at x at time t.

The wave function Ψ itself *does not* correspond to any measurable physical quantity. Only $|\Psi|^2$ has a physical meaning. In the Schrödinger equation, $U(x)$ is a function that describes the potential energy just like in Fig. 2.2 or 2.4. To better understand the wave function and probability density function, we will look at an example involving an 'infinite potential well'.

<u>Note for those interested</u>
Why do you need to take the square of the *absolute* value and not just simply square the wave function? The reason is that in most cases, the wave function turns out to be a *complex* quantity containing i (= $\sqrt{-1}$). For a *real* quantity x, $x^2 = |x|^2$ but for a *complex* quantity z, $z^2 \neq |z|^2$.

Infinite Potential Energy Well

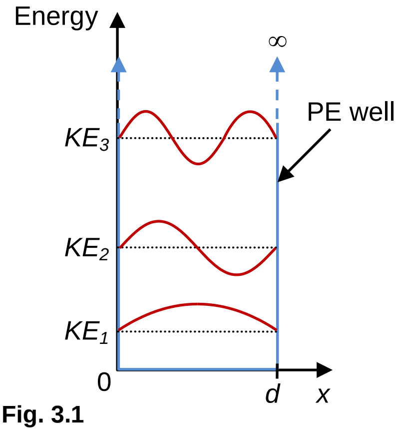
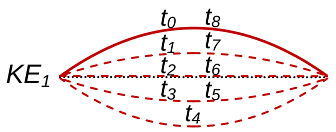


Fig. 3.1



$t_0 \rightarrow t_1 \rightarrow t_2 \rightarrow \ldots \rightarrow t_7 \rightarrow t_8$
is one cycle of the standing wave

Fig. 3.2

Consider a particle trapped inside a PE well that is infinitely deep and take the bottom of the well to be at zero energy. Mathematically,

$$U(x) = \begin{cases} \infty & \text{for} \quad x < 0 \\ 0 & \text{for} \quad 0 \le x \le d \\ \infty & \text{for} \quad d < x \end{cases}$$

The Schrödinger equation with the above $U(x)$ will produce a set of wave function solutions $\Psi(x,t) = \psi_s(x)\psi_T(t)$. $\psi_s(x)$ is the spatial part shown in Fig. 3.1 while $\psi_T(t)$ is a time varying part which in this case causes $\psi_s(x)$ to change periodically giving rise to standing waves (Fig. 3.2).

Thus each $\Psi(x,t)$ describes a stationary wave mode corresponding to an allowed kinetic energy. The first 3 allowed KE and $\psi_s(x)$ are shown in Fig.3.1.

Considering a given moment in time when $\Psi = \psi_s(x)$, Fig. 3.3 to 3.5 show how squaring the magnitude of the wave functions Ψ lead to their corresponding *probability density functions*.

