Class Notes for Modern Physics, Part 2

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The particle nature of matter

Most of you are already convinced that matter is composed of particles, but it is useful to at least briefly recall how our current understanding arose historically.

There were four major items in making this case:

1. Around 1833, Faraday performed a series of electrolysis experiments. these established three basic things:

   (a) that matter consists of molecules and that molecules consist of atoms;
   (b) that charge is quantized, because only integral numbers of charges are transferred between the electrolysis electrodes;
   (c) and that the subatomic parts of atoms carry positive and negative charges.

   However, he was unable to directly determine the masses of these subatomic particles, but it seemed clear that they were related to the atomic weights that were known from chemistry.

   Also, the absolute size of the charge of these subatomic particles could not be determined from electrolysis — only that charge was quantized.

Considerable time would pass before the next major input.

2. Around 1897, Thomson identified cathode rays as something with the same sign as the negative charges seen by Faraday.

   And, he found that all negative particles emitted from a cathode had identical e/m_e values, where e was the charge.

   He postulated that whatever this object was, it was probably a fundamental constituent of matter. We know it as the electron.

   A few years later, he was able to use measurements in a viscous cloud chamber to roughly determine the magnitude of the charge separately.

   He found that "e is the same in magnitude as the charge carried by the hydrogen atom in the electrolysis of solutions."

3. In 1909, Millikan was able to obtain a much more precise measurement of the electronic charge.

   This could be combined with the e/m_e value obtained by Thomson to obtain a value for m_e that was about 1000 times smaller than the mass of the Hydrogen atom (the latter being close to the proton mass, m_p), which had been known from atomic weights and chemistry.

4. **Finally, in 1913, Rutherford and co-workers established the nuclear model of the atom by scattering fast-moving α particles (charged Helium nuclei) from metal foil targets.**

   He showed that atoms consist of a compact positively charged nucleus (with diameter about $10^{-14}\ m$) surrounded by a swarm of orbiting electrons (with the electron cloud diameter being of order $10^{-10}\ m$.)

Here, I will try to say a few additional words about the Thomson and Rutherford experiments. Please read the material in the book on the Millikan experiment.

Thomson

The apparatus and schematic are shown below. We consider a $\vec{B}$ field pointing into the page and a $\vec{E}$ field in the plane of the page. When present, these produce forces $\vec{F}_E = -e\vec{E}$ (upwards) and $\vec{F}_B = -e(\vec{v}\times\vec{B})$ (downwards) on the e^-.

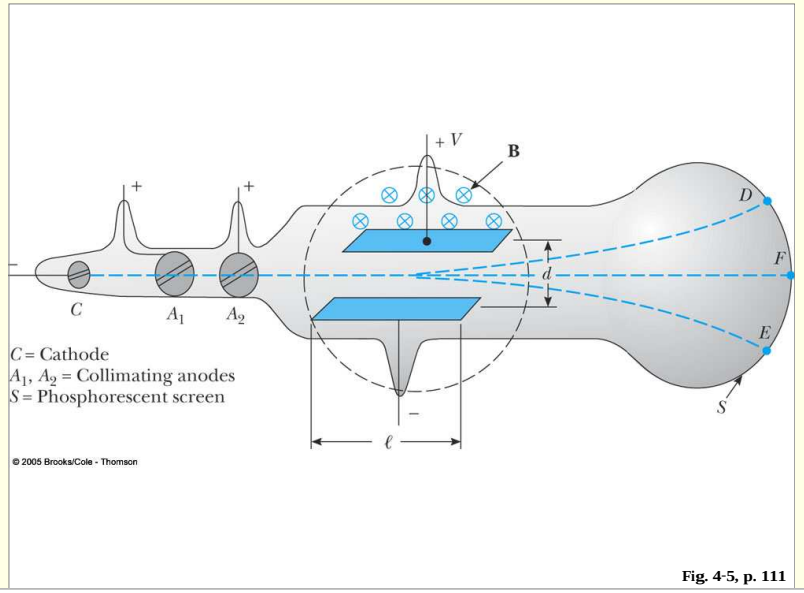


Fig. 4-5, p. 111

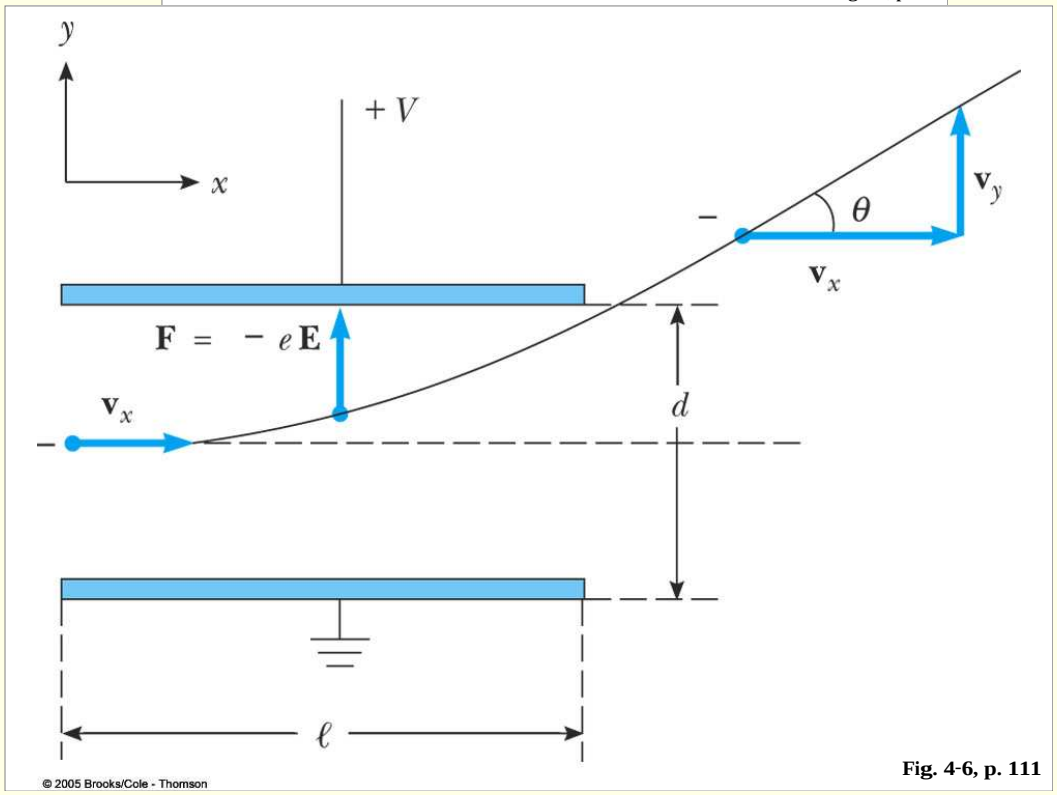


Fig. 4-6, p. 111

First, turn on just the $\vec{E}$ field. Initially, upon entering from the left, only v_x is non-zero, but upon exiting $v_y = a_y t$, where

$$a_y = \frac{F}{m_e} = \frac{eE}{m_e} = \frac{Ve}{m_e d} \quad \text{and} \quad t = \frac{l}{v_x}\,. \tag{1}$$

This gives

$$v_y = \frac{Vle}{m_e v_x d}\,, \quad \tan\theta = \frac{v_y}{v_x} = \frac{Vl}{v_x^2 d}\left(\frac{e}{m_e}\right)\,. \tag{2}$$

So a measurement of θ gives us a value for $\frac{e}{m_e}$ provided we can determine v_x. Thomson determined v_x, which remained the same if he kept his accelerating anodes at the same voltages, etc., by adding to $\vec{E}$ the $\vec{B}$ field. The forces exactly balance (and the e^- is undeflected) when (for any q, including $q = -e$)

$$qE = qv_x B\,, \quad \Rightarrow \quad v_x = \frac{E}{B} = \frac{V}{dB}\,. \tag{3}$$

Thus, using the $\vec{B}$ that gives exact balance, we get

$$\frac{e}{m_e} = \frac{v_x^2 d \tan\theta}{Vl} = \frac{V \tan\theta}{B^2 l d}. \tag{4}$$

Thomson obtained a result of $\sim 1.0 \times 10^{11}\ C/kg$ (vs. really accurate data of $1.76 \times 10^{11}\ C/kg$). This was clearly much larger than the electrolysis values which were probing $charge/proton\ mass$. Thomson had clearly demonstrated the existence of a new elementary particle with mass about 1000 times smaller than the mass of the proton (or hydrogen atom from the atomic weight / electrolysis point of view).

Rutherford

Based on his own experiments and those of others, in which it was clear that an atom was not a simple object, but had balancing negative and positive charged particles in it, with the negative one having a much smaller mass than the positive one, Thomson proposed the "plum-pudding" picture of the atom.

The atom was visualized as a homogeneous sphere of uniformly distributed mass and positive charge in which were embedded, like rasins in a plum pudding, negatively charged electrons, which just balanced the positive charge to make the atom electrically neutral.

Of course, this picture failed to explain the rich line spectra that people were finding for excited atoms, in particular even the simplest Hydrogen atom.

Rutherford and collaborators had noticed that a beam of α particles (i.e. Helium ions, $2p2n$) broadened upon passing through a metal foil, indicating that the foil was quite easily penetrated and yet at the same time caused significant scattering. This was hard to explain in the pudding model where the positive charge was spread all over the pudding.

After experimentation from 1909 to 1913, to be described, Rutherford concluded that all the positive charge, and most of the mass, was concentrated in a central nucleus of the atom. In particular, this picture was the only one that produced events in which the α particle was scattered at a very big angle, occassionally even backwards. The experimental apparatus and schematic picture of what is going on is depicted on the following page.

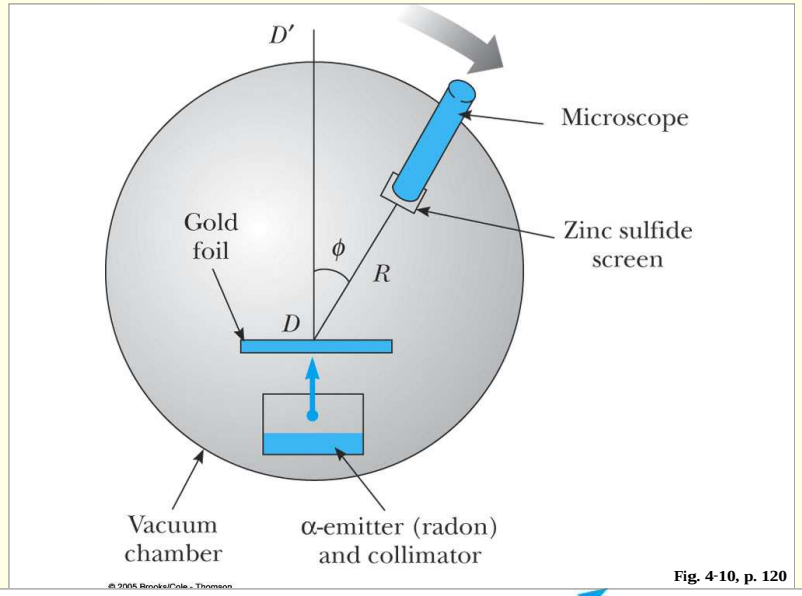


Fig. 4-10, p. 120

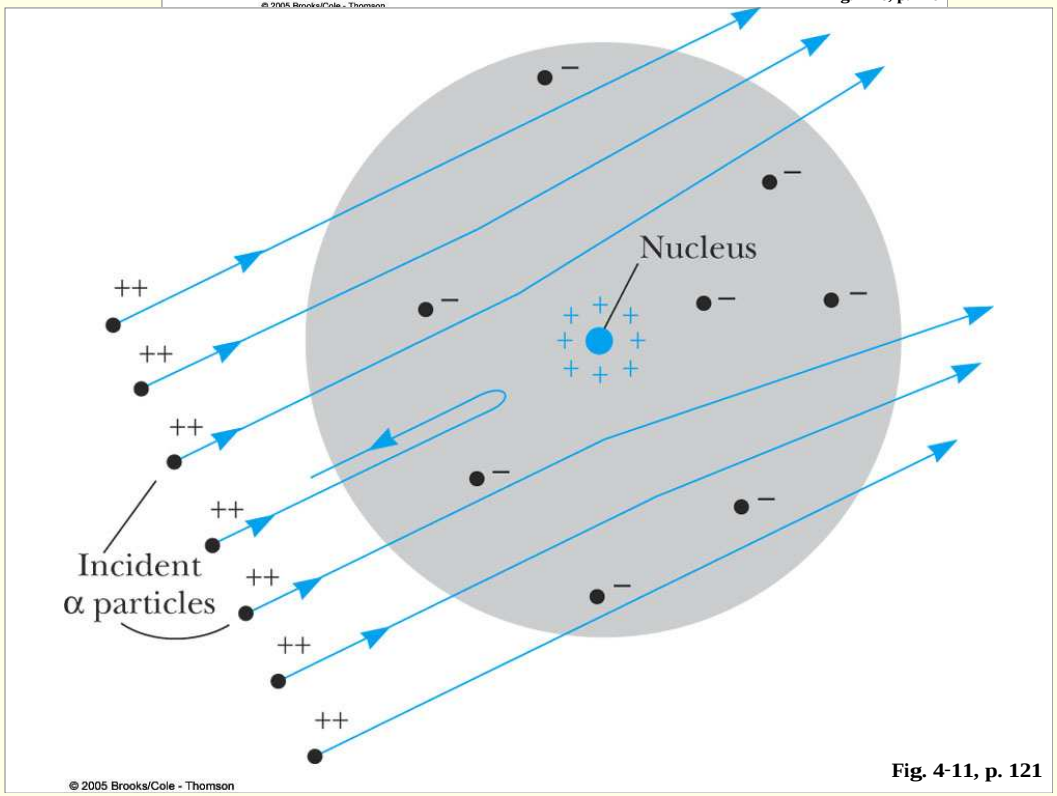


Fig. 4-11, p. 121

In order to account for the occassional large angle, including backwards, deflections, Rutherford pictured the atom as having a central charged nuclear core and employed nothing more than Coulomb's force law

$$F = k\frac{(2e)(Ze)}{r^2} \tag{5}$$

(where α has charge $2e$ in magnitude, the nucleus has charge Ze in magnitude, and k is Coulomb's constant). He predicted the following result for scattering:

$$\Delta n = \frac{k^2 Z^2 e^4 N n A}{4R^2(\frac{1}{2}m_\alpha v_\alpha^2)^2 \sin^4(\phi/2)}\,, \tag{6}$$

where R and ϕ appear in the figure, N is the number of nuclei per unit area of the foil (and is thus proportional to the foil thickness), n is the total number of α particles incident on the target per unit time, Δn is the number of α particles entering the detector per unit time at an angle ϕ, and A is the area of the detector. The velocity v_α is determined from the accelerating potential difference between the α emitter and the gold foil (or other) target: $K_\alpha = \frac{1}{2}m_\alpha v_\alpha^2 = (2e)V$ (non-relativistic ok here, and use charge of $\alpha = 2e$).

The agreement with the ϕ dependence was spectacular.

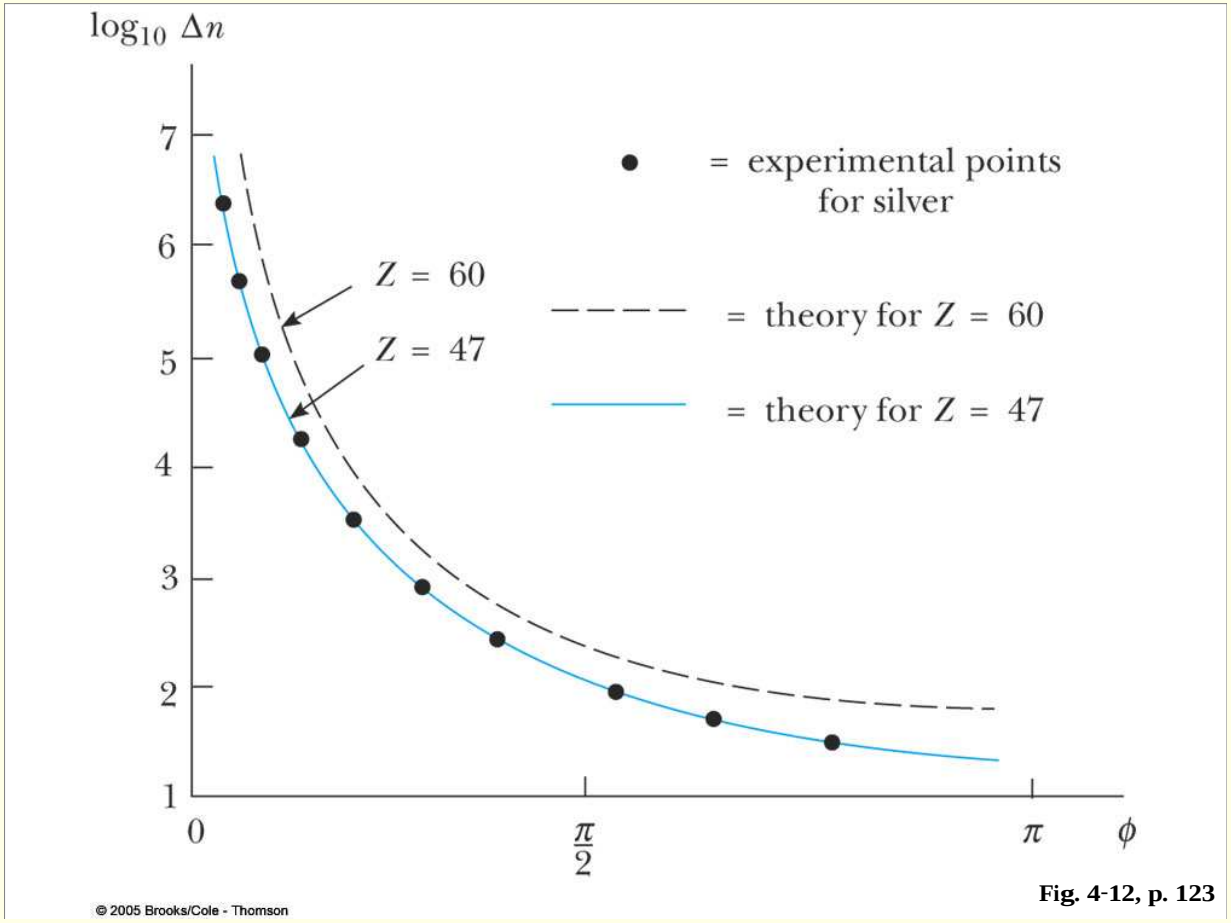


Fig. 4-12, p. 123

In fact, the normalization of the line allowed a determination of the then poorly determined Z values for different nuclei.

Rutherford also used the exactly back-scattered α particles to estimate the size of the nucleus. If d_{min} is the distance of closest approach of the α particle to the nucleus, and we know the kinetic energy of the α particle (which we do from the accelerating potential), then we may use

$$\frac{1}{2}m_\alpha v_\alpha^2 = k\frac{(Ze)(2e)}{d_{min}} \tag{7}$$

to solve for d_{min}. When Rutherford's prediction of eq. (6) starts to fail, the corresponding d_{min} presumably is the point at which the α is actually impinging into the nucleus itself rather than just Coulomb scattering from it.

Example

Estimate the radius of the Aluminum nucleus.

In 1919, Rutherford was able to show a breakdown in eq. (6) for 7.7 MeV α particles scattered at large angles from aluminum ($Z = 13$). Estimate the radius of the Al nucleus.

Answer: assume all the α kinetic energy, K_α, goes into potential energy

at d_{min}. Then,

$$\begin{aligned} d_{min} &= k\frac{2Ze^2}{K_\alpha} \\ &= (8.99 \times 10^9\ N \cdot m^2/C^2)\frac{2(13)(1.6 \times 10^{-10}\ C)^2}{(7.7 \times 10^6\ eV)(1.60 \times 10^{-19}\ J/eV)} \\ &= 4.9 \times 10^{-15}\ m\,. \end{aligned} \tag{8}$$

Spectral Lines and Balmer

As mentioned earlier, many spectral lines had been seen, coming from the sun, coming from excited atoms, and so forth. There was no explanation yet. ***Do spectral line demo.***

A particularly famous result was the one obtained by Balmer in 1885. He managed to "fit" the results of Angstrom's measurements of the wavelengths of the spectral lines from excited Hydrogen. These are displayed on the next page.

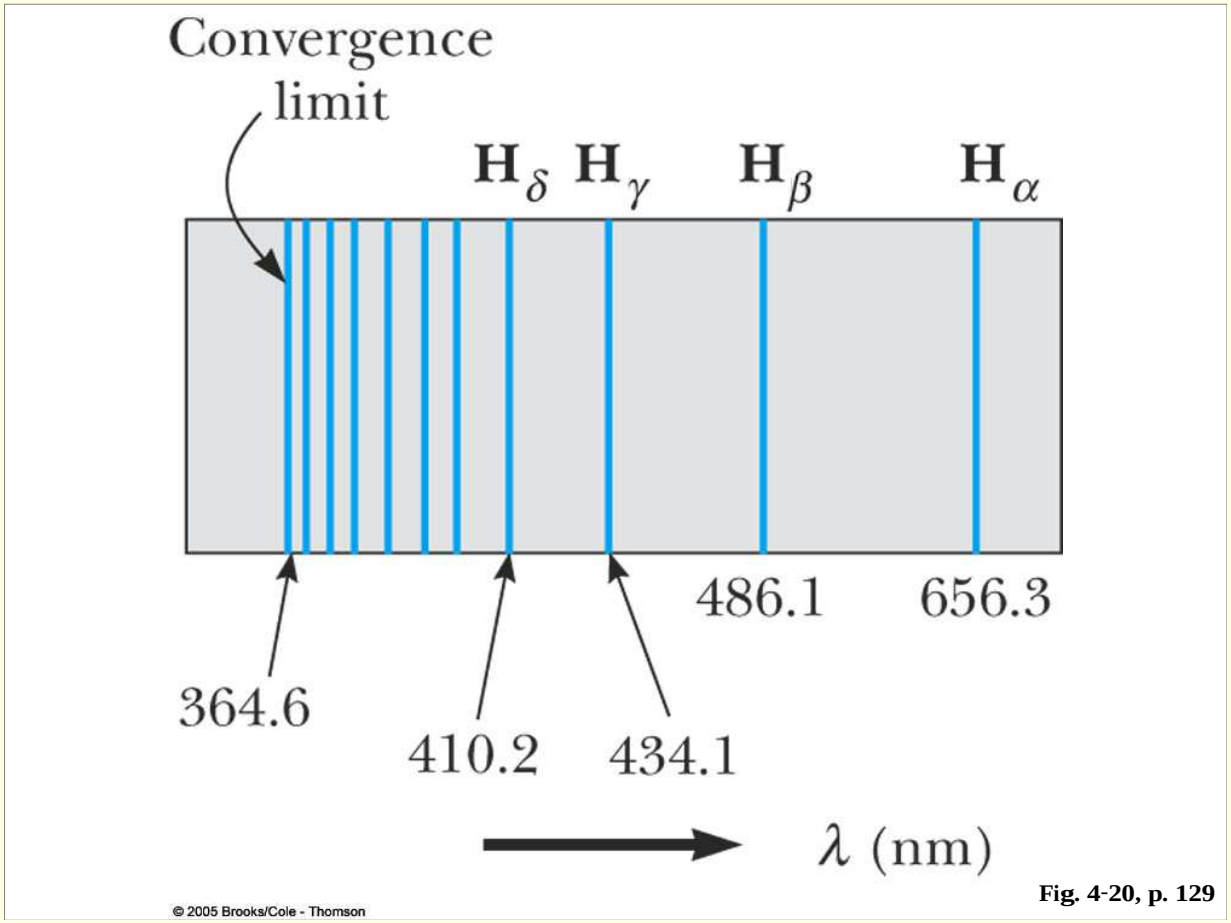


Fig. 4-20, p. 129

Balmer noted that the line wavelengths took the form:

$$\lambda(cm) = C_2 \left(\frac{n^2}{n^2 - 2^2} \right) , \quad n = 3, 4, 5, \ldots \tag{9}$$

where $C_2 = 3645.6 \times 10^{-8}\ cm$, a constant called the *convergence limit*

to which one tends as $n \to \infty$. He further speculated that there would be found other spectral line series of Hydrogen that would be fit by the general form (equivalent for $n_f = 2$ to the previous form)

$$\frac{1}{\lambda} = R\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) \tag{10}$$

where $n_i > n_f$ and $R = 1.0973732 \times 10^7\ m^{-1}$ is the Rydberg constant and is the same for all the different Hydrogen series lines. These series came to be named after the experimentalists that were first to see them: Balmer: $n_f = 2$ (visible and near UV); Lyman: $n_f = 1$ (more UV and harder to see); followed by Paschen, Brackett and Pfund ($n_f = 3, 4, 5$) in the IR.

The groundwork was now in place for

Bohr

To understand how revolutionary Bohr's ideas were, consider the conundrum that the atomic physics people found themselves in. The picture of a

positively charged nucleus with e^-'s circling around it was now firmly established.

But, according to classical Maxwell, the centripetal acceleration the e^-'s were continually undergoing would cause them to radiate $E\&M$ waves.

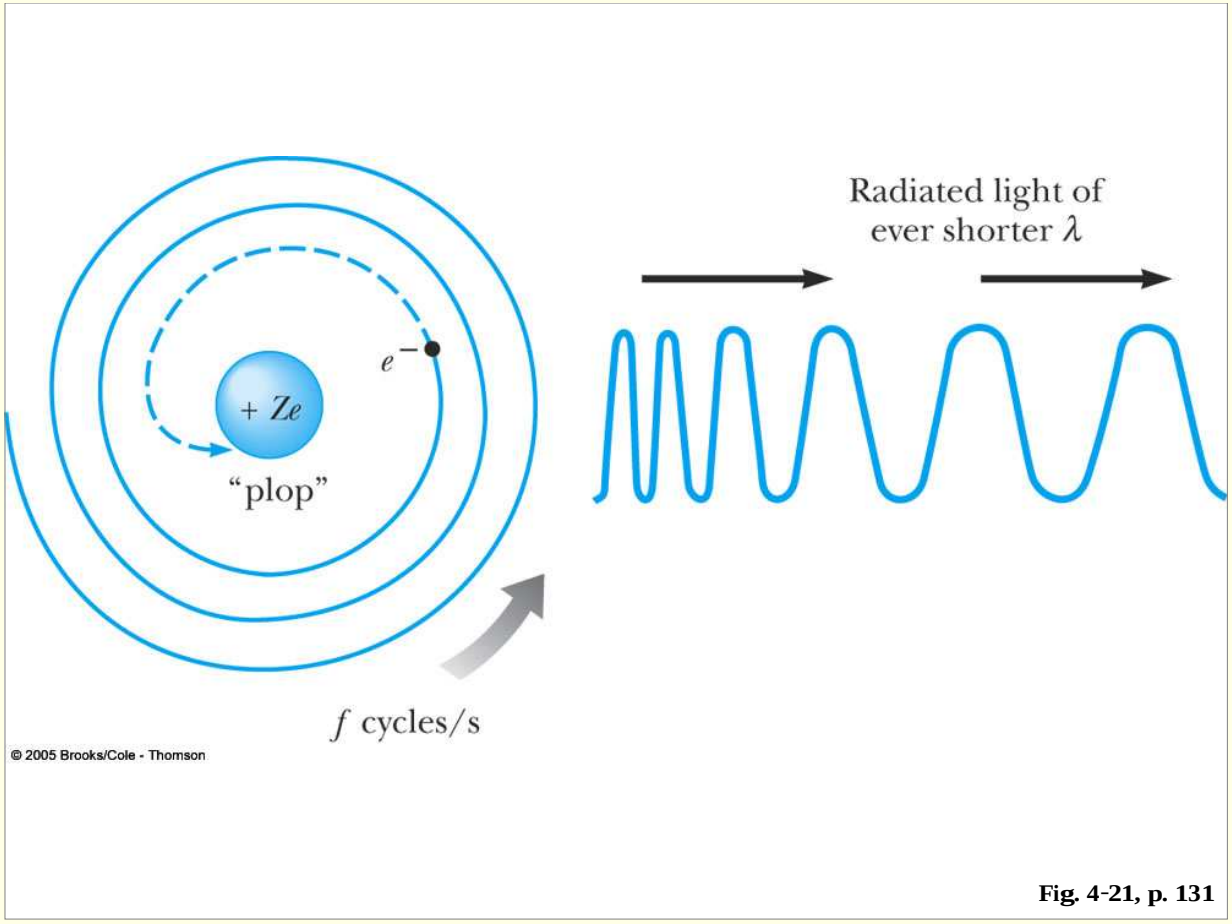


Figure 1: Classical model of the nuclear atom.

Classical theory would then imply that as the e^-'s lose energy they would move closer to the nucleus. Further, the spectrum of radiation from this continuous process would change continuously, and one should not see sharp spectral lines.

In fact, as the e^- gets closer to the nucleus it is moving faster and faster in a stronger and stronger Coulumb field and the frequency of the radiation would get higher and higher.

Of course, we would not be around to see all this in any case.

Bohr followed the lead of Planck and Einstein by assuming that if light was quantized then why shouldn't atomic electronic orbits be quantized in some way. Then, spectral lines could arise when an electron jumped from one such electronic orbit to another orbit (of lower energy) by emitting a photon of definite frequency given by $\Delta E = hf$.

Armed with the picture of the atom just developed by Rutherford, in 1913 Bohr published a 3-part paper in which he postulated that electrons in atoms are confined to stable, nonradiating energy levels and orbits known as stationary states.

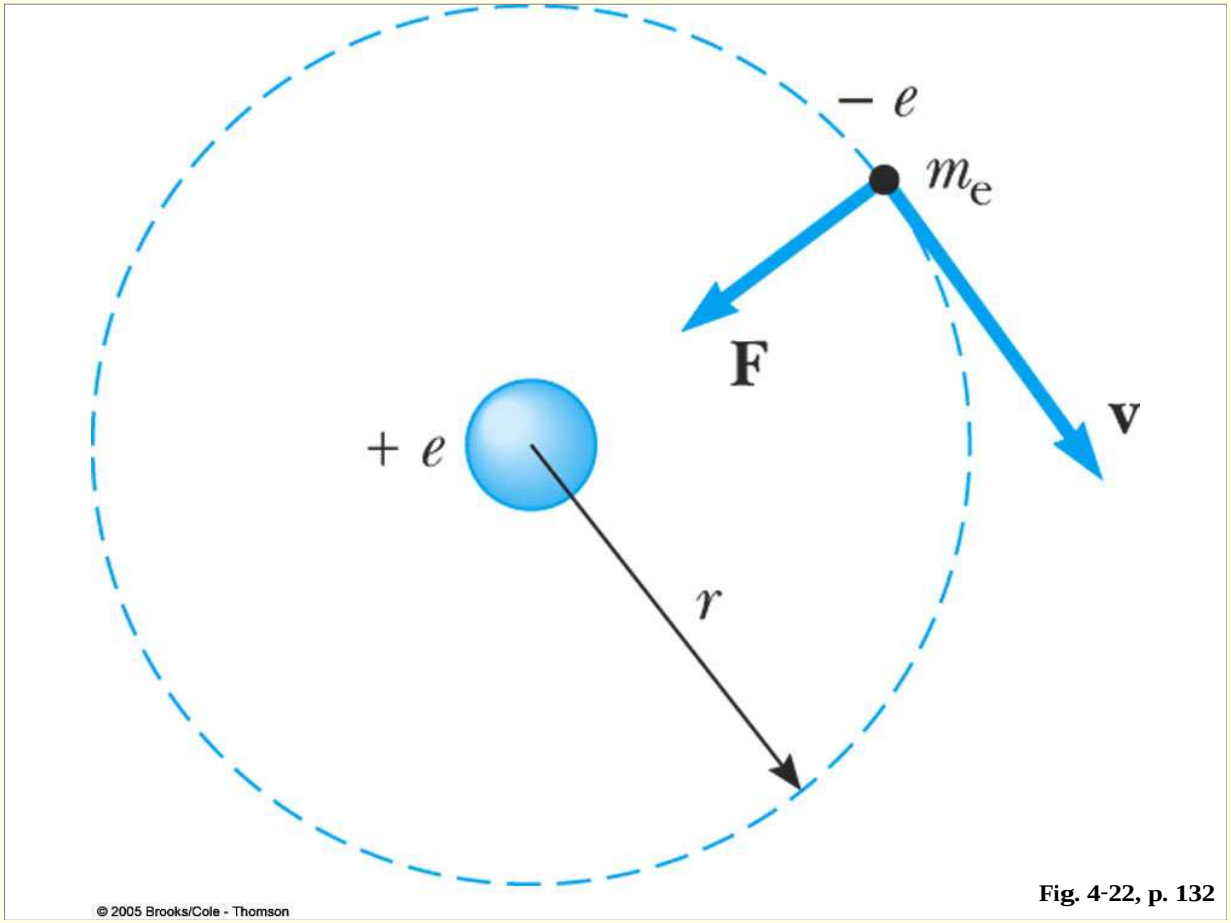


Figure 2: Bohr's model of the Hydrogen atom. The radius is assumed to be constant because of "quantization".

As just stated, Bohr realized that the spectral lines corresponded to photons of a definite wave length and definite frequency and so he knew that the separation between his stationary states should come in units of

$\Delta E = hf = h\frac{c}{\lambda}$.

The only remaining question was how to match this on to Balmer's formula. He discovered that this matching worked if he hypothesized that the electron's orbital angular momentum about the nucleus had to be an integral multiple of $\hbar \equiv \frac{h}{2\pi}$ (obviously, h had to be involved somehow)

$$m_e v r = n\hbar\,, \quad n = 1, 2, 3, \ldots \tag{11}$$

Let us see why this works. (For atoms, we can use non-relativistic procedures with adequate accuracy.)

1. The electric potential energy of the e^- is $U = -ke^2/r$, where $k = 1/(4\pi\epsilon_0)$.
2. The total energy of the atom is the sum of the potential and kinetic energies,
$$E = K + U = \frac{1}{2}m_e v^2 - k\frac{e^2}{r}\,. \tag{12}$$
3. Meanwhile, Newton's force law says force=centripetal acceleration, or

$$\frac{ke^2}{r^2} = m_e\frac{v^2}{r}\,, \quad \text{which} \Rightarrow \quad K = \frac{1}{2}m_e v^2 = \frac{ke^2}{2r}\,. \tag{13}$$

4. Putting this result into the equation for E, eq. (12), gives

$$E = -\frac{ke^2}{2r}\,. \tag{14}$$

5. Next, we solve for v in terms of n and r using the equations above, $m_e v r = n\hbar$ and $\frac{1}{2}m_e v^2 = \frac{ke^2}{2r}$, to obtain

$$r_n = \frac{n^2\hbar^2}{m_e k e^2}\,, \quad n = 1, 2, 3, \ldots \tag{15}$$

r_1 is often denoted by a_0, and is called the Bohr radius,

$$a_0 = \frac{\hbar^2}{m_e k e^2} = 0.0529\ nm\,. \tag{16}$$

6. Finally, substitute the form of r_n into the equation for E just above, *i.e.* eq. (14), to obtain

$$E_n = -\frac{ke^2}{2a_0}\left(\frac{1}{n^2}\right) = -\frac{13.6}{n^2}\ eV\,. \tag{17}$$

The values n are called the *quantum numbers* characterizing different states.

The lowest state $E_1 = -13.6$ eV is called the *ground* state.

The $n = 2$ state is the 1st *excited* state and has energy $E_2 = -3.4$ eV, and so forth.

At this point, we can explain the Balmer formula.

