Potential wells and barriers

Free particle

We start our discussions with a free particle of mass m for which $V = 0$. For a free particle the Hamiltonian is

$$\hat{H} = \frac{\hat{p}^2}{2m} \quad \text{- - - - - - - - (1)}$$

Note that $[\hat{H}, \hat{p}] = 0$, so that $\hat{H}$ and $\hat{p}$ have common eigenstates. The eigenvalue equation for $\hat{H}$ is

$$\hat{H} \, |E\rangle = E \, |E\rangle \quad \text{- - - - - - - (2)}$$

For a free particle, the energy E is positive and E can vary in a continuous manner. We would like to find the eigenkets, i.e., states with definite energy E.

First, we write Eq. (2) in coordinate representation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_E(x)}{dx^2} = E\,\psi_E(x)$$

or

$$\frac{d^2\psi_E(x)}{dx^2} + \frac{2mE}{\hbar^2}\psi_E(x) = 0 \qquad \cdots\cdots (3)$$

where $\psi_E(x) \equiv \langle x|E\rangle$ is the wave function of the eigenvector $|E\rangle$. We write Eq. (3) as

$$\frac{d^2\psi_E(x)}{dx^2} + \frac{p_E^2}{\hbar^2}\psi_E(x) = 0 \qquad \cdots\cdots (4)$$

where

$$p_E = +\sqrt{2mE}\ .$$

Eq. (4) has two linearly independent solutions

$$e^{ip_Ex/\hbar} \quad \text{and} \quad e^{-ip_Ex/\hbar}$$

so that the general solution is

$$\psi_E(x) = A\,e^{ip_Ex/\hbar} + B\,e^{-ip_Ex/\hbar}$$

where A and B are constants.

Now,

$$\hat{p}\, e^{ip_E x/\hbar} = -i\hbar \frac{\partial}{\partial x} e^{+ip_E x/\hbar} = p_E\, e^{ip_E x/\hbar}$$

$$\hat{p}\, e^{-ip_E x/\hbar} = -i\hbar \frac{\partial}{\partial x} e^{-ip_E x/\hbar} = -p_E\, e^{-ip_E x/\hbar}.$$

Therefore, $e^{ip_E x/\hbar}$ and $e^{-ip_E x/\hbar}$ represent states with definite momentum $p_E = \sqrt{2mE}$ and $-p_E$, respectively. ~~Tho~~ Both are eigenstates of $\hat{H}$ with eigenvalue E.

Therefore, E is doubly degenerate, i.e., there are two linearly independent eigenvectors corresponding to E. These eigenvectors are

$$|E,+\rangle = |p = \sqrt{2mE}\rangle \quad \text{------} \quad (5)$$

and

$$|E,-\rangle = |p = -\sqrt{2mE}\rangle \quad \text{------} \quad (6)$$

We adopt the following normalization for momentum eigenstates

$$\langle p | p' \rangle = \delta(p - p') \quad \text{.......} (7)$$

so that in coordinate representation

$$\langle x | p \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \quad \text{.....} (8)$$

Then

$$\psi_{E,\pm}(x) \equiv \langle x | E, \pm \rangle$$

$$= \frac{1}{\sqrt{2\pi\hbar}} e^{\pm i\sqrt{2mE}\, x/\hbar} \quad \text{....} (9)$$

<u>Orthonormality of $|E, \pm\rangle$</u>

We have

$$\langle E, \pm | E', \mp \rangle = 0 \quad \text{.....} (10)$$

and

$$\langle E, \pm | E', \pm \rangle = \langle \pm p = \sqrt{2mE} \, | \pm p' = \sqrt{2mE'} \rangle$$

$$= \delta(p - p')$$

$$= \delta\left(\sqrt{2mE} - \sqrt{2mE'}\right).$$

Now, we know

$$\delta\big(f(E)\big) = \frac{\delta(E-E')}{\left|\frac{df}{dE}\right|_{E=E'}}$$

where E' is a simple root of $f(E)$. Here we take

$$f(E) = \sqrt{2mE} - \sqrt{2mE'}$$

$$\therefore \quad \frac{df(E)}{dE} = \frac{\sqrt{2m}}{2\sqrt{E}} = \sqrt{\frac{m}{2E}}$$

$$\therefore \quad \delta\left(\sqrt{2mE} - \sqrt{2mE'}\right) = \sqrt{\frac{2E'}{m}}\,\delta(E-E') = \sqrt{\frac{2E}{m}}\,\delta(E-E'),$$

Hence

$$\langle E, \pm | E', \pm \rangle = \sqrt{\frac{2E}{m}}\,\delta(E-E') . \qquad \text{---- (11)}$$

Therefore, we can write compactly

$$\langle E, a | E', b \rangle = \delta_{ab}\sqrt{\frac{2E}{m}}\,\delta(E-E') \qquad \text{--- (12)}$$

where

$$a, b = \pm$$

Decomposition of identity

Momentum eigenstates $\{ |p\rangle ;\ -\infty < p < \infty \}$ and the energy eigenstates $\{ |E, a\rangle ;\ a = \pm,\ 0 < E < \infty \}$ form a complete sets of states. So we can write

$$\hat{1} = \int dp\ |p\rangle\langle p| \qquad \text{-------- (13)}$$

with

$$\langle p|p'\rangle = \delta(p-p') , \qquad \text{----- (14)}$$

or,

$$\hat{1} = \sum_{a=\pm}{}' \int dE \sqrt{\frac{m}{2E}}\ |Ea\rangle\langle Ea| \qquad \text{----- (15)}$$

with

$$\langle E a|E' b\rangle = \delta(E-E')\,\delta_{ab} . \qquad \text{---- (16)}$$

Propagator for a free particle.

The propagator $U(x,t;x_0,t_0)$ is defined as

$$U(x,t;x_0,t_0) = \langle x|\hat{T}(t,t_0)|x_0\rangle \quad \cdots \quad (17)$$

where $\hat{T}(t,t_0)$ is the time evolution operator of the state vectors in the Schrödinger picture. If the Hamiltonian operator is independent of time, then

$$\hat{T}(t,t_0) = e^{-i\hat{H}(t-t_0)/\hbar} \quad \cdots \quad (18)$$

and the propagator becomes

$$U(x,t;x_0,t_0) = \langle x|e^{-i\hat{H}(t-t_0)}|x_0\rangle \quad \cdots \quad (19).$$

Since, the eigenvalues and eigenvectors of the free Hamiltonian are completely known, we can easily calculate the propagator easily without taking recourse to the path integral method. Using the decomposition of identity once in Eq (19), either in the form Eq (13) or in the form Eq. (15), we find

$$U(x,t;x_0,t_0) = \left(\frac{m}{2\pi\hbar i(t-t_0)}\right)^{1/2} e^{-\frac{m(x-x_0)^2}{2\hbar i(t-t_0)}} .$$

Example

The wavefunction for a free particle at $t=0$ is

$$\psi(x,0) = N e^{i p_0 x/\hbar} e^{-x^2/2\Delta^2}$$

(a) Normalize the wavefunction

(b) Find Δx, Δp and $\Delta x \Delta p$ at $t=0$

(c) Find the wave function $\psi(x,t)$ at time t and calculate Δx. Comment on the spreading of the wave packet.

Ans

(a) $\langle \psi | \psi \rangle = 1$

or $\displaystyle\int_{-\infty}^{\infty} \psi^*(x,0)\, \psi(x,0)\, dx = 1$

or $\displaystyle |N|^2 \int_{-\infty}^{\infty} e^{-x^2/\Delta^2} dx = 0$

$\displaystyle\int_{-\infty}^{\infty} e^{-\alpha x^2} = \left(\frac{\pi}{\alpha}\right)^{1/2}$

Here $\alpha = \dfrac{1}{\Delta^2}$

or, $|N|^2 (\pi\Delta^2)^{1/2} = 1$

Choosing N to be real and positive

$$|N| = \frac{1}{(\pi\Delta^2)^{1/4}}$$

Thus, the normalized wavefunction is

$$\psi(x,0) = \frac{1}{(\pi\Delta^2)^{1/4}} e^{-x^2/2\Delta^2 + i p_0 x/\hbar}$$

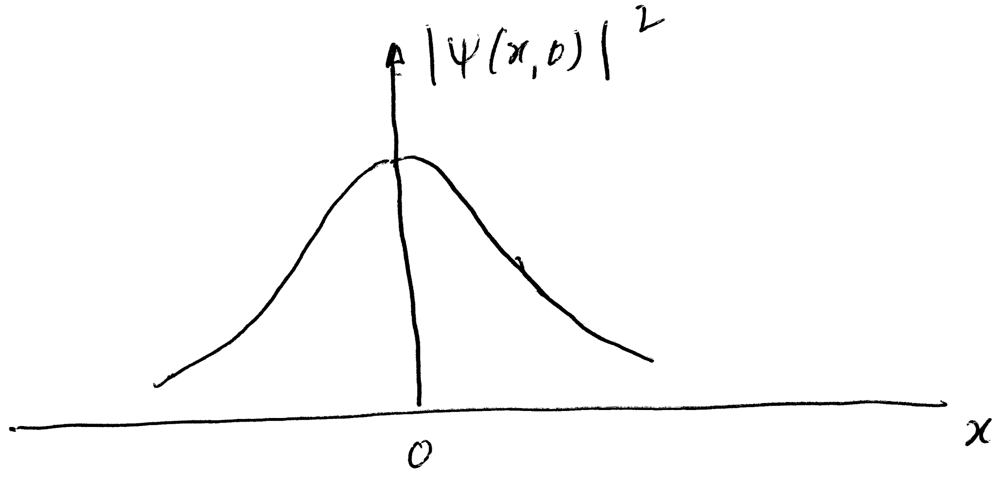
(b) The position probability density at $t=0$ is

$$|\psi(x,0)|^2 = \frac{1}{(\pi\Delta^2)^{1/2}} e^{-x^2/\Delta^2}$$

which is a Gaussian function of x.

The graph of $|\psi(x,0)|^2$ vs x is shown in the figure below.

(11



The position probability density is symmetric around $x=0$. Therefore

$$\langle x\rangle = 0$$

Now

$$(\Delta x)^2 = \langle (\hat{x} - \langle\hat{x}\rangle)^2\rangle$$

$$= \langle \hat{x}^2\rangle - \underbrace{\langle\hat{x}\rangle^2}_{=0}$$

$$= \langle \hat{x}^2\rangle$$

$$= \int_{-\infty}^{\infty} \Psi^*(x,0)\,x^2\,\Psi(x,0)\,dx$$

or,

$$(\Delta x)^2 = \frac{1}{(\pi \Delta^2)^{1/2}} \int_{-\infty}^{\infty} x^2 e^{-x^2/\Delta^2} dx$$

$$= \frac{1}{(\pi \Delta^2)^{1/2}} \cdot \frac{\Delta^2}{2} (\pi \Delta^2)^{1/2}$$

$$\int_{-\infty}^{\infty} x^2 e^{-\alpha x^2} dx = \frac{1}{2\alpha} \left(\frac{\pi}{\alpha}\right)^{1/2}$$

Here $\alpha = \frac{1}{\Delta^2}$.

$$= \frac{\Delta^2}{2}$$

$$\therefore \boxed{\Delta x \Big|_{t=0} = \Delta / \sqrt{2}}$$

We have found the uncertainty in position at $t=0$.

