Hooghly Women's College, Department of Physics
PHYH-C IX: ELEMENTS OF MODERN PHYSICS

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1 Quantum particle inside one dimensional infinitely rigid box

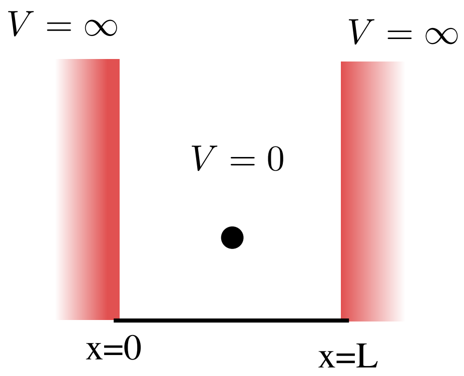

Figure 1: The potential inside the box is zero. Outside the box, the potential is infinite. The size of the box is from $0 < x < L$

The infinite square well of width L and infinte height is defined as

$$V(x) = 0, \quad for \ \ 0 \le x \le L \tag{1}$$
$$= \infty \quad otherwise \tag{2}$$

here E is the energy of particle of mass m inside the box, where the potential is $V(x) = 0$. You know how the Hamiltonian is coming:

$$\hat{p} = -i\hbar\frac{\partial}{\partial x} \tag{3}$$
$$\hat{H} = \hat{T} + \hat{V} = \frac{\hat{p}^2}{2m} + V(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \tag{4}$$

The Schrodinger ewquation in 1D is written as

$$\hat{H}\Psi(x) = E\Psi(x) \tag{5}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + V(x)\Psi(x) = E\Psi(x) \tag{6}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} = E\Psi(x) \tag{7}$$

$$\frac{d^2\Psi(x)}{dx^2} + \frac{2mE}{\hbar^2}\Psi(x) \tag{8}$$

$$\frac{d^2\Psi(x)}{dx^2} + k^2\Psi(x) \tag{9}$$

Where

$$k^2 = \frac{2mE}{\hbar^2} \tag{10}$$

Solving Eq.(9) we get

$$\Psi(x) = A\sin kx + B\cos kx \tag{11}$$

The boundary consditions are

$$\Psi(x=0) = 0; \qquad \Psi(x=L) = 0 \tag{12}$$

This gives us

$$B = 0; \qquad \sin(kL) = 0 \tag{13}$$

This Eq. (13) gives

$$kL = n\pi; \qquad k_n = \frac{n\pi}{L}; \qquad n = 1, 2, 3, \cdots \tag{14}$$

the wave vector k has an index n such that, k_n has discrete values. So we get

$$\Psi(x) = A\sin\left(\frac{n\pi x}{L}\right) \tag{15}$$

Now how to get the values for A. We know that the particle must stay inside the box, as there is no way it can escape the infinite wall where the potential is infinite. So total probability for the particle to be inside the box of length L is 1. Thus the wave function must be normalized. So the imposed condition is

$$P = \int_{x=0}^{L} |\Psi(x)|^2 dx = 1 \tag{16}$$

$$A^2 \int_0^L \sin^2\frac{n\pi x}{L} dx = 1 \tag{17}$$

This gives $A^2 = \frac{2}{L}$. (Do the above integration as home work problem)

$$\Psi_n(x) = \sqrt{\frac{2}{L}}\sin(\frac{n\pi x}{L}) \tag{18}$$

We get the discrete energy (eigen values) as

$$k_n^2 = \frac{n^2\pi^2}{L^2} = \frac{2mE_n}{\hbar^2} \tag{19}$$

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \tag{20}$$

Now you can ask me any questions... Like what is the nature of wave function and energy values if the box is from $-L/2$ to $L/2$.