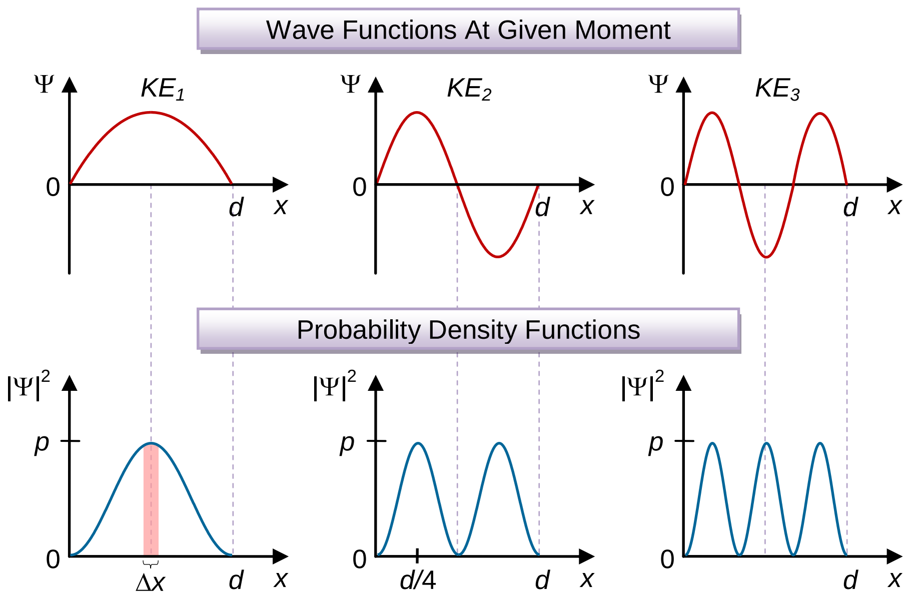


Fig. 3.3 **Fig. 3.4** **Fig. 3.5**

Given a 1D wave function $\Psi(x,t)$ the area under $|\Psi|^2$-x graph is *probability*.

$|\Psi|^2$-x graph shows where the particle is more likely to be found.

Here, $|\Psi|^2$ gives the probability *per unit length* along x. In Fig. 3.3, the probability of finding the particle at $x = d/2$ within the *tiny* segment Δx is given by the value $|\Psi(d/2)|^2\Delta x$ or $p\Delta x$ i.e. the probability is the shaded area. The total area is 1 since the particle has to be somewhere within the well.

The trapped particle can be found in *one* of the allowed energy levels and each level has a different probability density distribution function. It can be seen that the probability of finding the particle around $x = d/4$ is greater when the particle has KE_2 (Fig. 3.4) than when it has KE_1 (Fig. 3.3). We can also see that the particle has zero probability of being found in the regions $x < 0$ and $x > d$ which is no surprise since we expect the particle to be 'trapped' inside the well.

The particle trapped in an infinite potential well is quite similar to an electron trapped in an atom except that the potential well of an atom does not have the same shape and is not infinitely deep. In both cases, there are allowed energy levels or quantisation of energy associated with the formation of standing matter waves due to confinement by the well.

4 Heisenberg's Uncertainty Principle

$\Delta p_x \Delta x \geq \hbar/2$

In 1927 Werner Karl Heisenberg arrived at the uncertainty relation:

> The more precisely the *position* of a system is determined, the less precisely the *momentum* can be known *simultaneously*, and vice versa. Quantitatively, $\Delta p_x \Delta x \geq \hbar/2$ where $\hbar = h/2\pi$.

When we say 'position of a system is *determined*', we do not necessarily mean using a measuring instrument to 'find out' the position as a reading. It can also mean setting up the apparatus such that we 'know' the position of a system. Consider the double slit set-up (Fig. 4.1) from Quantum I.

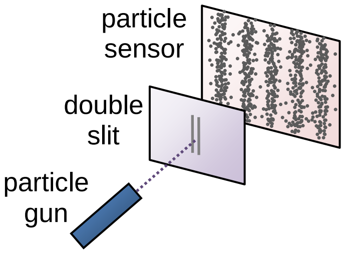


Fig. 4.1

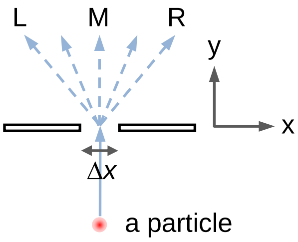


Fig. 4.2

Zooming in on one of the slits as in Fig. 4.2, the slit width's effect is to 'determine' the x-position of the passing particle with an uncertainty of Δx. According to the uncertainty relation, the particle must simultaneously have *minimum* uncertainty of Δp_x in the x-component momentum p_x whereby $\Delta p_x = \hbar/2\Delta x$. Since $\Delta p_x = m\Delta v_x$, this means that the particle will not necessarily go to M but could reach anywhere between L and R. Treating the particle as a matter wave would have led to the same outcome since waves diffract after passing through the slit.