To find Δp at $t=0$, we need the wave function in the momentum representation. ~~Ideas~~

$$\tilde{\psi}(p,0) = \langle p | \psi(t=0) \rangle$$

$$= \int \langle p | x \rangle \langle x | \psi(0) \rangle \, dx$$

$$= \int \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx} \psi(x,0) \, dx$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{(\pi\Delta^2)^{1/4}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \, e^{ip_0x/\hbar - x^2/2\Delta^2} \, dx$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{(\pi\Delta^2)^{1/4}} \int_{-\infty}^{\infty} e^{-x^2/2\Delta^2 - i(p-p_0)x/\hbar} \, dx.$$

We now use the standard integral

$$\int_{-\infty}^{\infty} e^{-ax^2 \pm ikx} \, dx = \left(\frac{\pi}{a}\right)^{1/2} e^{-k^2/4a}$$

and get

$$\tilde{\psi}(p,0) = \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{(\pi\Delta^2)^{1/4}} \left(2\pi\Delta^2\right)^{1/2} \exp\left[-\frac{\frac{(p-p_0)^2}{\hbar^2}}{4 \cdot \frac{1}{2\Delta^2}}\right]$$

$$\boxed{\tilde{\psi}(p,0) = \frac{\Delta}{(\pi\hbar^2\Delta^2)^{1/4}} \exp\left[-\frac{(p-p_0)^2\Delta^2}{2\hbar^2}\right]}$$

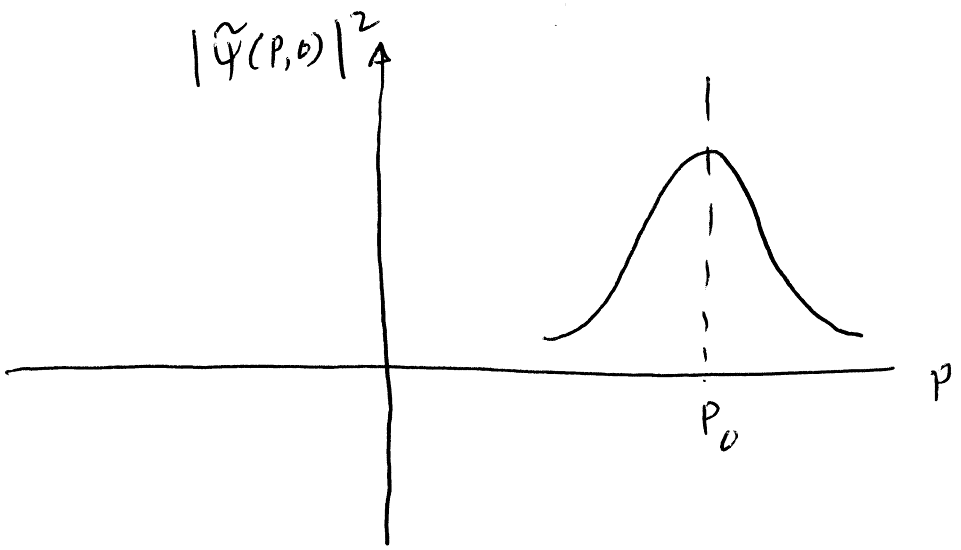
Therefore momentum probability density is

$$|\tilde{\psi}(p,0)|^2 = \frac{\Delta^2}{(\pi\hbar^2\Delta^2)^{1/2}} \exp\left[-\frac{(p-p_0)^2\Delta^2}{\hbar^2}\right]$$

or

$$\boxed{|\tilde{\psi}(p,0)|^2 = \frac{\Delta}{\pi^{1/2}\hbar} \exp\left[-\frac{(p-p_0)^2\Delta^2}{\hbar^2}\right]}$$

The plot of $|\tilde{\psi}(p,0)|^2$ vs p is shown in the figure below:



The momentum probability density is symmetric around p_0. Therefore

$$\langle \hat{p} \rangle = p_0 .$$

Next

$$(\Delta p)^2 = \langle (\hat{p} - \langle \hat{p} \rangle)^2 \rangle$$

$$= \langle \Psi(0) | (\hat{p} - \langle \hat{p} \rangle)^2 | \Psi(0) \rangle$$

$$= \int_{-\infty}^{\infty} \tilde{\Psi}^*(p,0)\, (p - p_0)^2\, \tilde{\Psi}(p,0)\, dp$$

$$= \int_{-\infty}^{\infty} (p - p_0)^2\, |\tilde{\Psi}(p,0)|^2\, dp$$

$$= \frac{\Delta}{\pi^{1/2}\hbar} \int_{-\infty}^{\infty} (p - p_0)^2 \exp\left[- \frac{\Delta^2 (p - p_0)^2}{\hbar^2} \right] dp$$

$$= \underbrace{\frac{\Delta}{\pi^{1/2}\hbar} \left(\frac{\pi \hbar^2}{\Delta^2} \right)^{1/2}}_{=1} \frac{1}{2\Delta^2/\hbar^2} = \frac{\hbar^2}{2\Delta^2}$$

Hence

$$\boxed{\Delta p\Big|_{t=0} = \frac{\hbar}{\sqrt{2}\,\Delta}}$$

Therefore, at $t=0$

$$\Delta x\,\Delta p = \frac{\Delta}{\sqrt{2}} \cdot \frac{\hbar}{\sqrt{2}\,\Delta}$$

or $$\boxed{\Delta x\,\Delta p = \frac{1}{2}\hbar},$$

i.e., the uncertainty product is minimum.

(c) Next, we find $\psi(x,t)$ from $\psi(x,0)$.

$$\psi(x,t) = \int_{-\infty}^{\infty} U(x,t,x',0)\,\psi(x',0)\,dx'$$

$$= \int_{-\infty}^{\infty} \left(\frac{m}{2\pi\hbar i t}\right)^{1/2} e^{im(x-x')^2/2\hbar t}$$

$$\times \frac{1}{(\pi\Delta^2)^{1/4}}\, e^{-x'^2/2\Delta^2 + i p_0 x'/\hbar}\, dx'$$

$$= \left(\frac{m}{2\pi\hbar i t}\right)^{1/2} \frac{1}{(\pi\Delta^2)^{1/4}} \int_{-\infty}^{\infty} e^{im(x-x')^2/2\hbar t \; - x'^2/2\Delta^2 + i p_0 x'/\hbar}\, dx'$$

This integral is straightforward but involves long ~~algebra~~ algebra. We obtain[+]

+ The integral is done in the appendix

$$\psi(x,t) = \left[\pi^{1/2}\left(\Delta + \frac{i\hbar t}{\Delta}\right)\right]^{-1/2}$$

$$\times \exp\left[\frac{i p_0}{\hbar}(x - p_0 t/2m)\right] \exp\left[-\frac{(x - p_0 t/m)^2}{2\Delta^2(1 + i\hbar t/m\Delta^2)}\right]$$

The position probability density is obtained as the absolute square of $\psi(x,t)$. Letting $\alpha = 1 + i\hbar t/m\Delta^2$, we have

$$|\psi(x,t)|^2 = \frac{1}{\pi^{1/2}(\Delta^2 + \hbar^2 t^2/\Delta^2)^{1/2}}$$

$$\times \exp\left[-\frac{(x - p_0 t/m)^2}{2\Delta^2}\left(\frac{1}{\alpha} + \frac{1}{\alpha^*}\right)\right]$$

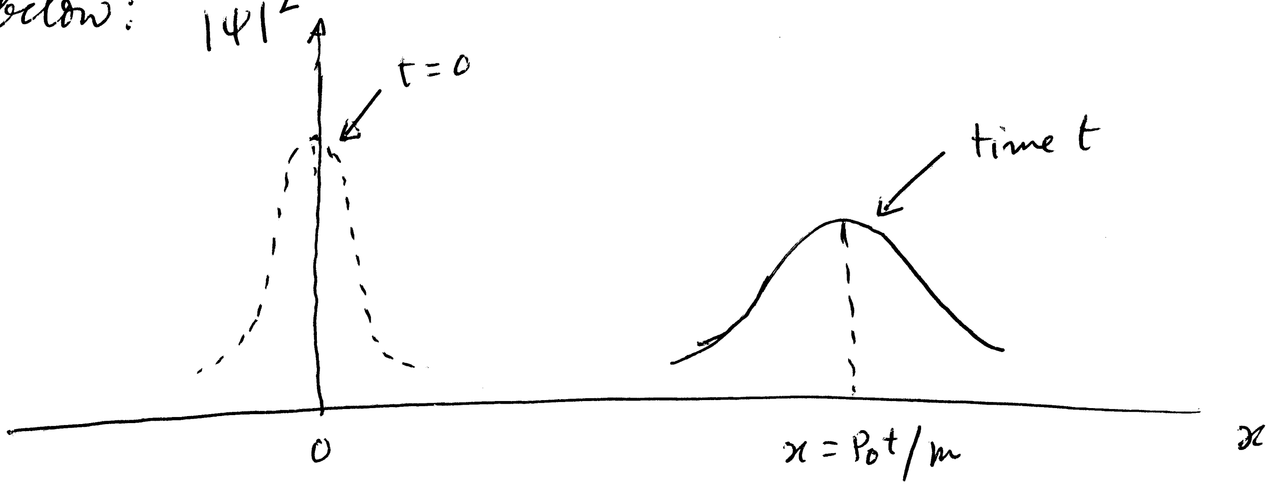
Now
$$\frac{1}{\alpha} + \frac{1}{\alpha^*} = \frac{\alpha + \alpha^*}{\alpha\alpha^*} = \frac{2\,\mathrm{Re}\,\alpha}{|\alpha|^2} \quad (\mathrm{Re}\,\alpha = 1)$$

$$= \frac{2}{(1 + \hbar^2 t^2/m^2\Delta^4)}$$

Hence

$$|\psi(x,t)|^2 = \frac{1}{\pi^{1/2}\left(\Delta^2 + \frac{\hbar^2 t^2}{\Delta^2}\right)^{1/2}} \exp\left[-\frac{(x - p_0 t/m)^2}{\Delta^2\left(1 + \frac{\hbar^2 t^2}{m^2 \Delta^4}\right)}\right]$$

We plot $|\psi(x,0)|^2$ and $|\psi(x,t)|^2$ in the figure below:



We see that the center of the wave packet has moved a distance $p_0 t/m$ in time t. Therefore, the group velocity of the wave packet is

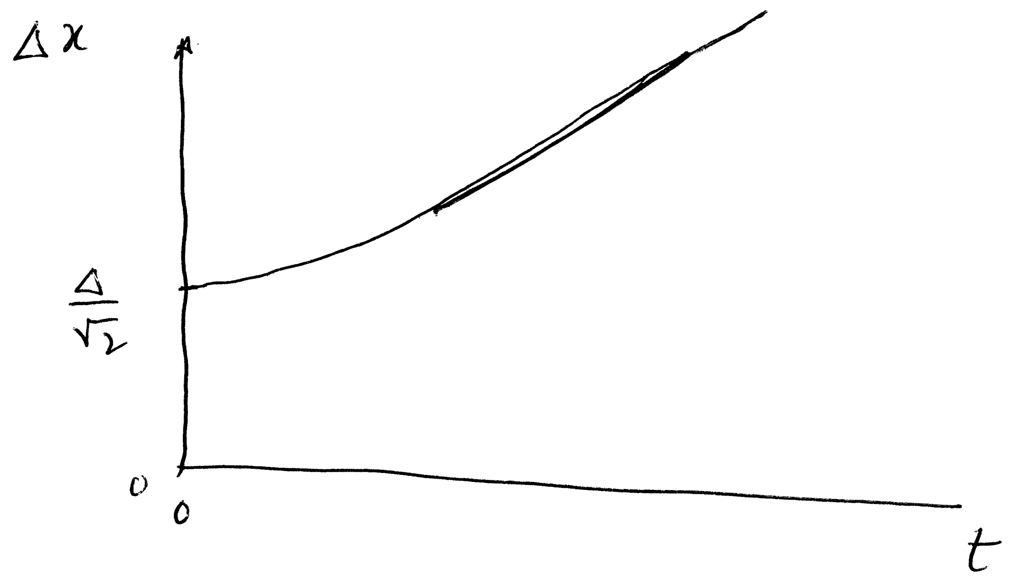
$v_g = p_0/m = \langle p \rangle/m$.

The wave packet also spreads because Δx increases. Noting that if $|\Psi|^2$ is of the form $\exp\left[-(x-\langle x\rangle)^2/\sigma^2\right]$, then $\Delta x = \sigma/\sqrt{2}$, we find

$$\Delta x(t) = \frac{\Delta\sqrt{1+\hbar^2t^2/m^2\Delta^4}}{\sqrt{2}}$$

$$= \Delta x(0)\sqrt{1+\hbar^2t^2/m^2\Delta^4}$$

$\Delta x(t)$ vs t is shown in the figure below



We can write $\Delta x(t)$ as

$$\Delta x(t) = \Delta x(0) \sqrt{1+(t/T)^2}$$

where

$$T = m\Delta^2/\hbar$$

is the characteristic time of the wave packet. When $t << T$, the spreading of the wave packet is negligible. At $t >> T$,

$$\Delta x(t) \approx \Delta x(0)\, t/T$$

i.e, ultimately the spread of the wave packet is directly propotional to time.