1. **A spectral photon is emitted when the atom drops from a state with a high $n = n_i$ to a state with more negative energy *i.e.* with smaller $n = n_f$.**
2. **The different series are obtained using $n_f = 1$, $n_f = 2$, . . . for the final lower-n state.**
3. **In other words, we have**

$$\frac{1}{\lambda} = \frac{f}{c} = \frac{E_i - E_f}{hc} = \frac{ke^2}{2a_0 h}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) . \tag{18}$$

One finds that $ke^2/(2a_0h) = R$, the Rydberg constant and one gets a theoretical post-diction of the Balmer formula.

This is depicted in Fig. 3.

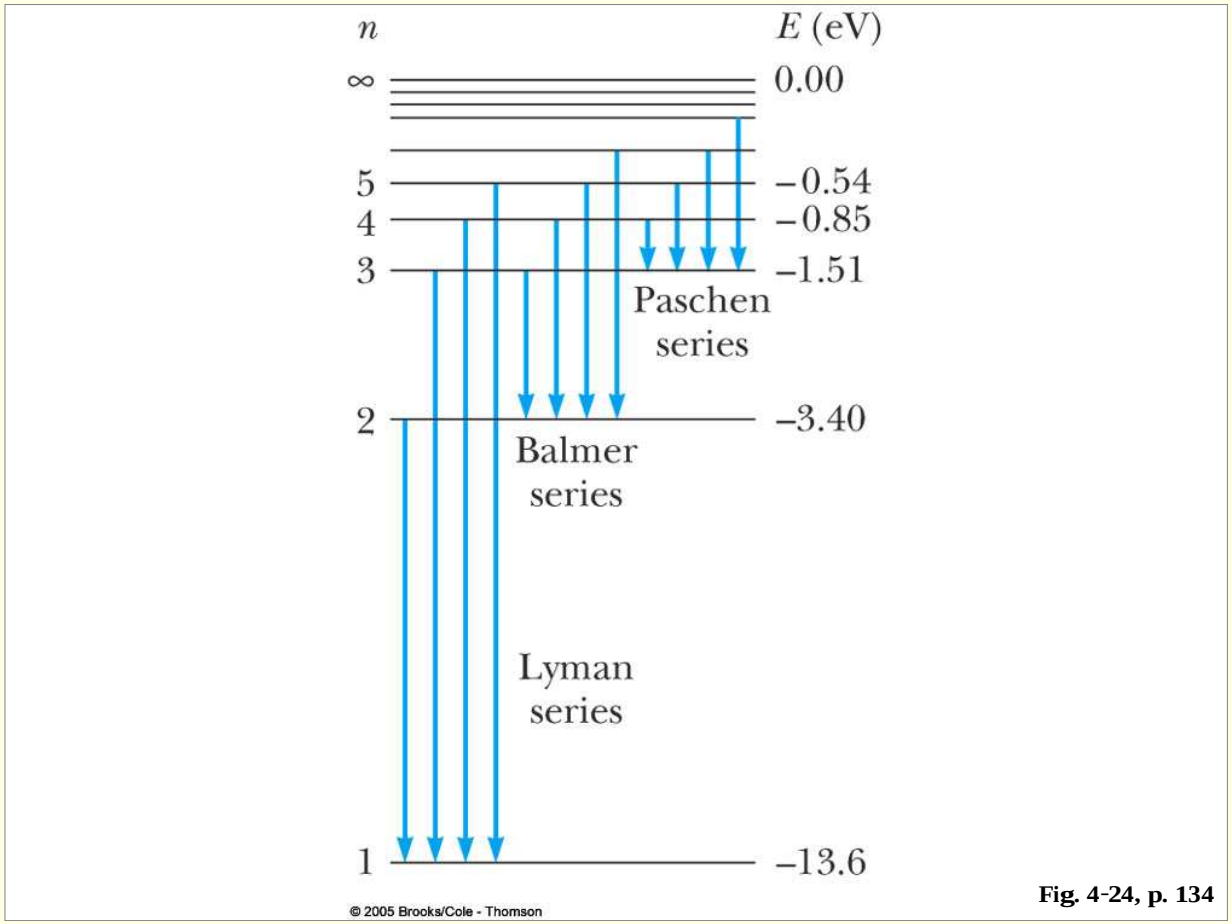


Figure 3: Bohr's explanation of the various Hydrogen spectral series.

An Example

Suppose the stellar atmosphere has a temperature of order $T = 79,000\ K$. (a) Is it reasonable to expect that a lot of the Hydrogen atoms

will be excited to the first excited state? (b) What is the wavelength of the light emitted when these excited atoms decay back to the $n = 1$ ground state level?

First, we compute the average thermal energy per atom:

$$\frac{3}{2}k_B T = (1.5)(8.62 \times 10^{-5}\ eV/K)(79000) = 10.2\ eV\,. \qquad (19)$$

This, we must compare to the energy of excitation,

$$E_2 - E_1 = -3.4\ eV - (-13.6\ eV) = 10.2\ eV\,. \qquad (20)$$

Since these are comparable, we expect substantial excitation.

The wavelength could either be obtained from the Balmer formula or we can return to Bohr's basic model according to which

$$\begin{aligned} hf &= E_2 - E_1 \quad \Rightarrow \\ \lambda &= \frac{hc}{E_2 - E_1} = \frac{(4.136 \times 10^{-15}\ eV \cdot s)(3 \times 10^8\ m/s)}{10.2\ eV} \\ &= 1.22 \times 10^{-7}\ m = 122\ nm\,, \end{aligned} \qquad (21)$$

well into the ultraviolet.

Bohr immediately realized that all of this could be extended to ions obtained from an element with a given nuclear charge Z by removing all but one of the e^-'s.

Such an ion has a single e^- orbiting about a nuclear charge of $+Ze$. Proceeding as above, but using the higher nuclear charge, one obtains

$$r_n = n^2 \frac{a_0}{Z}, \quad \text{implying} \quad E_n = -\frac{ke^2}{2a_0}\left(\frac{Z^2}{n^2}\right), \quad n = 1, 2, 3, \ldots \tag{22}$$

When applied to He^+, several previously unexplained spectral lines in radiation from the sun were explained.

An Example

Pickering, in 1896, observed unexpected spectral lines in the light from ξ-Puppis, a star.

He found that these lines fit the spectral formula

$$\frac{1}{\lambda} = R\left(\frac{1}{(n_f/2)^2} - \frac{1}{(n_i/2)^2}\right), \tag{23}$$

where R is the Rydberg constant. We can easily check that these lines are simply those associated with He^+ as follows.

Since He^+ has nuclear charge of $Z = 2$, we have energy levels given by

$$E_n = \frac{ke^2}{2a_0}\left(\frac{4}{n^2}\right) . \tag{24}$$

Using $hf = E_i - E_f$, we then have

$$\begin{aligned} \frac{1}{\lambda} &= \frac{f}{c} = \frac{E_i - E_f}{hc} \\ &= \frac{ke^2}{2a_0hc}\left(\frac{4}{n_i^2} - \frac{4}{n_f^2}\right) \\ &= \frac{ke^2}{2a_0hc}\left(\frac{1}{(n_i/2)^2} - \frac{1}{(n_f/2)^2}\right) \end{aligned} \tag{25}$$

where $ke^2/(2a_0hc) = R$ is precisely the Rydberg constant.

An interesting question from the class

During the lecture on this material, an interesting question was asked. This concerned why we don't see atoms absorbing starlight. Well, in fact we do. As we discussed, one should visualize a distant star sending light towards the earth, with some dust or gas cloud (for example) in between the star and the earth. If the cloud mainly contains Hydrogen, for example, then starlight with the right frequency to excite a Hydrogen atom from a low energy ($e.g.$ ground) state to a higher state will often get absorbed and not make it through the cloud. We get what are called absorption spectra (that can be used to help determine the red-shift of the star relative to the cloud and of the cloud relative to us).

The energy of the star radiation can even be sufficient to completely ionize the Hydrogen atom if the cloud is close to the star or the star is of a particularly energetic type.

A second question was why one doesn't get radiation, coming from the excited atom when it falls back to its ground state, that fills in the absorption line.

In fact, there is such radiation, but it goes in all directions (not just towards the earth) and so the amount headed towards earth is greatly

diminished.

An important dimensionless ratio

It turns out to be interesting to consider the ratio

$$\begin{aligned} \frac{v_{n=1}}{c} &= \frac{1}{c}\frac{\hbar}{m r_1} \quad \text{from } mvr = n\hbar \\ &= \frac{1}{c}\frac{k e^2}{\hbar} \quad \text{from } r_1 = \frac{\hbar^2}{m_e k e^2} \\ &= \frac{k e^2}{\hbar c} \equiv \alpha = \frac{1}{137}\,. \end{aligned} \tag{26}$$

Note how small v_1/c is. The non-relativistic approximation employed by Bohr was ok.

The quantitiy α is sometimes called the *fine structure constant*. It is a very useful characterization of the strength of the $E\&M$ force. Other forces, such as the strong and weak forces that we will learn more about late in the quarter, have different strengths.

Such dimensionless ratios constructed using known physical constants (here, $\hbar$, c, k and e) are typically of deep theoretical significance. To construct α, we needed the new fundamental constant $\hbar$.

The correspondence principle

One justification given by Bohr for his angular momentum quantization condition is that it is required if we demand a correspondence principle according to which

$$\lim_{n\to\infty} [\text{quantum physics}] = [\text{classical physics}] \tag{27}$$

where n is a typical quantum number of the system such that large n corresponds to a limit in which one should approach a classical type of situation, such as long wavelengths.

We will not go into the details of this in class.

Franck and Hertz

Of course, the critical assumption made by Bohr in his explanation of the spectral lines was that an electron could be in a higher n state and that when it "fell" down to a lower state it emitted a single photon.

A direct verification that the photon energies corresponded to the separation between energy levels of the electron of the atom was needed.

Franck and Hertz provided an explicit experimental demonstration that this was indeed the case.

They sealed some Mercury Hg inside a tube and accelerated e^-'s through the tube using a voltage $\overline{V}$. These e^-'s then collide with the Hg atoms inside the tube, possibly giving energy to them.

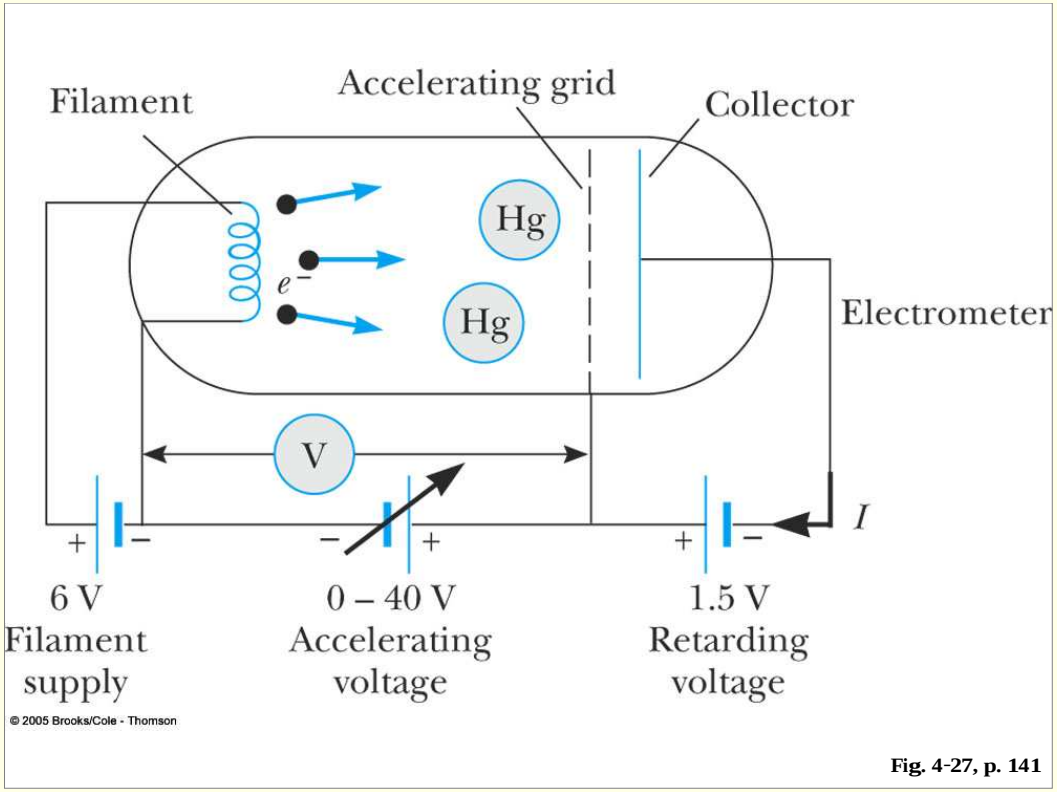


Figure 4: The Franck-Hertz apparatus.

For small $\overline{V}$, these collisions were elastic and the e^-'s retained most of

their kinetic energy (very little is taken by the much more massive Hg atoms in an average collision). Even after many collisions, the e^- arrives at the accleration grid with energy of about $e\overline{V}$.

Following this acceleration, their apparatus had a retarding voltage gap between the accelerating grid and the following collector plate of about $1.5\ V$. Thus, some e^-'s will be collected if $\overline{V} > 1.5\ V$.

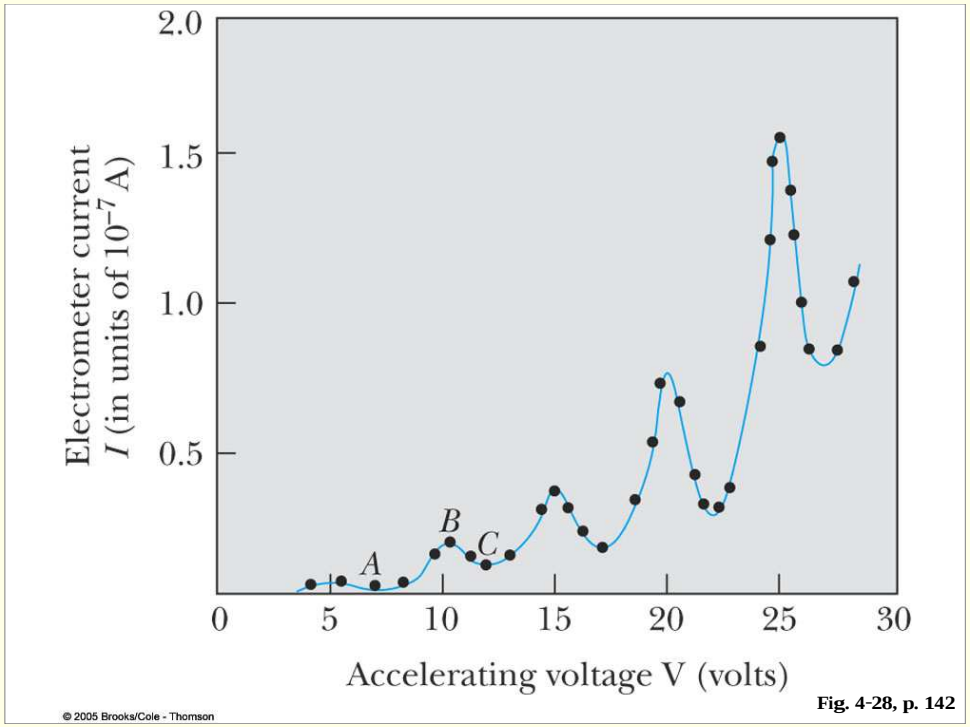


Figure 5: The Franck-Hertz current as a function of accelerating voltage $\overline{V}$.

As $\overline{V}$ is increased, more and more e^-'s make it to the collector until

the energy $e\overline{V}$ that the electrons have acquired matches the energy difference between two atomic energy levels. At this point, the collision between some of the accelerated e^-'s and the Hg can be inelastic — the Hg atom absorbs the $K = e\overline{V}$ energy of the e^- when one of its own electrons is excited to a higher n level.. There is a sudden dip in the current reaching the collector.

When $\overline{V}$ is increased further, more and more electrons reach the collector until once again the current suddenly dips. What is happening is that $\overline{V}$ is large enough for the accelerated e^-'s to have two inelastic collisions with two subsequent Hg atoms.

The separation between the dips was found to be $\Delta\overline{V} \sim 4.9\ V$. They interpreted $e\Delta\overline{V}$ as being the energy difference between the ground state of low n for one of the Mercury orbiting electrons and the next excited state of this same electron.

How could they check this? Well, if they really had excited the Hg atomic electron to a higher level, it should emit a photon of the corresponding frequency when this electron fell back down to its original lower level.

The expected wave length of the photon was therefore given by

$$e\Delta\overline{V} = \Delta E = hf = \frac{hc}{\lambda}, \quad \Rightarrow \quad \lambda = \frac{hc}{\Delta E} = \frac{1240\ eV \cdot nm}{4.9\ eV} = 253\, nm\,. \tag{28}$$

This is the precise wavelength they observed. In 1925, they were awarded the Nobel prize for this confirmation of Bohr's theory.

Connection of Bohr quantization to the wave nature of matter

The next big question was why should angular momentum be quantized in the manner proposed by Bohr?

What turns out to be the fundamental idea was that developed by de Broglie in 1925.

He speculated that if light, a wave phenomenon originally, also had a particle-like nature, then why not the reverse?

He also was looking for a way to explain the integers and quantization that emerged in Bohr's atomic theory, which concerned electrons circling a nucleus. The only way that integers had cropped up in the past was

in wave interference phenomena and normal modes of vibration (such as simple string standing waves). He decided that periodicity should be assigned to electrons under appropriate circumstances such as in atomic orbits.

For this, he needed a wavelength and a frequency to associate with particles. In analogy with light, he postulated

$$\lambda = \frac{h}{p} \quad \text{and} \quad f = \frac{E}{h}\,. \tag{29}$$

(We will return to the problem with this that arises if you compute wave velocity as $f\lambda = E/p$ using the relativistic formulae, $p = \gamma(u)m_0u$ and $E = \gamma(u)m_0c^2$, which would give $E/p = c^2/u > c$.)

De Broglie noticed that if we employ the photon-like formula $p = mv_e = h/\lambda$ and plug this into $m_evr = n\hbar$, we find

$$\frac{h}{\lambda}r = n\frac{h}{2\pi} \quad \Rightarrow \quad \frac{2\pi r}{\lambda} = n\,. \tag{30}$$

In other words, the circumference of the electron orbit must contain an integer number of electron wavelengths, which, in turn, implies that the

electron wave pattern will repeat by matching onto itself after going around a full orbit. In other words, an electron orbit should correspond to a standing, self-reinforcing wave pattern, much like a plucked guitar string.

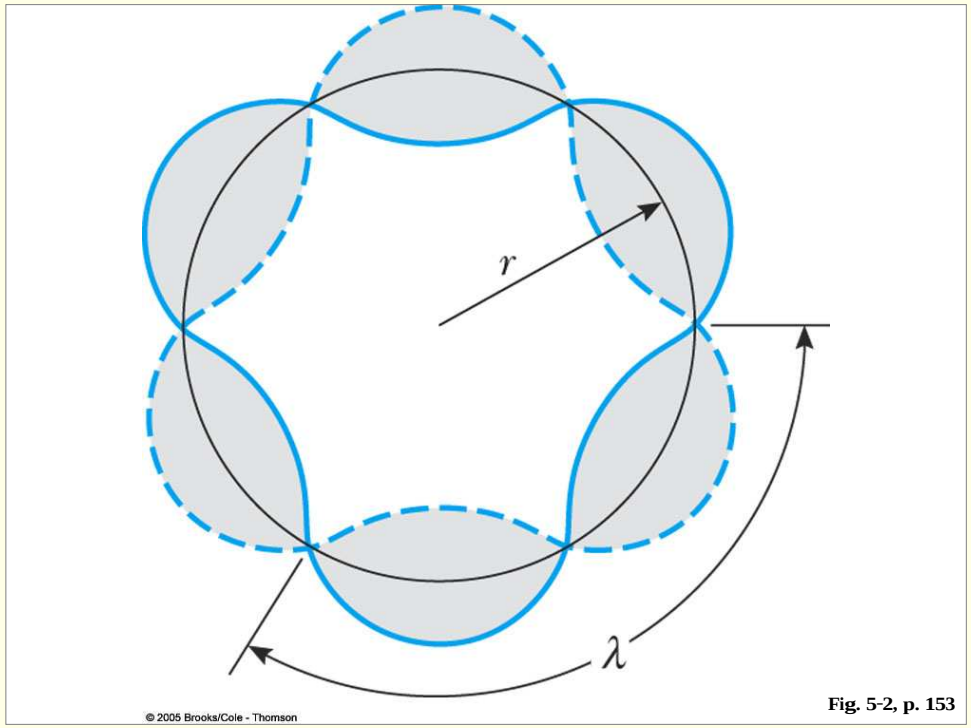


Figure 6: De Broglie's explanation of Bohr quantization for the case of $n = 3$, showing self-reinforcing standing wave pattern for an e^- around the nucleus with three wave lengths fitting into $2\pi r$ circumference.

We will soon turn to more discussion and eventual direct confirmation of

the association of a wavelength with a massive particle using $\lambda = h/p$.

In the end, we will see that this standing wave pattern and the whole Bohr picture is not an accurate point of view. However, it was very critical to developing the correct view that we now call Quantum Mechanics.

Wave Equations and Fourier Ideas

Since I want to make sure we are all on the same page, I will give a very brief review of wave equations and the $E\&M$ wave equation in particular. The latter material was in sections 32.2 and 32.3 of *University Physics* Part 2 by Young and Freedman, which is I believe the text employed for your earlier courses. Had you covered chapters 35 and 36 of this text, which I understand you probably did not, you would have seen a very detailed discussion for light of the interference phenomena and so forth that we have already talked about. But, you did, I believe, cover these phenomena for mechanical waves, which is where we begin.

First, recall the differential equation that you studied and understood for mechanical waves on a string or in water.

$$\frac{\partial^2 y(x,t)}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y(x,t)}{\partial t^2}\,, \tag{31}$$

where $y(x,t)$ is the displacement of the string, or ... at location x and time t, and v is the velocity with which the wave moves along the string.

Solutions of this equation take the form $f(x - vt)$ or $f(x + vt)$. In particular, denoting the argument of f as θ, for either $\theta = x - vt$ or $\theta = x + vt$ we have

$$\frac{\partial^2 f}{\partial x^2} = f''(\theta) \quad \text{and} \quad \frac{\partial^2 f}{\partial t^2} = v^2 f''(\theta) \quad \Rightarrow \frac{\partial^2 f}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 f}{\partial t^2}\,. \tag{32}$$

A particularly simple choice for f is one such that $f'' \propto f$. A possible example of this type is

$$f = \sin\left(\frac{2\pi}{\lambda}(x - vt)\right) \tag{33}$$

where, of course, you recognize λ as the wavelength such that if $x \longrightarrow x + \lambda$ the shape of the wave repeats. Of course, there is also a frequency of repetition intrinsic to the above form given by

$$\frac{2\pi}{\lambda}vT = 2\pi\,, \quad \text{or} \quad f = \frac{1}{T} = \frac{v}{\lambda}\,. \tag{34}$$

Often, it is more convenient to write

$$\frac{2\pi}{\lambda}(x - vt) \equiv kx - \omega t\,, \tag{35}$$

where $k \equiv 2\pi/\lambda$ and you can check that $\omega = 2\pi f$.

We should also recall that one can *superimpose* different solutions of the wave equation and still get a solution. For example,

$$e^{i(kx-\omega t)} \quad \text{and} \quad e^{-i(kx-\omega t)} \tag{36}$$

are both also solutions to the wave equation and the earlier $\sin$ form can be written as (using $e^{ib} = \cos b + i \sin b$)

$$\sin(kx - \omega t) = \frac{1}{2i}\left[e^{i(kx-\omega t)} - e^{-i(kx-\omega t)}\right]\,. \tag{37}$$

Of course, in the case of a real observable thing like the string displacement, when we superimpose these complex exponentials, we should always do so in such a way that the superposition has a real value. But, it is nonetheless convenient to use the complex exponentials. In

fact, as we shall see, matter waves are intrinsically complex and can be so because the waves have no direct physical manifestation. It is only their $|amplitude|^2$ that can be interpreted as $probability$.

We can also superimpose solutions with different wave lengths and frequencies (always holding $f\lambda = v$ fixed for a given wave velocity). This amounts to giving a Fourier representation of the wave solution: $e.g.$

$$f(x - vt) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dk \widetilde{f}(k) e^{ik(x-vt)} \,, \tag{38}$$

where k can run over negative as well as positive values and $\omega(k) = vk$ is implicitly required by this form. The functional form $\widetilde{f}(k)$ defines the Fourier decomposition of the wave solution $f(x - vt)$. The inverse $\sqrt{2\pi}$ is just a conventional choice.

The above might be complex. So, for a real observable like string displacement, we would take the real part of $f(x - vt)$. It will still be a solution of the wave equation since it will still be a function only of $x - vt$.

A useful example

Consider a "square-wave" shape for $\widetilde{f}(k)$

$$\widetilde{f} = 0, \quad k < k_0 - \frac{1}{2}\Delta k \tag{39}$$

$$\widetilde{f} = 1, \quad k_0 - \frac{1}{2}\Delta k \leq k \leq k_0 + \frac{1}{2}\Delta k \tag{40}$$

$$\widetilde{f} = 0, \quad k > k_0 + \frac{1}{2}\Delta k\,. \tag{41}$$

This $\widetilde{f}(k)$ is plotted below. (The book, Example 5.7, uses the notation $\widetilde{f}(k) = a(k)$.)

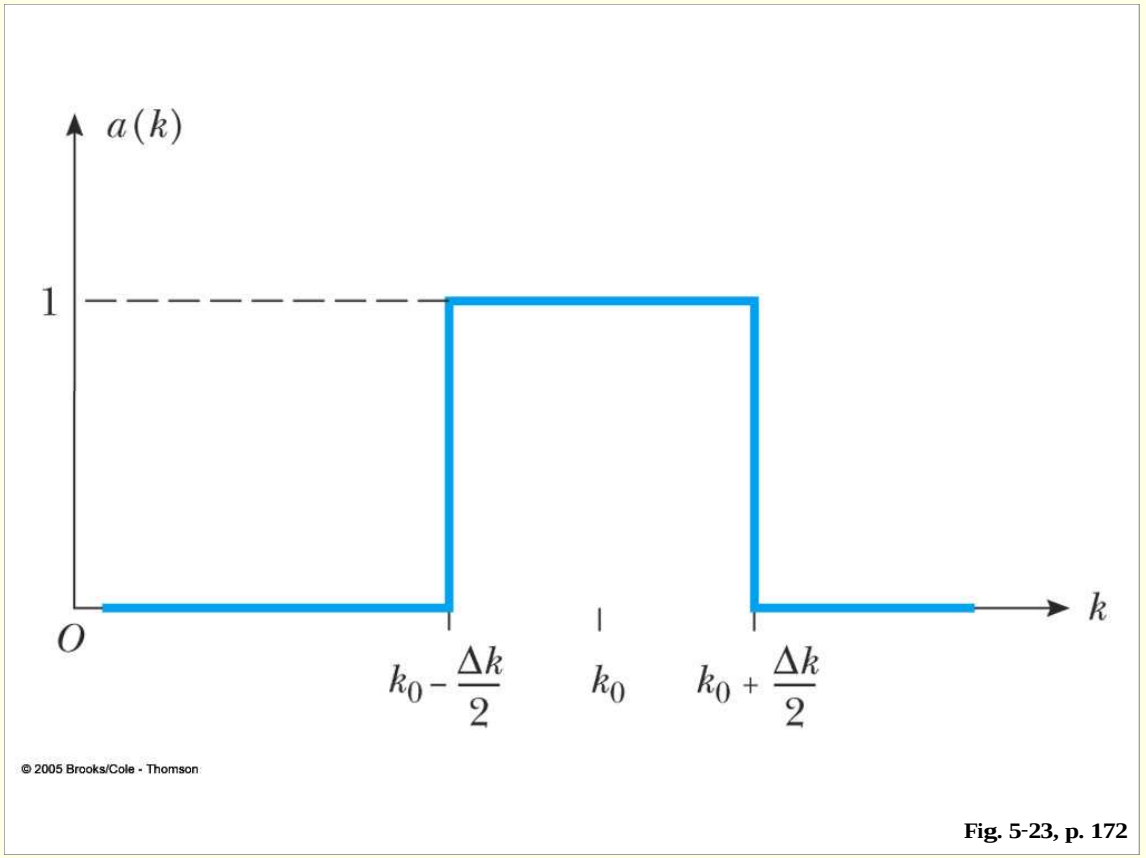


Figure 7: Input k-space function.

The resulting analytic form for $f(x - vt)$ at $t = 0$ (derived a bit later) is

$$f(x) = \frac{\Delta k}{\sqrt{2\pi}} \frac{\sin(\Delta k \cdot x/2)}{(\Delta k \cdot x/2)} e^{ik_0 x}\,, \tag{42}$$

the real part of which is plotted in the figure.

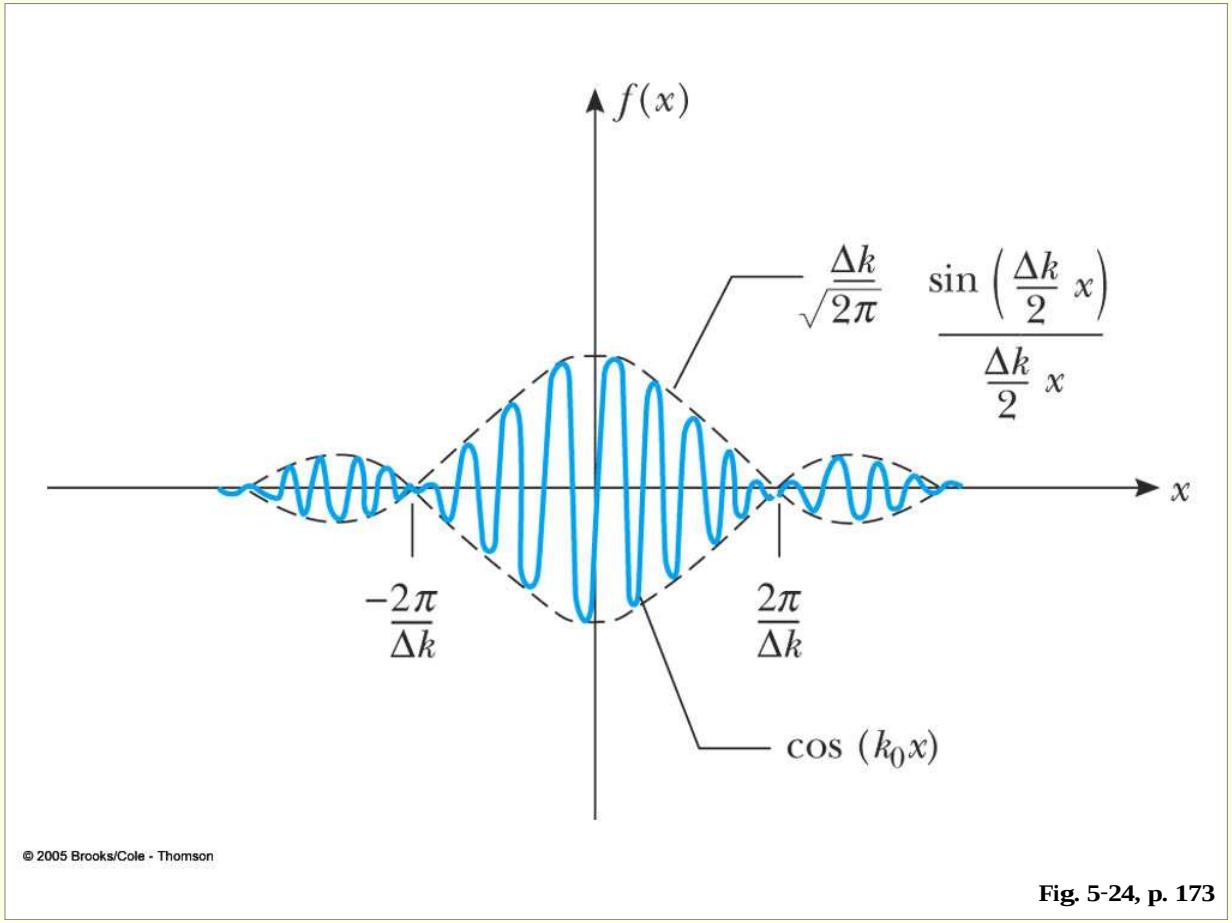


Figure 8: Output $\mathrm{Re}[f(x)]$ at $t = 0$.

What you see in the figure for $\mathrm{Re}[f(x)]$ is the rapid oscillation of the $\cos(k_0 x) = \mathrm{Re}[e^{ik_0 x}]$ factor within an envelope described by the $\sin(\Delta k\, x/2)/(\Delta k\, x/2)$ factor. The latter has its first nodes at $\Delta k\, x/2 = \pm\pi$, *i.e.* $x = \pm 2\pi/\Delta k$. (There is no node at $x = 0$ because

$\lim_{x\to 0} \sin x/x = 1$.) The full width between the two nodes is thus $\Delta x = 4\pi/\Delta k$.

What we wish to particularly point out is the relationship between the width of the input bump in k space to the width of the output wave form in x space. We have

$$\Delta x \Delta k = 4\pi\,. \tag{43}$$

The smallest value for this product occurs if a Gaussian form ($\widetilde{f}(k) \propto e^{-\frac{1}{2}(k-k_0)^2/(\delta k)^2}$) is employed. The output then has a similar Gaussian shape in x ($f(x) \propto e^{-\frac{1}{2}(x-x_))^2/(\delta x)^2}$), with $\delta x = 1/\delta k$, or $\delta x \delta k = 1$. With a certain "formal" defintion of Δx and Δk that we will come to, $\Delta x = \delta x/\sqrt{2}$ and $\Delta k = \delta k/\sqrt{2}$, and we obtain

$$\Delta x \Delta k = \frac{1}{2}. \tag{44}$$

Thus, for any possible form of $\widetilde{f}(k)$, we have

$$\Delta x \Delta k \geq \frac{1}{2}\,. \tag{45}$$

The Heisenberg Uncertainty Relation for Photon Waves

So what? What is the physical impact? First, as we shall remind ourselves in more detail in a moment. Light obeys the same kind of wave equation just considered, with $v = c$.

Next, let us input the light wave / photon relation that

$$k = \frac{2\pi}{\lambda} = \frac{2\pi p}{h} = \frac{p}{\hbar}\,, \tag{46}$$

eq. (45) can be rewritten as

$$\Delta x \Delta p \geq \frac{\hbar}{2}\,. \tag{47}$$

This is the famous Heisenberg uncertainty principle that was first proposed for matter, and only later was it realized that it was already present in the description of light waves as photon packets with $p = h/\lambda$.

We will return to a thorough discussion of the implications of this kind of uncertainty principle. However, you should at this point take note of the

fact that it is simply a mathematical result that follows from combining wave propagation ideas with quantization of the wave into particles, in the light case the particles being the photons.

We now derive $f(x)$ (at $t = 0$) using the input $\widetilde{f}(k)$. The only thing you need to know is that $\int e^{ak} dk = e^{ak}/a$, where $a = ix$ in our case.

$$\begin{aligned}
f(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \widetilde{f}(k) e^{ikx} dk \\
&= \frac{1}{\sqrt{2\pi}} \int_{k_0 - \Delta k/2}^{k_0 + \Delta k/2} e^{ikx} dk \\
&= \frac{1}{\sqrt{2\pi}} \frac{1}{ix} \left[e^{i(k_0 + \Delta k/2)x} - e^{i(k_0 - \Delta k/2)x} \right] \\
&= \frac{1}{\sqrt{2\pi}} \frac{e^{ik_0 x}}{x} 2 \sin\left(\frac{1}{2} \Delta k \, x \right) \\
&= \frac{\Delta k}{\sqrt{2\pi}} \frac{\sin(\Delta k \cdot x/2)}{(\Delta k \cdot x/2)} e^{ik_0 x} \, . \qquad (48)
\end{aligned}$$

Another way of understanding the uncertainty relation in the case of light waves / photons is to return to the single slit wave experiment. There, we "recalled" that a slit of size D gave a first diffraction minimum at $\theta \sim \lambda/D$.