If instead of the slit above, we have two instruments or set-ups for measuring the particle's momentum and position. Let's say we have very good instruments such that *individually* or *separately*, each has best limiting precision $\Delta p_x'$ and $\Delta x'$ respectively. It is theoretically possible that the product $\Delta p_x'\Delta x'$ is smaller than $\hbar/2$. However, the uncertainty principle or nature would dictate that *simultaneously* it is not possible for the instruments to yield measurements with uncertainties of $\Delta p_x'$ and $\Delta x'$. In other words, Δp_x and Δx in the uncertainty principle are not the limiting precisions of instruments. Δp_x and Δx are more like the *inherent* limits of our knowledge of the momentum and position.

The reason for the inherent limits was explained by Heisenberg using a 'thought experiment'. In this experiment, the position of an electron is to be determined by bouncing light off it into a microscope. As in all measurement processes, the measuring instrument has to interact with the system to be measured and thus inevitably change the system. To minimise the disturbance on the electron, imagine only one photon is bounced off the electron. It turns out that the shorter the wavelength, the more precise the position measurement. However, the shorter the wavelength, the greater the momentum of the photon ($p = h/\lambda$) and the greater the disturbance. Therefore, nature sets ultimate limits on the precisions of simultaneous measurements of position and momentum. Furthermore there are other similar pairs of quantities (a, b) which follow the uncertainty relation $\Delta a \Delta b \geq \hbar/2$.

The more precisely the *position* of a system is determined, the less precisely the *momentum* can be known *simultaneously*, and vice versa. Quantitatively, $\Delta p_x \Delta x \geq \hbar/2$ where $\hbar = h/2\pi$.

Δp_x and Δx in the uncertainty principle are not the limiting precisions of instruments. Instead, they are the *inherent* limits of our knowledge of the momentum and position when measured simultaneously.

$\Delta E \Delta t \geq \hbar/2$

Another uncertainty relation involves the energy and time pair - $\Delta E \Delta t \geq \hbar/2$. The E, t pair is not quite like the previous p, x pair. Here Δt is not the uncertainty in measuring or determining t. The interpretation of ΔE & Δt is dependent on context. Below are just two example scenarios:

The $\Delta E \Delta t \geq \hbar/2$ uncertainty relation has different interpretations in different situations.

Scenario 1 - Decay of Excited State

An excited state could be that of an atom. Excited states are unstable. If an atom stays in the excited state for 10^{-10} s before emitting a photon, 10^{-10} s would be the *lifetime* of the excited state. The energy-time uncertainty relation then says that the energy of the excited state will have an *inherent* uncertainty $\Delta E = \hbar/2(10^{-10})$. This means that the energy level is not a sharp line but has a small spread.

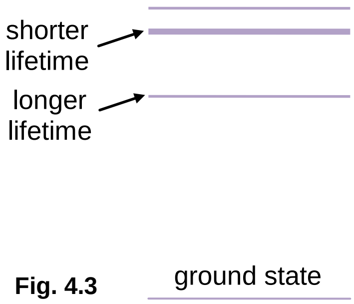


Fig. 4.3

When applied to the decay of an excited state Δt is the *lifetime* of the excited state while ΔE is the uncertainty in the energy of the state.

This inherent uncertainty cannot be reduced by using better equipment or procedures. There are other sources of uncertainties from measuring instruments and the motion of the atom but these can theoretically be reduced with better instruments or set-ups.

Another example of an excited state is found in some nuclear processes in which a virtual particle with very short lifetime is created. Thereafter, it decays to other particles. It has been found that the shorter the *lifetime* Δt of the virtual particle, the greater the inherent uncertainty ΔE of the energy of the particle.

Scenario 2 - Wave Pulse

A laser is able to produce a light beam with very precise frequency and hence photons of very uniform energy. However if the laser is fired in pulses of *duration* Δt, the energy and thus frequency of the photons ($E = hf$) will no longer be as uniform as before. Now there will be a range of photon energies ΔE and frequencies Δf such that $\Delta E \Delta t \geq \hbar/2$.