Let us calculate the time needed for the wave packet to double in size.

$$\Delta x(t) = \Delta x(0)\sqrt{1+\left(\frac{t}{T}\right)^2} \qquad \left(\Delta x(0) = \frac{\Delta}{\sqrt{2}}\right.$$

$$2 = \sqrt{1+t^2/T^2}$$

or, $t = \sqrt{3}\,T$.

We can write T in terms of $\Delta x(0)$.

$$T = \frac{m\Delta^2}{\hbar}$$

Since $\Delta x(0) = \dfrac{\Delta}{\sqrt{2}}$, we have

$$T = \frac{2m(\Delta x(0))^2}{\hbar}.$$

Consider an electron which at time $t=0$ is localized within a distance of 10^{-10} m, characteristic of atomic dimensions.

Therefore

$$T = \frac{2m\,(10^{-10}\,m)^2}{\hbar}$$

$m_{\text{electron}} = 9.1 \times 10^{-31}$ kg

$\hbar = 1.06 \times 10^{-34}$ J s

$$= \frac{(2)(9.1\times10^{-31}\,kg)(10^{-10}\,m)^2}{1.06\times10^{-34}\ J\,s}$$

$$= 1.7 \times 10^{-16}\ s$$

$\therefore$ Wave packet size doubles in

$$t = \sqrt{3}\,T = 2.97 \times 10^{-16}\ s$$

On the other hand, for a macroscopic particle of mass 1 g, whose position is initially defined within an accuracy of $\Delta x \simeq 10^{-6}$ m, we find that the width of the packet doubles after a time of $t \simeq 10^{19}$ s, which is larger than the estimated age of the universe.

A word of caution should be said about the interpretation of these results. Let us suppose that we have a wave packet representing an electron, which spreads so that the width of the packet is, for example, $\Delta x = 1$ km at a given time. If an electron detector is placed at a particular position at that time, it will record the presence or the absence of the 'complete' electron, since when the electron manifests itself in the detection process, it is indivisible. Before the electron is detected, the wave function determines the probability that the electron will be found at a certain place, at a given time. As soon as the electron has been detected, its location is of course known to within a precision $\Delta x' \ll \Delta x$, so that a new wave function (i.e., a new wave packet) must describe the situation. This change of the wave function upon measurement is called the 'collapse of the wave packet'.

Appendix

Here we show the details of the algebra encountered in calculating $\psi(x,t)$

$$\psi(x,t) = \int_{-\infty}^{\infty} U(x,t;x')\,\psi(x',0)\,dx'$$

$$= \left(\frac{m}{2\pi\hbar i t}\right)^{1/2} \int_{-\infty}^{\infty} e^{im(x-x')^2/2\hbar t} \cdot \frac{1}{(\pi\Delta^2)^{1/4}}\, e^{ip_0x'/\hbar - x'^2/2\Delta^2}\, dx'$$

$$= \left(\frac{m}{2\pi\hbar i t}\right)^{1/2} \frac{1}{(\pi\Delta^2)^{1/4}} \int_{-\infty}^{\infty} e^{im(x-x')^2/2\hbar t + ip_0x'/\hbar - x'^2/2\Delta^2}\, dx'$$

1 A PARTICLE IN A BOX

One of the key features of quantum physics is that the possible energies of a confined particle are quantized. Indeed, the familiar quantized energy levels of atomic, nuclear and particle physics are manifestations of confinement. We shall illustrate the connection between confinement and quantized energy levels by considering a particle confined to a box.

1.1 A one-dimensional box

We begin by considering a particle moving in one dimension with potential energy

$$V(x) = \begin{cases} 0 & \text{if } 0 < x < a \\ \infty & \text{elsewhere} \end{cases} \tag{1}$$

This infinite square-well potential confines the particle to a one-dimensional box of size a, as shown in Fig. (1).

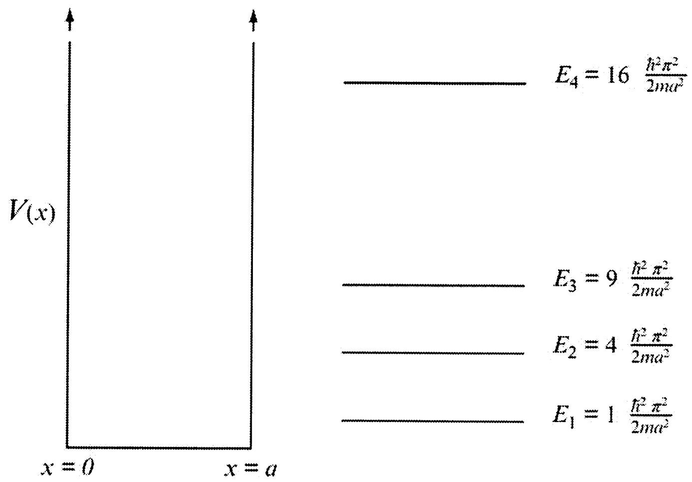


Figure 1: Low-lying energy levels of a particle of mass m confined by an infinite square-well potential $V(x)$ with width a

In classical physics, the particle either lies at the bottom of the well with zero energy or it bounces back and forth between the barriers at $x = 0$ and $x = a$ with any energy up to infinity. In quantum physics, more varied states exist. Each is described by a wave function $\Psi(x,t)$ which obeys the one-dimensional Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi \ . \tag{2}$$

However, when the particle has a definite value E, the wave function has the special form

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar} \ , \tag{3}$$

where $\psi(x)$ satisfies the energy eigenvalue equation

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x) \ . \tag{4}$$

We shall now seek physically acceptable solutions to Eq. (4). Because the potential energy $V(x)$ rises abruptly to infinity at $x = 0$ and at $x = a$, the particle is confined to the region $0 < x < a$ and outside this region the eigenfunction $\psi(x)$ is zero. Inside this region, the potential energy is zero and the eigenfunction is a solution of Eq. (4) with $V(x) = 0$. We shall simplify this equation by defining

$$k = \sqrt{\frac{2mE}{\hbar^2}} \ , \tag{5}$$

and rewriting the energy E as

$$E = \frac{\hbar^2 k^2}{2m} \tag{6}$$

to give

$$\frac{d^2\psi}{dx^2} = -k^2\psi \ . \tag{7}$$

Physically acceptable solutions of this differential equation are obtained by writing down the general solution

$$\psi(x) = M\,\cos kx + N\,\sin kx \ , \tag{8}$$

where M and N are constants and by imposing the boundary condition

$$\psi(0) = \psi(a) = 0 \ , \tag{9}$$

which ensures that the position probability density of the particle does not change abruptly at the end of the box.

We note that in order to have the wavefunction equal to zero at $x = 0$ we must choose $M = 0$. Next, for the wavefunction to be zero at $x = a$, the values of the wavenumber k cannot be arbitrary, rather k is such that

$$ka = 0 \,. \tag{10}$$

The values of k satisfying the above condition are discrete and are given by

$$k_n = \frac{n\pi}{a} \tag{11}$$

with $n = 1, 2, 3, \ldots$. Thus the possible eigenfunctions of the particle are

$$\psi_n(x) = N \sin k_n x \,, \tag{12}$$

where N is an arbitrary constant. The eigenfunctions of the energy operator is the wavefunction of the particle when the particle is in a definite energy state. We conclude that the possible energy levels of a particle in a one-dimensional box of width a are given by

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \,, \quad \text{with} \quad n = 1, 2, 3, \ldots \tag{13}$$

and that a particle with energy E_n has the time-dependent wavefunction of the form

$$\Psi_n(x,t) = N \sin k_n x \, e^{-iE_n t/\hbar} \,. \tag{14}$$

The eigenfunctions are shown in figure (8.2).

We note the following:

1. As shown in Fig. 1, the separation between the energy levels increases as the quantum number n increases. However, this separation as a fraction of the energy decreases; indeed

$$\frac{E_{n+1} - E_n}{E_n} \to \frac{2}{n} \quad \text{as } n \to \infty \,. \tag{15}$$

   This means that the discrete nature of the energy levels becomes less important when the energy is high.

2. The lowest possible energy, in contrast with classical physics, is not zero, but
$$E_1 = \frac{\hbar^2\pi^2}{2ma^2} \; . \tag{16}$$
We can understand this *zero-point energy* by using the Heisenberg uncertainty principle
$$\Delta x \Delta p \geq \hbar/2 \; .$$
If a particle is confined to a region of size a, it has an uncertain position $\Delta x \leq a$ and, hence, an uncertain momentum Δp which is at least of the order of $\hbar/2a$. Because the average magnitude of the momentum is always greater than Δp, the average kinetic energy of the particle is always greater than $(\Delta p)^2/2m$ which in turn is greater than $\hbar^2/8ma^2$.

3. The spatial shape of the wave function of a particle in a box with energy E_n is identical to the spatial shape of the normal mode of a string with angular frequency ω_n. As illustrated in Fig. 2, the number of nodes increases as the value of n increases

4. The wave function of a particle in a box, unlike the displacement of a string, is not observable, but it can be used to construct properties of the particle that are observable. The first step is to normalize the wave function so that
$$\int_0^a |\Psi(x,t)|^2 dx = 1 \; . \tag{17}$$
We can show that this condition is satisfied if $N = \sqrt{2/a}$. One can then calculate probability densities for position and momentum.

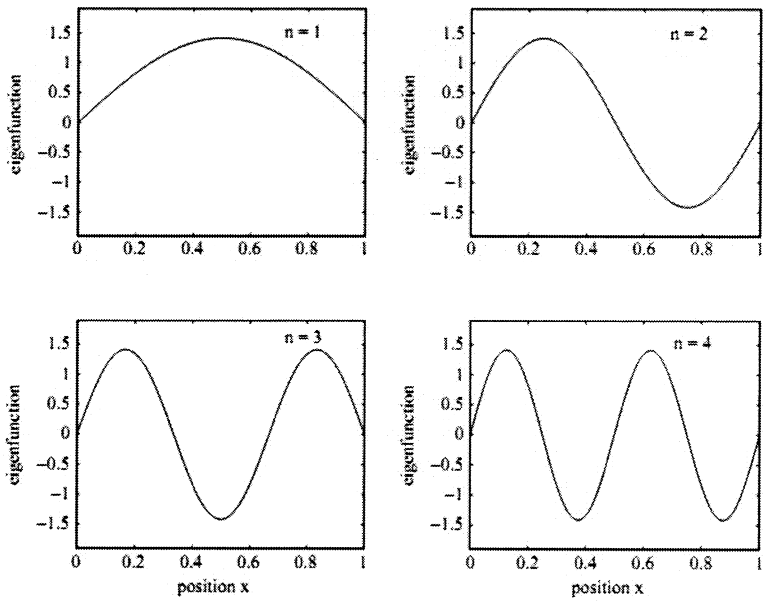


Figure 2: The spatial shapes of four eigenfunctions $\psi_n(x)$ in arbitrary units with $a = 1$. In classical physics, these eigenfunctions may describe the shape of a normal mode of vibration of a string with definite angular frequency. In quantum physics, they may describe the shape of a wave function of a particle in a box with definite energy.

2 A three-dimensional box

We shall now consider the more realistic problem of a particle confined in three dimensions. If the particle has definite energy E, its wave function has the form

$$\Psi(x, y, z, t) = \psi(x, y, z)e^{-iEt/\hbar}\,, \tag{18}$$

where $\psi(x, y, z)$ satisfies the energy eigenvalue equation

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(x, y, z)\right]\psi = E\psi\,. \tag{19}$$

We shall choose a potential energy function

$$V(x, y, z) = \begin{cases} 0 & \text{if } 0 < x < a,\ 0 < y < b,\ 0 < z < c \\ \infty & \text{elsewhere}\ , \end{cases} \tag{20}$$

which confines the particle to a box with sides a, b and c

The possible energy eigenfunctions and eigenvalues of the particle may be found by seeking solutions of Eq. (19) inside the box which are equal to zero on all six faces of the box. For example, the function

$$\psi(x, y, z) = N \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{\pi y}{b}\right) \sin\left(\frac{\pi z}{c}\right) \tag{21}$$

is zero on each of the faces defined by

$$x = 0, \quad x = a, \quad y = 0, \quad y = b, \quad z = 0, \quad z = c,$$

and it satisfies Eq. (19) inside the box where $V(x, y, z) = 0$, if

$$E = \frac{\hbar^2 \pi^2}{2m} \left[\frac{1}{a^2} + \frac{1}{b^2} + \frac{1}{c^2}\right] \ .$$

In general, there are an infinite set of eigenfunctions and eigenvalues labelled by three quantum numbers $n_x = 1, 2, 3, \ldots$, $n_y = 1, 2, 3, \ldots$ and $n_z = 1, 2, 3, \ldots$. The eigenfunctions have the form

$$\psi_{n_x, n_y, n_z}(x, y, z) = N \sin\left(\frac{n_x \pi x}{a}\right) \sin\left(\frac{n_y \pi y}{b}\right) \sin\left(\frac{n_z \pi a}{c}\right) \ , \tag{22}$$

and the energy eigenvalues are

$$E_{n_x, n_y, n_z} = \frac{\hbar^2 \pi^2}{2m} \left[\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right] \ . \tag{23}$$

Equation (23) shows how the quantized energy levels of a particle in a box depend upon the dimensions of the box, a, b and c. Most importantly, it shows that some energy levels may coincide when the box has particular dimensions. We illustrate this in Fig. 3 which shows that, for a particle in a cubical box with $a = b = c$, energy levels like $E_{1,1,2}$, $E_{2,1,1}$ and $E_{1,2,1}$ coincide.