Derivation

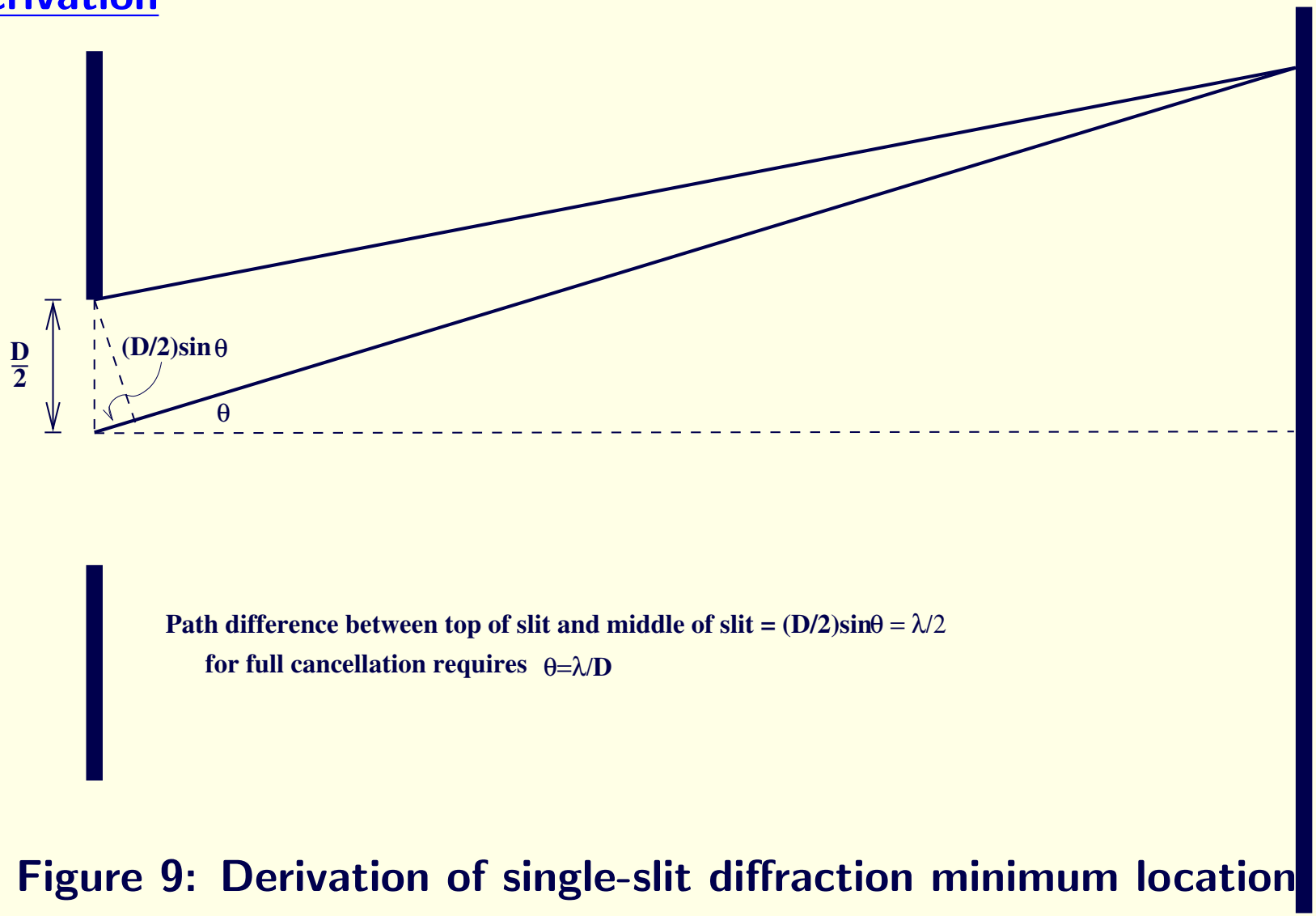


Figure 9: Derivation of single-slit diffraction minimum location

We can give a simple derivation based on Huygen's principle, something I hope you are familiar with. It says that the propagation of a wave can be constructed by dividing up the wave into many different little (circular in

a planar configuration) wavelets emanating from any well defined surface (curve in a planar configuration).

Using Huygen's principle, consider a wavelet emanating from the top of the slit and one from the midpoint of the slit. The diagram shows that these two wavelets will be precisely $1/2$ wavelength out of phase ($i.e.$ they will cancel) when $\sin\theta \sim \theta = \lambda/D$. The same will apply to a wavelet emanating from ϵ below top and ϵ below the midpoint, and so forth. Thus, $\theta \sim \lambda/D$ is the condition for a minimum in the diffraction pattern.

Demonstration

Take a red laser, $\lambda \sim 650\ nm = 0.65 \times 10^{-6}\ m$. Take a slit of order $D = 0.2\ mm = 2 \times 10^{-4}\ m$. The first minimum will be at $\theta \sim 0.0032$. Place a screen about $l = 10\ m$ away and the distance between the two first minima on either side of the maximum should be about $d = 2l\theta \sim 0.065\ m = 6.5\ cm$.

Implications for photon momenta

For the photon to have travelled there, it must pick up a momentum p_y perpendicular to the initial (upwards) momentum of $p_x \sim p = h/\lambda$.

Thus, we have

$$\theta \sim \frac{p_y}{p_x} \sim \frac{p_y \lambda}{h} \quad \Rightarrow \quad p_y \sim \frac{\theta\, h}{\lambda} \sim \frac{\lambda}{D}\frac{h}{\lambda} \sim \frac{h}{D} \tag{49}$$

from which we find (can't expect to get 2π type factors right here)

$$\Delta p_y \Delta y \sim p_y D \sim \frac{h}{D} D \sim h\,. \tag{50}$$

Once again, the uncertainty relationship emerges. Here, we have tried to confine the $E\&M$ wave to a location of size D in the y direction as it propagates to the right in the x direction, and, in so doing, we have generated a substantial uncertainty in p_y. The more we try to define the wave location in a certain direction, the greater the uncertainty in the momentum in that same direction.

Electromagnetic Waves

Let me now give a brief review of the $E\&M$ wave equation. Had I known that this was only given very brief attention in your previous course, I would have surely begun this quarter's lectures with the following review.

One starts with the two Maxwell equations:

$$\oint_C \vec{E} \cdot d\vec{l} = -\frac{d}{dt} \int_S \vec{B} \cdot \hat{n}\, dA \tag{51}$$

$$\oint_C \vec{B} \cdot d\vec{l} = \mu_0 \epsilon_0 \frac{d}{dt} \int_S \vec{E} \cdot \hat{n}\, dA \tag{52}$$

where the latter assumes no source current I, as appropriate for propagation in a vacuum. The vector $\hat{n}$ represents a unit vector normal to the surface S at any given point. The closed loop C runs along the boundary of the surface S, and the orientation of $\hat{n}$ relative to C is given by the right-hand rule.

In principle, you have read the material in University Physics Section 32 to learn that these reduce (for a wave traveling in the x direction with $\vec{E}$

pointing in the y direction and $\vec{B}$ pointing in the z direction) to

$$\frac{\partial E_y}{\partial x} = -\frac{\partial B_z}{\partial t} \tag{53}$$

$$\frac{\partial B_z}{\partial x} = -\mu_0\epsilon_0\frac{\partial E_y}{\partial t} \tag{54}$$

I give a brief derivation of the first equation. We apply eq. (51) to the case of $\vec{E} = \hat{y}E_y$ and $\vec{B} = \hat{z}B_z$. The equation says that a time varying B_z (using $\hat{n} = \hat{z}$ and very small size dx by dy loop in the x, y plane) can generate an $\vec{E}$ field that circulates around the small loop. Applying this to the $\vec{E} = \hat{y}E_y$ case, we find that E_y must vary with x. In short, the time varying B_z field is generating a spatial variation of E_y as a function of x. Of course, E_y will end up with time dependence that matches that of the time derivative of B_z. A figure showing how this application works is below.

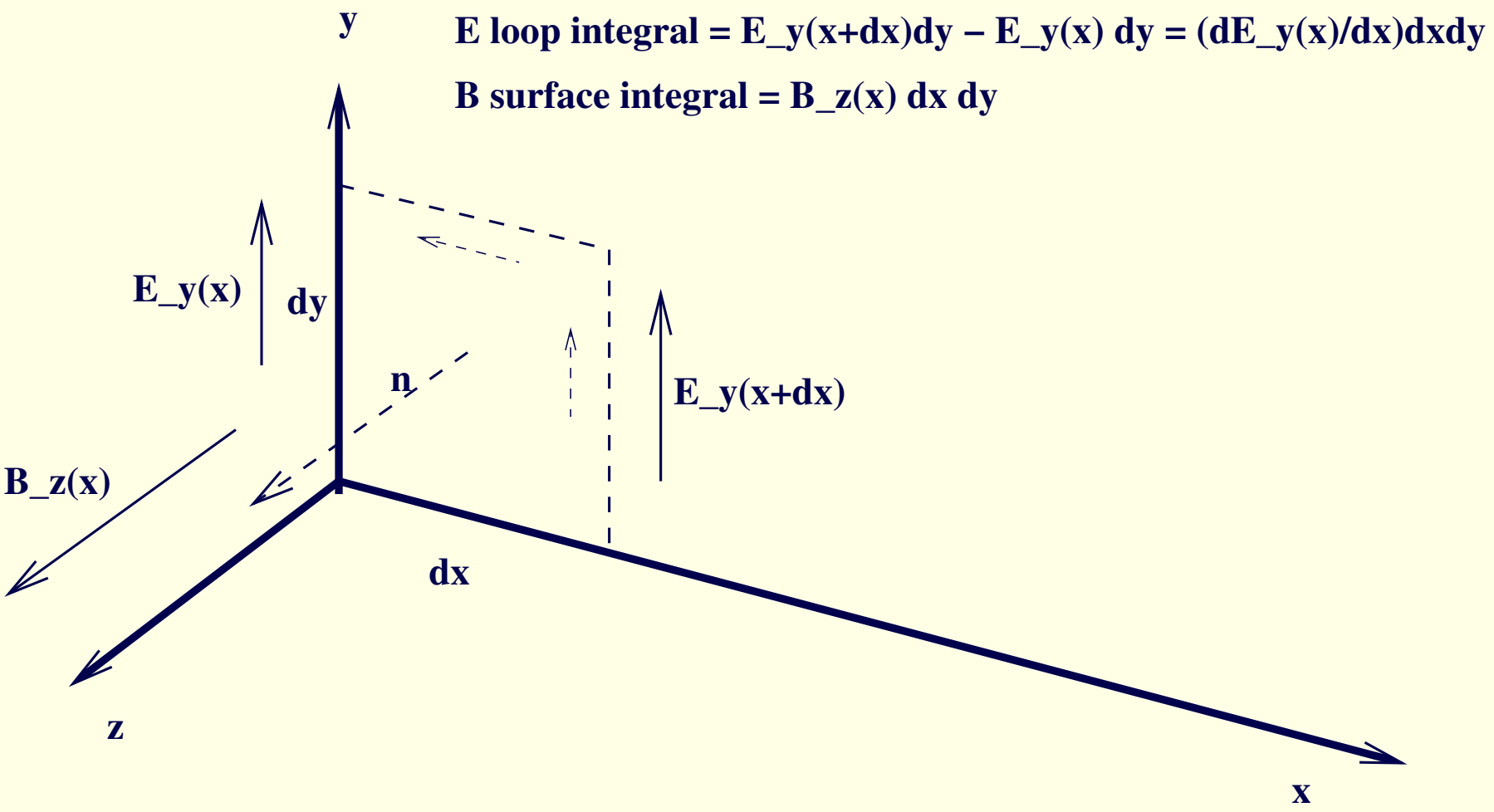


Figure 10: Set up for deriving eq. (53).

The 2nd of the integral-form Maxwell equations (applied with $\hat{n} = \hat{y}$ and a very small loop in the x, z plane of size dx by dz) implies that a spatial variation of B_z as a function of x will be generated by a time variation

of E_y. A set up analogous to that depicted in Fig. 10 would give you eq. (54).

Equivalently, you may have seen the two integral equations rewritten using the famous general theorem, called Stoke's theorem, which states:

$$\oint_C \vec{F} \cdot d\vec{l} = \int_S (\vec{\nabla} \times \vec{F}) \cdot \hat{n}\, dA \tag{55}$$

where $\vec{F}$ is any arbitrary vector "field" and $\vec{\nabla} \times \vec{F}$ denotes the "curl" of $\vec{F}$. The two important components of the definition of the curl are

$$(\vec{\nabla} \times \vec{F})_z = \frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y} \tag{56}$$

$$(\vec{\nabla} \times \vec{F})_y = \frac{\partial F_x}{\partial z} - \frac{\partial F_z}{\partial x}\,; \tag{57}$$

these will be needed in the differential forms of eqs. (51) and (52), respectively.

Using this theorem in eqs. (58) and (59) and the fact that the surface S, and its normal $\hat{n}$, can be thought of as being arbitrary, the integrands

must be equal so that eqs. (51) and (52) imply

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \tag{58}$$

$$\vec{\nabla} \times \vec{B} = \mu_0 \epsilon_0 \frac{\partial \vec{E}}{\partial t}\,, \tag{59}$$

respectively. We now assume, as above, that $\vec{B} = \hat{z} B_z$ only and $\vec{E} = \hat{y} E_y$ only. In this case, we are interested in the z component of eq. (58) and the y component of eq. (59). We then employ the curl defintions of eqs. (56) and (57) to obtain

$$(\vec{\nabla} \times \vec{E})_z = \frac{\partial E_y}{\partial x}\,, \quad (\vec{\nabla} \times \vec{B})_y = -\frac{\partial B_z}{\partial x}\,. \tag{60}$$

Substituting the above into eqs. (58) and (59), respectively, we get eqs. (53) and (54), repeated below.

$$\frac{\partial E_y}{\partial x} = -\frac{\partial B_z}{\partial t} \tag{61}$$

$$-\frac{\partial B_z}{\partial x} = \mu_0 \epsilon_0 \frac{\partial E_y}{\partial t} \tag{62}$$

Let us now consider the equation that can be derived from eqs. (53) and (54). Take $\frac{\partial}{\partial x}$eq. (53) $\Rightarrow \frac{\partial^2 E_y}{\partial x^2} = -\frac{\partial}{\partial t}\frac{\partial B_z}{\partial x}$ and substitute for $\frac{\partial B_z}{\partial x}$ using eq. (54), which states $\frac{\partial B_z}{\partial x} = -\mu_0\epsilon_0\frac{\partial E_y}{\partial t}$ to obtain:

$$\frac{\partial^2 E_y}{\partial x^2} = \mu_0\epsilon_0\frac{\partial^2 E_y}{\partial t^2}\,. \tag{63}$$

This matches the mechanical wave equation provided the velocity is $v^2 \equiv c^2 = \frac{1}{\mu_0\epsilon_0}$. Following a similar procedure we also find

$$\frac{\partial^2 B_z}{\partial x^2} = \mu_0\epsilon_0\frac{\partial^2 B_z}{\partial t^2}\,. \tag{64}$$

Thus, the E and B oscillations are continually feeding one another through Maxwell's laws and as a result the wave propagates in the x direction.

If we employ a form

$$E_y = A\sin(kx - \omega t)\,, \tag{65}$$

then we can check that the associated form for B_z must be

$$B_z = \frac{1}{c} A \sin(kx - \omega t)\,, \tag{66}$$

by employing either eq. (53) or eq. (54). For example, eq. (54) states that $\frac{\partial B_z}{\partial x} = -\frac{1}{c^2}\frac{\partial E_y}{\partial t}$. Substituting in the above forms we get

$$\begin{aligned}
\frac{\partial B_z}{\partial x} &= \frac{1}{c} A\, k \cos(kx - \omega t) \\
-\frac{1}{c^2}\frac{\partial E_y}{\partial t} &= -\frac{1}{c^2} A(-\omega) \cos(kx - \omega t) \\
&= \frac{1}{c} A \frac{\omega}{c} \cos(kx - \omega t) \\
&= \frac{1}{c} A\, k \cos(kx - \omega t) \quad \text{using } \omega/k = c\,.
\end{aligned} \tag{67}$$

The fact that E_y and B_z are exactly "in phase" all the time, is one of the remarkable features of $E\&M$ radiation. But, it had to be true in order for one to "feed" the other.

Energy carried by an $E\&M$ wave

It is also useful to remind ourselves about the amount of energy carried by an $E\&M$ wave. You need to remember that the energy density stored in the $\vec{E}$ and $\vec{B}$ fields is given by

$$u_E = \frac{1}{2}\epsilon_0 \vec{E}\cdot\vec{E}\,, \quad u_B = \frac{1}{2}\frac{\vec{B}\cdot\vec{B}}{\mu_0}\,, \tag{68}$$

respectively. As we have seen above, for the travelling wave, $|\vec{B}| = |\vec{E}|/c$. So, $u = u_E + u_B$ can be written in a variety of forms:

$$\begin{aligned} u &= \frac{1}{2}\epsilon_0|\vec{E}|^2 + \frac{1}{2}\frac{|\vec{B}|^2}{\mu_0} \\ &= \epsilon_0|\vec{E}|^2 \\ &= \frac{|\vec{B}|^2}{\mu_0} \\ &= \sqrt{\frac{\epsilon_0}{\mu_0}}|\vec{E}||\vec{B}|\,. \end{aligned} \tag{69}$$

And, we should also remember that for the $E\&M$ wave, travelling with velocity c, the amount of energy transported through a surface area perpendicular to the wave's direction of travel ($e.g.$ a surface in the y, z plane for travel in the x direction) is simply $S = cu$, which has the correct dimensions since $c = m/s$ while $u = energy/m^3$ so that $S = energy/m^2/s$.

An Example

Suppose the maximum $|\vec{E}|$ value for a traveling sinusoidal wave, moving in the x direction is $E_{max} = |\vec{E}| = 100\ N/C$ and occurs at $t = 0, x = 0$. Give a value for the amount of energy impacting a screen perpendicular to the x axis per unit area per unit time at $t = 0, x = (2/3) \times \lambda$.

Answer: Since the field is maximum at $t = 0, x = 0$, it is convenient to use the form $E_y = E_{max} \cos\left(\frac{2\pi}{\lambda}(x - ct)\right)$. Substituting $t = 0, x = (2/3)\lambda$ gives $E_y = E_{max} \cos(4\pi/3) = -\frac{1}{2}E_{max}$. From our earlier equations, we have

$$\begin{aligned} S &= cu = c\epsilon_0 E_y^2 \\ &= (3 \times 10^8\ m/s)(8.85 \times 10^{-12}\ C^2/N \cdot m^2)(-\frac{1}{2}100\ N/C)^2 \end{aligned}$$

$$= \quad 6.6375 \; J/(m^2 \cdot s) \, . \tag{70}$$

Of course, as time passes, at this same location, the S value will oscillate up and down and so the average energy per unit area per unit time will be $S_{average} = \frac{1}{2} S_{max} = \frac{1}{2} c \epsilon_0 E_{max}^2$. This is what we usually call the intensity of the $E\&M$ wave, but we see that a more accurate name would be *average* intensity.

We do not know how many photons this corresponds to (on average) until λ is specified. Also note that we could compute (at any instant) B_z using $B_z = E_y/c$.

Momentum Carried by an $E\&M$ wave

We have stated that the relation between the energy and the momentum carried by an $E\&M$ wave is $p = E/c$, where in the continuous wave vision E is the same as S. p will then be so much momentum per unit area per unit time.

To derive this relation between the energy and momentum carried by an $E\&M$ wave, is a bit of an exercise. I give it below in case you are interested.

Consider a test charge Q (of unit area) on which the wave impinges. The wave will start this test charge moving, to begin with in the y direction as a result of $F_y = QE_y$. Once Q has some v_y, the magnetic field of the wave will act on it to produce a force in the x direction

$$F_x\hat{x} = Qv_y\hat{y} \times B_z\hat{z} = \hat{x}Qv_yB_z\,. \tag{71}$$

Since $F_x = dp_x/dt$, we get momentum being fed to the charge at the rate of (using $B_z = E_y/c$, as above)

$$\frac{dp_x}{dt} = Qv_yB_z = Qv_y\frac{E_y}{c}\,. \tag{72}$$

Meanwhile, starting from $v_x = 0$ (so that F_x is not doing any x direction work yet) potential energy is being added to this charge, because it is moving against the electric field, according to

$$\Delta U = QE_y\Delta y\,, \quad \Rightarrow \quad \frac{dU}{dt} = QE_yv_y\,. \tag{73}$$

Substituting the result of solving this equation for v_y into the previous

equation gives

$$\frac{dp_x}{dt} = Q\left(\frac{dU/dt}{QE_y}\right)\frac{E_y}{c} = \frac{1}{c}\frac{dU}{dt}\,, \tag{74}$$

implying that on a per second basis the amount of energy being supplied by the $E\&M$ wave and the amount of x momentum being supplied by the wave must be related by $p = U/c$. But, the amount of energy being supplied by the $E\&M$ wave (all this is per unit area per unit time, recall) is simply $U = S$. We have been denoting S by E, which, to repeat, for a wave is the amount of energy per unit are per unit time passing a certain perpendicular plane. And, of course, if both the momentum and the energy are being carried by photons, then the energy per photon must be related to the momentum per photon by $p = E/c$.

Return to previous example

At $t = 0, x = (2/3)\lambda$, how much momentum is being transferred to the screen per unit area per unit time, assuming that all the radiation is being absorbed?

Answer: Using $E = S = cp$, we compute

$$p = \frac{S}{c} = \frac{6.6375 J/(m^2 \cdot s)}{3 \times 10^8\ m/s} = (2.212 \times 10^{-8}\ kg \cdot m/s)/(m^2 \cdot s)\,. \tag{75}$$

Hopefully, the demonstration of a little set of vanes inside a vacuum container is something you have seen?

General Lesson

Thus, just as in the case of a wave on a string, the $\vec{E}$ and $\vec{B}$ fields contained in a light wave have real physical implications. $\vec{E}$ could accelerate a charged test particle and $\vec{B}$ could deflect a moving charged test particle.

A Lesson in Wave Amplitudes and Probabilities

We have seen that a single slit will have a minimum at $\sin\theta = \lambda/D$ coming from the complete cancellation of various Huygen's wavelet amplitudes from different parts of the slit. At $\theta = 0$, all the wavelets arrive in phase at the central point of the screen and simply add up to give you a maximum E field, call this maximum E_0. E_0 will have some wave-like form, of course, and so will oscillate up and down as time passes according to some form like

$$E_0 = E_{max} \sin\left(\frac{2\pi}{\lambda}(x_{screen} - ct)\right) . \tag{76}$$

There will be an instantaneous intensity $I_0 = c\epsilon_0 |E_0|^2$ and the average intensity will be $\langle I_0 \rangle = \frac{1}{2} I_0^{max} = \frac{1}{2} c\epsilon_0 |E_{max}|^2$.

One can also add up the wavelets for any other θ. I will not go through the derivation, but the result is

$$E = E_0 \frac{\sin[\pi D(\sin\theta)/\lambda]}{\pi D(\sin\theta)/\lambda}, \quad \Rightarrow I = I_0 \left\{ \frac{\sin[\pi D(\sin\theta)/\lambda]}{\pi D(\sin\theta)/\lambda} \right\}^2 \qquad (77)$$

Now let us consider the case of $D \ll \lambda$. Then, since $\lim_{x\to 0} \frac{\sin x}{x} = 1$ we have $E = E_0$, independent of θ. That is, uniform intensity on the detecting screen.

Next consider the case of two such slits. If we cover up either one of the slits, we will get a uniform E_0 on the detecting screen and the corresponding $I_0 \propto |E_0|^2$, just as discussed above. But if we now open up both slits, we will get our two-slit interference pattern. Let us call the distance from the upper slit, slit $\#1$, to the screen L. Then the distance from the lower slit $\#2$ to the screen is $L + S\sin\theta$.

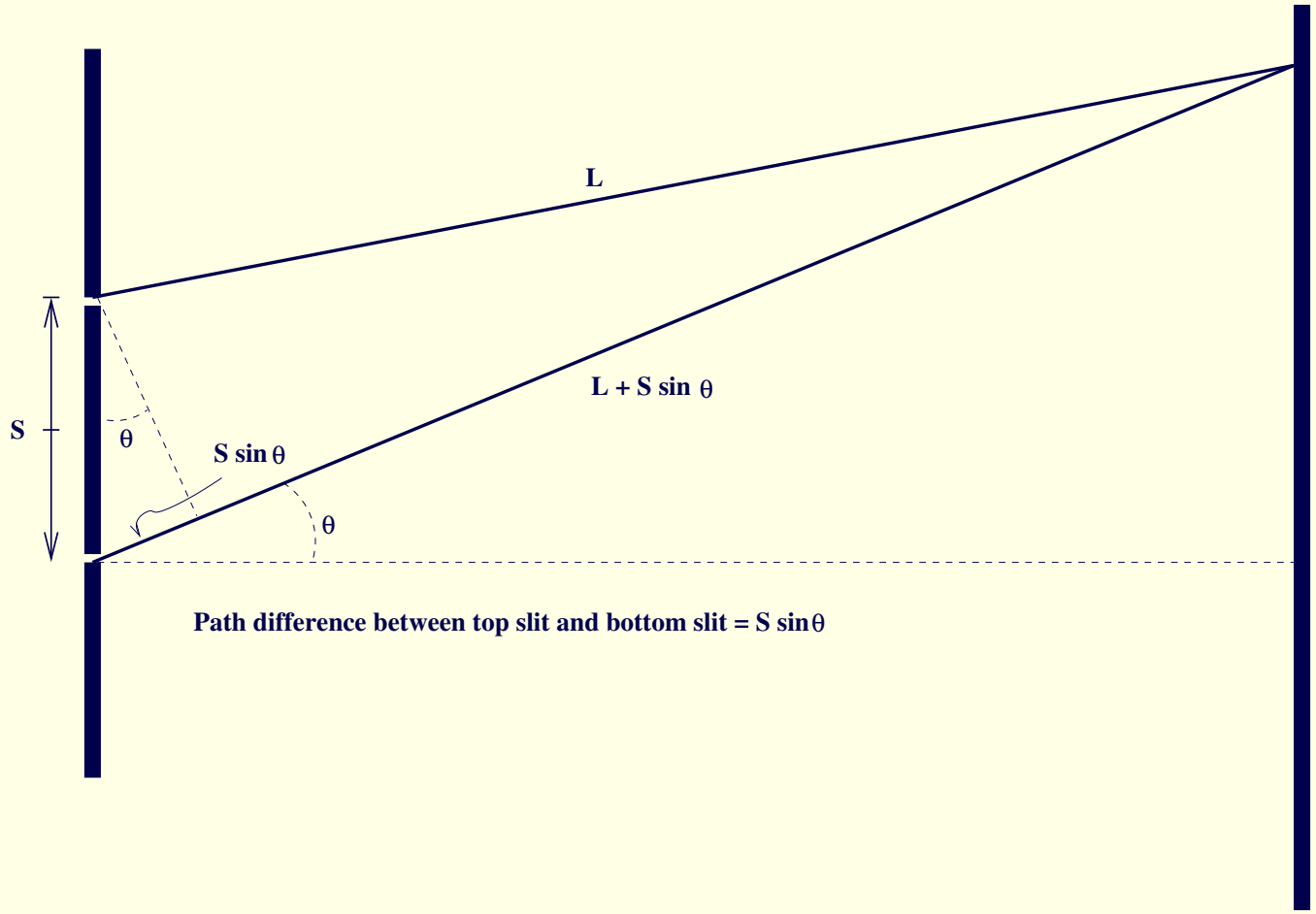


Figure 11: Two (narrow) slit interference.

From this picture, we obtain

$$\begin{aligned} E^{1+2} &= E^1 + E^2 \\ &= E_{max}\left[\sin\left(\frac{2\pi}{\lambda}(L-ct)\right) + \sin\left(\frac{2\pi}{\lambda}(L+S\sin\theta - ct)\right)\right] . \end{aligned}$$

First, let us note that the two waves cancel when $S\sin\theta = (n+\frac{1}{2})\lambda$,

since the arguments of the sin's would differ by π, *i.e.* one-half cycle. Thus, the two-slit pattern will have minima with zero intensity at such angles. Correspondingly, the two-slit pattern maxima occur at $S \sin\theta = n\lambda$. At such angles, constructive addition of the two waves is perfect.

Of course, for general θ, $L = x_{screen}/\cos\theta$, but this is not needed for the above discussion.

Now, let us return to the question posed at the end of the last class, for which we focus on the case of $\theta = 0$. Then,

$$E^{1+2} = 2E_{max} \sin\left(\frac{2\pi}{\lambda}(x_{screen} - ct)\right) , \quad \Rightarrow \quad I^{1+2} = 4c\epsilon_0 |E_0|^2 \tag{78}$$

implying that $I^{1+2} = 4I_0$, where I_0 is that from just one slit! Here, I_0 denotes the instantaneous intensity. For the average intensity, the same applies:

$$\langle I^{1+2} \rangle = 4\langle I_0 \rangle = 4\left[\frac{1}{2} I_0^{max}\right] . \tag{79}$$

What about matter waves?

In contrast, as I have said before, the matter waves that we shall come to do not have any such direct physical interpretation.

Matter waves are sort of like putting the $\vec{E}$ and $\vec{B}$ together in the form

$$\vec{F} = \vec{E} + ic\vec{B}\,. \tag{80}$$

If we take the absolute square of this $\vec{F}$, we get

$$|\vec{F}|^2 = (\vec{E} + ic\vec{B}) \cdot (\vec{E} - ic\vec{B}) = |\vec{E}|^2 + c^2|\vec{B}|^2 \tag{81}$$

which is indeed proportional to the intensity of the electromagnetic wave. We have learned that it is the intensity that tells us the probability of finding a photon at a certain point in space at a certain time.

For matter waves, the wave will usually be denoted by Ψ. Ψ can always be decomposed into its real and imaginary parts:

$$\Psi = \Psi_1 + i\Psi_2\,. \tag{82}$$

For matter waves, Ψ_1 and Ψ_2 do not have any direct physical manifestation analogous to the way in which $\vec{E}$ and $\vec{B}$ can impact a test charge. There is no test probe that one can employ. The only interpretation of Ψ is that

$$\text{Probability of finding particle} \propto |\Psi|^2 = |\Psi_1|^2 + |\Psi_2|^2 \,. \tag{83}$$

Ad hoc derivation of $E\&M$ wave equation

Before ending this "review", let me note an amusing "derivation" of the $E\&M$ wave equation.

First, we note again that the wave equation for X being either E_y or B_z takes the form

$$\frac{\partial^2 X}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 X}{\partial t^2} \,. \tag{84}$$

Suppose we write the energy momentum relationship for light in the form $p^2 = \frac{E^2}{c^2}$, multiply this times X and then make the replacements

$$E \longrightarrow i\hbar\frac{\partial}{\partial t} \quad \text{and} \quad p \longrightarrow \frac{\hbar}{i}\frac{\partial}{\partial x} \,. \tag{85}$$

Then,

$$p^2 X = \frac{E^2}{c^2} X \quad \Rightarrow \quad -\hbar^2 \left[\frac{\partial^2 X}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 X}{\partial t^2} \right] , \tag{86}$$

which contains our wave equation. A hand-waving motivation for these identifications is to note that for a wave solution of the type $e^{ik(x-ct)}$ (our general form for the case of $v = c$) that we were discussing earlier, it is certainly the case that

$$\frac{\hbar}{i} \frac{\partial}{\partial x} e^{ik(x-ct)} = \hbar k e^{ik(x-ct)} = p e^{ik(x-ct)} , \tag{87}$$

where we used

$$\hbar k = \frac{h}{2\pi} \frac{2\pi}{\lambda} = \frac{h}{\lambda} = p \tag{88}$$

for a photon within an $E\&M$ wave. Similarly,

$$i\hbar \frac{\partial}{\partial t} e^{ik(x-ct)} = \hbar k c e^{ik(x-ct)} = E e^{ik(x-ct)} , \tag{89}$$

where we used (see above)

$$\hbar k c = p c = E \tag{90}$$

for a photon within an $E\&M$ wave. (Note how we had to use a combination of wave and photon ideas for this little game.)

The replacements of eq. (85) turn out to also be applicable for particles with mass. In a very real sense, the replacements of eq. (85) are all that are required to formulate the theory of Quantum Mechanics that we now turn to. But, we will approach QM from the beginning and only come back to these considerations after a while.

More de Broglie

We have already discussed that $\lambda = h/p$ explains Bohr's quantization via $2\pi r = n\lambda$. This was a non-relativistic case. A natural question is whether we should use the relativistic momentum of Einstein in the more general situation. Answer=Yes!

For example, if we accelerate an electron through a large voltage V, it will acquire kinetic energy $K = eV$.

How do we get the momentum? Remember that $E = K + m_e c^2$ and that $cp = \sqrt{E^2 - m_e^2 c^4}$. Plugging in the form just given for E, we obtain (writing in a form that displays the small eV limit)

$$\begin{aligned} p &= \frac{1}{c}\sqrt{(eV + m_e c^2)^2 - m_e^2 c^4} = \frac{1}{c}\sqrt{e^2V^2 + 2eVm_e c^2} \\ &= \frac{\sqrt{2eVm_e c^2}}{c}\sqrt{\frac{eV}{2m_e c^2} + 1}\,. \end{aligned} \tag{91}$$

From this, we obtain

$$\begin{aligned} \lambda &= \frac{h}{p} = \frac{hc}{\sqrt{2eVm_ec^2}} \frac{1}{\sqrt{\frac{eV}{2m_ec^2}+1}} \\ &= \left(\frac{h}{\sqrt{2m_e \times 1eV}}\right) \frac{1}{\sqrt{V(volts)}} \frac{1}{\sqrt{\frac{eV}{2m_ec^2}+1}} \,. \end{aligned} \tag{92}$$

We evaluate the factor out in front as

$$\begin{aligned} \frac{h}{\sqrt{2m_e \cdot 1eV}} &= \frac{6.63 \times 10^{-34}\ J \cdot s}{\sqrt{2(9.11 \times 10^{-31}\ kg)(1.6 \times 10^{-19}\ J)}} \\ &= 1.227\ nm\,. \end{aligned} \tag{93}$$

To use the previous formula, V should be given in terms of volts, since $1V$ was taken inside the square root.

Remembering that $m_ec^2 = 0.511\ MeV$, we see that if the kinetic energy eV from acceleration is more than a small fraction of an MeV, we will need to use the full expression.

Davisson-Germer

The experimental confirmation of the de Broglie hypothesis was due to Davisson and Germer in 1927. Their apparatus is depicted below.