When applied to a wave pulse, Δt is the *duration* of the pulse while ΔE is the *range of energies* of the component waves

A continuous wave of a single frequency has spectrum as shown in Fig. 4.4. In contrast, a wave pulse can be constructed by superposing waves of a range of frequencies, leading to a spectrum as shown in Fig. 4.5. Again, the uncertainties represent *inherent* limits of nature that has nothing to do with precision of measuring instruments

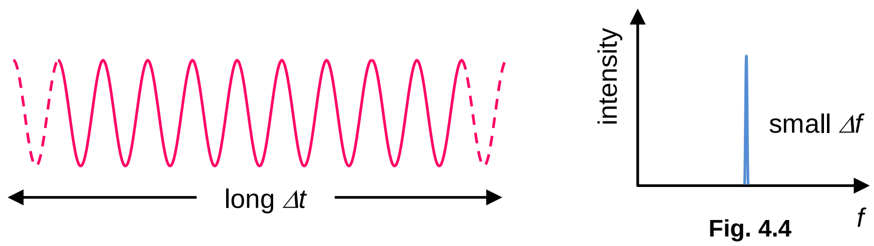


Fig. 4.4

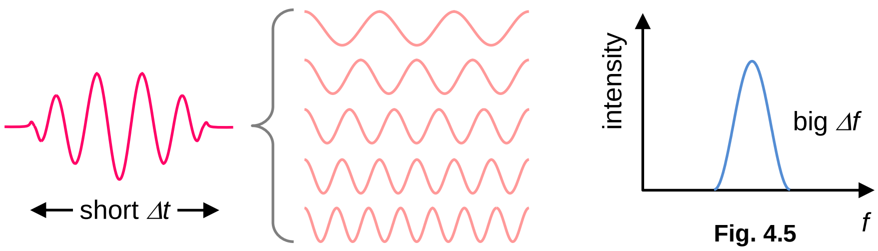


Fig. 4.5

[There is a lot more to the uncertainty principle. There are areas of confusion and issues of interpretation regarding the principle and quantum theory in general, so keep your mind open for further development in research.]

5 Quantum Tunnelling

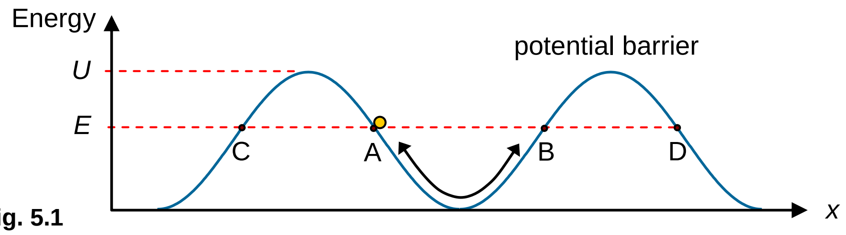


Fig. 5.1

In Fig 5.1, a ball between 2 hills is released from rest at point A with total energy E (KE = 0 and GPE = E). Assuming no energy loss, the ball can only roll back and forth between A and B. It is impossible for the ball to appear at C or D without further intervention. However at microscopic scale, a particle such as an electron with energy E lower than U can in fact be found at the other sides of the barriers at C or D! This is a quantum phenomenon, called *quantum tunnelling* that cannot happen according to classical physics.

In section 3, it was explained that in Schrodinger's equation $i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+U(x)\Psi$, $U(x)$ is a mathematical function which describes the shape of the potential energy between a particle of mass m and its environment. By using the appropriate $U(x)$ for a given situation, the equation can be solved. The solutions are wave functions Ψs whose magnitudes squared give the probability per unit length $P(x,t) = |\Psi(x,t)|^2$ of finding the particle at each position x. It turns out that at the microscopic scale, Ψ ($\therefore P$) is not zero inside and beyond the potential barrier as shown in Fig. 5.2 for a rectangular barrier. That means that the particle can be found inside and beyond the barrier i.e. particle can *tunnel* through the barrier.