When there are several states, or wave functions, with the same energy, the energy levels are said to be degenerate. Degenerate energy levels are very important in atomic, nuclear and particle physics. They arise because the interactions which confine electrons in atoms, nucleons in nuclei and quarks in hadrons, have specific symmetry properties. Indeed, the observed degeneracy of energy levels can be used to deduce these symmetry properties.

$$E_{2,2,2} = 16\,\frac{\hbar^2\pi^2}{2ma^2}$$

$$E_{1,1,3} = E_{3,1,1} = E_{1,3,1} = 11\,\frac{\hbar^2\pi^2}{2ma^2}$$

$$E_{1,2,2} = E_{2,2,1} = E_{2,1,2} = 9\,\frac{\hbar^2\pi^2}{2ma^2}$$

$$E_{1,1,2} = E_{2,1,1} = E_{1,2,1} = 6\,\frac{\hbar^2\pi^2}{2ma^2}$$

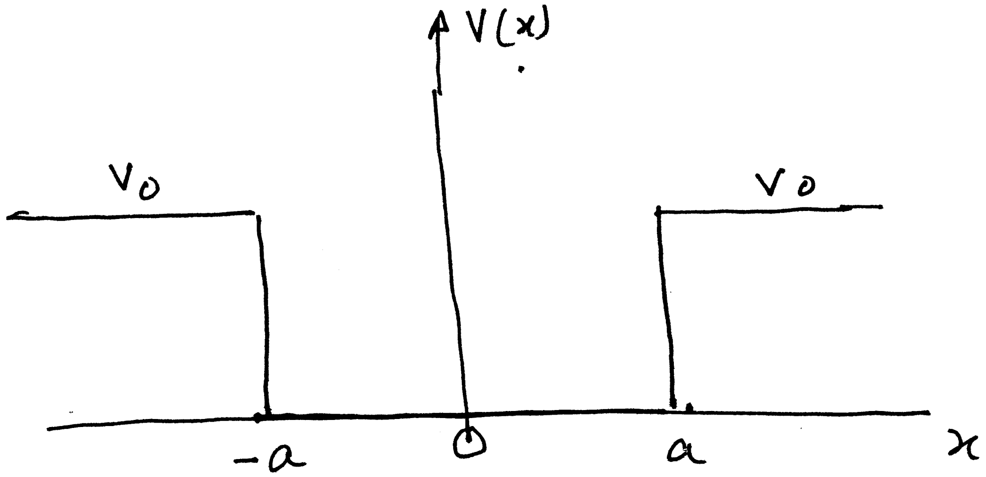
$$E_{1,1,1} = 3\,\frac{\hbar^2\pi^2}{2ma^2}$$

Figure 3: Low-lying energy levels of a particle of mass m confined in a cubical box with sides of length a. Note the degeneracy of the first, second and third excited state

Finite square well

Let us consider the potential

$$V(x) = \begin{cases} 0 & \text{for } -a < x < a \\ V_0 & \text{otherwise} \end{cases} \qquad (1)$$



We can look for two types of solutions of the time independent Schrödinger equation.

Unbound or scattering states

For these states $E > V_0$, i.e., total energy of the particle is greater than the potential energy for all x in the range $-\infty$ to ∞. Particles with energies $E > V_0$ ~~could~~ can exist even at $x = \pm\infty$. Eigenvalue spectrum of H for unbound states is continuous with $E > V_0$. Scattering states with definite energy are not normalizable to unity because they do not have finite norm.

Bound states

Bound states would occur for $0 < E < V_0$. These states are localized in the sense that for such states $\psi(x) \to 0$ as $x \to \pm\infty$. Therefore bound state wave functions are normalizable to unity unlike the scattering states. We will see that bound state energies are discrete.

Finally, acceptable solutions of the time independent Schrödinger equation ~~does~~ do not exist if $E < 0$. If the energy is less than the minimum of the potential, it would mean that the kinetic energy of the particle is $-$ve everywhere. Such a situation is physically meaningless.

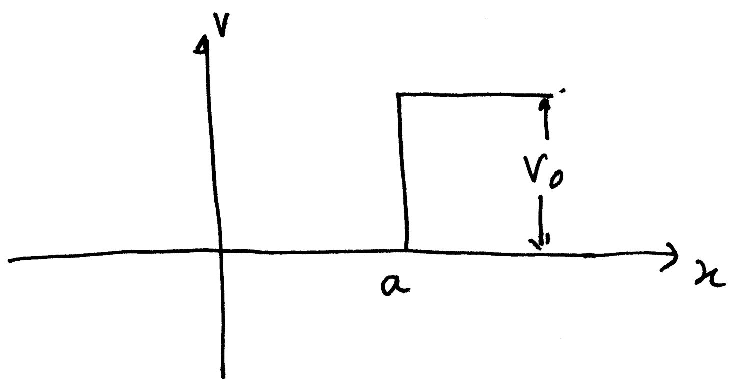
Boundary condition.

The finite square well potential (Eq (1)) has two discontinuities at $x = a$ and at $x = -a$.

For the finite square well, these two discontinuities are finite because potential changes abruptly at $x = \pm a$ by V_0 which is finite.

No matter whether the discontinuity of the potential is finite or infinite, $\psi(x)$ is always continuous at the discontinuities of the potential. ~~as of of course~~ However, $\psi'(x)$ would be continuous if the discontinuity in the potential is finite. If the discontinuity in the potential is infinite, then $\psi'(x)$ would be discontinuous.

To show this, consider the discontinuity of the square well potential at $x = a$. Let us integrate the Schrödinger equation from ~~x=~~ $a - \epsilon$ to $a + \epsilon$ where ϵ is an infinitesimal quantity which tends to zero.



Now the Schrödinger equation is

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

Integrating this equation from $a - \epsilon$ to $a + \epsilon$ we have

$$\int_{a-\epsilon}^{a+\epsilon} \frac{d^2\psi}{dx^2}\,dx = -\frac{2mE}{\hbar^2}\int_{a-\epsilon}^{a+\epsilon} \psi(x)\,dx + \frac{2m}{\hbar^2}\int_{a-\epsilon}^{a+\epsilon} V(x)\,\psi(x)\,dx$$

Noting that $\psi(x)$ is continuous at a (i.e., $\psi(x \to a^-) = \psi(x \to a^+)$) and $V(x)$ is continuous at a, we can write the above equation as

$$\psi'(x=a+\epsilon)-\psi'(x=a-\epsilon)$$

$$= \underbrace{-\frac{2m}{\hbar^2}\psi(a)\,2\epsilon}_{=0 \text{ as } \epsilon\to 0} + \frac{2m}{\hbar^2}\psi(a)\,\epsilon\left[V(x=a+\epsilon)+V(x=a-\epsilon)\right]$$

Now, taking the limit $\epsilon \to 0$, we have

$$\psi'(x=a^+)-\psi'(x=a^-)$$

$$= \frac{2m}{\hbar^2}\psi(a)\lim_{\epsilon\to 0}\epsilon\left[V(x\to a^+)+V(x\to a^-)\right] \quad \text{--(2)}.$$

Now, if the discontinuity in the potential is finite, then both $V(x\to a^+)$ and $V(x\to a^-)$ are finite (but different). Therefore, the right hand side goes to zero as $\epsilon\to 0$, i.e.

$$\psi'(x\to a^+)-\psi'(x=a^-) = 0$$

or, $\psi'(x)$ is continuous at $x=a$. However if the disconnity of the potential is infinite, then the right hand side of Eq. (2) will not vanish, i.e., $\psi'(x)$ would be discontinuous at $x=a$.

Parity

The time independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\,\psi(x) = E\,\psi(x) \quad \ldots\ldots (3)$$

Now make the following transformation of the coordinates

$$x \longrightarrow -x\,.$$

Such a transformation is called space inversion or parity transformation. Under this transformation Eq. (3) transforms to

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(-x)}{dx^2} + V(-x)\,\psi(-x) = E\,\psi(-x)\,. \quad \ldots (4)$$

Now suppose the potential energy function $V(x)$ is unchanged under the parity transformation, i.e.,

$$V(-x) = V(x)\,,$$

i.e., $V(x)$ is a symmetric function of x or an even function of x.

Thus for a potential symmetric under parity, the transformed Schrödinger equation, i.e., Eq. (4) can be written as

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(-x)}{dx^2} + V(x)\,\psi(-x) = E\,\psi(-x) \qquad \text{- - - - (5)}$$

Comparing Eqs. (3) and (5) we can conclude that if $\psi(x)$ is the eigenfunction of H with eigenvalue E, then $\psi(-x)$ is also an eigenfunction of H with the same eigenvalue provided the potential is a symmetric function of x.

Now, if the eigenvalue E is <u>nondegenerate</u>, there is only one linearly independent eigenvector corresponding to E. Therefore $\psi(x)$ and $\psi(-x)$ cannot be linearly independent of each other. Hence, $\psi(-x)$ can differ from $\psi(x)$ by at most a multiplicative constant, i.e.,

$$\psi(-x) = \pi\,\psi(x) \qquad \text{- - - - - - - (6).}$$

where π is a constant.

Replacing x by $-x$ in Eq.(6) we can also write

$$\psi(x) = \pi\,\psi(-x) \quad \text{- - - - - - . (7)}$$

Combining Eqs. (6) and (7), we have

$$\begin{aligned}\psi(x) &= \pi\,\psi(-x) \\ &= \pi\,(\pi\,\psi(x)) \\ &= \pi^2\,\psi(x)\end{aligned}$$

or,

$$\pi^2 = 1$$

i.e., $\boxed{\pi = +1 \text{ or } -1 .}$

Thus, we have either

$$\psi(-x) = \psi(x) \quad (\pi = 1)$$

i.e., the wave function is even, or

$$\psi(-x) = -\psi(x) \quad (\pi = -1)$$

i.e., the wave function is odd. When the wave function is even, we say that the corresponding state of the system has parity equal to +1 or even parity. Similarly, for odd wave function, the state of the system has odd parity, i.e., $\pi = -1$.

<u>Note</u> If $V(x)$ is unchanged under parity, i.e., if

$$V(-x) = V(x)$$

then

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

is also unchanged under parity because, obviously, $\frac{d^2}{dx^2}$ also remains invariant under $x \to -x$.

We say that the Hamiltonian is invariant under parity transformation if the Hamiltonian is unchanged under the transformation $x \to -x$.

<u>Theorem:</u> If the Hamiltonian of a system is invariant under the parity transformation, then the eigenfunction ϕ of the Hamiltonian belonging to a <u>nondegenerate</u> eigenvalue is either even or odd.