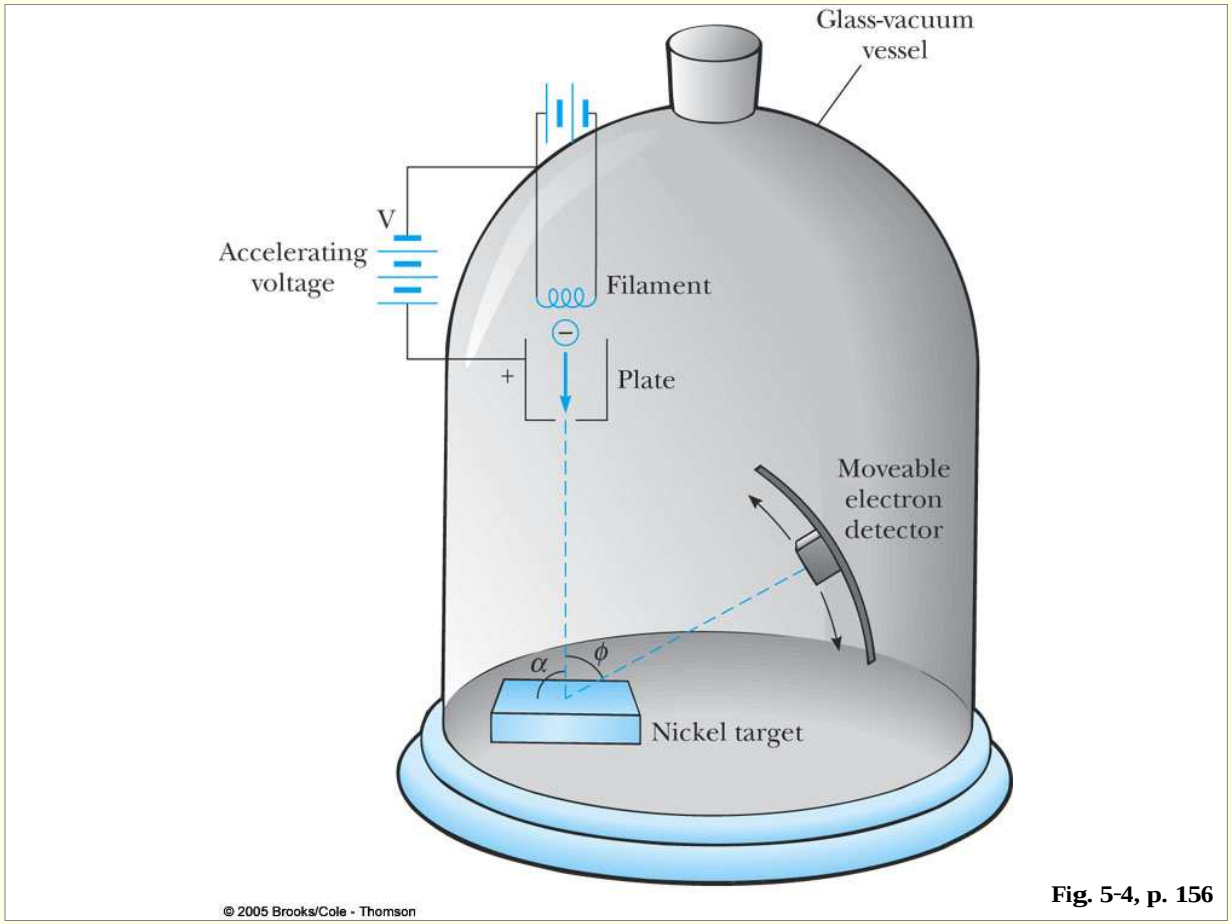


Figure 12: The Davisson-Germer apparatus.

Except for an accident in which they created a single large crystal at the surface of their Nickel target, they would never have seen the effect. Checking de Broglie was not actually the original goal of their experiment, but they were smart enough to realize what was going on when they saw sharp variations in the intensity of the "reflected" electrons.

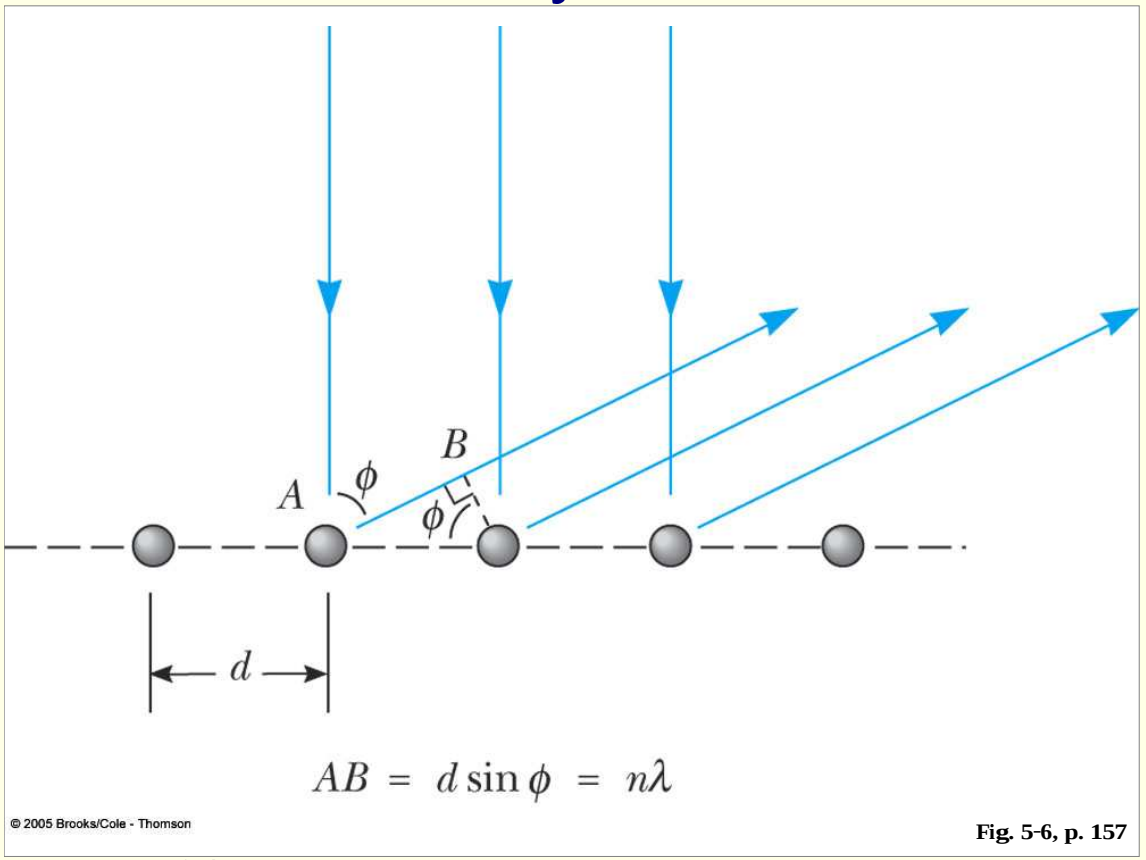


Figure 13: Electron scattering from an atomic lattice.

The correct picture is that the electron wave scatters off the top layer of Nickel atoms on the surface (the electrons had low energy and did

not penetrate beyond the surface). Because these were part of a single crystal, they had a very regular spacing, as depicted in the figure.

The electron waves arrive in phase (assuming 90° incident angle) and are then scattered at angle ϕ. As they leave the surface, the waves from different atoms are out of phase by an amount given by $\overline{AB} = d \sin\phi$. Only if $d \sin\phi = n\lambda$ will the different scattered waves all constructively interfere. Using the formula we just derived in the non-relativistic approximation, and an accelerating voltage of $54\ V$, the electron wavelength will be

$$\lambda = \frac{1.227\ nm}{\sqrt{54}} = 1.67 \times 10^{-10}\ m\,. \tag{94}$$

What did they see? From X-ray measurements DG knew that their atomic spacing was $d = 2.15 \times 10^{-10}\ m$. As illustrated in the next figure, they found constructive interference for $\phi = 50^\circ$ corresponding to

$$\lambda = d \sin\phi = 2.15 \times 10^{-10}\ m \sin 50.0^\circ = 1.65 \times 10^{-10}\,, \tag{95}$$

in excellent agreement (given experimental errors) with the prediction above of de Broglie's formula for λ for the given momentum.

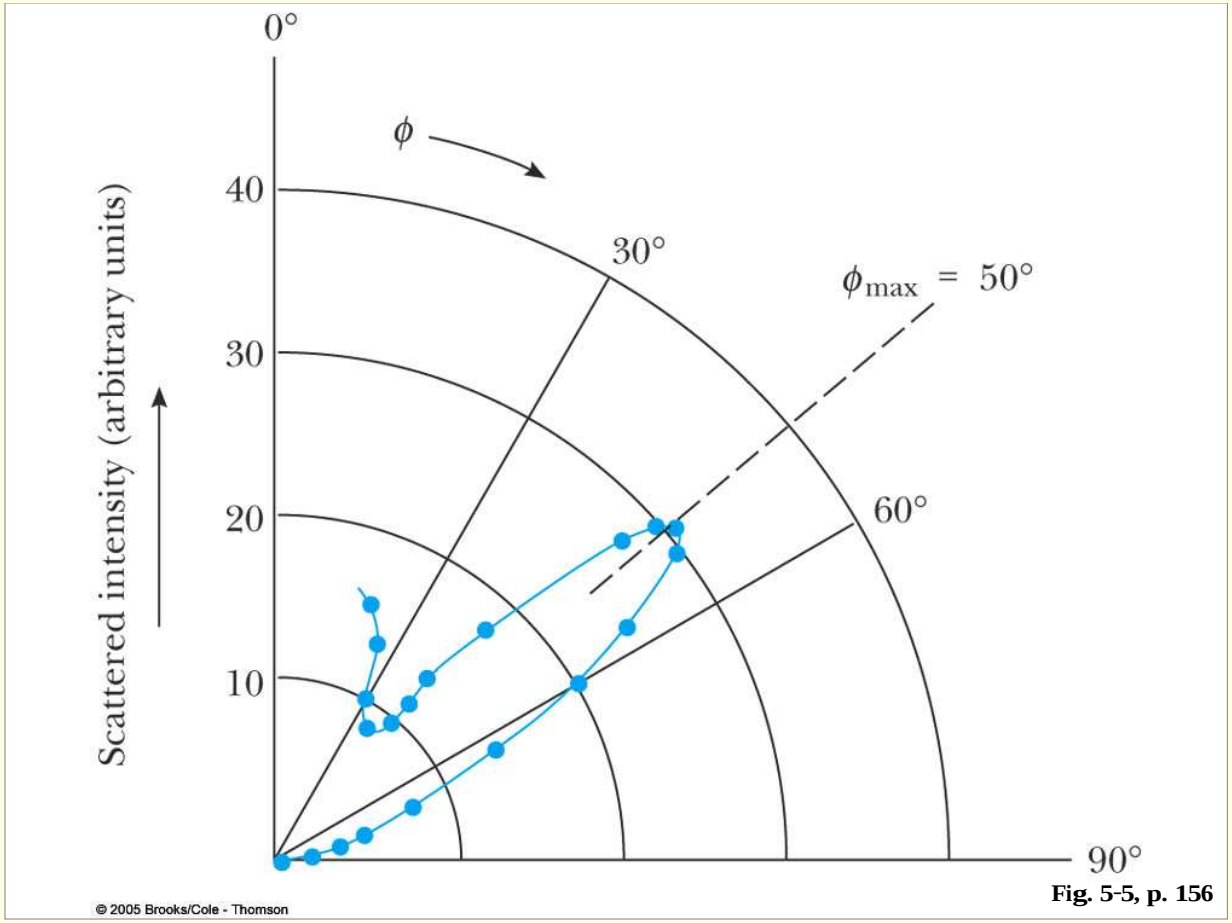


Figure 14: Scattered intensity vs. scattering angle for $54\ eV$ electrons incident at $90°$.

If one employs higher acceleration voltages, then the e^- will penetrate further into the surface, and the e^- waves will see many layers of the crystal structure. The picture is below.

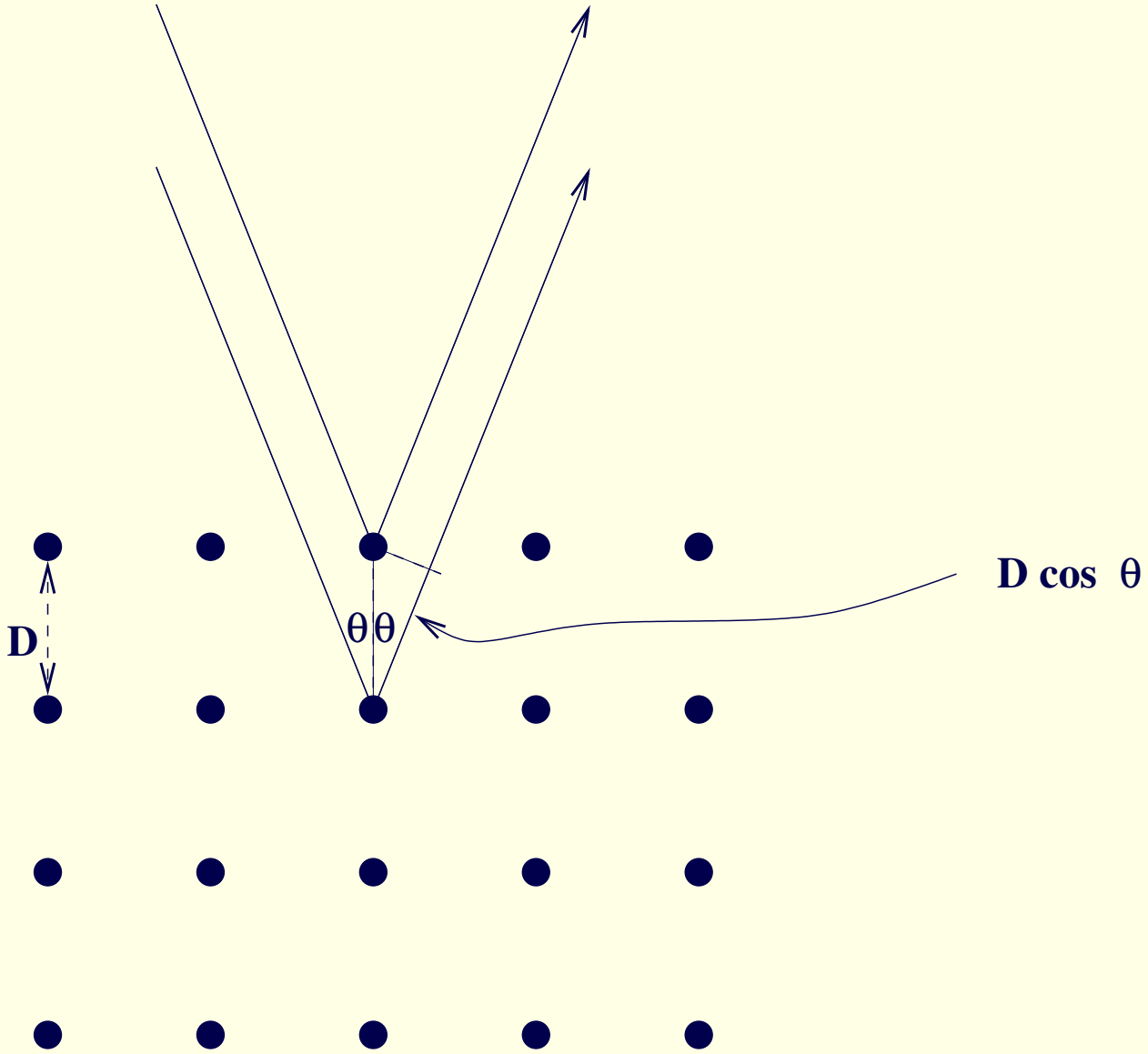


Figure 15: Multi-layer diffraction of deeply penetrating beam.

Because of equal entry and exit angles for the e^- (or any other particle, $e.g.$ neutron), the waves from any two atoms on any one horizontal crystal

layer will always be in phase. However, waves from atoms on different crystal layers are not necessarily in phase. The picture shows just one such pair of waves. There are many. One gets strong cancellation among the many unless the path differences are all an integer number of wave lengths. This leads to **Bragg's law**:

$$2D\cos\theta = m\lambda \tag{96}$$

The advantage of the multilayer diffraction type of probe is that the cancellation among the many different wavelets is so complete at any angles other than the Bragg angles that very precise information about the crystal structure can be obtained.

Indeed, crystal diffraction is an indispensable tool in the study of solids; the details of the diffraction patterns provide much information about the crystal's microscopic geometry.

An example of the very narrow constructive interference zones that emerge from e^-'s penetrating a thick crystal appears in the following figure.

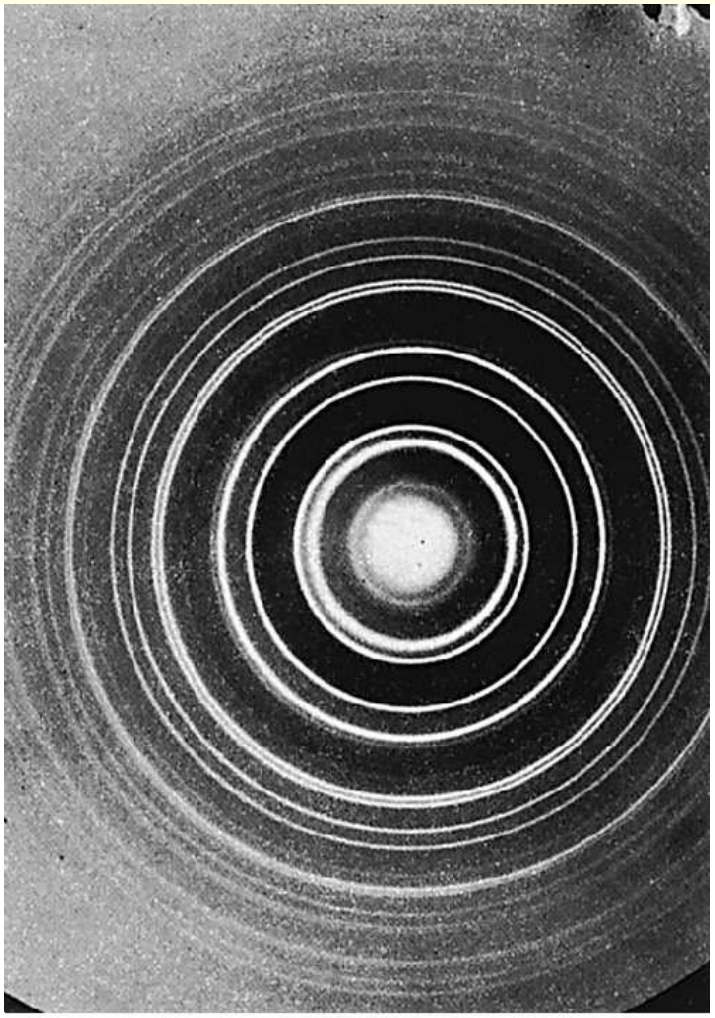


Figure 16: Bragg diffraction of $50\ keV$ electrons from a $4000\ nm$ thick single crystal of CU_3Au.

More Examples

(I) If moving with $v = 300\ m/s$, what would be the wavelength (a) of an $18,000\ kg$ airplane, and (b) of an electron?

Answer:

$$\lambda_{airplane} = \frac{6.63 \times 10^{-34}\ J \cdot s}{(18000\ kg)(300\ m/s)} = 1.23 \times 10^{-40}\ m$$

$$\lambda_{electron} = \frac{6.63 \times 10^{-34}\ J \cdot s}{(9.11 \times 10^{-31}\ kg)(300\ m/s)} = 2.43 \times 10^{-6}\ m . \quad (97)$$

The latter is something you can hope to measure using the kind of techniques just described. The former is not something you could ever measure — we do not need to worry about wavelengths and wave patterns in our everyday world!

(II) Consider a two-slit experiment using electrons. The slits are assumed to be very narrow compared to the wave-length of the electrons. Beyond the slits is a bank of e^- detectors. At the center detector, directly in the path the beam would follow if unobstructed, 100 electrons per second are detected. Suppose that as the detector angle varies, the number per

unit time of e^-'s arriving varies from a maximum of $100/s$ to a minimum of 0. Suppose the electrons have $K = 1.0\ eV$ of kinetic energy and the narrow slits are separated by $S = 0.020\ \mu m$. (a) At what angle, θ_X, is the detector X located where the minimum is reached? (b) How many electrons would be detected per second at the center detector if one of the slits were blocked? (b) How many electrons would be detected per second at the center detector and at detector X if one of the slits were narrowed to 36% of its original width?

Answers:

(a) At the minimum, we require $S \sin\theta_X = \frac{1}{2}\lambda$. We need, $\lambda = \frac{h}{p} = \frac{h}{mv}$ and we get v from

$$K = \frac{1}{2}m_e v^2\,, \quad \Rightarrow (1\ eV)\times(1.6\times10^{-19}\ J/eV) = \frac{1}{2}(9.11\times10^{-31}\ kg)v^2 \tag{98}$$

which gives $v = 5.93 \times 10^5\ m/s$. From this we get

$$p = mv = (9.11\times10^{-31}\ kg)(5.93\times10^5\ m/s) = 5.40\times10^{-25}\ kg{\cdot}m/s\,, \tag{99}$$

and

$$\lambda = \frac{h}{p} = \frac{6.63 \times 10^{-34}\ J \cdot s}{5.40 \times 10^{-25}\ kg \cdot m/s} = 1.23 \times 10^{-9}\ m. \qquad (100)$$

Inserting this into our requirements gives

$$\sin\theta_X \sim \theta_X = \frac{1}{2}\left(\frac{1.23 \times 10^{-9}\ m}{0.020 \times 10^{-6}\ m}\right) = 0.031 \quad \text{or} \quad 1.76^\circ. \qquad (101)$$

(b) In the discussion that follows, we do not write the wave form explicitly. But, there is always a wave form present. In the present case of e^- waves the wave form would be something like

$$Ae^{i(kx-\omega t)} = A\left[\cos(kx-\omega t) + i\sin(kx-\omega t)\right], \qquad (102)$$

initially, $i.e.$ before passing through a slit, and would afterwards be similar in form with $kx - \omega t$ replaced by $kr - \omega t$, where r is the distance from a slit. The important point will be that whatever the wave form, the two slits will have equivalent wave forms, that are in phase at a central

detector location, or exactly out of phase at the first minimum. The fluxes referred to below can be thought of as the average intensity of the oscillating waves.

With both slits open, the electron flux (electrons per second) is $100/s$ at the central detector. But, the electron flux is proportional to the probability of detection and therefore to the square of the amplitude of the total matter wave (from both slits):

$$|\Psi_T|^2 \propto 100/s \quad \Rightarrow \quad |\Psi_T| \propto 10\,. \tag{103}$$

Since the two slits are very narrow and the waves from the two slits add equally at this point of constructive interference, the amplitude of either individual wave must be half the total:

$$|\Psi_1| \propto 5 \quad \Rightarrow \quad |\Psi_1|^2 \propto 25/s\,. \tag{104}$$

With one slit closed, the electron flux at the central detector would be $1/4$ the two slit flux, or $25/s$. Note the importance of assuming that the slits are really narrow. In this case, this same flux would apply for all the electron detectors, regardless of angle, when only one slit is open.

You might say, *what happened to conservation of probability, or of the number of photons?*. **We have not violated anything here. The $100/s$ when both slits are open applies only to the central detector. As one moves away from the central detector, the intensity varies (see $E\&M$ two-slit discussion) from a maximum of 100 to a minimum of 0 so that averaging over the screen we get $50/s$. This is precisely $2\times$ the single-slit uniform intensity, as required by photon number conservation!**

(c) If one slit were open and its width (already very narrow) were reduced to 0.36 of its original size, all detectors would register an electron flux that is $0.36 \times 25/s$, or $9/s$. In equation form, this means that

$$|\Psi_1'|^2 = 0.36 \times |\Psi_1|^2 \propto 0.36 \times 25/s = 9/s\,, \quad \Rightarrow \quad |\Psi_1'| \propto 3. \quad (105)$$

This is 60% of the original amplitude.

With both slits open (but with slit $\#1$ at only 36% of its original size), we have two waves of different amplitudes, one proportional to 5 (slit $\#2$ of original width) and one proportional to 3 (slit $\#1$). At points of constructive interference, such as the central detector, where the waves

add, the total amplitude will be $\propto 5+3$:

$$|\Psi'_T|_{constructive} \propto 8\,, \quad \Rightarrow \quad |\Psi'_T|^2_{constructive} \propto 64/s. \tag{106}$$

At points of previously complete destructive interference, where the two waves are 180° out of phase, such as at detector X, the cancellation would no longer be complete. The waves still come in with opposite signs for the amplitudes so that the amplitude is proportional to $5-3$, leading to

$$|\Psi'_T|_{destructive} \propto 2\,, \quad \Rightarrow \quad |\Psi'_T|^2_{destructive} \propto 4/s\,. \tag{107}$$

The average electron flux is

$$\frac{1}{2}(64/s + 4/s) = 34/s\,, \tag{108}$$

i.e. **the sum of the $9/s$ and the $25/s$ expected from each slit alone.**

To repeat, to find the probability (or flux) at a given location, we do not add the probabilities (or fluxes) from each slit at that location; these

are always positive, so they cannot cancel. Rather, we add the wave amplitudes, which may add constructively or destructively, to find the total wave, and then square the total wave to find the probability.

*** There is a special problem assigned to cover this material: see web page. You will be tested on some quiz or exam on this kind of thing. ***

The electron microscope and related devices

Recall the formula for the e^- wavelength in terms of the acclerating voltage

$$\lambda_e = \frac{1.227\ nm}{\sqrt{V(volts)}} \frac{1}{\sqrt{\frac{eV}{2m_e c^2} + 1}}. \tag{109}$$

An electron microscope makes use of an accelerating voltage of $V \sim 100000\ volts$, leading to $\lambda_e \sim 0.003\ nm$, as compared to typical light wavelengths in the visible spectrum of $\sim several\ hundred\ nm$. Thus, electrons have the potential of far greater resolution capable of revealing much finer structures. Magnification, however, is not directly related to λ, being limited by other things such as appertures and "optics" of the device. In practice, the best that can be achieved is

a magnification of 10,000 to 100,000 with resolution of $0.2\ nm$, as compared to magnification and resolution of ~ 2000 and $\sim 100\ nm$ for optical microscopes. The electron microscope allows pictures of individual DNA strands, bacteria and the like. These developments were crucial to modern biology, ...

Other devices include *scanning electron microscope* **(SEM) and** *scanning tunneling microscope* **(STM) and** *atomic force microscope* **(AFM). These involve further applications of QM to which we shall turn in later chapters.**

The latest device for studying structures, especially of germanium crystals and other semi-conductors, is a *light source* **of very high energy γ-rays. These are beams of photons with energies beyond even the X-ray range. Typical energy is ~ 10 to $50 \times 10^9\ eV$. The wavelength that one is talking about is**

$$\lambda = \frac{ch}{E} \sim \frac{1.24 \times 10^3\ eV \cdot nm}{10 \times 10^9\ eV} = 1.24 \times 10^{-7}\ nm\,. \qquad (110)$$

More on the Heisenberg Uncertainty Principle

Let us review once more the HUP. We have found by example that for any wave pattern it is always true that

$$\Delta k \Delta x \geq \frac{1}{2}\,, \tag{111}$$

where I have stated that the minimum arises for Gaussian wave packets.

We then input either Planck (photons) or de Broglie (matter waves) via the relation

$$p = \frac{h}{\lambda} = \hbar\frac{2\pi}{\lambda} = \hbar k\,, \quad \Rightarrow \quad \Delta p \Delta x \geq \frac{1}{2}\hbar\,. \tag{112}$$

Another uncertainty relation involves the uncertainty in energy of a wave packet, ΔE, and the time, Δt, taken to measure that energy. Using Gaussian or other wave forms that are functions of $kx - \omega t$ and that are of finite extent in Δt, we can derive the wave result that

$$\Delta\omega \Delta t \geq \frac{1}{2}\,, \tag{113}$$

where once again the minimum is for Gaussian forms.

We now input the relation

$$E = hf = \hbar(2\pi f) = \hbar\omega\,, \quad \Rightarrow \quad \Delta E \Delta t \geq \frac{1}{2}\hbar\,. \tag{114}$$

This result states that the precision with which we can know the energy of some system is limited by the time available for measuring the energy.

The Mechanistic Point of View of the HUP

$\Delta p_x \Delta x$

Here we consider an idealized (thought) experiment in which we try to measure the position of a particle using photons. A more careful treatment is given in the book. Here, I just give the idea of the argument.

- The photon carries momentum given by $p = \frac{h}{\lambda}$.
- The matter particle tends to pick up some portion of this momentum (depending upon angle of incidence which is determined by size of lens

of microscope employed — see book) so

$$(\Delta p)_{\text{particle being probed}} \sim \frac{h}{\lambda}\,. \tag{115}$$

- Also, the position of the particle can not be determined to any greater precision than the wavelength λ of the light:

$$(\Delta x)_{\text{particle being probed}} \gtrsim \lambda\,. \tag{116}$$

- Multiplying, we get

$$(\Delta p \Delta x)_{\text{particle being probed}} \gtrsim h\,. \tag{117}$$

This shows in a mechanistic way that any attempt to improve your measurement of Δx by employing smaller λ necessarily increases the amount of momentum that the photon will typically transfer to the particle being probed (the direction being unpredictable) as a result of the higher momentum being carried by each photon.

The key physics ideas that lead to the uncertainty principle from the mechanistic point of view are:

1. There is an indivisible nature of the light particles (photons) and nothing less than one photon can be used to perform a measurement of the momentum or energy of another particle.
2. There is a wave nature of light that even a single photon cannot evade.
3. These lead to the impossibility of predicting or measuring the precise (classical) path that a single scattered photon will follow, which in turn implies inability to determine precisely the momentum transferred to the electron.

$\Delta E \Delta t$

A similar argument is possible for the $\Delta E \Delta t$ relation.

- Consider a wave of frequency f incident on a particle at rest.
- Suppose that the minimum uncertainty in the number of waves we can count is 1 wave.
  Since $f = \frac{\#\text{ we count}}{\text{time interval}}$, we get

$$\Delta f = \frac{1}{\Delta t}\,, \tag{118}$$

where Δt is the time interval available for counting the waves.

- We now wish to employ the photon scattering off the particle to determine the particle's energy. The photon is bringing in an amount of energy that is uncertain by the amount (from Planck formula for photon)

$$\Delta E = h\Delta f = h\frac{1}{\Delta t}, \quad \Rightarrow \quad \Delta E \Delta t \sim h\,. \tag{119}$$

Another approach to this same energy-time uncertainty is the following:

- a photon with $E = cp = \frac{hc}{\lambda}$ hits a particle in a powerful microscope.
- The best that you can do to determine $time$ is specified by the arrival of the photon wave front. When this wave front arrives is known no better than $\frac{\lambda}{c}$ ($i.e.$ the time separation between two bumps in the light wave intensity). Thus,

$$\Delta t \sim \frac{\lambda}{c} \tag{120}$$

  is the smallest amount of time that you are using to perform your energy measurement.
- Meanwhile, the photon impact changes the energy of the particle it is probing by an amount of order

$$\Delta E \sim \frac{hc}{\lambda}; \tag{121}$$

i.e. **if you want to not change the energy of the particle the photon is probing, you must keep λ large. But, then this means it takes longer for the wave front arrival to be clearly defined. The result is**

$$\Delta E \Delta t = \frac{hc}{\lambda}\frac{\lambda}{c} \sim h\,. \tag{122}$$

Heisenberg Uncertainty Principle (HUP) Examples

e^- in a Hydrogen atom

Is there any relation between the energy levels of the Hydrogen atom and the uncertainty principle? Let's see.

We suppose that the electron is confined in a one-dimensional sense to a region of order Δx. Then, let us employ the HUP in the form $\Delta p_x \sim \hbar/\Delta x$. (I have chosen the numerical factor to give me the prettiest results.) The associated kinetic energy is

$$K \geq (K)_{\Delta p_x} \equiv \frac{(\Delta p_x)^2}{2m_e} > \frac{\hbar^2}{2m_e(\Delta x)^2}\,. \tag{123}$$

Let us demand that this kinetic energy not exceed significantly the negative potential energy associated with this same distance scale.

$$(K)_{\Delta p_x} \sim \frac{\hbar^2}{2m_e(\Delta x)^2} \sim \left| -\frac{ke^2}{\Delta x} \right| . \tag{124}$$

This gives us,

$$\Delta x \sim \frac{\hbar^2}{2km_e e^2} = \frac{a_0}{2} . \tag{125}$$

What this is telling us is that it is very difficult to confine the electron to a distance much smaller than a_0 using the electromagnetic force. If we scale up the potential energy using Z for a charged ion, the Δx cannot decrease faster than $1/Z$ without violating the HUP. The same argument would give us $\Delta x > \frac{a_0}{2}\frac{1}{Z}$. Plugging this into $-\frac{ke^2Z}{\Delta x}$ gives us energy levels that should scale as Z^2, as they do.

We can actually go further. It is apparent that the typical potential energy for an e^- confined to a region of size Δx is

$$U = -\frac{ke^2}{\Delta x} , \tag{126}$$

which can be combined with our minimum K for the particle to compute the total energy:

$$E = K + U = \frac{\hbar^2}{2m_e(\Delta x)^2} - \frac{ke^2}{\Delta x}\,. \tag{127}$$

Note that $E \to 0$ for $\Delta x \to \infty$, has a minimum somewhere and then $E \to +\infty$ for $\Delta x \to 0$. The most likely value of Δx is the value that minimizes E. Taking derivatives, this gives

$$\frac{\partial E}{\partial \Delta x} = 0 = -2\frac{\hbar^2}{2m_e(\Delta x)^3} + \frac{ke^2}{(\Delta x)^2} \tag{128}$$

which is solved by

$$\Delta x = \frac{\hbar^2}{m_e k e^2} = a_0\,, \tag{129}$$

which, after substitution into the above form for E gives

$$E = -\frac{k^2 e^4 m_e}{2\hbar^2} \tag{130}$$

which is precisely the E_0 energy level of the first Bohr orbit.

The Unstable Z boson

The Z boson is an unstable ($i.e.$ a particle that decays) with mass $m_Z \sim 91 \times 10^9\ eV$. The average lifetime of the Z is

$$\tau_Z = 2.9 \times 10^{-25}\ s\,. \tag{131}$$

This lifetime is determined by how many different types of particles it can decay into and what the strengths of those decays are. One important type of particle is something called a "neutrino", ν. There are potentially many different types of neutrinos. The more $Z \longrightarrow \bar{\nu}\nu$ channels there are, the shorter the Z lifetime. Since we cannot see ν's directly (they are very weakly interacting and have zero charge), it is important to determine the Z lifetime to indirectly determine how many ν's there are.

However, the above τ_Z is far too short to actually measure directly. So, how do we determine it. Answer: use Heisenberg uncertainty principle for theoretically predicted shape of "mass spectrum".

If we attempt to measure the mass of the Z by using $e^+e^- \longrightarrow Z$ collisions with different values of the e^+e^- total energy, what do we

expect to see? The HUP says we should expect to see a distribution of mass values of a certain shape.