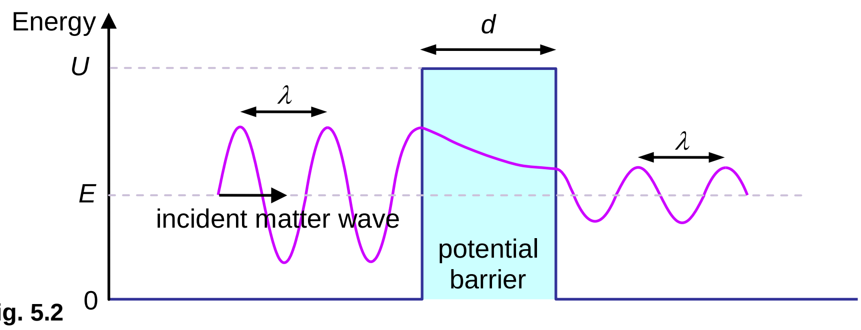


Fig. 5.2

On either side of the barrier, the particle's kinetic energy is E.

$E = ½ mv^2$
$= p^2/2m$ as $p = mv$
$= h^2/2m\lambda^2$ de Broglie's relation $p = h/\lambda$

Thus, shorter wavelength of matter wave corresponds to greater particle KE. Fig. 5.2 shows the same wavelength and thus KE before and after tunnelling. Quantum tunnelling is definitely not like a bullet tunnelling through a wall as the bullet will have lesser KE upon emerging from the other side.

Referring to Fig. 5.2, the probability that a particle of mass m can tunnel through a barrier of width d and potential energy U is given by:

$$\boxed{\begin{array}{l} T \approx e^{-2kd} \\ T + R = 1 \end{array} \quad \text{where } k=\sqrt{\frac{8\pi^2 m(U-E)}{h^2}}}$$

T - *transmission coefficient* or *probability*. R - *reflection probability*.

Transmission probability T at a rectangular barrier is

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

$T + R = 1$

Notice the following intuitively reasonable features of the formula:

1. As the barrier gets thicker (d larger), T gets smaller.
2. As the mass m increases, T gets smaller.
3. As the barrier gets higher (larger U), T gets smaller.
4. As E increases ($E < U$), T increases.

One key idea in this section is that 'the solution Ψ shows that a particle can tunnel through a barrier'. Does the statement really explain why? Indeed, physics merely *describes* how nature behaves according to some rules without telling us why the rules are the way they are and how they come about. Therefore, an exam question asking you to 'explain why' is really asking you to show how some theories, laws, principles or ideas can be used to derive a certain outcome or result. In the end, quantum tunnelling is just how nature behaves and its weirdness is due to it being an uncommon encounter. For particles with larger masses, Ψ will decrease exponentially more quickly inside the barrier, hence just like most quantum phenomena, tunnelling is only observed at microscopic scales.

Tunnelling Examples

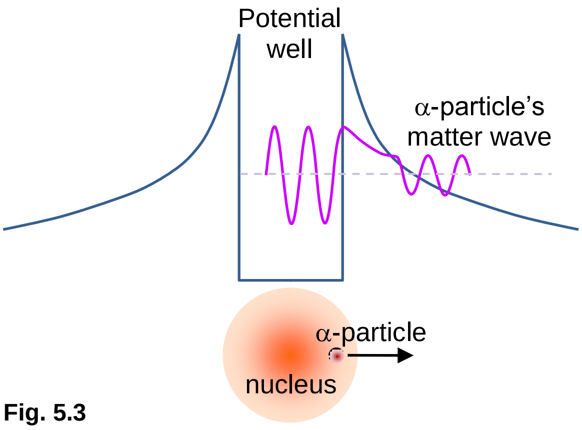


Fig. 5.3

In radioactive decay of α particle, the particle can be seen as trapped inside a potential well created by the rest of the nucleus. The α particle, made up of 2 neutrons and 2 protons, does not have sufficient energy according to classical physics to escape from the nucleus but it does so by quantum tunnelling.

Examples of quantum tunnelling
- α-decay
- fusion of protons in star.