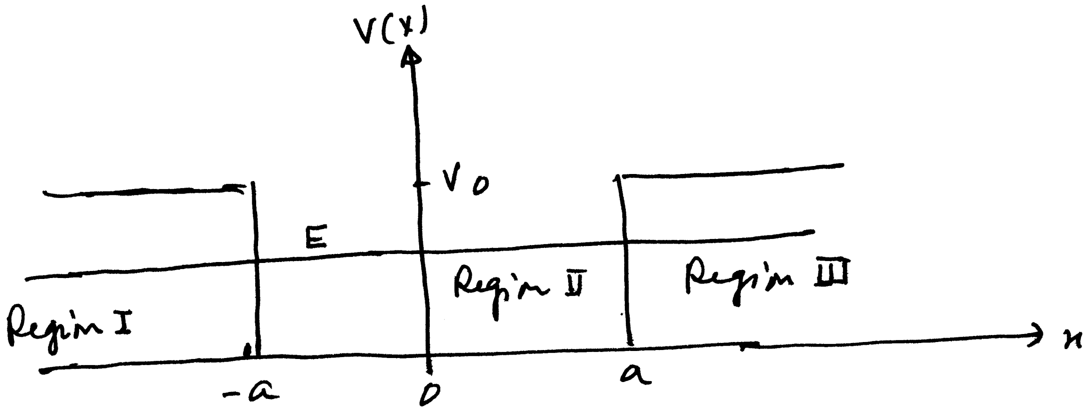
Now, we can show (see notes on harmonic oscillator) that the eigenvalues of H for bound states are nondegenerate, i.e., for every bound state of definite energy E there corresponds only one linearly independent eigenvector. Therefore, if the potential is symmetric, then the bound state wave functions are either even or odd.

Bound states in a finite square well.

The potential is given by Eq. (1), i.e.,

$$V(x) = \begin{cases} 0 & \text{if } -a < x < a \\ V_0 & \text{otherwise.} \end{cases}$$

The plot of the potential is shown below:



We are looking for bound state eigenfunctions of H, i.e, we are looking for solutions of the time-independent Schrödinger equation with E in the range $0 < E < V_0$.

Now, the Schrödinger equation is

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}(E-V)\psi(x) = 0 \quad \text{-----(7)}$$

We divide the x-axis into three regions (figure above):

$x < -a$ Region I

$-a < x < a$ Region II

$x > a$ Region III.

In region II, $V = 0$, so the Schrödinger equation is

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0$$

or

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad (\text{Region II}) \quad \ldots\ldots (8)$$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}} \quad \ldots\ldots (9)$$

Region I and III

In these two regions $V = V_0$ with $V_0 > E$. The Schrödinger equation is

$$\frac{d^2\psi}{dx^2} - \frac{2m}{\hbar^2}(V_0 - E)\psi = 0$$

or

$$\frac{d^2\psi}{dx^2} - K^2\psi = 0 \quad \ldots\ldots (10)$$

with

$$K = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

Solutions of the Schrödinger equation.

Even solutions

In region II, the solution of the Schrödinger equation (Eq. 8) is of the form

$$\psi_{II}(x) = A\cos kx + B\sin kx$$

If we want to retain only even solutions, we must have

$$\psi_{II}(x) = A\cos kx.$$

In regions I & III, the general solutions are of the form

$$\psi_{I,III}(x) = Ce^{\kappa x} + De^{-\kappa x}.$$

Since $\psi(x)$ has to be finite everywhere, we have to choose $D=0$ in region I and $C=0$ in region III. Thus, acceptable solutions in regions I & III are

$$\psi_I(x) = Ce^{\kappa x} \qquad (x \leq -a)$$

and

$$\psi_{III}(x) = De^{-\kappa x} \qquad (x > a).$$

Since we are looking for even solutions, we must choose $D = C$. Thus, the even solutions are of the form

$$\psi(x) = \begin{cases} C e^{\kappa x} & x < -a \quad \text{Region I} \\ A \cos kx & -a < x < a \quad \text{Region II} \\ C e^{-\kappa x} & x > a \quad \text{Region III} \end{cases} \tag{11}$$

Next, continuity of $\psi(x)$ at $x = a$ gives

$$A \cos ka = C e^{-\kappa a} \quad \cdots\cdots (12)$$

and the continuity of $\psi'(x)$ at $x = a$ gives

$$-kA \sin ka = -\kappa C e^{-\kappa a}. \quad \cdots\cdots (13)$$

Dividing (13) by (12) we get

$$k \tan ka = \kappa$$

or

$$\boxed{ka \tan ka = \kappa a} \quad \cdots\cdots (14)$$

for even solutions.

Odd solutions

We now look for the odd solutions. In region II, we have to take $\sin kx$ as the solution;

$$\psi_{II}(x) = A \sin kx . \quad (-a < x < a)$$

Also $\psi_I(x)$ and $\psi_{III}(x)$ are of the form

$$\psi_I(x) = C e^{Kx} \quad (x < -a)$$

$$\psi_{III}(x) = D e^{-Kx} \quad (x > a).$$

Since $\psi(x)$ is odd, we must now choose $D = -C$.

Therefore

$$\psi(x) = \begin{cases} C e^{Kx} & x < -a \quad \text{Region I} \\ A \sin kx & -a < x < a \quad \text{Region II} \\ -C e^{-Kx} & x > a \quad \text{Region III}. \end{cases} \quad \text{--- (15)}.$$

The continuity of $\psi(x)$ and $\psi'(x)$ at $x = a$ yields

$$A \sin ka = -C e^{-Ka}$$
$$kA \cos ka = KC e^{-Ka}$$

or

$$k \cot ka = -K$$

or

$$\boxed{ka \cot ka = -Ka} \quad \text{. . . . . . (16)}$$

(odd solutions).

for

Energy levels.

We have obtained two transcendental equations, Eqs. (14) and (16) valid for even solutions and odd solutions, respectively. We rewrite these equations here

$$ka \tan ka = \kappa a \quad \text{(even)} \quad \cdots\cdots (14)$$

$$ka \cot ka = -\kappa a \quad \text{(odd)}. \quad \cdots\cdots (15)$$

The variables k and κ are defined as

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

and

$$\kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

Hence k and κ are not independent of each other. They are related by

$$(ka)^2 + (\kappa a)^2 = \frac{2mV_0 a^2}{\hbar^2} \quad \cdots\cdots (16)$$

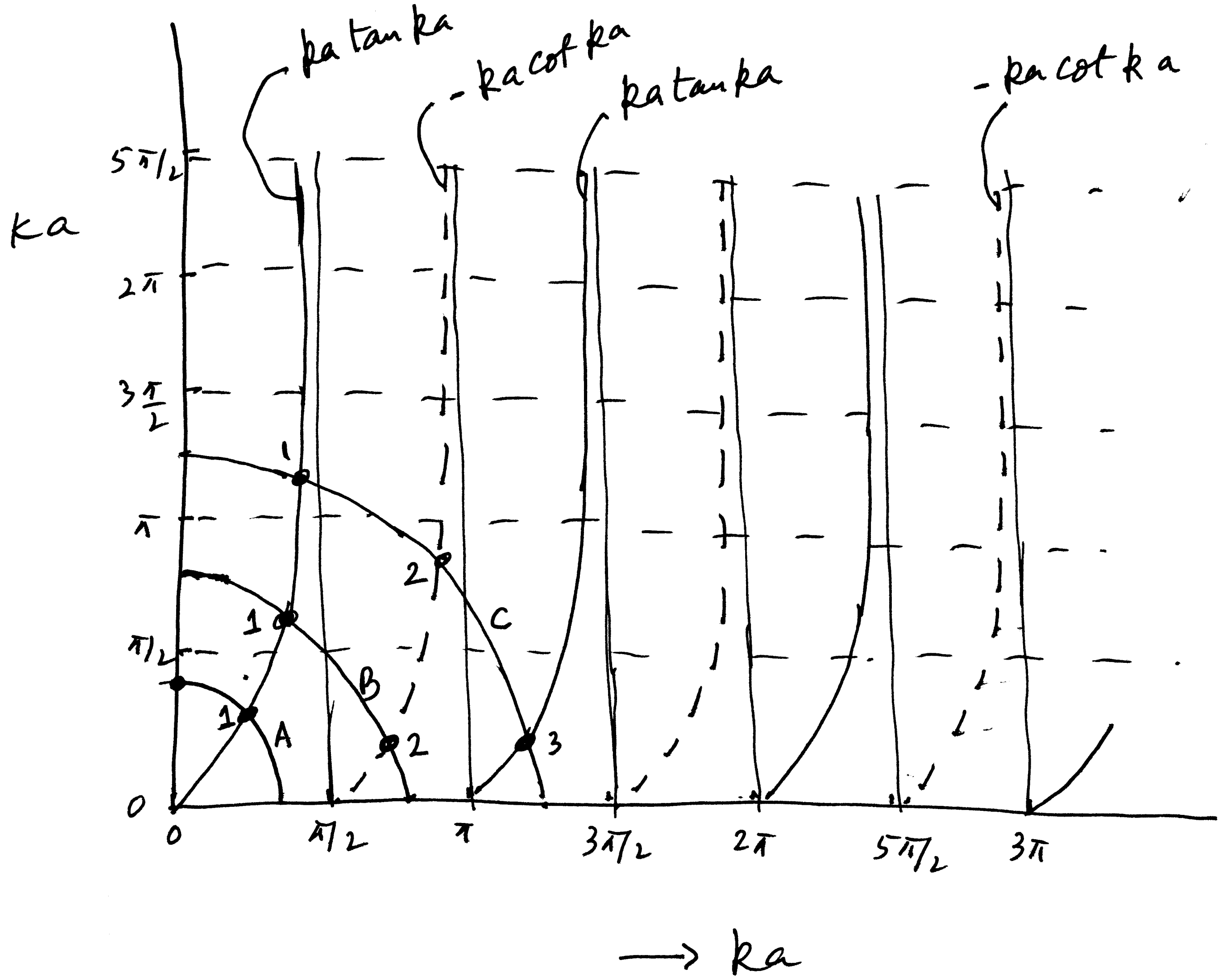
Note that in the $ka - \kappa a$ plane, Eq. (16) represents a circle of radius $\sqrt{2mV_0a^2/\hbar^2}$.

Graphical solutions for the energy levels.

To get the energy levels for the even parity states we plot Eqs. (14) and (16) in the $\kappa a - ka$ plane. The points of intersection give the possible values of k and hence the energy of the even parity states.

Similarly, to get the energy of the odd parity states we plot Eqs. (15) and (16) in the $\kappa a - ka$ plane and the points of intersections would then give us the possible energy values.

In the figure below, we have plotted both Eqs. (14) and (15) and Eq. (16). We have put κa along the y-axis and ka along the x-axis. Note that Eq. (16) are circles with radius $\sqrt{2mV_0a^2/\hbar^2}$.



Eq. (16) are represented by circles – circles A, B, C ..., in the plot. The radius of the circles are given by the formula

$$R = \sqrt{\frac{2mV_0a^2}{\hbar^2}}.$$

Depending upon the values of V_0a^2, different circles would have different radii. The quantity V_0a^2 is a measure of the strength of the potential. For a 'strong' potential, the value of V_0a^2 will be large, and consequently

The radius of the circle would be large too. Circles A, B, C, ... in the plot above correspond to square well potentials of increasing strength $V_0 a^2$.

First, suppose that the strength of the potential is not too large so that the radius of the circle is less than $\pi/2$ (circle A). For this potential

$$\sqrt{\frac{2mV_0a^2}{\hbar^2}} < \pi/2$$

or

$$\frac{2mV_0a^2}{\hbar^2} < \frac{\pi^2}{4}$$

or,

$$V_0a^2 < \frac{\pi^2\hbar^2}{8m}. \qquad \cdots\cdots (17)$$

For potential strengths satisfying (17), there is only one point of intersection (labelled by 1 in circle A). Thus there is only one bound state. To find the energy of the bound state we have to ~~read~~ read off the value of $y_1 \equiv ka$ for the point of intersection and the calculate E_1 according the formula

$$E_1 = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 y_1^2}{2ma^2}.$$

For circle A, the bound state is an even parity ~~states~~ state because the circle only intersects the curve $\kappa a = ka \tan ka$ which corresponds to even parity states.

Now imagine increasing the strength of the the potential such that so that the radius of the circle increases to a value between $\pi/2$ and π (circle B). For circle B

$$\pi/2 < \sqrt{\frac{2mV_0a^2}{\hbar^2}} < \pi$$

or

$$\frac{\pi^2}{4} < \frac{2mV_0a^2}{\hbar^2} < \pi^2 .$$

or

$$\frac{\pi^2\hbar^2}{8m} < V_0 a^2 < \frac{\pi^2\hbar^2}{2m} . \qquad \text{---- (18)}$$

Now there are two points of intersection marked 1 and 2 on circle B. So there are now two bound states. The state with lower energy (intersection 1) has even parity and the state with higher energy has odd parity.