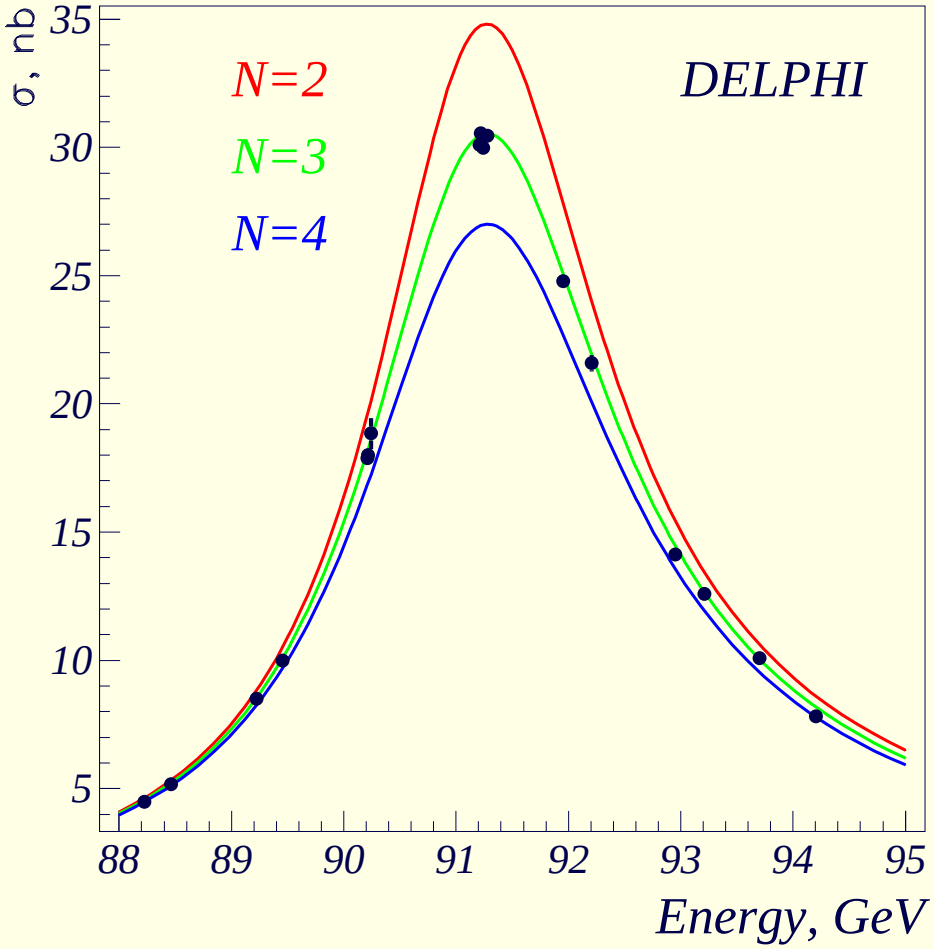


Figure 17: $e^+e^- \rightarrow hadrons$ as a function of $M_{e^+e^-}$. The Z peak is centered about $m_Z = 91.13 \times 10^9\ eV = 91.13$ GeV and has a width of roughly 2 to $3 \times 10^9\ eV$.

The resonance picture shows that we cannot make a precise determination of the mass. As stated, this is required by the uncertainty principle which says that we would need an infinite amount of time to get a precise mass determination, whereas the resonance disappears quickly. The HUP says

$$\Delta E \equiv \Delta m_Z \sim \hbar \frac{1}{\tau_Z} = \frac{6.582 \times 10^{-16}\ eV \cdot s}{2.9 \times 10^{-25}\ s} \sim 2.3 \times 10^9\ eV = 2.3\ \mathrm{GeV}\,, \tag{132}$$

and this is what is explicitly seen in the plot. The plot also shows how the peak would get narrower (broader), relative to its height, if certain decay modes are eliminated (added).

Relation of HUP to Two-Slit Interference Pattern

Things we know

Assume equal slit widths.

1. It is only when we have both slits open that the interference pattern develops.
2. Even if we send only one e^- at a time, if both slits are open the e^- hits at the detector bank will accumulate where the interference wave

prediction has a maximum and no e^-'s will hit at the destructive wave pattern cancellation minima.

3. We cannot be sure where any given e^- will end up; only the final average pattern can be predicted with certainty.
4. If we close one slit, the accumulation pattern changes to approximately uniform (for very narrow slits).

Now try to do better.

1. Suppose you have both slits open, but you try to measure unambiguously which slit a given e^- passes through.
   $\Rightarrow$ you disturb the e^-.
2. For example, place some detecting particles on the right side of the slit. Use the recoil of one of these particles to determine which slit the e^- goes through.
3. To decide which slit, need to measure the detecting particle's position with $\Delta y \ll D$ (D in the figure is the separation between slits, not the size of an individual slit).
4. During the collision, the detecting particle suffers a change in momentum Δp_y, equal and opposite to the change in momentum experienced by the e^- passing through the slit.

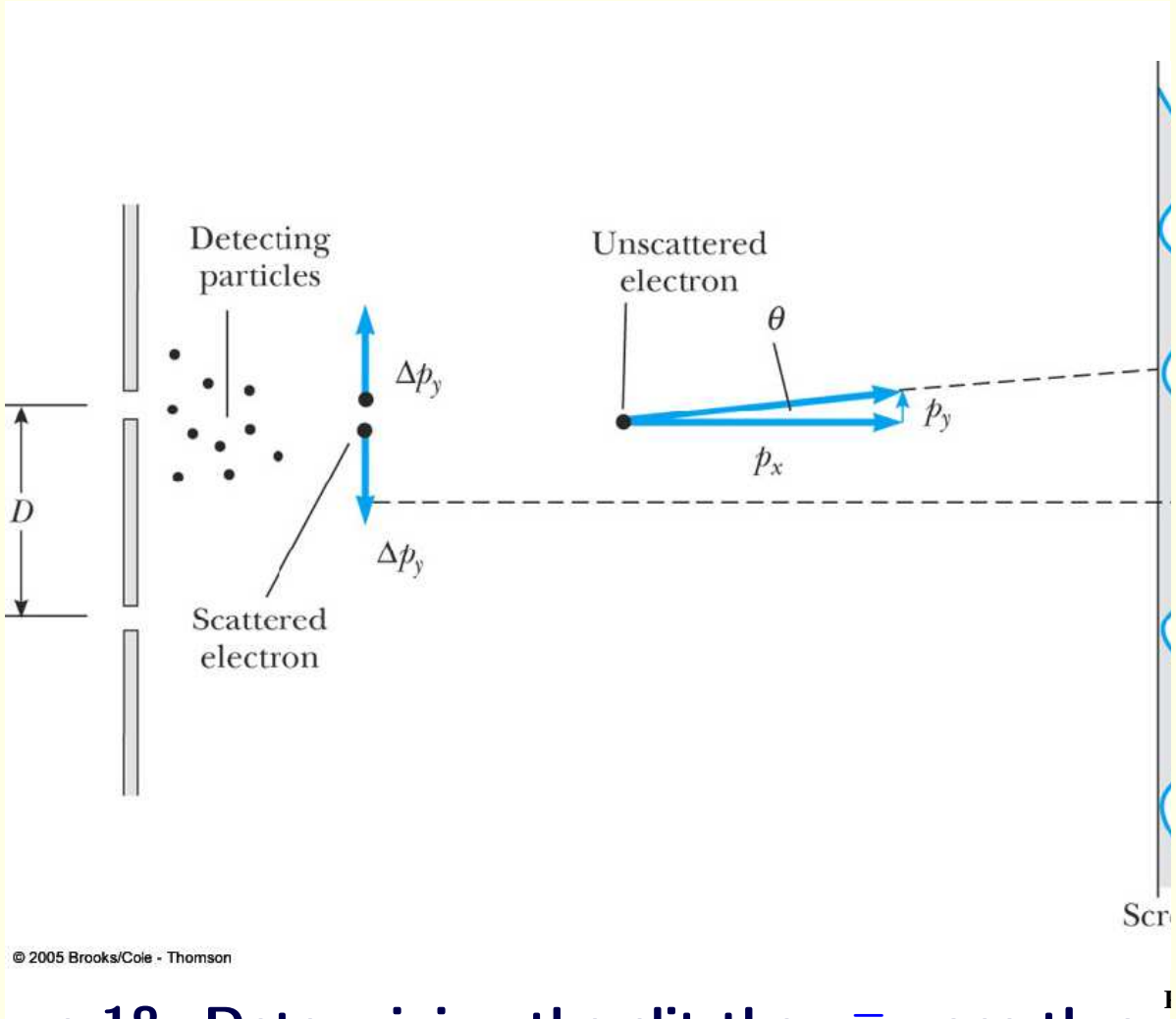


Figure 18: Determining the slit the e^- goes through.

5. **An undeviated e^- landing at the first minimum** *and producing an interference pattern* **has**

$$\tan\theta \sim \theta = \frac{p_y}{p_x} = \frac{h}{2p_x D}\,. \tag{133}$$

(This is our old $\frac{1}{2}\lambda$ path difference requirement.)

6. Thus, we require that an e^- scattered by a detecting particle has

$$\frac{\Delta p_y}{p_x} \ll \theta = \frac{h}{2p_x D} \quad \text{or} \quad \Delta p_y \ll \frac{h}{2D} \tag{134}$$

if the interference is to not be distorted.

7. Because

$$(\Delta p_y)_{e^-} = -(\Delta p_y)_{\text{detecting particle}}\,, \tag{135}$$

$$(\Delta p_y)_{\text{detecting particle}} \ll \frac{h}{2D} \tag{136}$$

is also required.

8. Altogether, for the detecting particle, we require

$$(\Delta p_y \Delta y)_{\text{detecting particle}} \ll \frac{h}{2D} \cdot D = \frac{h}{2}\,. \tag{137}$$

This is in clear violation of the uncertainty principle.
If Δy is small enough to determine which slit the electron goes through, Δp_y will be so large that the e^-'s will be deflected all over the place and the interference pattern will be destroyed.

Matter Probability Waves and the Schroedinger Equation

I will be, and have been for that matter, kind of combining the material appearing in Chapters 5 and 6. You should read this material as a unit. For example, I have set up the ingredients for writing down the Schroedinger equation that first appears in Sec. 6.3, where it is introduced more or less by fiat. I will now go a little bit beyond just simply writing it down and tell you one way that you can kind of understand it.

The Schroedinger Equation

The Schroedinger equation is the wave equation for matter probability waves when the non-relativistic limit is appropriate. A different equation must be used if the matter particles are in a situation where they typically have relativistic velocities.

Recall the game we played for "deriving" the light-wave equations. We wrote $E^2 = c^2p^2$, multiplied this equation by some E_y or B_z

electromagnetic field and then replaced

$$p_x = \frac{\hbar}{i}\frac{\partial}{\partial x}\,, \quad E = i\hbar\frac{\partial}{\partial t}\,. \tag{138}$$

In this case, we write (non-relativistically and neglecting any potentials or such for the moment — $i.e.$ we consider a "free" particle)

$$\begin{aligned} E &= m_0c^2 + \frac{p^2}{2m}\,, \quad \Rightarrow \quad E\Psi = \left(m_0c^2 + \frac{p^2}{2m}\right)\Psi \\ &\Rightarrow \quad i\hbar\frac{\partial\Psi}{\partial t} = m_0c^2\Psi - \frac{\hbar^2}{2m_0}\frac{\partial^2\Psi}{\partial x^2}\,. \end{aligned} \tag{139}$$

In the text, the constant m_0c^2 is absorbed into an overall redefinition of the energy scale in this NR limit, but this is really misleading when it comes to considering how the particle is moving, as we shall see.

The very simplest solution to this equation is the exponential form:

$$\Psi = Ae^{i(kx-\omega t)}\,, \tag{140}$$

where we compute $\omega(k)$ from the SE (Schroedinger equation) requirement

$$i\hbar(-i\omega(k))Ae^{i(kx-\omega(k)t} = \left(m_0c^2 - \hbar^2(ik)^2\right)Ae^{i(kx-\omega(k)t)}\,, \qquad (141)$$

implying

$$\omega(k) = \frac{m_0c^2}{\hbar} + \frac{\hbar k^2}{2m}\,. \qquad (142)$$

Note how this is consistent with the de Broglie / Planck relations

$$k = \frac{2\pi}{\lambda} = \frac{2\pi p}{h} = \frac{p}{\hbar}\,, \quad \text{and} \quad \omega = 2\pi f = 2\pi\frac{E}{h} = \frac{E}{\hbar} \qquad (143)$$

or equivalently

$$p = \frac{h}{\lambda} = \hbar\frac{2\pi}{\lambda} = \hbar k\,, \quad E = hf = \hbar 2\pi f = \hbar\omega \qquad (144)$$

being substituted into $E = m_0c^2 + p^2/2m$:

$$E = \hbar\omega = m_0c^2 + \frac{(\hbar k)^2}{2m_0}\,. \qquad (145)$$

The $m_0c^2/\hbar$ part of $\omega(k)$ is normally dropped in the non-relativistic limit, as it amounts to an irrelevant redefinition of the absolute energy scale. In the relativistic limit, it cannot be dropped.

Note that a $\sin$ or $\cos$ function form does not solve the SE. For example, if we tried the $\sin$ function form, the single time derivative would give us a $\cos$ function, whereas the double space derivative would give us back $-\sin$. In the free-particle case at any rate, we **must** employ the intrinsically complex "plane wave" form

$$Ae^{i(kx-\omega t)} = A\cos(kx-\omega t) + iA\sin(kx-\omega t)\,. \tag{146}$$

This is still a traveling complex wave moving in the $+x$ direction because of the $kx-\omega t$ argument which says that if I move in the direction x by an amount Δx then I can compensate by advancing t by an amount $\Delta t = k\Delta x/\omega$. We shall soon consider whether the velocity that you might compute from

$$\frac{\Delta x}{\Delta t} = \frac{\omega(k)}{k} = \frac{m_0c^2}{\hbar k} + \frac{\hbar k}{2m_0} = \frac{m_0c^2}{p} + \frac{p}{2m_0} \tag{147}$$

has any meaning. The answer is no. We will have to deal with **wave**

packets and the concepts of phase and group velocity to which we shortly turn.

The HUP (again).

As stated, the above $e^{i(kx-\omega t)}$ solution to the SE is called a *plane wave* solution.

The particle described by this solution has a precisely defined momentum (in the x direction) of $p = \hbar k$, as computed above.

If the HUP is correct, Δx should be infinite! and it is!

This is because

$$|\Psi|^2 = A^2 \tag{148}$$

is completely independent of x and so the particle has a uniform probability of being anywhere along the x axis! Obviously, it is nonsense to discuss the velocity of a uniform probability distribution.

How fast is the matter particle moving?

We must now face the subtle issue of how to construct a wave form that can describe an actual physical particle and how it is we determine the velocity of the particle. This will bring us to consider the difference between group and phase velocity.

We considered in Fig. 8 and surrounding material how to create a photon-like object by adding together $E\&M$ type wave patterns. There, the group and phase velocities were both equal to c and we did not distinguish or even discuss. For massive particles one must be careful.

The book has a discussion using two $\sin$ waves. However, I prefer to use the plane wave form we have just been discussing, which is an actual solution of the SE (unlike the $\sin$ or $\cos$ forms alone).

To define a "particle" we clearly cannot use a single plane-wave solution for which the particle has no preferred location.

We must superimpose a least two plane-wave solutions.

Let us begin with exactly two and see what happens.

- **Write**

$$\Psi(x,t) = Ae^{i(k_1 - \omega_1 t)} + Ae^{i(k_2 - \omega_2 t)} \tag{149}$$

where we have taken in to account the fact that when k changes a little bit then so must ω.

- **Let us assume we only change k by a small amount and write**

$$k_1 = k_0 + dk\,, \quad k_2 = k_0 - dk\,, \quad \omega_1 = \omega_0 + d\omega\,, \quad \omega_2 = \omega_0 - d\omega\,. \tag{150}$$

- **Then,**

$$\begin{aligned} \Psi &= A\left[e^{i[(k_0+dx)x-(\omega_0+d\omega)t]} + e^{i[(k_0-dx)x-(\omega_0-d\omega)t]}\right] \\ &= Ae^{i(k_0-\omega_0 t)}\left[e^{i[(dk)x-(d\omega)t]} + e^{-i[(dk)x-(d\omega)t]}\right] \\ &= Ae^{i(k_0 x-\omega_0 t)} 2\cos\left[(dk)x - (d\omega)t\right]\,. \end{aligned} \tag{151}$$

- **We have a complex exponential that moves at speed**

$$v_p \equiv \frac{\omega_0}{k_0} = \frac{\hbar\omega_0}{\hbar k} = \frac{E_0}{p_0}\,, \tag{152}$$

where v_p is called the phase velocity appropriate to these central values, modulated by a cosine function that moves at speed

$$v_g \equiv \frac{d\omega}{dk}\,, \tag{153}$$

which is called the group velocity.

- It is this latter term that defines the envelope of the wave and tells us where the probability is. Indeed,

$$|\Psi|^2 = 4A^2\cos^2\left[(dk)x - (d\omega)t\right]. \tag{154}$$

The phase velocity has disappeared. Since a physical particle moves with its probability, the actual physical speed of the particle is v_g.

- Of course, this two-plane-wave superposition is still a bit too simple. It is really a sequence of peaks that we observe passing by. To get a localized wave form we have to form the kind of superposition discussed earlier:

$$\Psi(x,t) = \int_{-\infty}^{\infty} \widetilde{\psi}(k)e^{i(kx-\omega(k)t)}dk\,. \tag{155}$$

We will do another explicit construction of this type shortly. The important point is that since the sum must include plane waves of

various k ($= p/\hbar$) and various $\omega(k)$ ($= E(p)/\hbar$) values, neither the momentum nor the energy of the group is well defined.

- All of this applies to photon waves as well as particle waves. It's just that $\omega(k) = ck$ for a photon wave is a much simpler formula than $\omega(k) = \frac{m_0c^2}{\hbar} + \frac{\hbar k^2}{2m_0}$ which is the formula that applies for a NR particle with mass. For $E = pc$, $v_p = E/p = c$ and for $\omega = ck$, $v_g = d\omega/dk = c$ also.
- It is useful to next generalize to the proper relativistic result:

$$E(p) = \sqrt{p^2c^2 + m_0^2c^4}\,. \tag{156}$$

The phase velocity is, as above,

$$v_p = \frac{E(p)}{p} = c\sqrt{1 + \left(\frac{m_0c}{p}\right)^2} = c\sqrt{1 + \left(\frac{m_0c}{\hbar k}\right)^2}\,. \tag{157}$$

From this we see that for a massless photon, $v_p = c$, but that for a massive particle $v_p > c$. However, this is not a problem since v_p does not describe where the probability is!

- Instead, we must look at $v_g = d\omega/dk$. We have (using our time-tested relation $f = E/h$)

$$\begin{aligned} \omega(k) &= 2\pi f = \frac{E(p=\hbar k)}{\hbar} = \frac{1}{\hbar}\sqrt{\hbar^2 k^2 c^2 + m_0^2 c^4}\,, \\ &\Rightarrow \\ v_g &= \frac{d\omega(k)}{dk} = \frac{1}{\hbar}\frac{\hbar^2 k c^2}{\sqrt{\hbar^2 k^2 c^2 + m_0^2 c^4}} \\ &= \frac{c}{\sqrt{1 + \left(\frac{m_0 c}{\hbar k}\right)^2}} = \frac{c^2}{v_p}\,, \end{aligned} \tag{158}$$

  implying that $v_g < c$, given that $v_p > c$ as just derived above.
- We can now check that v_g is the actual speed of the particle by using

$$v_p = \frac{E}{p} = \frac{\gamma(u) m_0 c^2}{\gamma(u) m_0 u} = \frac{c^2}{u} \quad \Rightarrow \quad v_g = \frac{c^2}{v_p} = u\,! \tag{159}$$

More on wave functions and propagating waves

It was Max Born who in 1925 zeroed in on the interpretation of Ψ as a probability amplitude.

He had in mind in particular the case where we want to describe a single particle that is sufficiently localized (unlike our nice plane wave solution, more like our wave packet type solutions) that you can (and should) define a normalizable probability. Then, he said that

$$P(x)dx = |\Psi(x,t)|^2 dx \tag{160}$$

should be the probability that the particle will be found in the infinitesimal interval dx about the point x. Once again, I stress that Ψ itself is not something you can observe and even $|\Psi|^2$ is only observable in a probabilistic sense.

Because of its relation to probabilities, we will typically insist on the following.

1. Ψ should be single valued and a continuous function of x and t. In this way, no ambiguities will arise concerning the predictions of the theory.
2. In fact, we will typically require that not only should Ψ be continuous, but it should also be *smooth* in the sense that its first derivatives are finite.

However, there are certain specialized situations where this is not appropriate. But, for most of the physical situations we shall discuss in this course, this requirement should be met. The exception is when there is some discontinuity in some potential.

3. Next, the total probability of finding a particle somewhere should be unity. Since $|\Psi|^2$ is the probability distribution for the particle in question, this means

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1 \quad \text{for any } t\,. \tag{161}$$

Similarly,

$$P_{ab} = \int_a^b |\Psi(x,t)|^2 dx \tag{162}$$

should be the probability of finding the particle in the interval $a \leq x \leq b$.

In this formulation of QM, the fundamental problem of QM is the following: Given the wavefunction at some initial instant, say $t = 0$, what is the wavefunction at any subsequent time t.

To answer this question requires a dynamical equation for $\Psi(x,t)$. We

have already written this dynamical equation down. It is Schroedinger's (wave) equation.

We have discussed it in the free-particle case, mostly focusing on the free-particle plane wave solution. However, the function $\Psi = Ae^{i(kx-\omega t)}$ is not normalizable in the way we would like. There is uniform probability everywhere.

However, we have also learned how to proceed. We form an appropriate superposition of plane waves, sometimes called a *wave packet*. As stated earlier, the Gaussian type of superposition is the most ideal. Let us go through the details now.

1. We start with
$$\Psi(x,0) = \int_{-\infty}^{\infty} \widetilde{\Psi}(k) e^{ikx} dk \tag{163}$$
with $\widetilde{\Psi}(k) = (C\alpha/\sqrt{\pi})\exp[-\alpha^2 k^2]$.
Since $\widetilde{\Psi}(k)$ is centered about $k = 0$, we will be constructing a wave packet that has a central momentum and velocity of 0 (motionless particle), although there will be a spread of velocities and momenta about this central value.
2. We can perform the k integral if we carefully examine it and use the

process called "square completion". We need

$$\begin{aligned}\Psi(x,0) &= \frac{C\alpha}{\sqrt{\pi}}\int_{-\infty}^{\infty} dk e^{-\left(\alpha k-\frac{ix}{2\alpha}\right)^2-\frac{x^2}{4\alpha^2}} \\ &= \frac{C}{\sqrt{\pi}}e^{-x^2/4\alpha^2}\int_{-\infty}^{\infty} e^{-z^2}dz \quad \text{defining} \quad z=\alpha k - ix/(2\alpha) \\ &= Ce^{-x^2/4\alpha^2} = Ce^{-(x/2\alpha)^2}. \end{aligned} \tag{164}$$

Above, we used $\int_{-\infty}^{\infty} e^{-z^2}dz = \sqrt{\pi}$ — see any integral table.

A Gaussian form has begot another Gaussian form.

3. We now state that the appropriate way to define the width of a Gaussian form is to take the probability and write it in the form

$$P(x) \propto e^{-x^2/2(\Delta x)^2}, \quad \text{or} \quad P(k) \propto e^{-k^2/2\Delta k)^2}, \tag{165}$$

for distributions centered about $x=0$ and $k=0$.
So, using $|\widetilde{\Psi}(k)|^2 \propto e^{-2\alpha^2k^2}$ and $|\Psi(x,0)|^2 \propto e^{-2x^2/(4\alpha^2)}$ we identify

$$2\alpha^2k^2 = \frac{k^2}{2(\Delta k)^2}, \quad \text{and} \quad 2\frac{1}{4\alpha^2}x^2 = \frac{x^2}{2(\Delta x)^2} \tag{166}$$

from which we find

$$\Delta k = \frac{1}{2\alpha}\,, \quad \text{and} \quad \Delta x = \alpha\,, \tag{167}$$

implying $\Delta k \Delta x = \frac{1}{2}$. That these are the appropriate definitions of Δk and Δx will be left until a later time. But, assuming this, we are back to our minimum HUP after multiplying by $\hbar$ and converting to $p = \hbar k$.

4. Finally, we can normalize this $\Psi(x,0)$ by requiring

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} |\Psi(x,0)|^2 dx \\ &= \int_{-\infty}^{\infty} C^2 e^{-2x^2/4\alpha^2} dx \\ &= C^2(\sqrt{2}\alpha)\int_{-\infty}^{\infty} e^{-y^2} dy \quad \text{using } y = x/(\sqrt{2}\alpha) \\ &= C^2(\sqrt{2}\alpha)\sqrt{\pi}\,, \quad \Rightarrow \quad C = \frac{1}{(2\pi)^{1/4}\sqrt{\alpha}}\,, \end{aligned} \tag{168}$$

where we have claimed that $\alpha = \Delta x$ for an appropriate definition of Δx.

We should now discuss how it is that this wavepacket evolves with time.

We find that it disperses, getting broader in space as time passes. This is because it was initially made up of plane waves with many different k values (both positive and negative).

The steps and results are as follows:

1. For $t \neq 0$, use

$$\begin{aligned}
\Psi(x,t) &= \int_{-\infty}^{\infty} \widetilde{\Psi}(k) e^{i(kx-\omega(k)t)} \\
&= \int_{-\infty}^{\infty} \widetilde{\Psi}(k) e^{i\left(kx-\frac{\hbar k^2}{2m_e}t\right)} dk \\
&= \frac{C}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-\alpha^2 k^2 + ikx - i\hbar t k^2/(2m_e)} dk \qquad (169)
\end{aligned}$$

   where we inserted the expression for $\omega(k)$ that is required by Schroedinger's equation.
2. We can again complete the square. In the exponent we have

$$ikx - k^2[\alpha^2 + i\hbar t/(2m_e)]$$
$$= -\left(k\sqrt{\alpha^2 + \frac{i\hbar t}{2m_e}} - \frac{ix}{2\sqrt{\alpha^2 + \frac{i\hbar t}{2m_e}}}\right)^2 - \frac{x^2}{4\left(\alpha^2 + \frac{i\hbar t}{2m_e}\right)} \quad (170)$$

I will not go through the details of the variable shift and integration. The fact that the k^2 coefficient is complex is not any particular problem. You just have to trust your square completion process and use the standard $\int_{-\infty}^{\infty} \exp[-y^2]dy = \sqrt{\pi}$ at the appropriate point.

3. The important component of interest is the residual coming from the last term above which says that

$$\Psi(x,t) \propto \exp\left[-\frac{x^2}{4\left(\alpha^2 + \frac{i\hbar t}{2m_e}\right)}\right] . \quad (171)$$

4. As always, in defining a width we are interested in the probability and

not the amplitude. We have

$$
\begin{aligned}
|\Psi(x,t)|^2 &\propto \exp\left[-\frac{1}{4}\frac{x^2}{\alpha^2+\frac{i\hbar t}{2m_e}}\right]\times\exp\left[-\frac{1}{4}\frac{x^2}{\alpha^2-\frac{i\hbar t}{2m_e}}\right] \\
&= \exp\left[-\frac{1}{4}x^2\left(\frac{1}{\alpha^2+i\hbar t/(2m_e)}+\frac{1}{\alpha^2-i\hbar t/(2m_e)}\right)\right] \\
&= \exp\left[-\frac{1}{4}x^2\left(\frac{2\alpha^2}{\alpha^4+\left[\frac{\hbar t}{2m_e}\right]^2}\right)\right] \\
&= \exp\left[-\frac{1}{2}\frac{x^2}{\alpha^2+\left[\frac{\hbar t}{2m_e\alpha}\right]^2}\right] \\
&\equiv \exp\left[-\frac{1}{2}\frac{x^2}{[\Delta x(t)]^2}\right] \\
\Rightarrow\quad [\Delta x(t)]^2 &= [\Delta x(0)]^2+\left[\frac{\hbar t}{2m_e\Delta x(0)}\right]^2, \qquad (172)
\end{aligned}
$$

where we used $\alpha = \Delta x(0)$. In getting from the 2nd to the 3rd line

above, we used

$$\frac{1}{a+ib}+\frac{1}{a-ib}=\frac{2a}{a^2+b^2}\,. \tag{173}$$

Non-stationary case

If we want a particle whose central location is moving, we simply modify our input form of $\widetilde{\Psi}(k)$ so that it is a Gaussian (or other choice) centered about $k=k_0$. The packet would then move with a group velocity given, in the NR case, by

$$v_g=\left[\frac{d\omega(k)}{dk}\right]_{k=k_0}=\left[\frac{d}{dk}\left(\frac{\hbar k^2}{2m_0}\right)\right]_{k=k_0}=\frac{\hbar k_0}{m_0}\,. \tag{174}$$

The wave packet would, just as in the $k_0=0$ case discussed above, spread out as time passed due to the presence of a distribution of momenta and velocities for individual subcomponents of the wave packet.

Definition of Δx?

So, let us now use the probability interpretation of $\Psi(x,0)$ to actually

define an appropriate definition of Δx. We employ (from eq. (164))

$$P(x) = |\Psi(x,0)|^2 = \left|Ce^{-x^2/4\alpha^2}\right|^2 = C^2 e^{-x^2/2\alpha^2}\,. \tag{175}$$

We could then define the average value of x as

$$\langle x\rangle \equiv \int_{-\infty}^{\infty} x\,P(x)\,dx\,, \quad \Rightarrow \quad \langle x\rangle = 0 \tag{176}$$

for the particular form of $P(x)$ above due to the fact that $P(x)$ is even in $x \to -x$, whereas as x changes sign under $x \to -x$.

We now come to the "standard" definition of Δx:

$$(\Delta x)^2 = \langle (x - \langle x\rangle)^2\rangle = \langle x^2\rangle - 2\langle x\langle x\rangle\rangle + \langle x\rangle^2 = \langle x^2\rangle - \langle x\rangle^2\,. \tag{177}$$

Let us compute $\langle x^2\rangle$.

$$\langle x^2\rangle \equiv \int_{-\infty}^{\infty} x^2\,P(x)\,dx$$

$$
\begin{aligned}
&= \int_{-\infty}^{\infty} x^2 C^2 e^{-x^2/2\alpha^2}\, dx \\
&= C^2\sqrt{2\pi}\alpha^3 \quad \text{using } \textstyle\int_{-\infty}^{\infty} e^{-ax^2}dx = \sqrt{\pi}/(2a^{3/2}) \\
&= \alpha^2 \quad \text{using } C^2 = 1/(\sqrt{2\pi}\alpha)\,. \qquad (178)
\end{aligned}
$$

Thus, using this definition of Δx, we do indeed find that $\Delta x = \alpha$ as claimed earlier.

You should remember how we proceeded here. We could compute other average values using $P(x)$, and these will have real physical meaning in various situations, just as Δx really describes the size of a wave packet in a quantitative way.

Another example: a structure localized in time

This time, we consider a probability that is somewhat localized in time. In particular, we consider the case of an unstable particle produced at $t = 0$ which then decays according to a probability distribution

$$P(t) \equiv \frac{dN}{dt} = N_0 e^{-t/\tau}\,, \qquad (179)$$

where by convention τ is referred to as the particle lifetime.

Of course, we must remember that $P(t)$ is not the amplitude, but rather the probability. The amplitude will be $f(t) \propto \sqrt{P(t)} \propto e^{-t/2\tau}$.

If we are talking about solutions to the SE, it must be that this time structure is a superposition of plane-wave type solutions (these are all we have — they form a *complete set*). In the case of a time structure, this means that there must exist a $\widetilde{f}(\omega)$ such that

$$f(t) = \int_{-\infty}^{\infty} d\omega \widetilde{f}(\omega) e^{-i\omega t} \,. \tag{180}$$

The appropriate $\widetilde{f}(\omega)$ is found by the inverse relation

$$\widetilde{f}(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt e^{i\omega t} f(t) \tag{181}$$

as we easily show.

Proof

We use a "dummy" variable t' to define the $\widetilde{f}(\omega)$ integral form and then write:

$$\begin{aligned}
f(t) &=? \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega \left[\int_{-\infty}^{\infty} dt' e^{i\omega t'} f(t')\right] e^{-i\omega t} \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} dt' f(t') \lim_{W\to\infty}\int_{-W}^{W} d\omega e^{i\omega(t'-t)} \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} dt' f(t') \lim_{W\to\infty} \frac{e^{iW(t'-t)} - e^{-iW(t'-t)}}{i(t'-t)} \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} dt' f(t') \lim_{W\to\infty} \frac{2\sin[W(t'-t)]}{t'-t} \\
&= f(t)\,. \qquad (182)
\end{aligned}$$

The last step takes a bit of work. Note that if $t' \neq t$ then the $\sin[W(t'-t)]$ is very rapidly oscillating as a function of t' (for very large W) and in the large W limit nothing will survive in the $\int dt'$ integral for any tiny dt' interval where $t' \neq t$. Assuming that $f(t)$ is a smoothly

varying function on the scale of $1/W$, this allows us to write

$$\begin{aligned}
\frac{1}{2\pi}\int_{-\infty}^{\infty} dt' f(t') \lim_{W\to\infty} \frac{2\sin[W(t'-t)]}{t'-t} \\
&= f(t)\frac{1}{2\pi}\lim_{W\to\infty}\int_{-\infty}^{\infty} dt' \frac{2\sin[W(t'-t)]}{t'-t} \\
&= f(t)\,, \qquad (183)
\end{aligned}$$

where for the last step we have simply looked up the integral in a table and found that its value is 2π *independent of* $t'-t$ *and* W.

QED

So, now let us return to the computation of interest:

$$\begin{aligned}
\widetilde{f}(\omega) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} dt e^{i\omega t} f(t) \\
&\propto \frac{1}{2\pi}\int_{0}^{\infty} dt e^{i\omega t} e^{-t/2\tau} \\
&= \frac{1}{2\pi}\int_{0}^{\infty} dt e^{t(i\omega - 1/2\tau)}
\end{aligned}$$

$$= \frac{1}{2\pi}\left[\frac{e^{t(i\omega-1/2\tau)}}{i\omega-1/2\tau}\right]_0^\infty$$
$$= \frac{1}{2\pi}\left[\frac{1}{1/2\tau-i\omega}\right]. \quad (184)$$

From this we compute the $P(\omega)$ distribution as

$$P(\omega) = |\widetilde{f}(\omega)|^2 \propto \frac{1}{\omega^2+\frac{1}{4\tau^2}}. \quad (185)$$

If we want to make connection with the Z resonance example given earlier, see Fig. 17, we would write $\hbar\omega = E - m_Z c^2$ and the functional form given above is precisely that used to draw the plotted curves, one of which fits perfectly (for the correct choice of $\tau = \tau_Z$) the experimental data. The quantity $\hbar/\tau$ that determines the width of the E distribution is sometimes written as $\Gamma = \hbar/\tau$. For the precise τ_Z given earlier we have

$$\Gamma_Z = \frac{\hbar}{\tau_z} = 2.3 \text{ GeV}, \quad (186)$$

as computed earlier, eq. (132).

The Schroedinger Equation in the Presence of Forces/Potentials

We begin by following our previous route of writing an equation for the energy, but now including a potential energy term, $U(x)$, which is associated with a force, $F(x) = -dU/dx$:

$$E = \frac{p^2}{2m_0} + U\,. \tag{187}$$

We will consider only cases where $U = U(x)$. Now, multiply by $\Psi(x,t)$ and make the replacements $E \to i\hbar\frac{\partial}{\partial t}$, $p \to \frac{\hbar}{i}\frac{\partial}{\partial x}$ to obtain the SE:

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m_0}\frac{\partial^2\Psi(x,t)}{\partial x^2} + U(x)\Psi(x,t)\,. \tag{188}$$

Although we have motivated the above replacements on the basis of the HUP and wave ideas and analogies to $E\&M$ wave regarding momentum

and energy, the SE and the probability interpretation of Ψ must really be regarded as a basic new law that we must repeatedly test against experiment.

Is there a solution analogous to $e^{i(kx-\omega(k)t)}$ to the SE in the presence of U?

When U does not depend explicitly on t, we can always write

$$\Psi(x,t) = \psi(x)\phi(t) \tag{189}$$

which is to say the time and space dependence can be separated. (In the $U = 0$ case, $\psi(x) = e^{ikx}$ and $\phi(t) = e^{-i\omega t}$.) Substituting this form into eq. (188) and dividing by $\psi\phi$, we obtain (I will drop the subscript 0 on m_0, and simply write m in what follows.)

$$-\frac{\hbar^2}{2m}\frac{\psi''(x)}{\psi(x)} + U(x) = i\hbar\frac{\phi'(t)}{\phi(t)}\,. \tag{190}$$

The lhs depends only on x and the rhs depends only on t. This is only possible if both sides are equal to the same constant, which we call E

(of course). We can immediately integrate the rhs:

$$i\hbar\frac{d\phi(t)}{dt} = E\phi(t) \; : \quad \Rightarrow \quad \phi(t) = e^{-i\frac{E}{\hbar}t} = e^{-i\omega t} \, . \tag{191}$$

This leaves us with solving the time-independent lhs

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x) \, , \tag{192}$$

which is often rewritten in the form

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}[U(x) - E]\psi(x) \, . \tag{193}$$

If $U = 0$, this reduces to our free-particle situation with $\psi(x) = e^{ikx}$ and $E = \hbar^2 k^2/(2m)$. Even in the case of $U \neq 0$, E will be the total energy, and will be a constant describing the state in which the particle resides.