In stars, nuclear fusion of two protons is also a quantum tunnelling process. When protons get near to each other, they experience a dominant repulsive Coulomb force but when they are even nearer, they will experience a dominant attractive nuclear force. The resulting potential energy curve looks quite similar to Fig. 5.2 except that now, a proton is trying to get into the well instead of out.

Scanning Tunnelling Microscope

STM makes use of quantum tunnelling for microscopy.

The STM (Scanning Tunnelling Microscope) makes use of an extremely small pointed tip to scan over the surface of a conductor (Fig. 5.4a). The tip is maintained at a distance of a few atomic diameters from the surface so that electrons can tunnel across the gap. In one mode of operation, the tip is moved across the sample at a fixed level as shown in Fig. 5.4b. When the tip is right above an atom e.g. A or B, the tunnelling current will be bigger than when the tip is between A and B because the gap (or barrier width) between the tip and sample is smaller when right above A and B. The variation of current with position reveals the profile of the surface (Fig. 5.4c).

The surface profile can be revealed by either scanning at constant height or current.

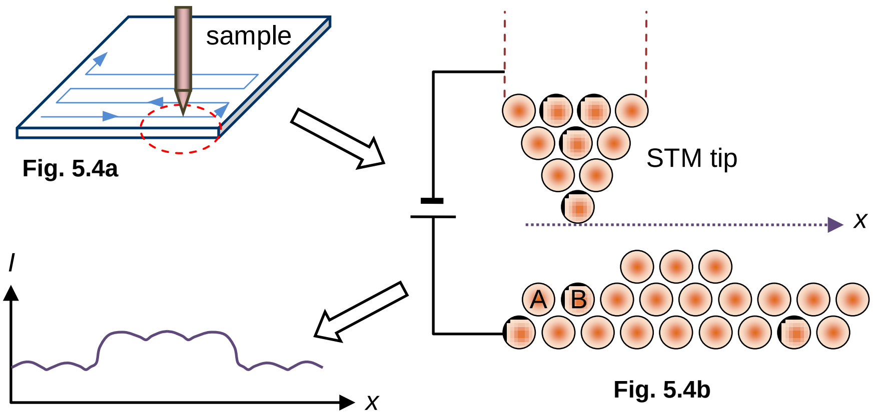


Fig. 5.4a **Fig. 5.4b** **Fig. 5.4c**

In a second mode, the STM tip is moved across the surface while keeping the tunnelling current constant by moving the tip up or down (Fig. 5.4d). The variation of the tip's height with position reveals the surface profile (Fig. 5.4e)

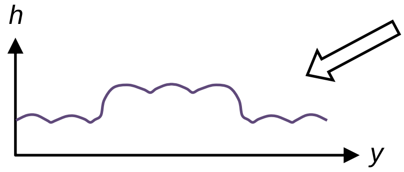


Fig. 5.4e

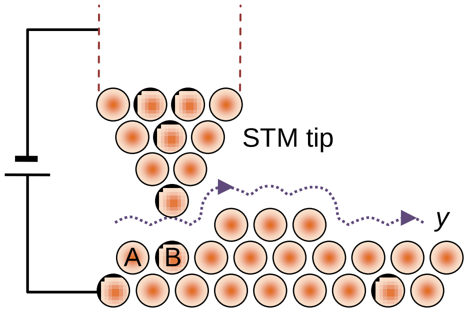
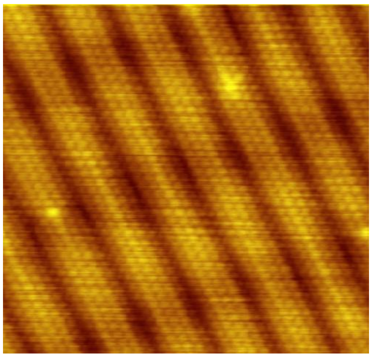


Fig. 5.4d



The data collected is usually processed by a computer into colour coded pictures such as the one to the left in which individual gold atoms could be seen.

(Picture in public domain. Author: Erwinrossen)