Next, let us increase the strength of the energy even further, so that the circle has a radius between π and $3\pi/2$ (circle C), i.e

$$\pi < \sqrt{\frac{2mV_0 a^2}{\hbar^2}} < 3\frac{\pi}{2}$$

or $$\pi^2 < \frac{2mV_0 a^2}{\hbar^2} < \frac{9}{4}\pi^2$$

or $$\frac{\pi^2\hbar^2}{2m} < V_0 a^2 < \frac{9}{4}\cdot\frac{\pi^2\hbar^2}{2m} \quad \cdots\cdots (19)$$

For the potential with 'strength' $V_0 a^2$ lying in the range given in Eq. (19), there are three points of intersection, marked 1, 2 and 3 on circle C. So there are three bound states.

The state with lowest energy (intersection 1) has even parity, the state with next higher energy (intersection 2) has odd ~~even~~ parity, and the state with the highest energy (intersection 3) has again even parity. Thus the parity of the states alternates ~~be~~ between even and odd, starting with ~~the~~ even parity for the ground state.

From the above analysis it is clear that, if we keep on increasing ~~that~~ the strength of the potential, $V_0 a^2$, either making the well deeper and/or by making it broader, the potential can support an increasing number of bound states.

Finally, we note that if the potential is very weak, even then there is at least one bound state. This ~~fact is~~ statement is true only for one-dimensional potentials. In three dimensions, the potential strength of the potential has to exceed a certain value before a bound state can be supported.

Wave function

Previously we have written down the even wave functions in Eq (11) where the constant C is related to constant A according to Eq (12) which was obtained from the continuity of the wave function at $x = a$. Thus, we can write

$$\psi_{even}(x) = \begin{cases} A e^{\kappa a} \cos ka \, e^{\kappa x} & , \; x < -a \\ A \cos kx & , \; -a < x < a \\ A e^{\kappa a} \cos ka \, e^{-\kappa x} & , \; x > a \end{cases} \quad \text{---} (20)$$

There is one as yet undetermined constant A. This constant A is an overall multiplicative factor in the wave function. The value A can be found by normalizing the wave function to unity.

The odd wave functions are written down in Eq. (15). We can write

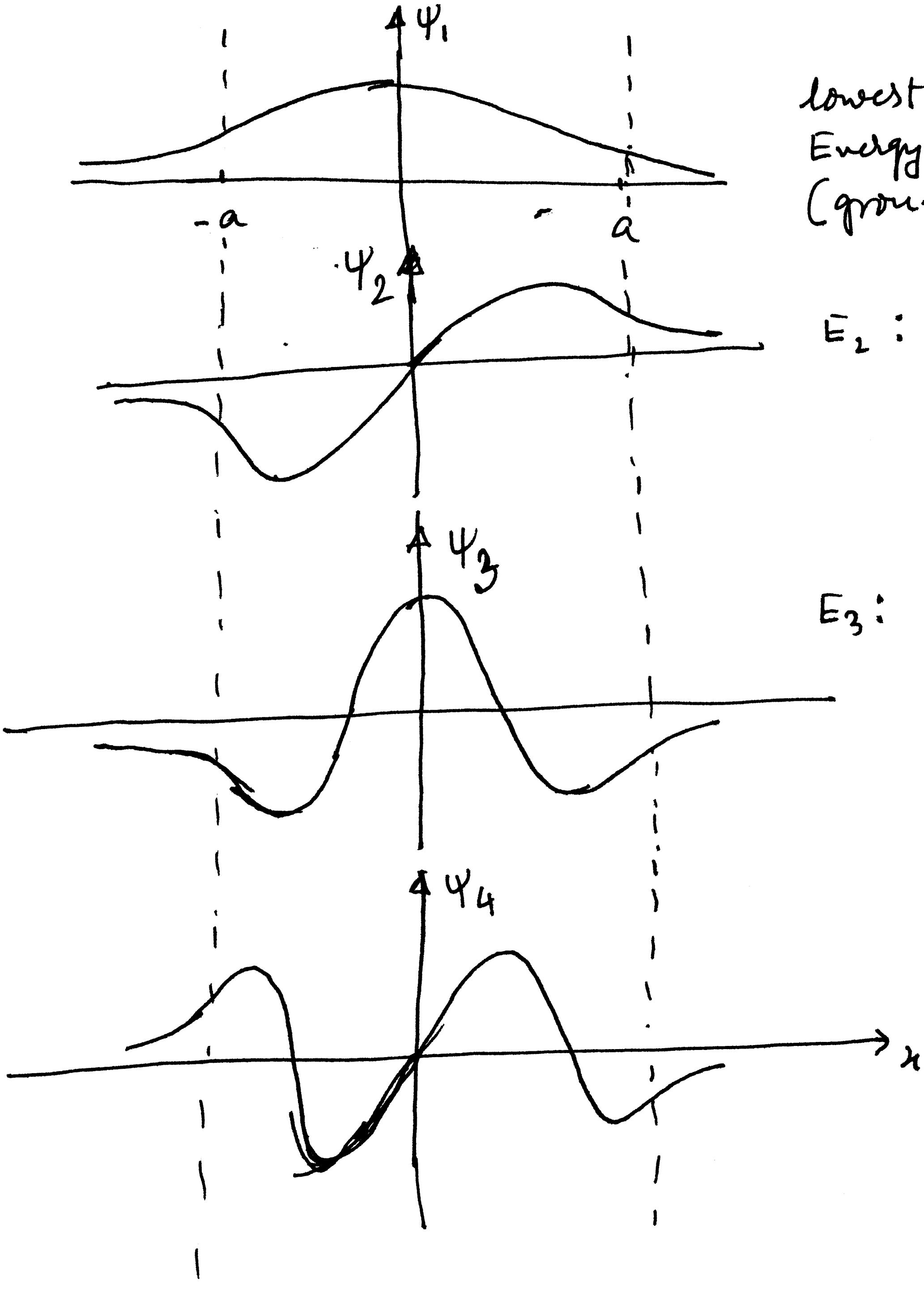
$$
\psi_{odd}(x) = \begin{cases} -A \sin ka \, e^{\kappa a} e^{\kappa x} & \text{for } x < -a \\ A \sin kx & \text{for } -a < x < a \\ A \sin ka \, e^{\kappa a} e^{-\kappa x} & \text{for } x > a \end{cases}
$$

where, as for the even wave functions, the constant A has to be found by normalizing the wave function.

For a potential of a certain strength $V_0 a^2$, there will be a finite number of bound states; exactly how many that depends on within what range of values $V_0 a^2$ lies. These states have discrete energies.

In the figure below we show qualitative plots of the bound states.

Graph of wave functions



lowest energy state * Energy E_1. (ground state)

E_2 : 1st excited state

E_3 : 2nd excited state

E_4 : Third excited state.

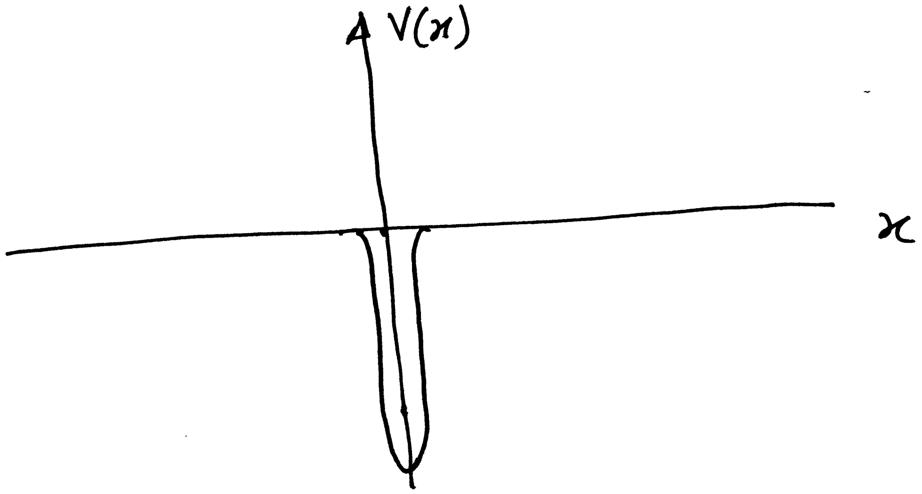
Note that there are no nodes in the wave function for the ground state. The wave function for the first excited state has one node, the wave function for the next higher state has two nodes. Thus higher the energy of the state, the larger the number of nodes in the wavefunction of that state.

Note also that the ground state wave function is even, for the next higher state the wave function is odd and so on. The parity of the states alternate between even and odd starting with even parity for the ground state.

Bound state in a delta function potential

Let us consider a potential of the form

$$V(x) = -a\,\delta(x) \qquad \cdots\cdots (1)$$



The Schrödinger equation for the delta-function potential reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} - a\,\delta(x)\,\psi(x) = E\,\psi(x) \qquad (2)$$

We will be looking for bound state solutions with $E < 0$.

In the region $x<0$ and $x>0$, $V(x)=0$. So the Schrödinger equation is

$$\frac{d^2\psi}{dx^2} = \underbrace{-\frac{2mE}{\hbar^2}}_{+ve}\psi(x) = K^2\psi(x) \qquad (3)$$

where

$$K = \sqrt{-\frac{2mE}{\hbar^2}} \; . \quad \text{-------- (3a)}$$

Note that K is real and positive since E is negative.

<u>$x<0$</u>

In the region $x<0$, the general solution of Eq. (3) is of the form

$$\psi(x) = Ae^{-Kx} + Be^{Kx} \quad \text{------ (4)}$$

The first term blows up as $x\to-\infty$. So we must choose $A=0$, so that

$$\psi(x) = Be^{Kx} \quad (x<0). \quad \text{---- (5)}$$

$x > 0$

In the region $x > 0$, $V(x)$ is again zero. The general solution of (3) for $x > 0$, is

$$\psi(x) = F e^{-kx} + G e^{kx}.$$

The second term blows up as $x \to \infty$. So we must choose $G = 0$, so that for ~~[illegible]~~, $x > 0$ the wave function is

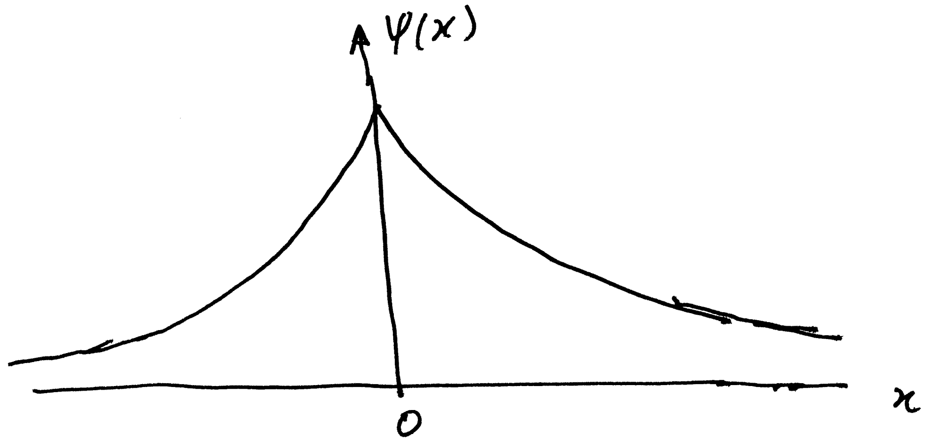
$$\psi(x) = F e^{-kx} \quad (x > 0). \quad \ldots\ldots \quad (6)$$

Boundary condition

The wave function $\psi(x)$ is continuous everywhere. Continuity of $\psi(x)$ at $x = 0$ implies $F = B$. Thus the wave function is

$$\psi(x) = \begin{cases} B e^{kx}, & x < 0 \\ B e^{-kx} & x > 0. \end{cases} \qquad (7)$$

The plot of the wave function is shown below



The derivative of ψ, $\psi'(x)$ is continuous everywhere except at points where the potential is infinite. We see that $\psi'(x)$ has a discontinuity at $x=0$ where the potential has an infinite discontinuity.