The solution $\psi(x)$ will depend upon U, but for $P(x) = |\psi(x)|^2$ to be physically interpretable, $\psi(x)$ should be finite everywhere, single-valued

and continuous. Further, $\psi(x)$ should be smooth in that $\frac{d\psi}{dx}$ should be normally be continuous. (Just from the SE itself, $\frac{d^2\psi}{dx^2}$ can only be infinite if U is infinite.)

Finally, note that since $|\phi(t)|^2 = 1$, we have

$$P(x,t) = |\Psi(x,t)|^2 = |\psi(x)|^2 \tag{194}$$

which is to say that $P(x,t)$ is independent of time. This is why such solutions are referred to as stationary states — all probabilities are static.

Particle in a box

We envision an electron or other particle confined absolutely to a region between $x = 0$ and $x = L$ by a potential

$$U(x) = \begin{cases} 0\,, & 0 \le x \le L \\ \infty\,, & x < 0 \quad \text{or} \quad x > L \end{cases} . \tag{195}$$

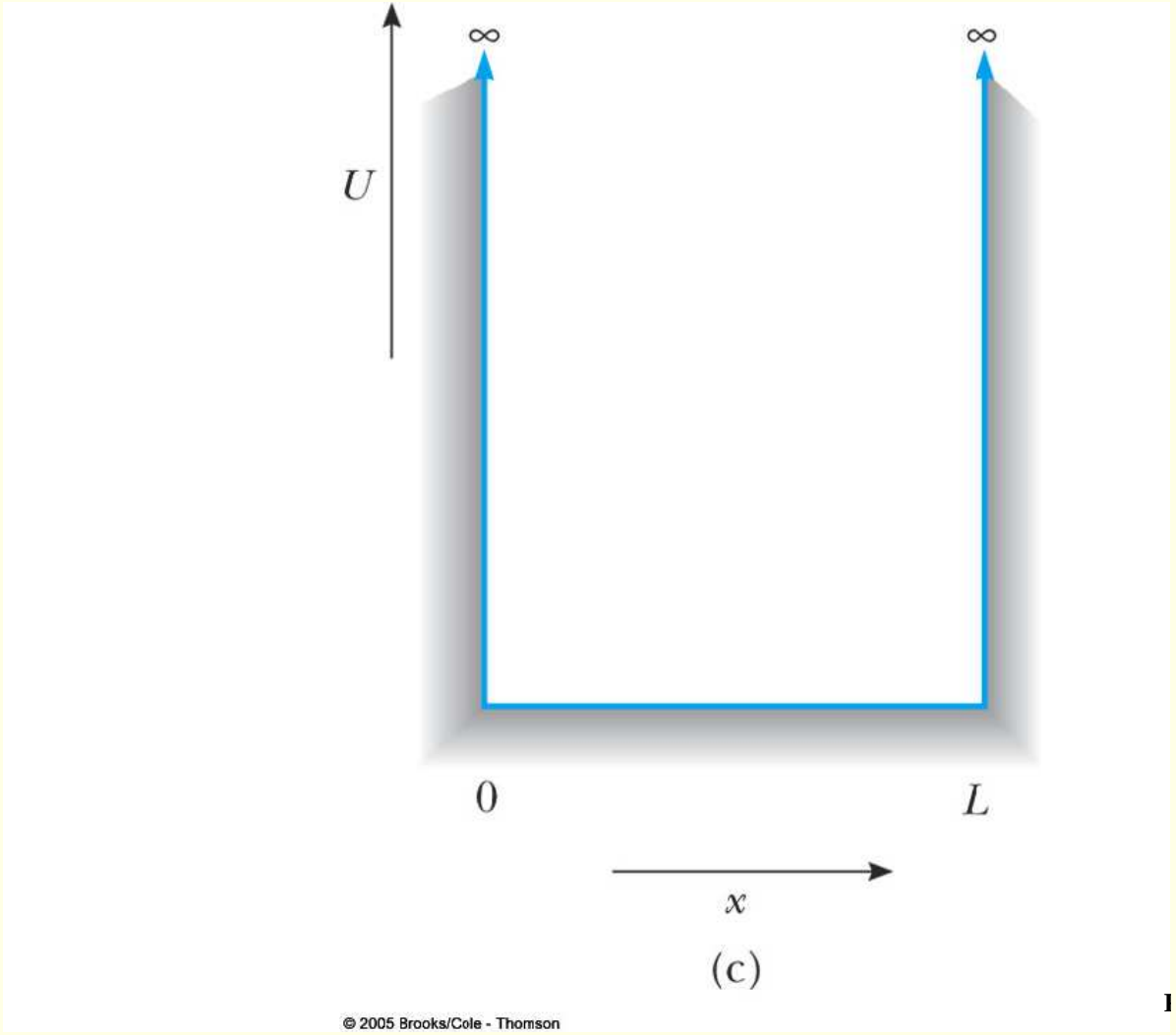


Figure 19: The infinite square-well potential.

1. **Because the particle is absolutely confined by the infinite potential, we must have $\psi = 0$ for $x < 0$ and $x > L$.**
2. **By continuity, we must then have $\psi = 0$ at $x = 0$ and $x = L$.**

3. For $0 \leq x \leq L$, $U = 0$ and we must solve (defining $E = \hbar^2 k^2/(2m)$ as usual in the NR case)

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi(x) = -k^2\psi(x)\,. \tag{196}$$

4. The solution can be a combination of $\sin kx$ and $\cos kx$:

$$\psi(x) = A\sin kx + B\cos kx\,, \quad \text{for} \;\; 0 < x < L\,. \tag{197}$$

5. At $x = 0$, $\psi(0) = 0 \Rightarrow B = 0$.
At $x = L$, with $B = 0$, and assuming $A \neq 0$, $\psi(L) = 0 \Rightarrow kL = n\pi$.
This latter condition can be written in what should now be a not-unexpected manner. Namely:

$$kL = n\pi \quad \Rightarrow \quad k = \frac{n\pi}{L} \quad \Rightarrow \quad \frac{2\pi}{\lambda} = \frac{n\pi}{L} \quad \rightarrow \quad \frac{n}{2}\lambda = L\,, \tag{198}$$

which is to say that we must fit a half-integer number of wave-lengths in between the box edges.

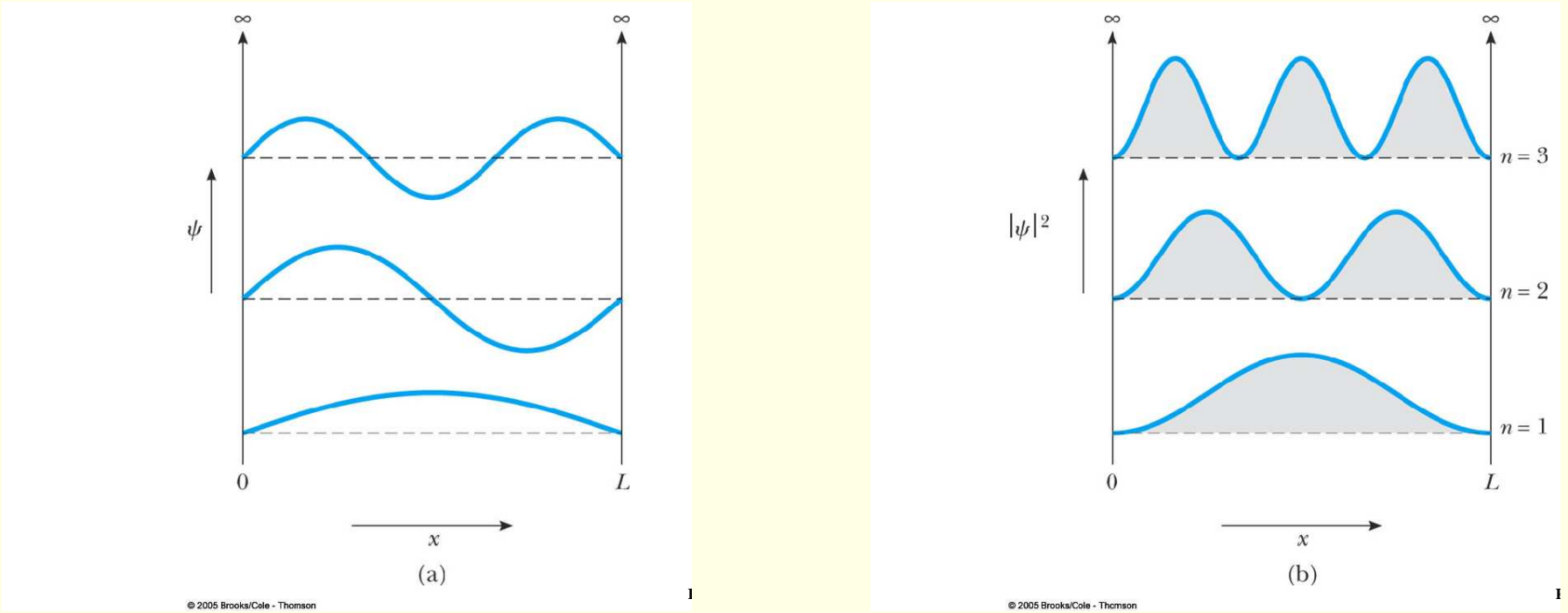
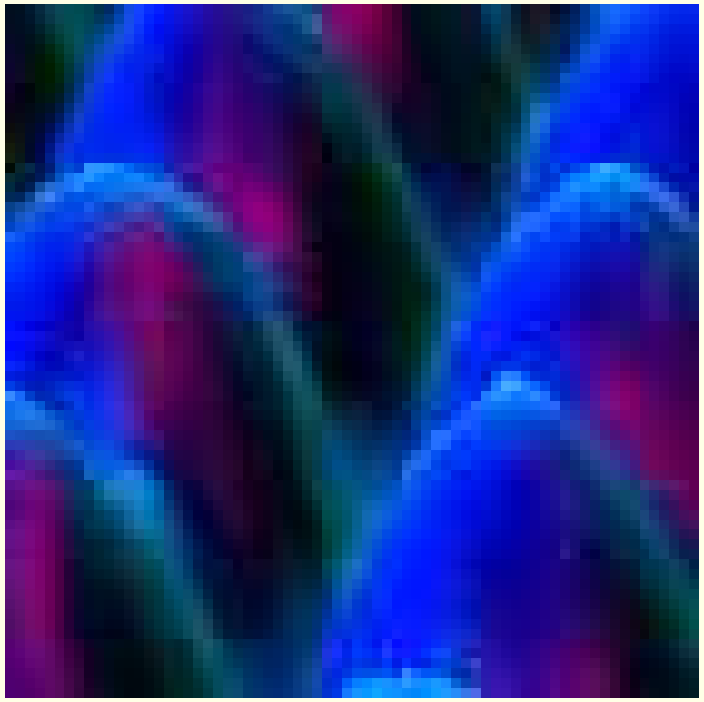


Figure 20: The infinite square-well potential wave-functions and probabilities.

The wave functions are:

$$\psi_n(x) = A \sin\left(\frac{n\pi x}{L}\right), \quad \text{for } 0 < x < L \text{ and } n = 1, 2, \ldots \tag{199}$$

To normalize, we require $\int_0^L |\psi_n(x)|^2 dx = 1$ which gives $A = \sqrt{2/L}$.



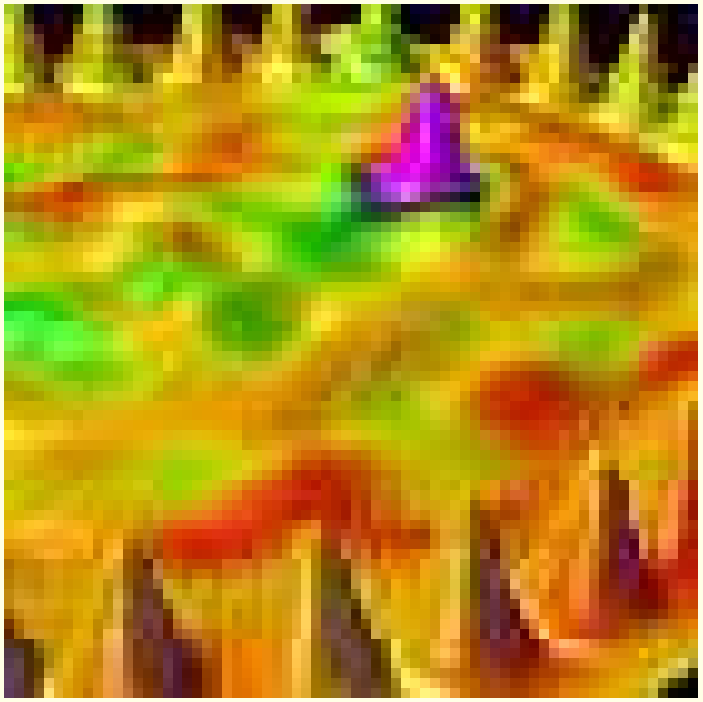


Figure 21: Scanning tunneling microscope (STM) pictures of electron patterns in approximately infinite well set ups.

Above, are two pictures of the electron density for two approximately infinite well set ups. For example, the 2nd picture has a one-dimensional oval well set up. The regular peaks along the ring of atoms that create a "well" like our square well are the STM measurements of the electron density. Note the wave pattern. So, you should believe this stuff!

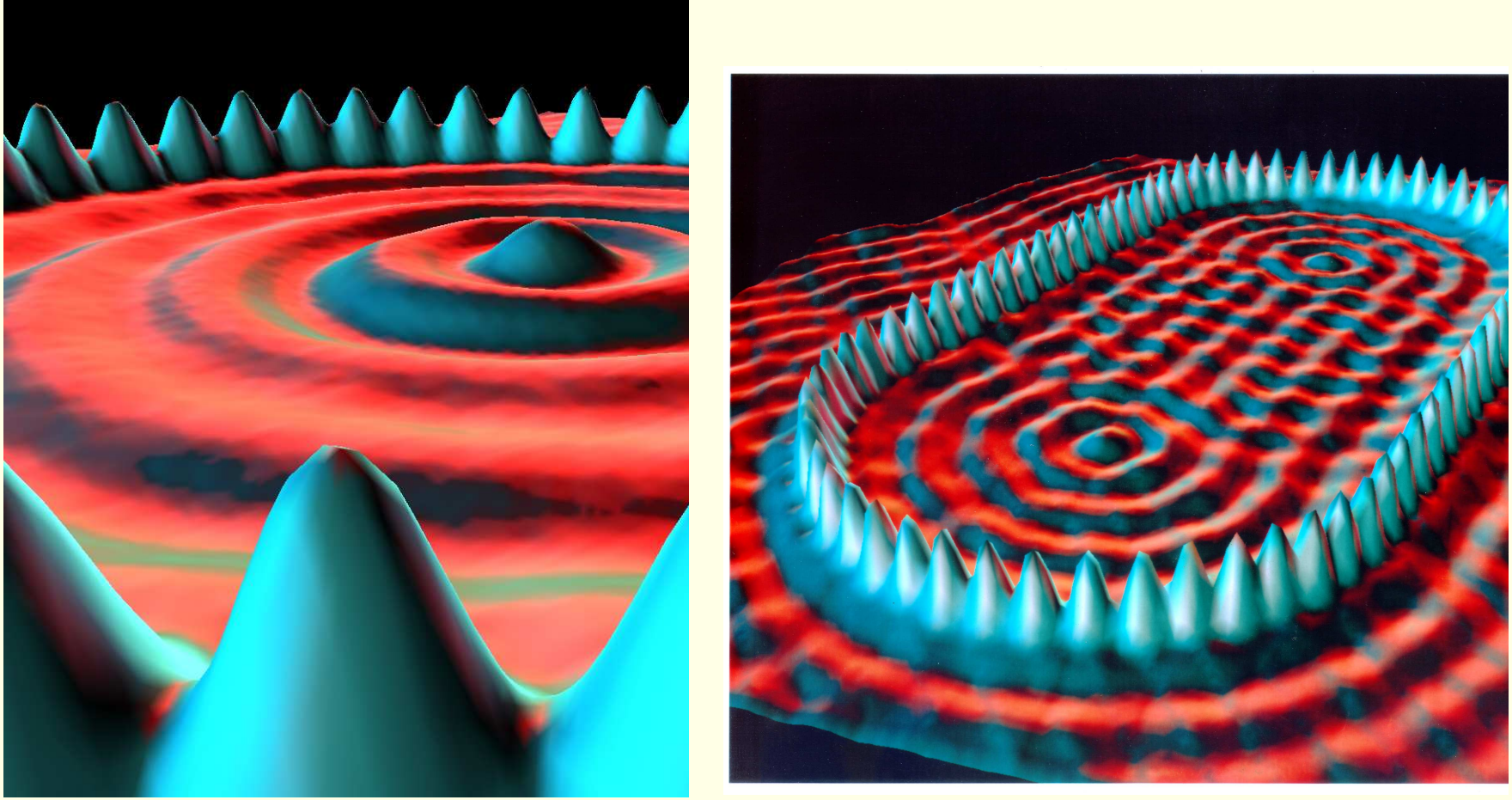


Figure 22: (a) The discovery of the STM's ability to image variations in the density distribution of surface state electrons created a compulsion to have complete control of not only the atomic landscape, but the electronic landscape also. Here we have positioned 48 iron atoms into a circular ring in order to "corral" some surface state electrons and force them into "quantum" states of the circular structure. The ripples in the ring of atoms are the density distribution of a particular set of quantum states of the corral. The STM measured distributions agree with those found for the corral by solving the classic eigenvalue problem in quantum mechanics – a particle in a hard-wall box. (b) Here we have another STM measurement where iron atoms are shaped into a stadium shaped structure.

6. The corresponding energy values are:

$$E = \frac{\hbar^2 k^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2mL^2}, \quad n = 1, 2, \ldots \tag{200}$$

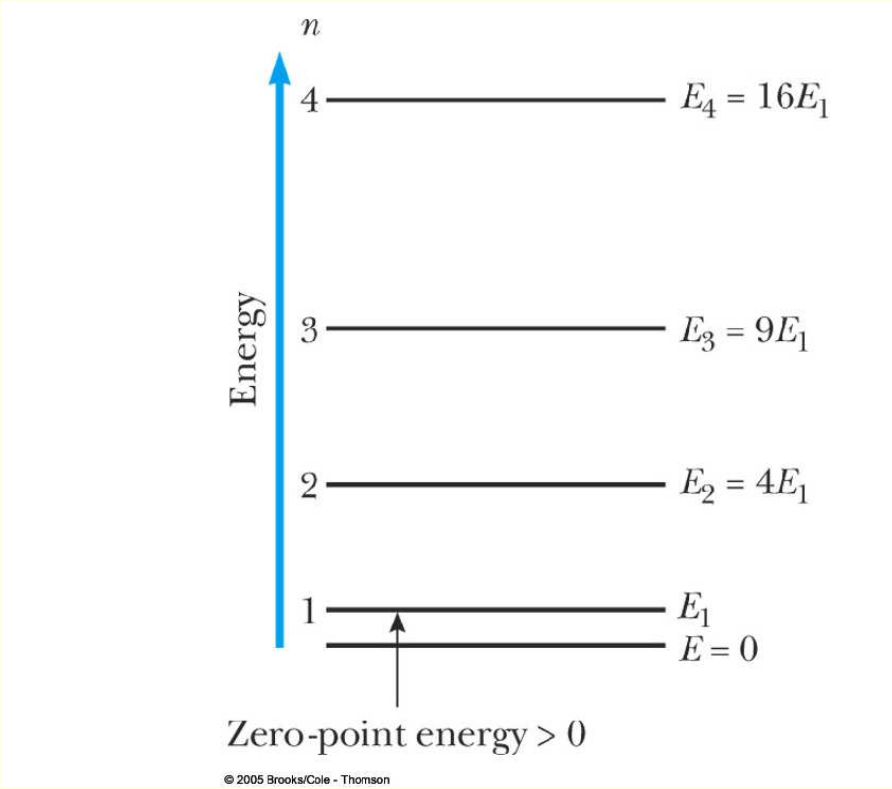


Figure 23: The infinite square-well potential energy levels.

The lowest energy level is the $n = 1$ state, which we call the ground

state.

$$E_1 = \frac{\pi^2 \hbar^2}{2mL^2}\,. \tag{201}$$

7. Note that $n = 0$, corresponding to $E = 0$ is not a possible solution. This means the particle can never be at rest.
   This is what we expect from the HUP. A particle confined to $\Delta x \sim L$, should have $\Delta p \sim \hbar/L$ and $K \sim (\hbar/L)^2/(2m)$, which is precisely the kind of result that we get!
   E_1 is sometimes referred to as the zero-point energy.

Example 1

Could we ever expect to see any of this stuff for a macroscopic object? Answer: no!

For example, consider a $1.00\ mg$ object confined to move between two rigid walls separated by $1.00\ cm$. (a) Calculate the minimum speed of the object. (b) If the speed of the object is (an observable amount of) $3.00\ cm/s$, find the corresponding, value of n.

Solution:

(a) Treating this as a particle in a box, the energy of the particle can

only be one of the values given by Eq. (6.17), or

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} = \frac{n^2h^2}{8mL^2}\,. \tag{202}$$

The minimum energy results from taking $n = 1$. For the above m and L, we calculate

$$E_1 = \frac{(6.626 \times 10^{-34}\ J \cdot s)^2}{8.00 \times 10^{-10}\ kg \cdot m^2} = 5.49 \times 10^{-58}\ J\,. \tag{203}$$

Because the energy is all kinetic ($U = 0$ inside well), $E_1 = \frac{1}{2}mv_1^2$, or

$$v_1 = \sqrt{2(5.49 \times 10^{-58}\ J)/(1.00 \times 10^{-6}\ kg)} = 3.31 \times 10^{-26}\ m/s\,, \tag{204}$$

an immeasurably small speed. The object would take $3 \times 10^{23}\ s$, or about 1 million times the present age of the universe, to move the $1.00\ cm$ between the walls.

(b) If the speed is $v = 3.00\ cm/s$, then the particle's energy is

$$E = K = \frac{1}{2}mv^2 = \frac{1}{2}(1.00\times10^{-6}\,kg)(3.00\times10^{-2}\,m/s)^2 = 4.50\times10^{-10}\,J\,. \tag{205}$$

This too, to be allowed, would have to be one of the E_n values. To determine which one, we solve for n, and obtain

$$n = \frac{\sqrt{8mL^2E}}{h} = \sqrt{(8.00\times10^{-10}\ kg\cdot m^2)(4.50\times10^{-10}\ J)} = 9.05\times10^{23}\,. \tag{206}$$

This is an enormous number. Indeed, the value of n is so large that we would never be able to distinguish the quantized nature of the energy levels. The difference between the energies for $n = 9.05\times10^{23}$ and $n' = 9.05\times10^{23}+1$ is only about $10^{-33}\ J$, much too small to be detected experimentally.

This is an example that illustrates Bohr's correspondence principle, which asserts that quantum predictions must agree with classical results for large masses and lengths.

Example 2

An electron is confined in an infinite well of $30\ cm$ width.

(a) What is the ground-state energy?

$$E_1 = \frac{(1)^2\pi^2(1.055 \times 10^{-34}\ J \cdot s)^2}{2(9.11 \times 10^{-31}\ kg)(0.3\ m)^2} = 6.77 \times 10^{-37}\ J\,. \tag{207}$$

(b) In this state, what is the probability that the e^- would be found within $10\ cm$ of the left-hand wall?

We have $P(x) = |\psi(x)|^2$. For the general case,

$$|\psi_n(x)|^2 = \left(\sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L}\right)^2\,. \tag{208}$$

So,

$$\begin{aligned} P\left(0 \le x \le \frac{L}{3}\right) &= \int_0^{L/3} \frac{2}{L}\sin^2\frac{n\pi x}{L}dx \\ &= \int_0^{L/3} \frac{2}{L}\left[\frac{1}{2}\left(1 - \cos\frac{2n\pi x}{L}\right)\right]dx \end{aligned}$$

$$= \frac{2}{L}\left[\frac{x}{2} - L\frac{\sin\frac{2n\pi x}{L}}{4n\pi}\right]_0^{L/3} = \frac{2}{L}\left[\frac{L}{6} - L\sin\frac{\frac{2n\pi(L/3)}{L}}{4n\pi}\right]$$
$$= \frac{1}{3} - \frac{1}{2n\pi}\sin\frac{2n\pi}{3}. \quad (209)$$

The width L has canceled as we know it must on dimensional grounds.

For $n = 1$, we find a result of $1/3 - 0.137 = 0.196$. This is to be expected since $P(x)$ for $n = 1$ peaks in the center of the well. In fact, the probability for the electron to be in the center $1/3$ is $1 - 2 \times 0.196 = 0.609$.

(c) If the e^- instead has an energy of $1.0\ eV$, what is the probability that it would be found within $10\ cm$ of the left-hand wall?

We must first determine the n value for this energy by solving

$$1.0\ eV \times 1.6 \times 10^{-19}\ J/eV = \frac{n^2\pi^2(1.055 \times 10^{-34}\ J \cdot s)^2}{2(9.11 \times 10^{-31}\ kg)(0.3\ m)^2} \quad (210)$$

which yields $n = 4.89 \times 10^8$. Then, using the general result above, we

find

$$P(0 \le x \le L/3) = \frac{1}{3} - \frac{1}{2(4.89 \times 10^8)\pi} \sin \frac{2(4.89 \times 10^8)\pi}{3} \simeq \frac{1}{3}\,. \tag{211}$$

Clearly, we are approaching a classical limit, even for an electron of modest energy.

(d) For the $1\ eV$ electron, what is the distance between nodes and the minimum possible fractional decrease in energy?

The distance between nodes of the $\sin \frac{n\pi x}{L}$ function is L/n. For $n = 4.89 \times 10^8$, this is

$$\frac{0.3\ m}{4.89 \times 10^8} \simeq 0.6\ nm\,. \tag{212}$$

This a very fine spacing indeed and would be very hard to detect.

The fractional spacing between energy levels is

$$\frac{E_{n-1} - E_n}{E_n} = \frac{\frac{(n-1)^2\pi^2\hbar^2}{2mL^2} - \frac{n^2\pi^2\hbar^2}{2mL^2}}{\frac{n^2\pi^2\hbar^2}{2mL^2}} = \frac{(n-1)^2 - n^2}{n^2} = -\frac{2}{n} + \frac{1}{n^2}$$

$$\simeq \quad -\frac{2}{4.89 \times 10^8} \simeq -4 \times 10^{-9} \,. \tag{213}$$

Thus, the energy levels are very densely spaced and it would be very difficult to detect a transition from one to the next at high n.

Interpreting The Wavefunctions

Notice that for $n \geq 2$ there are places where $|\psi_n(x)|^2 = 0$. This means we can never find the particle at such a location.

You could ask, *how can a particle get from one side of a box to the other without passing such a zero-probability point?*

The answer is that you cannot picture a particle moving in the classical way that this question envisages. The wave picture is in contradiction to such a particle picture.

Of course, for very large n, there are many zeroes but also many maxima. These are so closely spaced that you cannot resolve the minima and maxima, and you can only in practice see an average value of the probability. Thus, what you will see will look like the particle can be at any location it likes and can travel back and forth between the walls, but that is not really what is correct at the underlying level.

Expectation Values and Wave Functions

We have also seen that the wave functions and associated probabilities can be used to compute expectation values, such as that we considered when computing $(\Delta x)^2 \equiv \langle (x - \langle x \rangle)^2 \rangle$. In general, any such average is an average of some dynamical property that can be measured, such as position, momentum, energy, ... We always define

$$\langle Q \rangle = \int_{\text{all } x} \Psi^*(x,t) \widehat{Q} \Psi(x,t) dx. \tag{214}$$

The symbol $\widehat{Q}$ stands for the operator associated with the observable Q; for each observable there is a unique operator. For position it is simply x. But, in many cases $\widehat{Q}$ is a differential operator. Thus, its location above is absolutely critical.

We have already seen two examples of derivative operators when we constructed the Schroedinger Equations:

$$\widehat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}, \quad \widehat{E} = i\hbar \frac{\partial}{\partial t}. \tag{215}$$

We will not go through it here, but it can be shown that (dropping the time dependent part of the wave function)

$$\int dx \psi^*(x) \frac{\hbar}{i} \frac{\partial}{\partial x} \psi(x) = \int dk \widetilde{\psi}(k) \hbar k \widetilde{\psi}(k) \,. \tag{216}$$

This means that $\widehat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$ is the appropriate x-space representation for the momentum operator $\hbar k$, where the latter is the obvious choice in the k-space integral form on the rhs above. Another way of deciding that the lhs above is a correct way of computing $\langle p \rangle$ is to write

$$\langle p \rangle = m \frac{d\langle x \rangle}{dt} = m \frac{d}{dt} \int \Psi^*(x,t) x \Psi(x,t) dx \tag{217}$$

then use the SE to evaluate $\frac{d\Psi}{dt}$ and $\frac{d\Psi^*}{dt}$ in terms of $\frac{\partial^2 \Psi}{\partial x^2}$ and $\frac{\partial^2 \Psi^*}{\partial x^2}$, and then do some partial integrations.

Let us use $\widehat{p}$ to compute $\langle p \rangle$ and $\langle \frac{p^2}{2m} \rangle$ for the $n = 1$ ground state of the infinite well.

$$\langle p \rangle \quad = \quad \int \psi^*(x) \frac{\hbar}{i} \frac{\partial}{\partial x} \psi(x) dx$$

$$
\begin{aligned}
&= \int_0^L \left(\sqrt{\frac{2}{L}}\sin\frac{\pi x}{L}\right)\frac{\hbar}{i}\frac{\partial}{\partial x}\left(\sqrt{\frac{2}{L}}\sin\frac{\pi x}{L}\right)dx \\
&= \int_0^L \left(\sqrt{\frac{2}{L}}\sin\frac{\pi x}{L}\right)\frac{\hbar}{i}\frac{\pi}{L}\left(\sqrt{\frac{2}{L}}\cos\frac{\pi x}{L}\right)dx \\
&= \frac{\hbar}{i}\frac{2\pi}{L^2}\int_0^L \sin\frac{\pi x}{L}\cos\frac{\pi x}{L}dx = 0 \qquad (218)
\end{aligned}
$$

which is the answer we expected since the particle is not going anywhere. Classically, it is just bouncing back and forth. Quantum mechanically, the particle is a stationary wave form in a fixed box.

Now let us compute

$$
\begin{aligned}
\langle p^2\rangle &= \int \psi^*(x)(-\hbar^2)\frac{\partial^2}{\partial x^2}\psi(x) \\
&= \int_0^L \left(\sqrt{\frac{2}{L}}\sin\frac{\pi x}{L}\right)(-\hbar^2)\frac{-\pi^2}{L^2}\left(\sqrt{\frac{2}{L}}\sin\frac{\pi x}{L}\right)dx \\
&= \frac{\pi^2\hbar^2}{L^2}\int_0^L \left(\sqrt{\frac{2}{L}}\sin\frac{\pi x}{L}\right)^2
\end{aligned}
$$

$$= \frac{\pi^2\hbar^2}{L^2} \times 1\,, \tag{219}$$

where the 1 just comes from the fact that the remaining integral is just the total probability integral.

First, let us note that this result implies that

$$\langle E \rangle = \langle \frac{p^2}{2m} \rangle = \frac{\hbar^2\pi^2}{2mL^2} = E_1 \tag{220}$$

as we expect.

Next, we note that since $\langle p \rangle = 0$, we have

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \frac{\pi\hbar}{L}\,. \tag{221}$$

With some work, we could compute

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{L^2\left(\frac{1}{3} - \frac{1}{2\pi^2}\right) - \left(\frac{1}{2}L\right)^2} = 0.181L \tag{222}$$

Combining, we find

$$\Delta x \Delta p = 0.181 L \frac{\pi \hbar}{L} = 0.568 \hbar \,, \tag{223}$$

which is pretty close to the smallest (Gaussian wave function) result. Of course, as n increases, $\Delta x \Delta p$ increases, with

$$\lim_{n \to \infty} \Delta x = \frac{L}{\sqrt{12}} \,. \tag{224}$$

This latter limit is the same as the classical limit, in which we would compute $\langle x^2 \rangle$ using the uniform probability $P = \frac{1}{L}$

$$\begin{aligned} \langle x^2 \rangle &= \int_0^L \frac{1}{L} x^2 \, dx = \frac{1}{3} L^2 \,, \\ \langle x \rangle &= \int_0^L \frac{1}{L} x \, dx = \frac{L}{2} \\ &\Rightarrow \quad \Delta x = L \sqrt{\frac{1}{3} - \frac{1}{4}} = \frac{L}{\sqrt{12}} \,. \end{aligned} \tag{225}$$

Eigenvalues and eigenstates

This discussion of the operator $\widehat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$ allows us to introduce the concept of an eigenstate and an eigenvalue.

In general, we say that some wavefunction Ψ is an eigenstate of an operator $\widehat{Q}$ if

$$\widehat{Q}\Psi = q\Psi\,, \tag{226}$$

where q is just some constant number, called the eigenvalue. Using our infinite square well wave functions, we can illustrate using the operator $\widehat{p}$.

$$\widehat{p}\psi_n(x) = \frac{\hbar}{i}\frac{\partial}{\partial x}\sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L} = \frac{\hbar}{i}\frac{n\pi}{L}\sqrt{\frac{2}{L}}\cos\frac{n\pi x}{L}\,. \tag{227}$$

The change of the function form means these wave functions are not eigenstates of $\widehat{p}$. What about $\widehat{p^2} = \widehat{p}\widehat{p}$. Using the result above, we have

$$\begin{aligned}\widehat{p}\widehat{p}\psi_n(x) &= \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\left[\frac{\hbar}{i}\frac{n\pi}{L}\sqrt{\frac{2}{L}}\cos\frac{n\pi x}{L}\right] \\ &= (-\hbar^2)\left(\frac{n\pi}{L}\right)^2\sqrt{\frac{2}{l}}\sin\frac{n\pi x}{L}\end{aligned}$$

$$= \quad -\frac{\hbar^2 n^2 \pi^2}{L^2}\psi_n(x) \tag{228}$$

which is a constant times the original wavefunction. Thus, ψ_n is an eigenstate of $\widehat{p^2}$ with eigenvalue $-\frac{\hbar^2 n^2 \pi^2}{L^2}$.

Note the general result that if Ψ is an eigenstate of $\widehat{Q}$, then $\langle \widehat{Q}^2 \rangle = q^2 = \langle \widehat{Q} \rangle^2$ implying that

$$(\Delta Q)^2 = \langle \widehat{Q}^2 \rangle - \langle \widehat{Q} \rangle^2 = 0\,. \tag{229}$$

Similar manipulations apply for the energy operator. For stationary states, energy is always an eigenvalue. Our time dependence is $\Psi(x,t) = \psi(x)\phi(t) = \psi(x)e^{-i\omega t}$ for which

$$\widehat{E}\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \hbar\omega\Psi(x,t)\,, \tag{230}$$

in agreement with the standard energy-frequency relationship. In contrast, $\widehat{p}^{\,2}$ does not always give a definite eigenvalue when operating on a stationary state. It just happens to for this infinite well case, where $U = 0$ is a constant inside the well.