2 Quantum dot as example of 1D box

To my students: Read yourself how to realize potential inside an infinitely rigid box experimentally in laboratory. Smartest humankind of this earth have created single particle or few particle inside a tight confinement. Read some science journal and ask me if something not clear. I suggest to read Americal Physical Society articles (specially Phys Rev B), APS View Point, New Journal of Physics, Nature Physics article (not nature.com its narute physics.com) etc. This is one of my research interest. Hope you too come to this vast field and do your PhD in this topic rather than Astro Physics Black Hole Sring theory etc.

3 Step potential & Rectangular potential barrier

Quantum mechanical scattering and tunnelling in one dimension

Example-1: Problem of Step Potential

There is a step with energy V_0, which is starting at $x = 0$ in the positive x axis. Region 1 is $x < 0$ and region 2 is where $x > 0$.

The time independent Schroedinger equation is written as

$$H\psi = E\psi \tag{21}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi \qquad \textbf{Region 1} \tag{22}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V_0\psi(x) = E\psi(x) \qquad \textbf{Region 2} \tag{23}$$

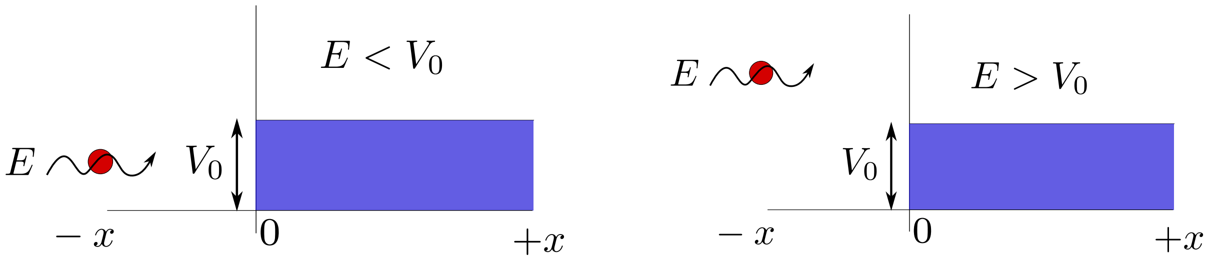

Figure 2: Step potential in the positive x axis. A particle with energy E is incident from left, and the energy of the particle can be less or higher than the step size.

We shall solve the above equations for two cases. (i) When the energy of the particle is below the step height. So $E < V_0$. See figure above. (ii) When the energy oa the particle is greated than the step potential height. $E > V_0$. See figure. To remind you the solution means, how the wave function $\psi(x)$ looks like in these two regions. The main idea is to find the wave function which is sinlge valued, well defined, continuous and finite everywhere. Let us solve for case by case.

Case 1: $E < V_0$

In region 1 , left side of the step $(x < 0)$. the Schrodinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \tag{24}$$

$$\frac{d^2\psi(x)}{dx^2} + k_1^2\psi(x) = 0; \qquad where\ \ k_1^2 = \frac{2mE}{\hbar^2} \tag{25}$$

$$\psi_I(x) = Ae^{ik_1x} + Be^{-ik_1x} \tag{26}$$

first term is for particle going to right and second term in for particle coming back after reflecting at $x = 0$. As the particle is coming from left, there is probability that the particle be reflected at the step as $E < V_0$. And there is also some probability that the particle be transmitted through the potential step.

In region 2: The particle can penetrate through the step potential and come to right side i.e. inside the potential step, we have $x > 0$. So the Schrodinger equation looks like