To find the discontinuity of $\psi'(x)$ at $x=0$, integrate the Schrödinger equation from $-\epsilon$ to ϵ. We have

$$-\frac{\hbar^2}{2m}\int_{-\epsilon}^{\epsilon}\frac{d^2\psi}{dx^2}\,dx + \int_{-\epsilon}^{\epsilon} V(x)\,\psi(x)\,dx = E\int_{-\epsilon}^{\epsilon}\psi(x)\,dx$$

Since $\psi(x)$ is continuous, the integral on the right hand side of this equation is zero. So we find

$$\lim_{\epsilon \to 0}\left[\frac{\partial \psi}{\partial x}\bigg|_{+\epsilon} - \frac{\partial \psi}{\partial x}\bigg|_{-\epsilon}\right] = \frac{2m}{\hbar^2}\lim_{\epsilon \to 0}\int_{-\epsilon}^{\epsilon} V(x)\,\psi(x)\,dx$$

$$= \frac{2m}{\hbar^2}\lim_{\epsilon \to 0}\int_{-\epsilon}^{\epsilon}\left(-a\,\delta(x)\right)\psi(x)\,dx$$

$$= -\frac{2ma}{\hbar^2}\,\psi(0)$$

or $\quad \Delta\left(\frac{\partial \psi}{\partial x}\right) = -\frac{2ma}{\hbar^2}\,\psi(0) \quad \cdots\cdots (9)$

Using $\psi(x)$ given in Eq. (7), Eq. (9) becomes

$$-KB - KB = -\frac{2ma}{\hbar^2}\,B$$

or $\quad 2K = \frac{2ma}{\hbar^2}$

or $\quad \boxed{K = \frac{ma}{\hbar^2}} \quad \cdots\cdots (10)$

Now, K is related to E as in Eq. (3a). Therefore, the energy of the bound state is

$$E = -\frac{\hbar^2 K^2}{2m} = -\frac{\hbar^2}{2m}\left(\frac{ma}{\hbar^2}\right)^2$$

or $\quad \boxed{E = -\frac{ma^2}{2\hbar^2}} \quad \cdots\cdots (11)$

Finally, we normalise $\psi(x)$.

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 2|B|^2 \int_0^{\infty} e^{-2Kx}$$

$$= 2|B|^2 \cdot \frac{1}{2K} = \frac{|B|^2}{K} = 1$$

$$\therefore \quad B = \sqrt{K} = \frac{\sqrt{ma}}{\hbar} \quad \text{- - - - - - -} (12)$$

Evidently, the delta function potential well regardless of its strength a, has exactly one bound state. In summary, the energy of the bound state and the corresponding normalized wave function is

$$\boxed{\begin{aligned} E &= -\frac{ma^2}{2\hbar^2} \\ \psi(x) &= \frac{\sqrt{ma}}{\hbar} e^{-m\alpha|x|/\hbar} \end{aligned}} \quad \text{- - -} (13)$$

Unbound (i.e., scattering) states in a potential well.

1. Transmission and reflection from a step potential.

Consider the step potential

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \quad \text{Region I} \\ V_0 & \text{for } x > 0 \quad \text{Region II} \end{cases} \quad \text{---} (1)$$

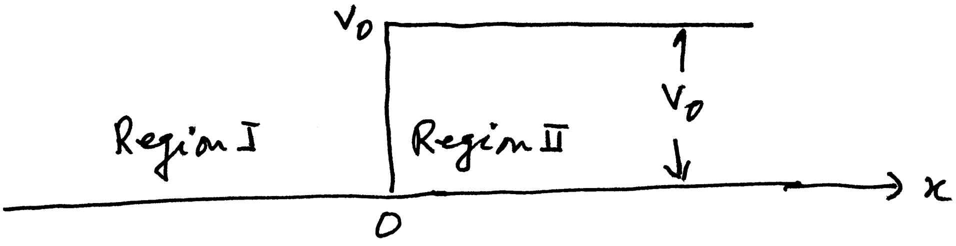


Fig: The step potential

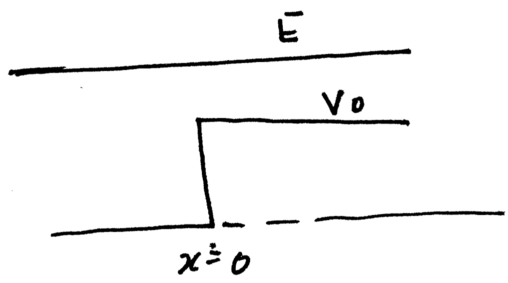
Consider the behaviour of a particle sent from the left of the plot with energy E. Classically we know the answer: If $E > V_0$ then the particle goes over the barrier and if $E < V_0$ the particle is reflected back. We would like to know what happens quantum mechanically.

Time independent Schrödinger equation is

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

We consider two cases:

• Case 1 $\quad E > V_0$



For a given energy we consider solutions independently in Regions I and II.

Region I $\quad$ In region I, $V=0$ and Eq. (2) becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \qquad (3)$$

or

$$\frac{d^2\psi}{dx^2} = -k^2\psi \qquad (4)$$

where we have defined

$$k = +\sqrt{\frac{2mE}{\hbar^2}} \, . \qquad (5)$$

There are two linearly independent solutions of Eq. (4). We can take these solutions to be e^{ikx} and e^{-ikx}

or, $\sin kx$ and $\cos kx$. We can write down the wave function in region I $(x<0)$ in a physically motivated way as

$$\psi(x) = \underbrace{e^{ikx}}_{\text{incoming}} + \underbrace{A e^{-ikx}}_{\text{reflected}} \qquad (6)$$

where A is the amplitude of the reflected wave. In other words, we set up the incoming (i.e., right moving) wave e^{ikx} and we want to calculate how much of the wave is reflected back as left moving e^{-ikx}. The functions e^{ikx} and e^{-ikx} are called right moving and left moving respectively, since they are eigenfunctions of the momentum operator $\hat{p}$ with eigenvalues $+\hbar k$ and $-\hbar k$ respectively.

In region I there is a probability current heading in the $+x$ direction. The probability current is

$$J_I = \frac{\hbar}{2mi}\left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx}\right)$$

$$= \frac{\hbar}{m} \operatorname{Im}\left(\psi^* \frac{d\psi}{dx}\right)$$

$$= \frac{\hbar}{m} \operatorname{Im}\left[\left(e^{-ikx} + A^* e^{ikx}\right) \frac{d}{dx}\left(e^{ikx} + A e^{-ikx}\right)\right]$$

$$= \frac{\hbar}{m} \operatorname{Im}\left[\left(e^{-ikx} + A^* e^{ikx}\right) ik\left(e^{ikx} - A e^{-ikx}\right)\right]$$

$$= \frac{\hbar}{m} \operatorname{Im}\left[ik\left(1 - |A|^2 - A e^{-2ikx} + A^* e^{2ikx}\right)\right]$$

$$= \frac{\hbar}{m} \operatorname{Im}\left[ik\left(1 - |A|^2 + 2i \operatorname{Im}\left(A^* e^{2ikx}\right)\right)\right]$$

$$= \frac{\hbar k}{m}\left(\underbrace{1}_{J_{inc}} - \underbrace{|A|^2}_{J_{ref}}\right) \qquad \text{.....(7)}$$

$$= J_{inc} - J_{ref}$$

where

$$J_{inc} = \frac{\hbar k}{m}$$

and

$$J_{ref} = \frac{\hbar k}{m} |A|^2 \quad \text{- - - - - (8)}$$

Here J_{inc} is the current carried by the right moving wave and J_{ref} is the reflected current carried by the left moving wave. If $|A| = 1$, then the total current is zero, i.e., everything is reflected back.

• Region II

In this region $V = V_0$ and the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = (E - V_0)\psi \quad \text{- - - - - (9)}$$

Since $E > V_0$, let us define

$$q = +\sqrt{\frac{2m(E-V_0)}{\hbar^2}} > 0 \quad \text{- - - - - (10)}$$

So we get

$$\frac{d^2\psi}{dx^2} = -q^2\psi(x) \quad \text{- - - - - (11)}$$

which is also oscillatory.

Since there is no left moving wave in region II, the general solution is

$$\psi(x) = \underbrace{B e^{iqx}}_{\text{transmitted}} \qquad (12)$$

where B quantifies the amplitude of the transmitted wave. The current can be calculated as usual, and it is

$$J_{\mathrm{II}} = J_{\text{transmitted}} = \frac{\hbar q}{m} |B|^2 \qquad (13)$$

We want to find A and B as functions of k and q by matching solutions at $x = 0$. The wave function $\psi(x)$ is continuous at $x = 0$. Since the potential has only a finite discontinuity at $x = 0$, the derivative of the wave function is also continuous at $x = 0$.

Now, the wave function is of the form: (Eqs. (6) and (12))

$$\psi(x) = \begin{cases} e^{ikx} + A e^{-ikx} & , x < 0 \\ B e^{iqx} & , x > 0 . \end{cases}$$

Therefore continuity of ψ and ψ' at $x=0$ gives us

$$1 + A = B \quad \text{.......} (14)$$

and

$$ik(1-A) = iq\, B \quad \text{.......} (15).$$

Substituting the value of B from Eq. (14) into Eq. (15) we get

$$ik(1-A) = iq(1+A)$$

or

$$A = \frac{k+q}{k-q} . \quad \text{.......} (16)$$

Substituting this expression for A in Eq. (15) we get

$$B = \frac{2k}{k+q} \quad \text{.......} (17)$$

We define reflectivity and transmissivity as

$$R = \frac{J_{ref}}{J_{inc}}$$

and

$$R = \frac{J_{trans}}{J_{inc}}$$

Using Eqs. (8) and (13) we get

$$R = |A|^2 = \left(\frac{k-q}{k+q}\right)^2 \quad \cdots\cdots (18)$$

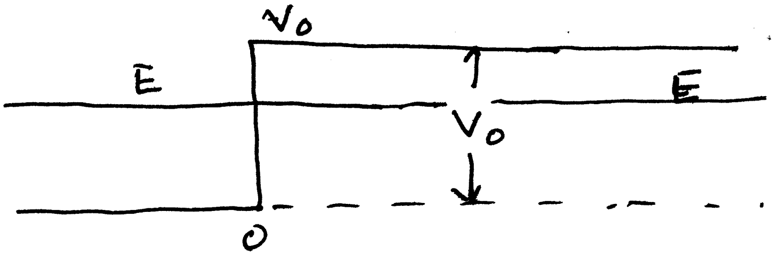
and

$$T = \frac{\frac{\hbar q}{m}|B|^2}{\frac{\hbar k}{m}} = \frac{q}{k}\,\frac{4k^2}{(k+q)^2} = \frac{4kq}{(k+q)^2}. \quad (19)$$

So, as E becomes very large, i.e., $E \gg V_0$, $q \to k$ and $R = 0$ and $T = 1$. Note that even when ~~~~ $E > V_0$, there is a non-zero chance of particles being reflected, unlike the classical case. Note also that

$$R + T = 1. \quad \cdots\cdots (20)$$

Case 2 $E < V_0$



In region I, the solution is as before, i.e.,

$$\psi_I(x) = e^{ikx} + A e^{-ikx} \quad (x<0) . \quad \text{---}(21)$$

In region II, the Schrödinger equation is

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}(V_0 - E)\,\psi$$

Since $V_0 - E$ is positive, define the quantity K as

$$K = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

This equation has the solution

$$\psi_{II}(x) = B e^{-Kx} + C e^{Kx} \quad (x>0)$$

Since $e^{Kx} \to \infty$ as $x \to \infty$, we must choose $C = 0$.

Therefore

$$\psi_{II}(x) = B e^{-Kx} \quad (x>0) . \quad \text{----}(22)$$

i.e., the wave function decays as it penetrates the barrier.

Now, we can find A and B as functions of k and K by applying the boundary conditions at $x=0$ and then ~~B~~ find R and T.