The Heisenberg Uncertainty and Operators

If a wave function, Ψ is such that both the momentum and the position are well defined, in operator language this means that Ψ should be an eigenstate of both the momentum and the position operators:

$$\widehat{p}\Psi = \frac{\hbar}{i}\frac{\partial \Psi}{\partial x} = p\Psi\,, \quad \widehat{x}\Psi = x\Psi\,. \tag{231}$$

In this case, it should not matter in which order we operate the momentum and position operators on the wave function. That is, we would for consistency have

$$\widehat{p}\widehat{x}\Psi = \widehat{x}\widehat{p}\Psi\,, \quad \Rightarrow \frac{\hbar}{i}\frac{\partial}{\partial x}[x\Psi] = x\left[\frac{\hbar}{i}\frac{\partial}{\partial x}\Psi\right]\,,. \tag{232}$$

But, by explicit calculation this is not true. Instead, we find

$$\frac{\hbar}{i}\frac{\partial}{\partial x}[x\Psi] = \frac{\hbar}{i}\Psi + x\left[\frac{\hbar}{i}\frac{\partial}{\partial x}\Psi\right] \tag{233}$$

which we write in terms of what is called a **commutator** ($[\widehat{a}, \widehat{b}] = \widehat{a}\widehat{b} - \widehat{b}\widehat{a}$) that applies whenever the particular combination of operators on a wave function.

$$[\widehat{p}, \widehat{x}] = \left[\frac{\hbar}{i}\frac{\partial}{\partial x}, x\right] = \frac{\hbar}{i}\,. \tag{234}$$

This non-zero commutator implies that momentum and position cannot be simultaneously perfectly well-known. In other words, it encodes the Heisenberg Uncertainty Principle for position and momentum.

A similar computation gives

$$[\widehat{E}, \widehat{t}] = \left[i\hbar\frac{\partial}{\partial t}, t\right] = i\hbar \tag{235}$$

implying that energy and time cannot be both precisely known, since a wave function $\Psi(x,t)$ cannot simultaneously have precise $\widehat{E}$ and $\widehat{t}$ eigenvalues.

The Finite Square Well

How does all this change if we make the well finite?

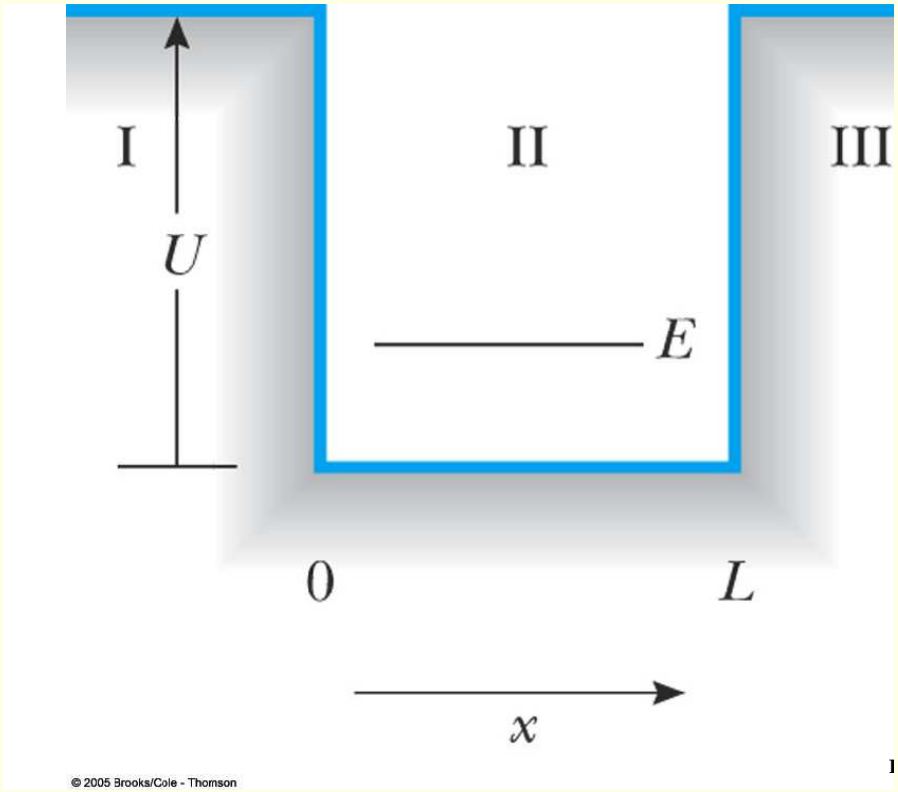


Figure 24: The finite square-well potential.

We write

$$\psi(x) = \begin{cases} Ae^{+\alpha x}\,, & x < 0 \\ C\sin kx + D\cos kx\,, & 0 < x < L \\ Be^{-\alpha x}\,, & x > L \end{cases} \quad . \tag{236}$$

1. In the region $x < 0$, the time-independent SE takes the form

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}(U - E)\psi \tag{237}$$

which, for $E < U$, is solved by

$$\psi(x) = e^{\alpha x}\,, \quad \text{with} \quad \alpha = [2m(U - E)/\hbar^2]^{1/2}\,. \tag{238}$$

The form $e^{-\alpha x}$ is also a solution of the equation, but becomes infinite if $x \to -\infty$. This choice would not allow us to normalize the wave function — the net probability integral would diverge. Thus, we must choose only the $e^{+\alpha x}$ form for $x < 0$.

2. In the region $x > L$, we have exactly the same SE, but now we must only have the $e^{-\alpha x}$ solution which decays exponentially for $x \to +\infty$.

3. In the $0 < x < L$ region, we have the same SE as for the infinite well with the same possible $\sin kx$ and $\cos kx$ solutions with $\hbar^2 k^2/(2m) = E$. Note that E must be the same for all these different regions.

So, we now impose our continuity and smoothness requirements.

1. Continuity of ψ at $x = 0 \Rightarrow A = D$.
2. Continuity of $\frac{d\psi}{dx}$ at $x = 0 \Rightarrow \alpha A = kC$.
3. If we divide the 2nd result above by the first, A is eliminated and we find
$$\frac{C}{D} = \frac{\alpha}{k}. \tag{239}$$
4. Continuity of ψ at $x = L \Rightarrow C \sin kL + D \cos kL = Be^{-\alpha L}$.
5. Continuity of the derivative at $x = L \Rightarrow kC \cos kL - kD \sin kL = -\alpha B e^{-\alpha L}$.
6. Dividing the equation just above by the preceding equation eliminates B and we may also replace C/D by α/k to obtain
$$\frac{(\alpha/k)\cos kL - \sin kL}{(\alpha/k)\sin kL + \cos kL} = -\frac{\alpha}{k}, \tag{240}$$
which we rewrite as
$$\tan kL \left(1 - \frac{\alpha^2}{k^2}\right) = \frac{2\alpha}{k}. \tag{241}$$

For specified U and L, this equation can only be solved for very special values of E (which is contained in both α and k).

Given a value of E that solves eq. (241), let us examine the behavior of ψ. The crucial point is that ψ "leaks" into the $x < 0$ and $x > L$ regions where classically the particle cannot go. The distance, δ, from one of the side boundaries of the well at which ψ declines to $1/e$ of its value at the boundary is called the penetration depth. That is, δ is defined by

$$e^{-\alpha\delta} = e^{-1}\,, \tag{242}$$

implying

$$\delta = \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m(U-E)}}\,. \tag{243}$$

Note that δ gets increases as E increases in magnitude towards U.

Example

An electron is in a potential well with $L = 0.200\ nm$ and $U = 100\ eV$. Find the possible values of E for which the electron is bound to the well. We are looking for values of $E < U$ that solve eq. (241). The left and right hand sides of eq. (241) are plotted below.

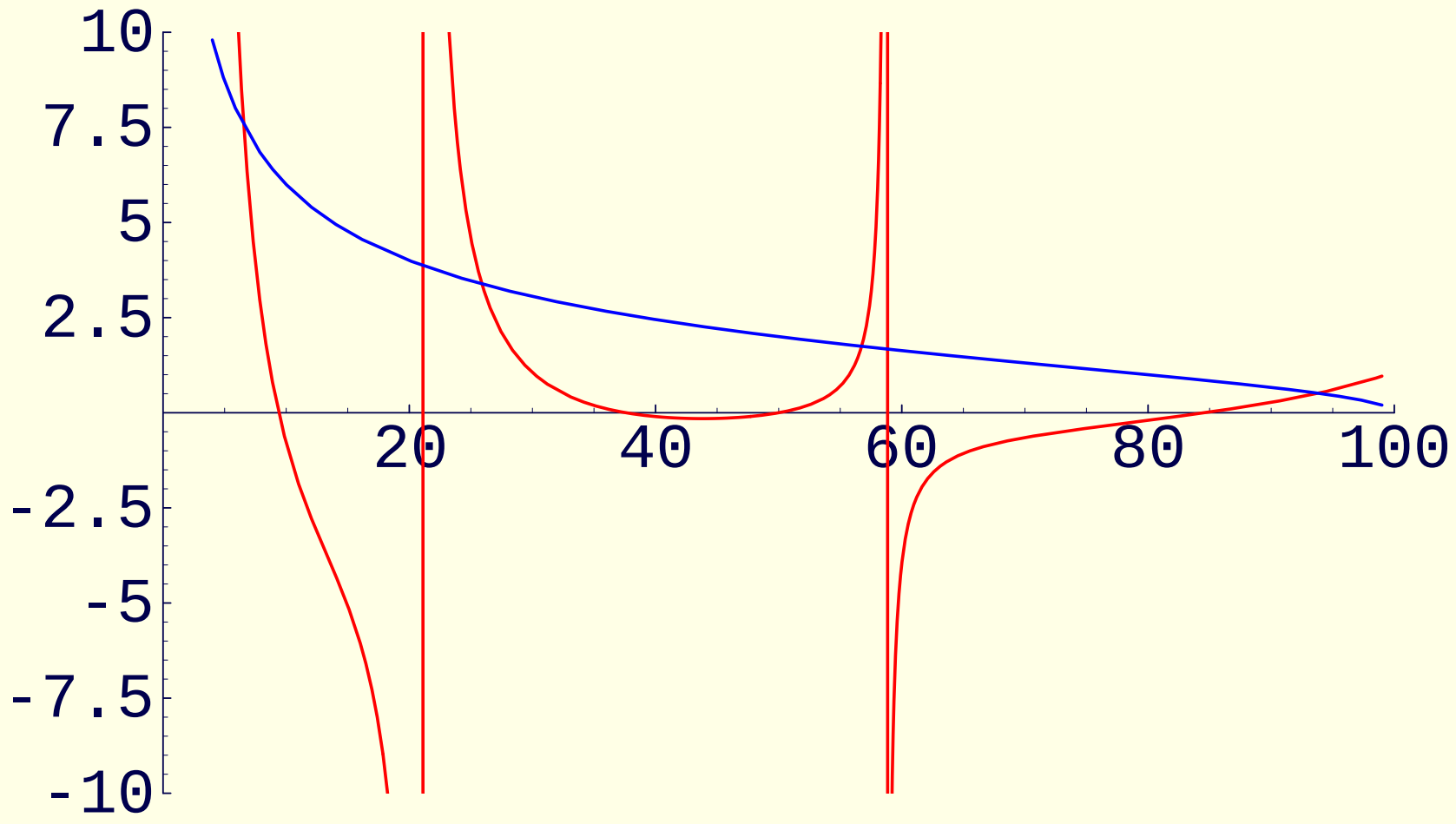


Figure 25: Plot of left (red) and right (blue) sides of eq. (241). The horizontal axis is E in eV.

Solutions correspond to points of intersection between the blue curve and the (non-vertical) branches of the red curve. The corresponding

values of the energy are $E = 6.555, 25.900, 56.735, 93.833\ eV$. (We note that the iterative technique outlined in the book does not converge to the precise lowest energy value given above.)

Thus, there are only 4 possible bound state energy levels. For the largest E value, we have

$$\begin{aligned} \delta &= \frac{\hbar}{\sqrt{2m(U-E)}} = \frac{(197.3\ eV \cdot nm/c)}{\sqrt{2(511 \times 10^3\ eV/c^2)(100\ eV - 93.833\ eV)}} \\ &= 0.07859\ nm\,, \end{aligned} \tag{244}$$

a rather substantial fraction of the basic well width of $0.2\ nm$.

Once we have an allowed E value, we would get the shape of the wave function by setting $A = 1$ (temporarily — eventually we would determine the magnitude of A that would give us $\int_{-\infty}^{\infty} |\psi(x)|^2 = 1$). Condition 1 then gives $D = A = 1$. Condition 2 then gives $C = (\alpha/k)D = \alpha/k$ (both of which are known once E is determined). Condition 4 then gives $B = e^{\alpha L}\left[(\alpha/k)\sin kL + \cos kL\right]$. (Recall that k, L, and α are all known.) The wave function shape is now determined. We would then integrate the square of this shape to determine the appropriate value of A^2.

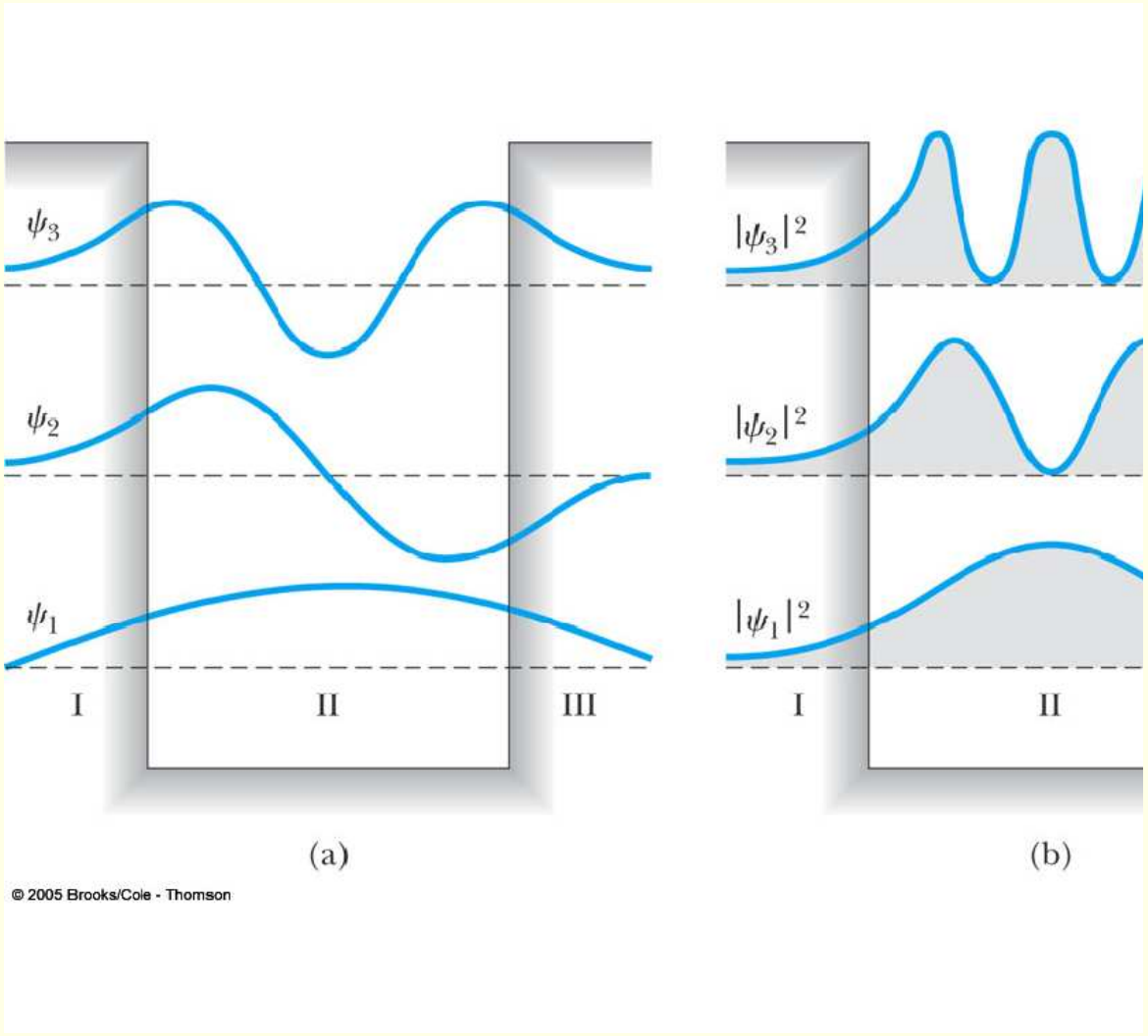


Figure 26: The finite square-well potential wavefunctions. Note the continuity of the wave function and its leakage into classically forbidden regions.

We should now ask what happens if $E > U$. Classically, this is a situation in which the particle can escape the potential well. In the QM approach,

this should be, and is, apparent. For example, for $x < 0$, if we solve

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}(U - E)\psi\,, \tag{245}$$

with $E > U$, the solutions are now of the form e^{ilx} or e^{-ilx} (it will prove more convenient to use these exponential forms than the equivalent $A\sin lx$ and $B\cos lx$ forms), with $l^2 = \frac{2m}{\hbar^2}(E-U)$. Similar results apply to $x > L$. In both regions we have oscillatory behavior and there is no damping for $|x| \to \infty$. We will have more to say about related situations in the next chapter.

The Harmonic Oscillator

This is a very important example. The restoring force for a harmonic oscillator is $F = -kx$, corresponding to $U = \frac{1}{2}kx^2$.

Not only is this one of the few cases for which an exact solution can be obtained, but this particular case has repeated applications in all kinds of contexts. In particular, anytime a potential $U(x)$ has a local minimum, for small excursions relative to this minimum at point $x = a$, one can

approximate the shape of $U(x)$ using the harmonic form:

$$U(x) = U(a) + \frac{1}{2}k(x-a)^2\,, \quad \text{where} \quad k = \left.\frac{d^2U}{dx^2}\right|_{x=a} \tag{246}$$

We can then agree to redefine our energy scale so that we reference to $U(a)$ and redefine our coordinate axis so that the minimum is located at $x = 0$.

Classically, for $U(x) = \frac{1}{2}kx^2$, the particle would oscillate about $x = 0$ with an angular frequency $\omega = \sqrt{k/m}$ and with maximum amplitude, or excursion in x from $x = 0$, set by the initial conditions. Let the maximum excursion correspond to $x = \pm A$. The total energy would be conserved and would be $E = \frac{1}{2}kA^2$. We could take A to be as small as we like, implying that there should be no minimum for E.

So, let us see what happens in QM. The time-independent SE takes the form

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}(\frac{1}{2}m\omega^2x^2 - E)\psi(x)\,. \tag{247}$$

The general solutions of this equation can be obtained in closed form, but the techniques go beyond what we wish to cover in this course. We

focus on obtaining the solution that corresponds to the lowest possible energy, $i.e.$ the ground state.

1. **We have seen that a typical ground state has no "nodes" where ψ vanishes.**
2. **Also, the gs wavefunction typically is symmetric for a symmetric potential, and so $\psi = f(x^2)$.**
3. **Of course, for a confined solution, ψ should vanish as $|x| \to \infty$.**

Let us try

$$\psi(x) = C_0 e^{-\alpha x^2} . \tag{248}$$

For this form

$$\frac{d^2\psi}{dx^2} = \frac{d}{dx}\left[C_0(-2\alpha x)e^{-\alpha x^2}\right] = C_0[-2\alpha + 4\alpha^2 x^2]e^{-\alpha x^2} \tag{249}$$

which has the same structure as the other side of the SE equation,

$$\frac{2m}{\hbar^2}\left(\frac{1}{2}m\omega^2 x^2 - E\right) C_0 e^{-\alpha x^2} , \tag{250}$$

provided

$$4\alpha^2 = \frac{2m}{\hbar^2}(\frac{1}{2}m\omega^2)\,, \quad \textbf{or} \quad \alpha = \frac{m\omega}{2\hbar}$$
$$\frac{2mE}{\hbar^2} = 2\alpha = \frac{m\omega}{\hbar}\,, \quad \textbf{or} \quad E = \frac{1}{2}\hbar\omega\,. \tag{251}$$

In short, we have

$$E_0 = \frac{1}{2}\hbar\omega\,, \quad \psi_0(x) = C_0 e^{-\frac{m\omega x^2}{2\hbar}}\,, \tag{252}$$

where C_0 is to be determined by normalizating the integrated probability to 1. ψ_0 and its square are depicted below.

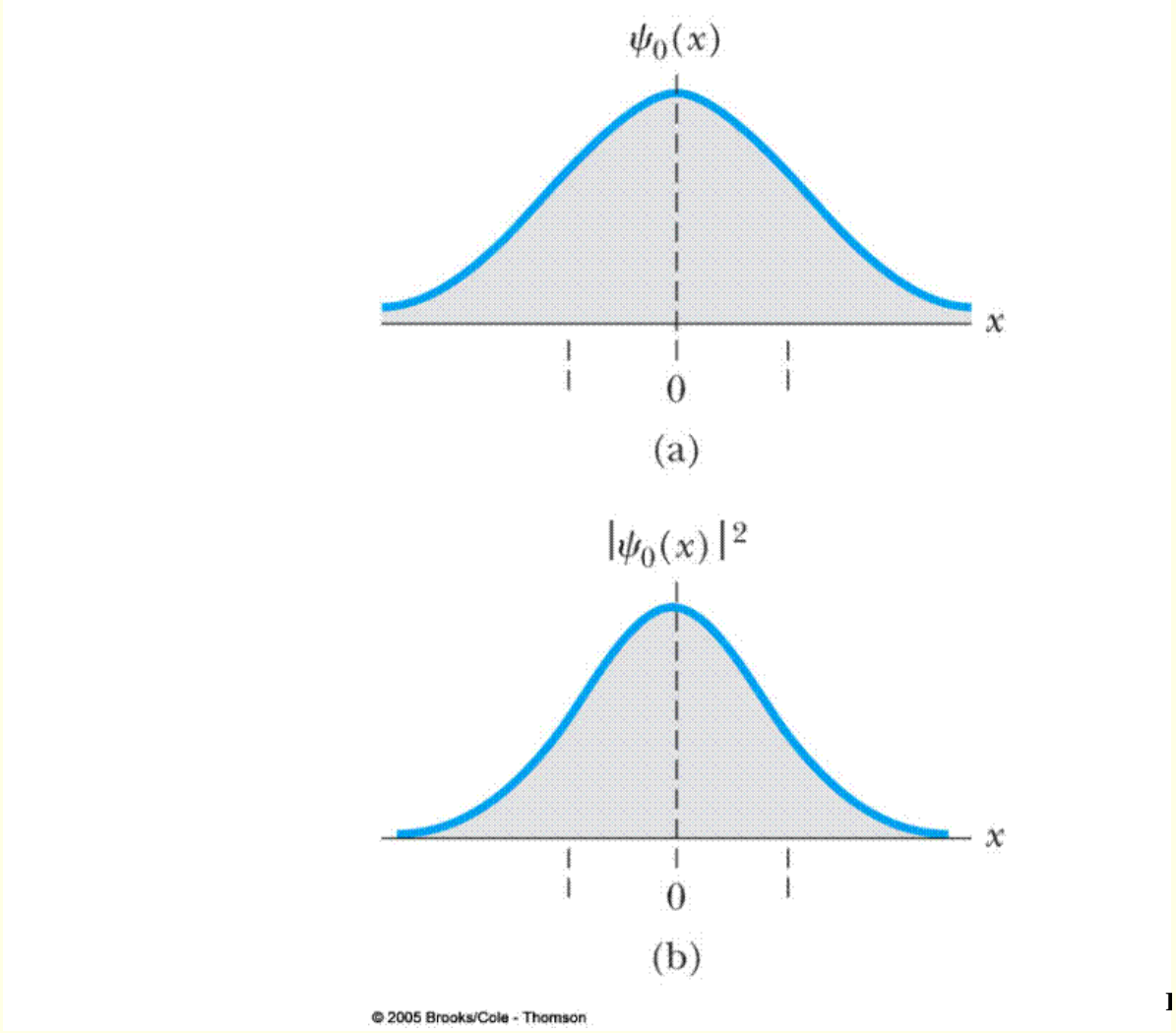


Figure 27: Ground state wavefunction and probability density.

The most important point about the ground state is that $E_0 \neq 0$. That is, there is a minimum energy for the QM oscillator state. This energy is sometimes called the zero-point energy. It has important implications. It means for example that a crystal lattice of ions, each of which can be

thought of as being trapped relative to its presumed fixed location by a harmonic oscillator type potential, is actually "humming" with the energy of this huge number of harmonic oscillators in their ground states.

Should we have expected such a minimum energy? The answer is that the HUP requires it. Suppose we say that the electron is confined to $|x| \leq A$. Then, the HUP requires minimum $p_x \sim \hbar/A$. This will imply an excursion in x such

$$K \sim \frac{p_x^2}{2m} \sim \frac{\hbar^2}{2mA^2} \sim \frac{1}{2}m\omega^2 x_{max}^2\,, \quad \Rightarrow |x_{\rm max}|^2 \sim \frac{\hbar^2}{m^2\omega^2 A^2}\,. \tag{253}$$

Requiring, $|x_{max}|^2 \lesssim A^2$ (for consistency with our input assumption) leads to

$$|x_{max}|^2 \sim \frac{\hbar^2}{m^2\omega^2 A^2} \lesssim A^2\,, \quad \Rightarrow \quad A^2 \gtrsim \frac{\hbar}{m\omega}\,, \tag{254}$$

which corresponds to $\alpha \sim m\omega/\hbar$ (as found) and minimum energy

$$E_0 \gtrsim \frac{1}{2}m\omega^2\left[\frac{\hbar}{m\omega}\right] = \frac{1}{2}\hbar\omega\,. \tag{255}$$

We can continue this guessing game to the first excited level fairly easily. $\psi_1(x)$ should have just one node, and be antisymmetric, suggesting $\psi_1(x) \propto x \exp(-\alpha x^2)$. Substituting into the SE we find this form works if α is the same as before ($\alpha = m\omega/(2\hbar)$) and $E = \frac{3}{2}\hbar\omega$.

The general result is

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega\,. \tag{256}$$

This is depicted in the following figure.

The important aspect of this prediction is the equal spacing of the energy levels. For this system, if the state is in a $n \neq 0$ state, when it decays to its next lowest state, the frequency of the radiation will always be given by $hf = \hbar\omega$, no matter what the starting n value.

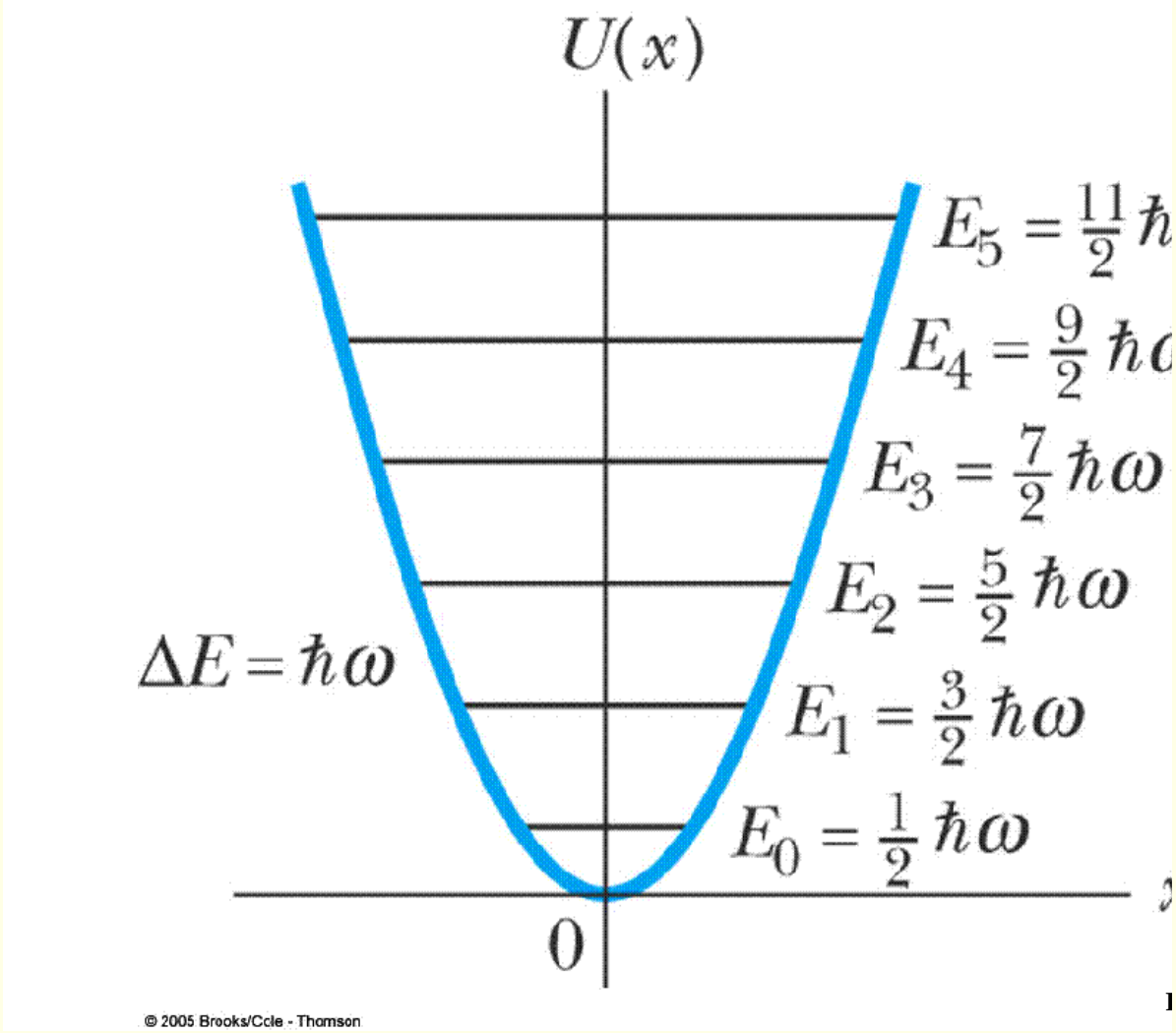


Figure 28: Harmonic oscillator quantum energy levels.

Plots of the probability densities associated with these energy levels are given in the next figure, where the dashed lines show the classical probabilities for the same energy values. Note how the average classical and quantum distributions get closer as n gets large.

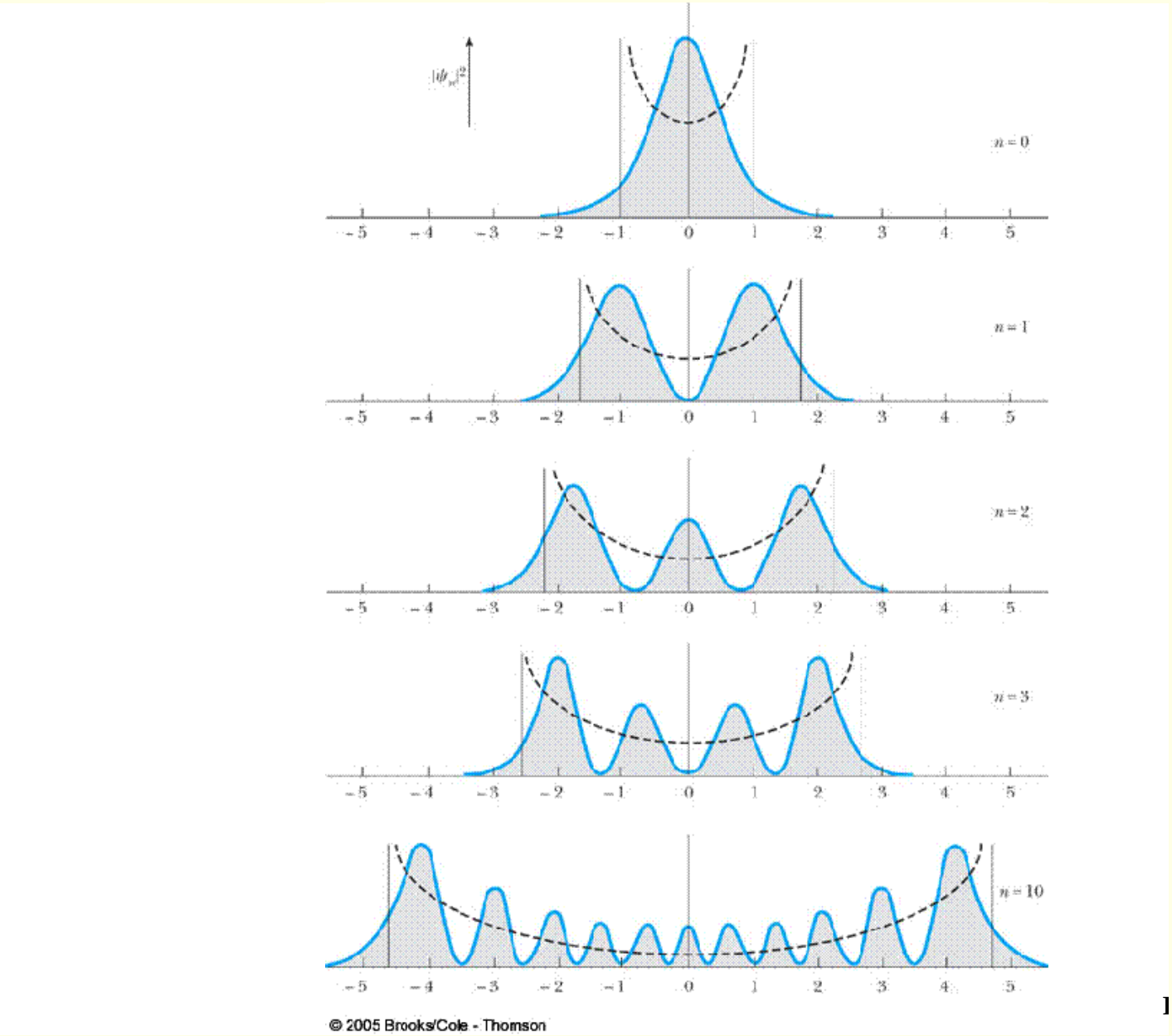


Figure 29: Harmonic oscillator probability densities, compared to classical probabilities (dashed lines).

Tunneling Phenomena

The square barrier

The classic example of a tunneling situation is the square barrier, depicted in Fig. 30.