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V_0\psi(x) = E\psi(x) \tag{27}$$

$$\frac{d^2\psi(x)}{dx^2} - \frac{2m}{\hbar^2}(V_0 - E)\psi(x) = 0 \tag{28}$$

$$\frac{d^2\psi(x)}{dx^2} - k_2^2\psi(x) = 0; \qquad where \;\; k_2^2 = \frac{2m}{\hbar^2}(V_0 - E) > 0 \tag{29}$$

$$\psi(x) = Ce^{k_2 x} + De^{-k_2 x} \tag{30}$$

There is no chance, both classically or quantum mechanically, the particle can reflect back from inside the step as there is no wall and the potential is extended upto infinite. The physical situation is the wave function must be finite everywhere , so at $x = +\infty$, to have finite wave function we set $D = 0$. Thus

$$\psi_{II}(x) = Ce^{-k_2 x} \tag{31}$$

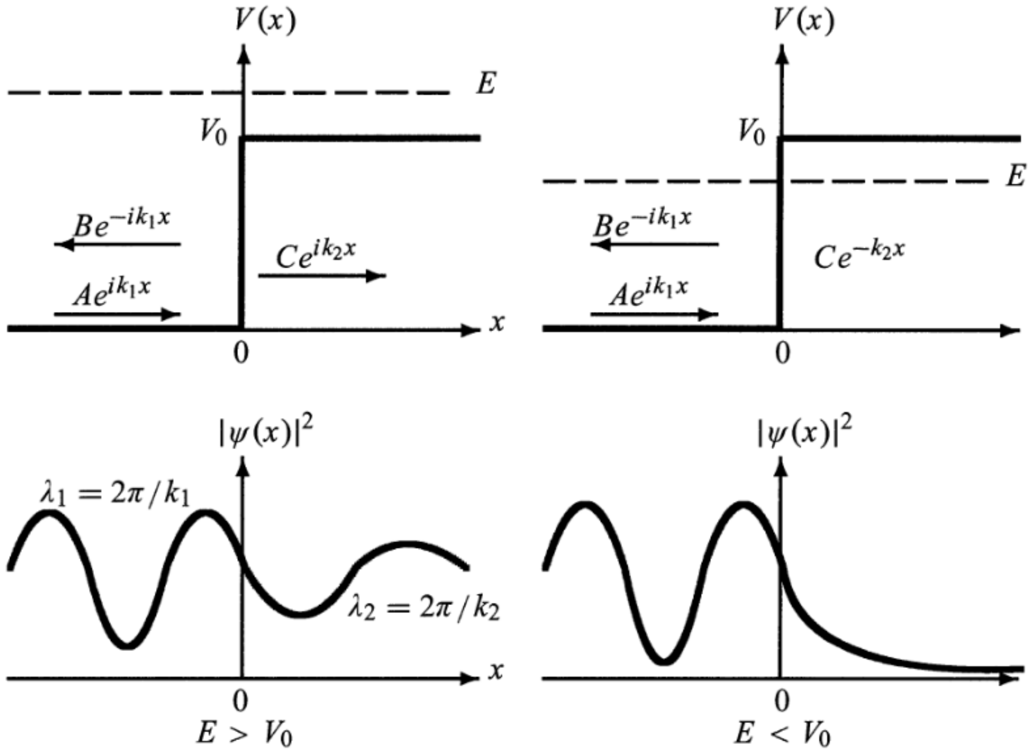

Figure 3: Potential step and propagation directions of the incident, reflected and transmitted waves, plus their probability densities $|\psi(x)^2|$ when $E > V_0$ and $E < V_0$. Figure taken from Zettili, Quantum Mechanics book.

Let us write the wavefunctions once again

$$\psi_I(x) = Ae^{ik_1 x} + Be^{-ik_1 x}; \qquad x < 0 \tag{32}$$

$$\psi_{II}(x) = Ce^{-k_2 x}; \qquad x > 0 \tag{33}$$

$$\tag{34}$$

Now we are in a position to find the transmission coefficient T and reflection coefficient R. And theoretically

$$R + T = 1 \tag{35}$$

The reflection coefficint (R) and transmission coefficients (T) are defined as

$$R = \frac{reflected\ current\ density}{incident\ current\ density} = \frac{J_{refl}}{J_{in}} \tag{36}$$

$$T = \frac{transmitted\ current\ density}{incident\ current\ density} = \frac{J_{trans}}{J_{in}} \tag{37}$$