However we can use our previous solutions in the case $E > V_0$ (Eqs. (16) and (17)) and substitute $q \to iK$, to find the coefficients

$$A = \frac{k - iK}{k + iK}, \quad B = \frac{2k}{k + iK}. \quad \cdots (23)$$

The current in region II vanishes

$$J_{II} = \frac{\hbar}{2mi}\left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx}\right) = 0$$

meaning that no particle is ~~trans~~ transmitted, i.e., $T = 0$. What about the reflectivity R? Since $|A|^2 = 1$,

$$J_{ref} = J_{inc}$$

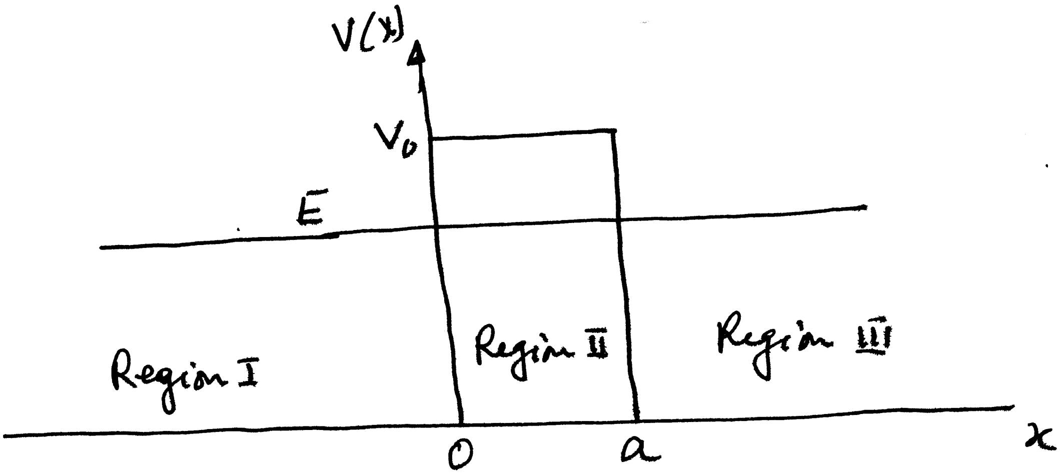
and

$$R = 1.$$

The Barrier Potential : Tunneling

Consider the potential barrier

$$V(x) = \begin{cases} V_0 & \text{for } 0 < x < a \\ 0 & \text{otherwise} . \end{cases} \quad \ldots (1)$$



In the previous example of the step potential, we saw that even if $E < V_0$, the wave function penetrates into the barrier and decays exponentially as long as the barrier is in place. Now, what happens if after some distance a, the potential again drops to zero as shown in the figure above? The wave function falls until it hits $x = a$, and then suddenly it is no longer suppressed by the potential and is free to propagate. Physically this means that there is a non-zero probability of finding the particle on the other side of the barrier — we say that the particle has ~~tunnelled~~ tunneled through the barrier, and this phenomenon is called Tunneling.

We will demonstrate tunneling through the potential barrier (Eq. (1)) by assuming that $E < V_0$. As before we define the variables

$$k = \sqrt{\frac{2mE}{\hbar^2}} \quad \text{and} \quad K = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \, . \qquad (2)$$

The wave function can be written down immediately

$$\psi(x) = \begin{cases} e^{ikx} + Ae^{-ikx}, & x < 0 \quad \text{Region I} \\ Be^{-Kx} + Ce^{Kx}, & 0 < x < a \quad \text{Region II} \\ De^{ikx}, & x > a \quad \text{Region III} \end{cases} \qquad (3)$$

At boundary $x=0$ continuity conditions imply

$$1+A = B+C \quad \cdots\cdots (4)$$

$$ik(1-A) = K(-B+C) \quad \cdots\cdots (5)$$

whilst at $x=a$ we get

$$Be^{-Ka} + Ce^{Ka} = De^{ika} \quad \cdots\cdots (6)$$

$$-KBe^{-Ka} + KCe^{Ka} = ikDe^{ika} \quad \cdots\cdots (7)$$

We then do a bunch of tedious algebra for A, B, C and D. Since we are interested in the transmitted current, we look for D.

Solution for D

Multiply Eq(6) by K.

$$KBe^{-Ka} + KCe^{Ka} = KDe^{ika} \quad \cdots\cdots (8)$$

Now, add Eq (7) and Eq (8). We get

$$2KCe^{Ka} = D(K+ik)e^{ika}$$

or

$$C = \frac{1}{2}D\left(1+\frac{ik}{K}\right)e^{ika-Ka} \quad \cdots\cdots (9)$$

Next, subtract (7) from (8), i.e., (8) − (7).

$$2\kappa B e^{-\kappa A} = D(\kappa - ik)e^{ika}$$

or $$B = \frac{1}{2} D\left(1 - i\frac{k}{\kappa}\right)e^{ika+\kappa a} \quad \ldots\ldots (10)$$

Next, (5) is written as

$$1 - A = -i\frac{\kappa}{k}(-B + C)$$

$$1 - A = i\frac{\kappa}{k}B - i\frac{\kappa}{k}C \quad \ldots\ldots (11)$$

Now add Eq (4) and Eq. (11)

$$2 = \left(1 + i\frac{\kappa}{k}\right)B + \left(1 - i\frac{\kappa}{k}\right)C \quad \ldots (12)$$

Next, substitute Eq. (10) and Eq. (9) in Eq. (12).

$$2 = \frac{1}{2}De^{ika}\left[\left(1 + i\frac{\kappa}{k}\right)\left(1 - i\frac{k}{\kappa}\right)e^{\kappa a} + \left(1 - i\frac{\kappa}{k}\right)\left(1 + i\frac{k}{\kappa}\right)e^{-\kappa a}\right]$$

or $$2 = \frac{1}{2} D e^{ika} \left[\left\{ 2 + i\left(\frac{K}{k} - \frac{k}{K}\right) \right\} e^{Ka} + \left\{ 2 - i\left(\frac{K}{k} - \frac{k}{K}\right) \right\} e^{-Ka} \right]$$

or $$2 = \frac{1}{2} D e^{ika} \left[2\left(e^{Ka} + e^{-Ka}\right) + i\left(\frac{K}{k} - \frac{k}{K}\right)\left(e^{Ka} - e^{-Ka}\right) \right]$$

or $$2 = D e^{ika} \left[2\left(\frac{e^{Ka} + e^{-Ka}}{2}\right) + i\,\frac{K^2 - k^2}{Kk}\left(\frac{e^{Ka} - e^{-Ka}}{2}\right) \right]$$

or $$2 = D e^{ika} \left[2\cosh Ka + i\,\frac{(K^2 - k^2)}{Kk} \sinh Ka \right]$$

or $$D = \frac{2 e^{-ika}}{2\cosh Ka + i\,\frac{(K^2 - k^2)}{Kk} \sinh Ka}$$

or $$\boxed{D = \frac{2Kk\, e^{-ika}}{2Kk\cosh Ka + i\,(K^2 - k^2)\sinh Ka}} \quad (13)$$

The incident and the transmitted flux are

$$J_{inc} = \frac{\hbar k}{m}$$

$$J_{trans} = J_{III} = \frac{\hbar k}{m} |D|^2 .$$

Therefore the transmissivity is

$$T = \frac{J_{trans}}{J_{inc}} = \frac{(\hbar k/m)\,|D|^2}{(\hbar k/m)}$$

or $$T = |D|^2$$

or $$\boxed{T = \frac{4K^2k^2}{(K^2-k^2)^2 \sinh^2 Ka + 4K^2k^2 \cosh^2 Ka}} \qquad (14)$$

So the transmissivity is not zero.

We will rewrite Eq (14) in a slightly different way. We know

$$\cosh^2 x - \sinh^2 x = 1 \Rightarrow \cosh^2 x = 1 + \sinh^2 x$$

$\therefore$ Eq (14) can be rewritten as

$$T = \frac{1}{\cosh^2 Ka + \frac{(K^2 - k^2)^2}{4K^2k^2} \sinh^2 Ka}$$

$$= \frac{1}{1 + \left(1 + \frac{(K^2 - k^2)^2}{4K^2k^2}\right) \sinh^2 Ka}$$

$$\boxed{T = \frac{1}{1 + \frac{(K^2 + k^2)^2}{4K^2k^2} \sinh^2 Ka}} \qquad (15)$$

Next we will express T in terms of E & V_0.

We have

$$K = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

$$k = \sqrt{\frac{2m}{\hbar^2}E}$$

Therefore

$$\frac{(K^2+k^2)^2}{4K^2k^2} = \frac{(V_0 - E + E)^2}{4(V_0-E)E} = \frac{V_0^2}{4E(V_0-E)}$$

Hence

$$\boxed{T = \frac{1}{1 + \frac{V_0^2}{4E(V_0-E)}\sinh^2 Ka}} \quad \text{----(16)}$$

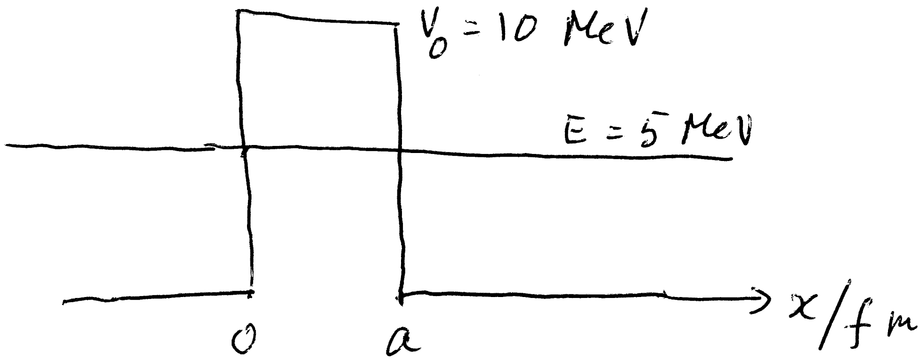
Now, it is usually ~~that~~ the case that κa is large. This factor is large if κ and a are large. κ is large if $E \ll V_0$ and large a means that the width of the barrier is large. For large κa, we can make the following approximation

$$\sinh \kappa a = \frac{e^{\kappa a} - e^{-\kappa a}}{2} \approx \frac{1}{2} e^{\kappa a}$$

i.e. $\sinh \kappa a$ is large. The factor multiplying the $\sinh^2 \kappa a$ in the denominator of Eq. (16) is of the order of unity. So the factor 1 in the denominator can be neglected. We then get

$$\boxed{T \approx \frac{16 E (V_0 - E)}{V_0^2} \, e^{-2\kappa a} \quad (\kappa a \gg 1)} \qquad \cdots\cdots (17)$$

<u>Ex</u> Consider a 5 MeV proton incident upon a rectangular barrier of height 10 MeV and width 10 fm. What is the probability that the proton would tunnel through the barrier?



The transmission coefficient is

$$T = 16\left(\frac{E}{V_0}\right)\left(1-\frac{E}{V_0}\right)e^{-2Ka} \qquad (Ka \gg 1)$$

Now

$$K = \sqrt{\frac{2m(V_0-E)}{\hbar^2}} = \sqrt{\frac{2\times\overset{940}{\cancel{470}}\text{ MeV}\times 5\text{ MeV}}{(197\text{ MeV fm})^2}}$$

$$= 0.49\text{ fm}^{-1}$$

$$\therefore Ka = 0.49\text{ fm}^{-1}\times 10\text{ fm} = 4.9$$

Note that κa is sufficiently large so that

$\sinh \kappa a \approx \frac{1}{2} e^{\kappa a}$,

The transmission coefficient (or transmissivity or transmission probability) is then

$$T = 16\left(\frac{E}{V_0}\right)\left(1-\frac{E}{V_0}\right)e^{-2\kappa a}$$

$$= 16 \times \frac{1}{2} \times \left(1-\frac{1}{2}\right) e^{-2\times 4.9}$$

$$= 4 \times e^{-9.8}$$

$$= 2.2 \times 10^{-4}$$

Calculational notes.

- Mass of proton $m = 1.673 \times 10^{-27}$ kg

$\therefore mc^2 = 1.673 \times 10^{-27}$ kg $\times (3.0 \times 10^8 \text{ m s}^{-1})^2$

$= 1.506 \times 10^{-10}$ J

$= 940$ MeV

| 1 eV $= 1.60 \times 10^{-19}$ J
| 1 MeV $= 1.60 \times 10^{-13}$ J

$\therefore \boxed{m = 940 \text{ MeV}/c^2}$

- $\hbar = 1.0546 \times 10^{-34}$ J s

$c = 3.0 \times 10^8 \text{ m s}^{-1}$

$\therefore \hbar c = (1.05 \times 10^{-34} \text{ J s})(3.0 \times 10^8 \text{ m s}^{-1})$

$= 3.15 \times 10^{-26}$ J m

$= (3.15 \times 10^{-26}) \left(\frac{1}{1.60 \times 10^{-13}} \text{ MeV}\right) \times (10^{15} \text{ fm})$

| 1 MeV $= 1.60 \times 10^{-13}$ J
| $\therefore 1 \text{ J} = \frac{1}{1.60 \times 10^{-13}}$ MeV
| 1 m $= 10^{15}$ fm

$= 196.9$ MeV fm

≈ 197 MeV fm.

——— X ———

END