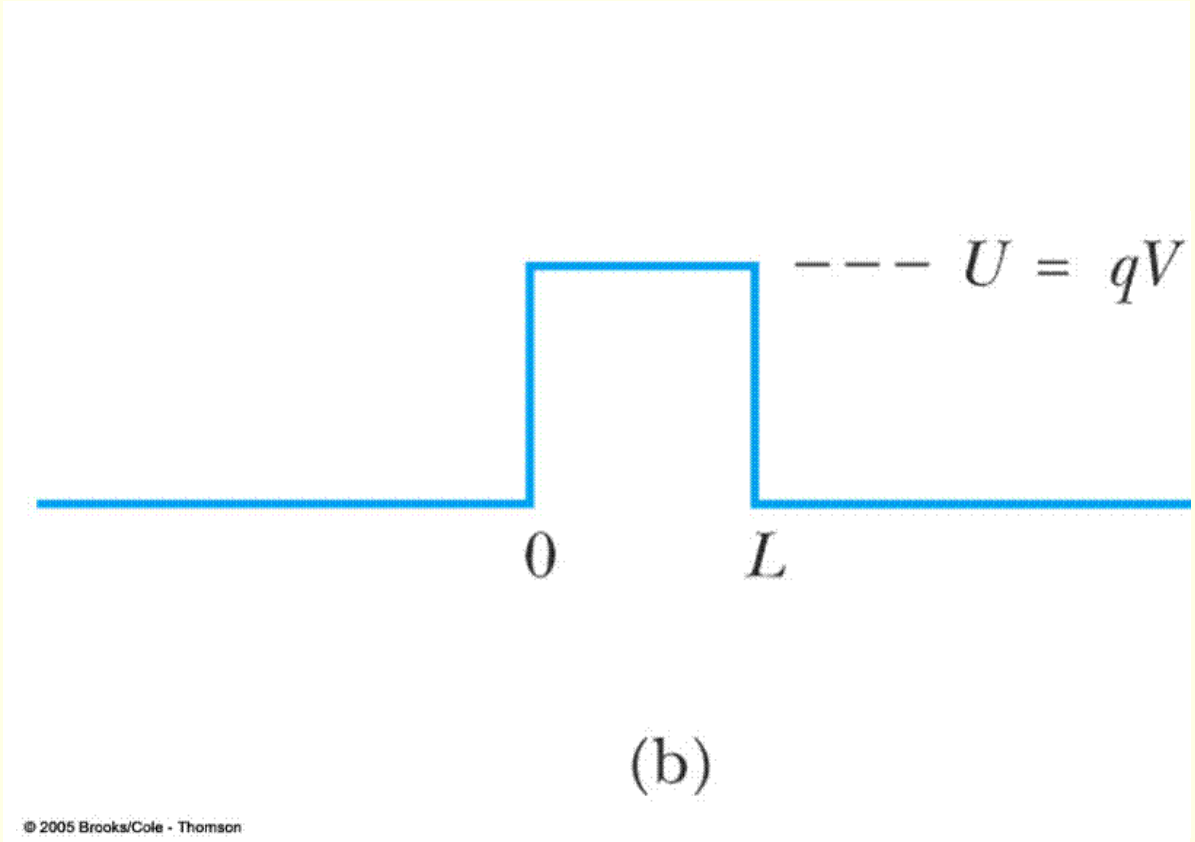


Figure 30: The square barrier.

Imagine a particle incident on the barrier from the left. Classically, if $E > U$, then the particle will temporarily have reduced velocity as it passes the barrier (there is a force to slow it down at the left-hand edge of the barrier), but it will regain its initial velocity once it has passed the barrier (there is a force to speed it up at the far right-hand edge of the barrier).

If $E < U$, the particle cannot penetrate the barrier classically and the particle will simply bounce off the barrier and reverse direction.

In QM, all regions are accessible to the particle **even if** $E < U$. The QM penetration of the barrier is called **tunneling**.

To explore this quantitatively, we must set up the situation and impose appropriate boundary condition requirements at the edges of the barrier. We will imagine:

1. A wave is coming in from the left.
2. It hits the barrier.
3. Some of the wave is reflected, but some penetrates into the barrier.
4. The penetrating wave can make it over to the right-hand side of the barrier with some reduced amplitude.
5. There is thus some wave moving to the right in the region past the

barrier.

This is all depected in the figure below.

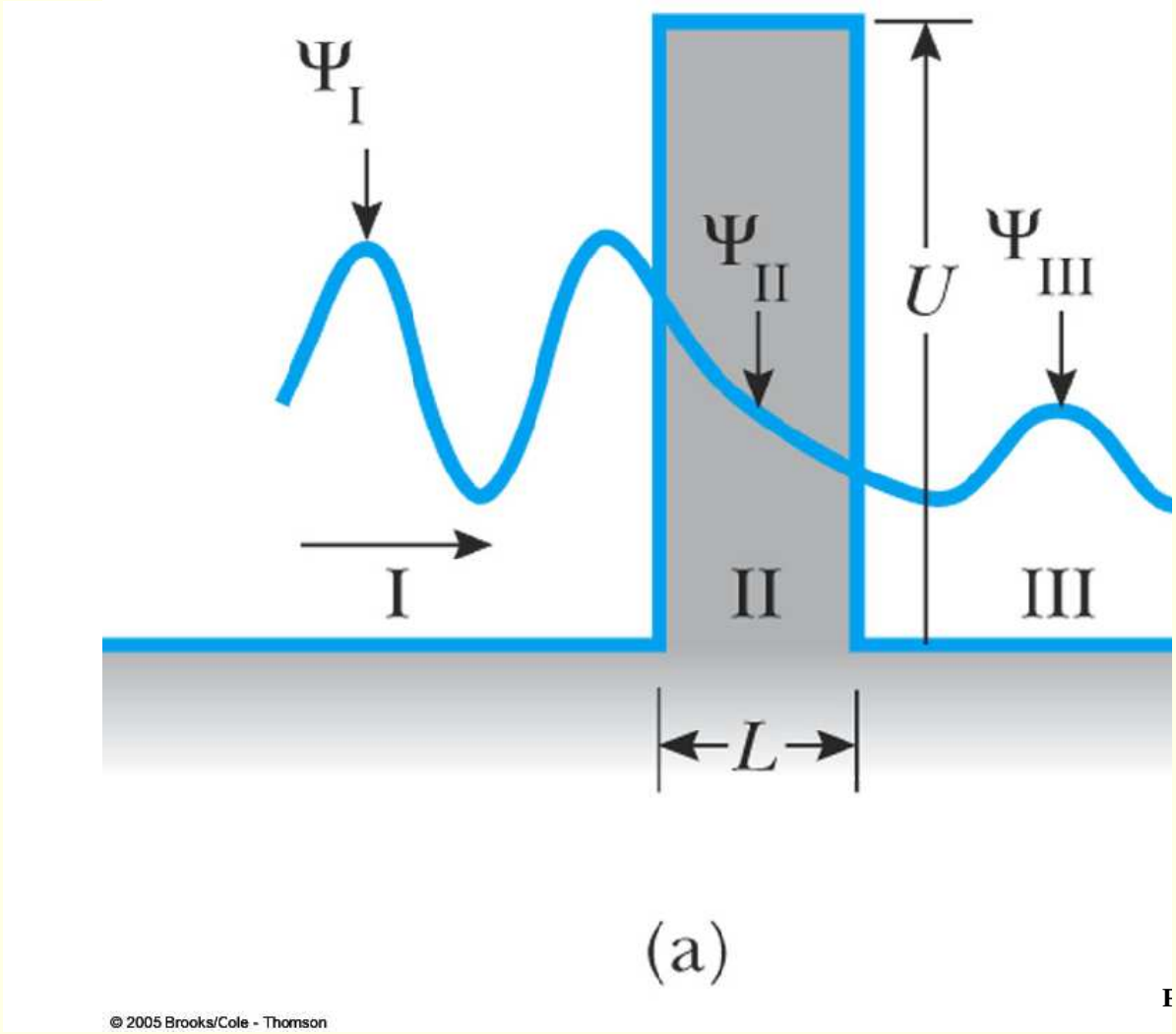


Figure 31: Transmission and reflection for the square barrier.

The above set-up is realized using the plane wave solutions of the SE as

follows. See the figure below.

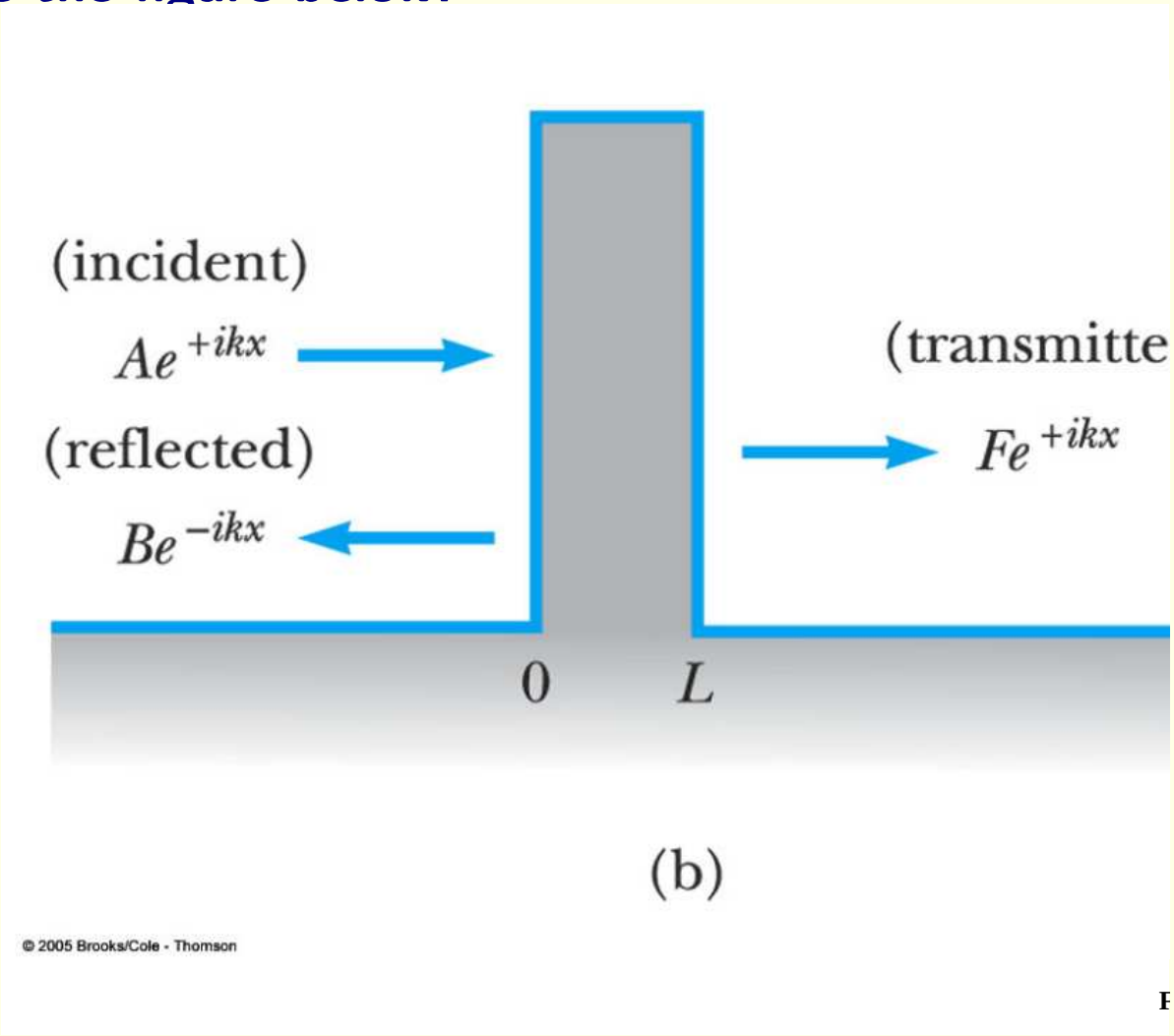


Figure 32: Transmission and reflection: plane wave set up

First, we must recall that a plane wave with perfectly defined momentum moving to the right is proportional to $e^{i(kx-\omega t)}$, where $\hbar k$ is the momentum and $E = \hbar\omega = \hbar^2 k^2/(2m)$ is the energy.

Similarly, a plane wave moving to the left is proportional to $e^{i(-kx-\omega t)}$.

Thus, on the left side of the barrier, where we have both incident and reflected waves, we write

$$\Psi(x,t) = Ae^{i(kx-\omega t)} + Be^{i(-kx-\omega t)}\,, \quad x<0\,. \tag{257}$$

If reflection were complete, then $|B| = |A|$. In general, reflection is not complete and we define the reflection coefficient by

$$R = \frac{(\Psi^*\Psi)_{reflected}}{(\Psi^*\Psi)_{incident}} = \frac{B^*B}{A^*A} = \frac{|B|^2}{|A|^2}\,. \tag{258}$$

To the right side of the barrier, the physical setup envisioned means that we should allow only the wave moving to the right:

$$\Psi(x,t) = Fe^{i(kx-\omega t)}\,, \quad x>L\,. \tag{259}$$

The corresponding transmission coefficient is then given by

$$T = \frac{(\Psi^*\Psi)_{transmitted}}{(\Psi^*\Psi)_{incident}} = \frac{F^*F}{A^*A} = \frac{|F|^2}{|A|^2}\,. \tag{260}$$

Since a given particle is either transmitted or reflected, these probabilities should sum to unity:

$$R + T = 1 \tag{261}$$

is as sum rule that should emerge from the mathematics.

When the wave is in the barrier region itself, the SE takes a different form.

$$\frac{d^2\psi}{dx^2} = \frac{2m(U-E)}{\hbar^2}\psi(x) \equiv \alpha^2\psi(x)\,, \tag{262}$$

where we are considering the situation with $U > E$ so that the α^2 on the rhs above is positive (as opposed to the negative $\frac{-2mE}{\hbar^2}$ that applies outside the barrier region). The solutions of this equation are exponential decay or increase. We should allow for both by writing

$$\Psi(x,t) = \psi(x)e^{-i\omega t} = Ce^{-\alpha x - i\omega t} + De^{+\alpha x - i\omega t} \quad 0 \le x \le L\,. \tag{263}$$

Setting up the mathematics: boundary conditions

We employ continuity of Ψ and of $\frac{\partial\Psi}{\partial x}$ at the right and left sides of the

barrier to obtain:

$$\begin{aligned}
A + B &= C + D\,, && \text{(continuity of } \Psi \text{ at } x = 0) \\
ikA - ikB &= \alpha D - \alpha C\,, && \text{(continuity of } \tfrac{\partial \Psi}{\partial x} \text{ at } x = 0) \\
Ce^{-\alpha L} + De^{+\alpha L} &= Fe^{ikL}\,, && \text{(continuity of } \Psi \text{ at } x = L) \\
(\alpha L)e^{+\alpha L} - (\alpha C)e^{-\alpha L} &= ikFe^{ikL}\,, && \text{(continuity of } \tfrac{\partial \Psi}{\partial x} \text{ at } x = L)
\end{aligned} \tag{264}$$

These equations can be solved. It takes a number of pages. Perhaps I will include the algebra in these notes at a later time. What one finds is that

$$T(E) = \frac{1}{1 + \frac{1}{4}\left[\frac{U^2}{E(U-E)}\right]\sinh^2 \alpha L}\,, \quad E < U\,. \tag{265}$$

And, we can check that the sum rule $R + T = 1$ is true. In the above, $\sinh x = (e^x - e^{-x})/2$. Note that for this case of $E < U$ we find $T(E) < 1$ always. If $E > U$, the wave behavior in the barrier region is oscillatory, and there will generally be a series of E values for which $T(E) = 1$. These are called transmission resonances.

Example

Two wires are separated by an insulating layer. Modeling the latter as a

square barrier of height $10\ eV$, estimate the transmission coefficient for penetration by $7\ eV$ electrons: (a) for $L = 5\ nm$ and (b) for $L = 1\ nm$.

We first must compute α.

$$\alpha = \frac{\sqrt{2m(U-E)}}{\hbar} = \frac{\sqrt{2(511 \times 10^3\ eV/c^2)(3.00\ eV)}}{1.973 \times 10^3\ eV \cdot \mathring{A}/c} = 0.8875\ \mathring{A}^{-1}. \tag{266}$$

The transimission coefficient is then

$$T = \frac{1}{1 + \frac{1}{4}\left[\frac{10^2}{7\times 3}\right] \sinh^2(0.8875\ \mathring{A}^{-1}\ L)}. \tag{267}$$

For $L = 50\ \mathring{A}$ ($i.e.\ 5\ nm$), we get $T = 0.963 \times 10^{-38}$, a very small number.

For $L = 10\ \mathring{A}$, we get $T = 0.657 \times 10^{-7}$. Changing the barrier thickness by just a factor of 5 has a huge effect.

Now suppose that we have the above situation and that a $1\ mA$ current of electrons is incident on the insulating barrier layer. How much of

this current passes through the layer to the adjacent wire if the electron energies are $7\ eV$ and the layer thickness is $1\ nm$.

Answer: Each of the e^-'s in the current has the probability given by $T = 0.657 \times 10^{-7}$ to pass through the insulating layer. The cumulative effect will be a transmitted current of

$$T \times 1\ mA = 0.657 \times 10^{-7} \times 1\ mA = 0.657 \times 10^{-7}\ mA = 6.57 \times 10^{-11}\ A\,. \tag{268}$$

Heisenberg Uncertainty Intuition

Another way to understand the tunneling phenomenon is to focus on the most important component of $T(E)$, namely the exponential suppression factor for large L from the $\sinh$ function:

$$T(E) \sim e^{-2\alpha L} \times \text{less important factors} \sim e^{-2L\sqrt{2m(U-E)}/\hbar} \sim e^{-2L/\delta}\,. \tag{269}$$

Here, δ has the same meaning as in the finite well bound state situation; it is the length scale describing penetration of the wave into a forbiddne

region. (The factor of 2 in the exponent is because T is the probability rather than the amplitude.)

If we regard δ as a kind of Δx over which we try to restrict the wave, the HUP says $\Delta p \sim \hbar/\delta$, leading to

$$\Delta K = \frac{\Delta p^2}{2m} = \frac{\hbar^2}{2m\delta^2} = \frac{\hbar^2}{2m\left(\frac{\hbar^2}{2m(U-E)}\right)} = U - E\,. \qquad (270)$$

This is just the right amount of kinetic energy to get the particle over the $U - E$ barrier; if $\delta = \Delta x$ were any bigger then $\Rightarrow$ not enough K to get over barrier.

Example: large αL limit

It is possible to solve the boundary condition equations fairly easily in the

case where $e^{+\alpha L}$ is a big number. I repeat those equations here.

$$\begin{aligned} A + B &= C + D\,, && \text{(continuity of } \Psi \text{ at } x = 0) \\ ikA - ikB &= \alpha D - \alpha C\,, && \text{(continuity of } \tfrac{\partial \Psi}{\partial x} \text{ at } x = 0) \\ Ce^{-\alpha L} + De^{+\alpha L} &= Fe^{ikL}\,, && \text{(continuity of } \Psi \text{ at } x = L) \\ (\alpha L)e^{+\alpha L} - (\alpha C)e^{-\alpha L} &= ikFe^{ikL}\,, && \text{(continuity of } \tfrac{\partial \Psi}{\partial x} \text{ at } x = L) \end{aligned} \tag{271}$$

If $e^{+\alpha L}$ is large, then D (but not $De^{\alpha L}$) must be small (from 3rd b.c. equation). The first two equations are then easily solved. Setting $A = 1$ (A normalization just sets overall flux), we find very easily (multiply 1st equation by ik and add to 2nd equation to eliminate B terms) that

$$C = \frac{2ik}{ik - \alpha} = \frac{2}{1 - \frac{\alpha}{ik}}\,. \tag{272}$$

If we define $C' \equiv Ce^{-\alpha L}$ and $D' \equiv De^{+\alpha L}$, then the 3rd of the b.c. equations (271) + $\frac{1}{ik}\times$ 4th b.c. equation yields

$$C' + D' \;=\; \frac{1}{ik}(-\alpha C' + \alpha D')\,, \quad \Rightarrow \quad D' = C'\frac{\frac{\alpha}{ik} + 1}{\frac{\alpha}{ik} - 1}$$

$$\Rightarrow$$

$$C' + D' = C' \frac{\frac{2\alpha}{ik}}{\frac{\alpha}{ik} - 1} = \left(\frac{2}{1 - \frac{\alpha}{ik}} e^{-\alpha L} \right) \left(\frac{\frac{2\alpha}{ik}}{\frac{\alpha}{ik} - 1} \right) \tag{273}$$

Armed with this result, we can easily compute (see 3rd b.c. equation)

$$|F|^2 = |C' + D'|^2 = \frac{\left(\frac{4\alpha}{k}\right)^2}{\left(1 + \frac{\alpha^2}{k^2}\right)^2} e^{-2\alpha L} = \left(\frac{4k\delta}{1 + (k\delta)^2} \right)^2 e^{-2L/\delta} . \tag{274}$$

Of course, the thing that is a bit tricky for you is all the use of absolute squares of complex numbers. I go through this example so that you can see that this complex stuff is essential for actual computations in QM.

In any case, you can now see that my earlier approximation of keeping only the exponential factor is only a rough approximation. However, for large L/δ, and $(k\delta)^2 = E/(U - E) \sim \mathcal{O}(1)$, dropping the multiplicative factor is a small perturbation on the very small exponential, thereby justifying the use of

$$T(E) \sim e^{-2L/\delta} = e^{-2L\sqrt{2m(U-E)}/\hbar} . \tag{275}$$

Scanning Tunneling Microscope

The idea is simple. We want to examine the surface structure of a metal.

Inside the metal is an e^- with some wave behavior inside metal.

There is a barrier that prevents e^- from escaping the metal. This is characterized by the $U - K = e\phi$ work function that we have discussed.

However, the real view is that the e^- wave function actually penetrates for a distance of order δ into the region outside the metal.

The e^- has $K = E$ inside the metal, so $\delta = \frac{\hbar}{\sqrt{2m(U-E)}}$.

The STM uses a probe to look at the exponential decay in this region outside the metal.

This is depicted in the following figure.

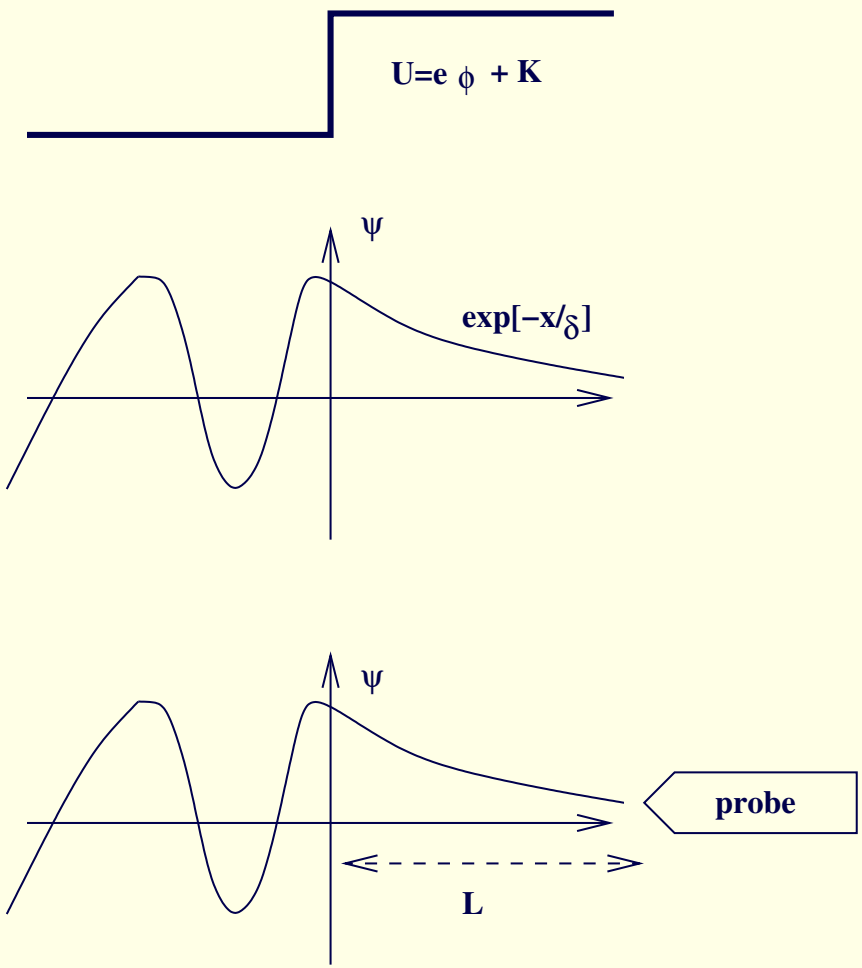


Figure 33: Scanning Tunneling Miscroscope setup. ϕ=work function. Ψ= wave function.

Typical numbers would be $U = 9\ eV$ and $E = 5\ eV$, $\Rightarrow U - E = 4\ eV$.

Then

$$\begin{aligned}\delta &= \frac{\hbar}{\sqrt{2m(U-E)}} = \frac{\hbar c}{\sqrt{2mc^2(U-E)}} \\ &= \frac{1.973\ keV\cdot\mathring{A}}{\sqrt{2(511\ keV)(4\times 10^{-3}\ keV)}} \simeq 1\mathring{A}\,. \end{aligned} \tag{276}$$

A "bias" voltage V would be introduced between the metal surface and the probe to ensure that the probe is probing the metal and not the reverse. The tunneling current would be given by

$$i = \frac{e^2V}{4\pi^2L\delta\hbar}e^{-2L/\delta}\,, \tag{277}$$

and if L changes by even a small amount ($i.e.$ if there is variation in the surface defined by the e^- wave functions), we will see a change in i.

In the above example, if $L \longrightarrow L + 0.01\mathring{A}$ then i changes by a fractional amount of $e^{-0.01\times 2/1\ \mathring{A}} \simeq 0.98$. Such a 2% change in i is measurable using appropriate amplification techniques. Thus, one can have sensitivity to surface details at the $0.01\mathring{A}$ level.

Varying $U(x)$

In most physical cases, U is not actually a constant, but rather has some non-trivial x dependence. We will do the example of α decay shortly.

The generalization of our approximate formula for $T(E)$ that applies in this case is

$$T(E) \sim \exp\left[-\frac{2\sqrt{2m}}{\hbar}\int_{barrier}\sqrt{U(x)-E}\,dx\right]. \qquad (278)$$

This reduces to our previous expression if the barrier region has length L and $U(x) = U$ is a constant in that region.

α decay simplified

Many nuclei heavier than lead naturally emit an α particle, but emission rates vary by factors of 10^{13}, whereas the energies of the α's range only from 4 to $8\ MeV$. Why?

The basic picture is below.

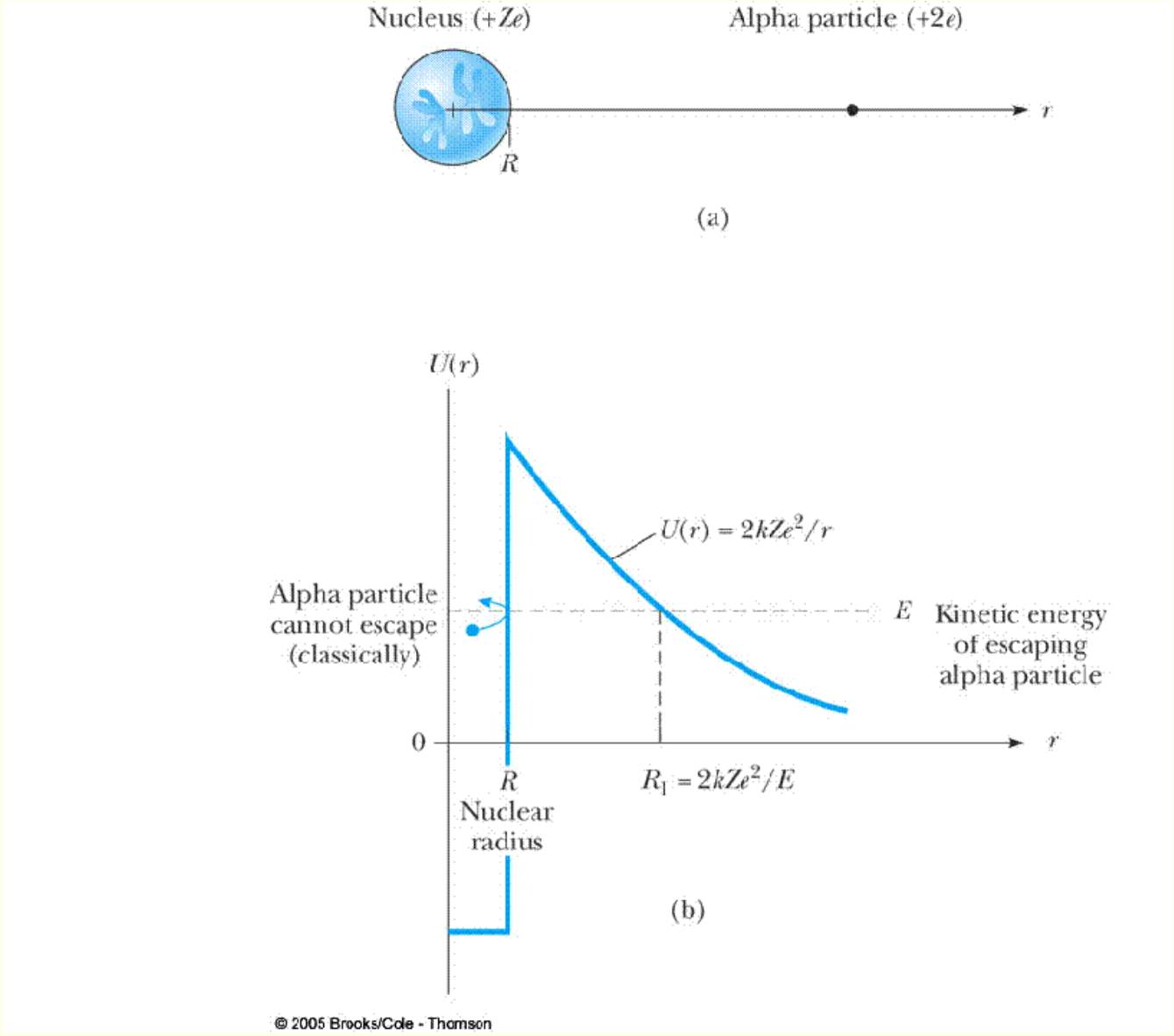


Figure 34: Picture of α decay.

Consider the α-particle emission of ^{238}U (nuclear charge of 92) which turns into an unstable isotope of Th by emitting a $4.2\ MeV$ α particle, *i.e.* $E_{escape} = 4.2\ MeV$.

We know that $R_{nucleus} \sim 7 \times 10^{-15}\ m$. This means that there is a barrier height at R coming from the Coulomb attraction that is of order (Z is the charge of the daughter nucleus in what follows))

$$\begin{aligned} V_{coulomb}(R) &= \frac{2kZe^2}{R} \\ &= \frac{2(90)(1.6 \times 10^{-19}\ C)^2(9 \times 10^9\ N \cdot m^2/C^2)}{7 \times 10^{-15}\ m} \\ &\quad \times \frac{10^{-6}\ MeV}{1.6 \times 10^{-19}\ J} \\ &= 37\ MeV\,. \end{aligned} \tag{279}$$

The α must tunnel through to radius

$$\begin{aligned} R_1 &= \frac{2kZe^2}{E} = \frac{2(9 \times 10^9\ N \cdot m^2/C^2)(90)(1.6 \times 10^{-9}\ C)^2}{4.2\ MeV} \\ &= \frac{37\ MeV \times R}{4.2\ MeV} = 6.2 \times 10^{-14}\ m = 62\ fm\,. \end{aligned} \tag{280}$$

Very crudely (see book for more precise formulae), assume

$$\begin{aligned} \textbf{average potential height} &= \frac{37\ MeV}{2} \sim 18\ MeV\,, \\ \textbf{average barrier width} &= \frac{R_1 - R}{2} = \frac{(62-7)\ fm}{2} \sim 28\ fm\,. \end{aligned} \tag{281}$$

Then,

$$\begin{aligned} T(E) &= \frac{1}{1 + \frac{1}{4}\left[\frac{U^2}{E(U-E)}\right] \sinh^2 \alpha L} \\ &\sim 16 \frac{4.2\ MeV}{18\ MeV}\left(1 - \frac{4.2\ MeV}{18\ MeV}\right) \exp\left[-2(2.8 \times 10^{-14}\ m)/\delta\right]\,, \end{aligned} \tag{282}$$

where

$$\delta = \frac{\hbar}{\sqrt{2m_\alpha(V-E)}} = \frac{6.58 \times 10^{-22}\ MeV \cdot s}{\sqrt{2(3727\ MeV/c^2)(18-4.2)\ MeV}}$$

$$= \quad 6 \times 10^{-16}\ m = 0.6\ fm\,. \tag{283}$$

This gives

$$e^{-2\cdot 28/0.6} = 2.9 \times 10^{-41}\,, \quad \Rightarrow \quad T = 1.6 \times 10^{-41}\,. \tag{284}$$

So, you might say how can it ever escape?

The point is that the above is the probability for tunneling in a single collision of the α particle with the barrier. We must ask how many collisions there are per second.

Inside the nucleus, the e^- kinetic energy is roughly

$$\begin{aligned} K &= \frac{1}{2}mv^2\,, \quad \Rightarrow \\ v &= \sqrt{\frac{2K}{m}} = \sqrt{\frac{2(4.2\ MeV)}{3727\ MeV/c^2}} = 0.047\ c = 1.4 \times 10^7\ m/s \end{aligned} \tag{285}$$

where we should note that the output v implies that the NR approximation is ok.

Now, the nuclear diameter is $2R \sim 1.4 \times 10^{-14}\ m$, so the α crosses the nucleus in a time of about

$$t_{crossing} \sim \frac{1.4 \times 10^{-14}\ m}{1.4 \times 10^{7}\ m/s} = 10^{-21}\ s\,. \tag{286}$$

Now the lifetime, τ of the nucleus in the presence of α decay is given by the point at which (# of times = number of collisions of the α particle with the barrier for which the probability of one penetration becomes equal to unity)

$$T(E) \times \#\text{ of times} = 1\,, \tag{287}$$

where

$$\#\text{ of times} = \frac{\tau}{t_{crossing}}\,. \tag{288}$$

Plugging this into the equation just above gives

$$\frac{T(E)\tau}{t_{crossing}} = 1\,, \quad \Rightarrow \quad \tau = \frac{10^{-21}\ s}{10^{-41}} \sim 10^{20}\ s\,. \tag{289}$$

The actual ^{238}U lifetime is $\tau = 4.5 \times 10^{9}\ yr \sim 10^{17}\ s$. Thus, our first estimate, while very crude, is in the right ballpark.

To get a more precise result (in better agreement with experiment), one must actually carry out the integral

$$T(E) \sim \exp\left[-\frac{2\sqrt{2m}}{\hbar}\int_{barrier}\sqrt{U(x)-E}\,dx\right]\,. \qquad (290)$$

using the potential drawn. This gives (to a good approximation)

$$T(E) = \exp\left[-4\pi Z\sqrt{\frac{E_0}{E}}+8\sqrt{\frac{ZR}{r_0}}\right]\,, \qquad (291)$$

where $r_0 = \frac{\hbar^2}{m_\alpha k e^2}$ is a kind of a $Z=1$ Bohr radius for the α particle: $r_0 \sim a_0/7295 \sim 7.25\ fm$ since $m_\alpha \sim 7295 m_e$, and the associated $Z=1$ kinetic energy is

$$E_0 = \frac{ke^2}{2r_0} = \frac{ke^2}{2a_0}\frac{a_0}{r_0} = 13.6\ eV \times 7295 = 0.0993\ MeV\,. \qquad (292)$$

The more precise formulation of the lifetime is to use

$$\tau_{\text{half life}} \equiv \tau_{1/2} = \frac{\ln 2}{f_{crossing} T(E)} \tag{293}$$

where $f_{crossing} = 1/t_{crossing} = 10^{21}\ Hz$.

Example

As an example of using the precise formula, consider Th which ejects an α particle with energy $E = 4.05\ MeV$. The nuclear radius is $R = 9.00\ fm$.

The daughter atomic number is $Z = 88$. We compute

$$\begin{aligned} T(E) &= \exp\left[-4\pi(88)\sqrt{\frac{0.0993}{4.05}} + 8\sqrt{88\frac{9.00}{7.25}}\right] \\ &= \exp[-89.542] = 1.3 \times 10^{-39}\,. \end{aligned} \tag{294}$$

Taking the collision frequency to be $f_{crossing} = 10^{21}$ (as is more or less

applicable for all these heavy nuclei) then we find

$$f_{crossing}T(E) = 1.3 \times 10^{-18}/s \tag{295}$$

and

$$\tau_{1/2} = \frac{0.693}{f_{crossing}T(E)} = \frac{0.693}{1.3 \times 10^{-18}} = 5.4 \times 10^{17}\ s = 1.7 \times 10^{10}\ yr\,. \tag{296}$$

which compares favorably with the actual value of $1.4 \times 10^{10}\ yr$.