we recall the probability current density expression from last chapter

$$J = \frac{i\hbar}{2m}\left(\psi\frac{\partial\psi^\star}{\partial x} - \psi^\star\frac{\partial\psi}{\partial x}\right) \tag{38}$$

please note that, the reflected part of the incident wave is $\psi_{refl} = Be^{-ik_1x}$, the incoming part of the incident wave which is going to right hand side is $\psi_{in} = Ae^{ik_1x}$ and the trnamitted part of the wave function is $\psi_{trans} = Ce^{-k_2x}$

> Home Work:
>
> Calculate the J_{trans}, J_{in} and J_{refl} and then calculate R and T for the case 1 described above. (i.e. particle coming from left hand side and incident at a step potential with enegy E lower than the step height.)

Case 2: $E > V_0$

If the particle has energy greater than the height of the step height, then there is always some reflection and transmission coefficients.

Calculate the wave functions and R and T for this problem as home work excercise. This is a lengthy problem and should be done carefully. If problem occurs, ask me in the class.

See the left panel of the figure (3)

Example-2: Problem of Potential Barrier

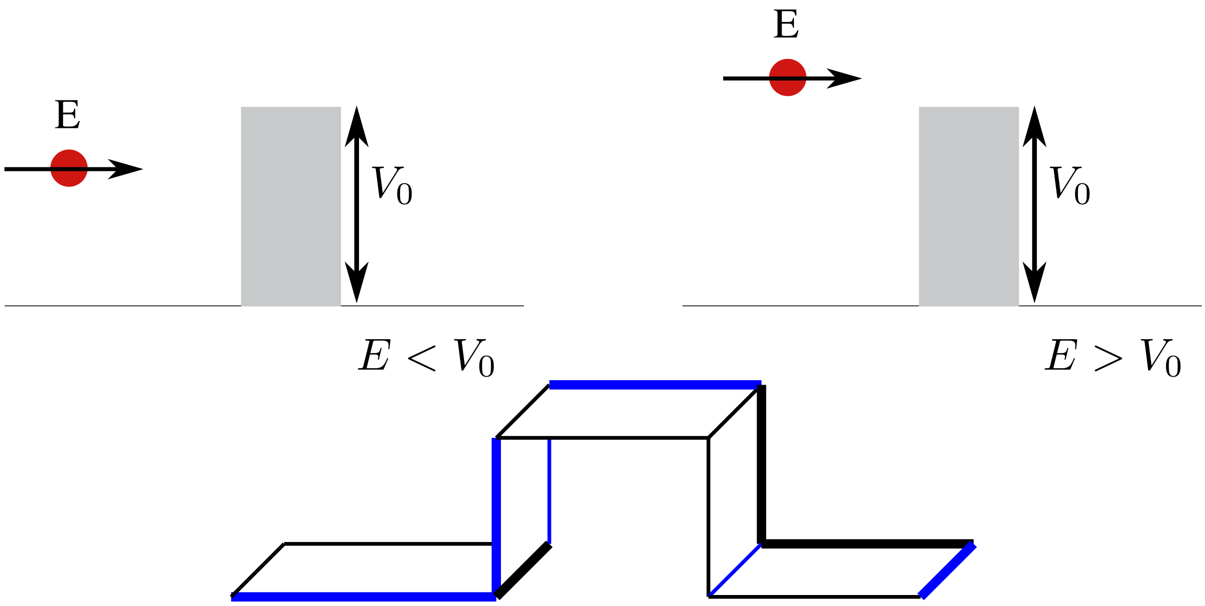

Figure 4: The particle in incident from left hand side and striking a potential barrier of with L. There may be two cases, when the energy (E) of the particle less than or greater than the height of the barrier V_0. The 3D potential barrier figure at bottom is created Using Latex PSTRICKS

Notes will be updated in future: