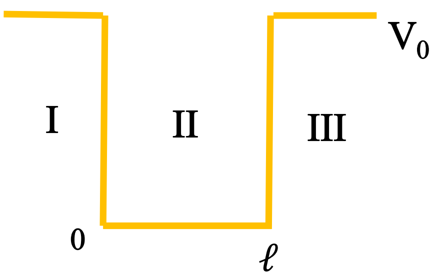
Particle in a Finite Box



$$V = V_0, \quad x < 0$$

$$V = 0, \quad 0 \le x \le \ell$$

$$V = V_0, \quad x > \ell$$

We know the form of the wave function in each of the three regions

$$\psi_{\mathrm{I}} = C e^{\sqrt{\frac{2m(V_0 - E)}{\hbar^2}}x}, \quad \psi_{\mathrm{III}} = G e^{-\sqrt{\frac{2m(V_0 - E)}{\hbar^2}}x}$$

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

$$\psi_{\mathrm{II}} = A\cos\left[\left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}} x\right] + B\sin\left[\left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}} x\right]$$

If we require ψ and its 1st derivative to be continuous then

$$\psi_{\mathrm{I}}(0)=\psi_{\mathrm{II}}(0),$$
$$\psi_{\mathrm{I}}'(0)=\psi_{\mathrm{II}}'(0)$$

and

$$\psi_{\mathrm{II}}(\ell)=\psi_{\mathrm{III}}(\ell),$$
$$\psi_{\mathrm{II}}'(\ell)=\psi_{\mathrm{III}}'(\ell)$$

To simplify, lets switch to atomic units and set m = 1, ħ = 1

$$\psi_{\mathrm{I}}=Ce^{\sqrt{2(V_0-E)}x}$$

$$\psi_{\mathrm{II}}=Acos\left(\sqrt{2E}x\right)+Bsin\left(\sqrt{2E}x\right)$$

$$\psi_{\mathrm{III}}=Ge^{-\sqrt{2(V_0-E)}x}$$

Consider first the case with E < V_0

$$\text{At } x = 0 \quad \psi_{\text{I}}(0) = \psi_{\text{II}}(0)$$

$$\Rightarrow C = A$$

$$\psi_{\text{I}}'(0) = \psi_{\text{II}}'(0)$$

$$\Rightarrow C\sqrt{2(V_0 - E)} = -\sqrt{2E}A\sin(0) + \sqrt{2E}B\cos(0)$$

$$= \sqrt{2E}B$$

So $B = \dfrac{\sqrt{V_0 - E}}{\sqrt{E}}C = \dfrac{\sqrt{V_0 - E}}{\sqrt{E}}A$

At $\quad x = \ell \quad \psi_{\text{II}}(\ell) = \psi_{\text{III}}(\ell)$

$$\Rightarrow A\cos\left(\sqrt{2E}\ell\right) + B\sin\left(\sqrt{2E}\ell\right) = Ge^{-\sqrt{2(V_0 - E)}\ell}$$

$$\psi_{\text{II}}'(\ell) = \psi_{\text{III}}'(\ell)$$

$$-A\sqrt{2E}\sin\left(\sqrt{2E}\ell\right) + B\sqrt{2E}\cos\left(\sqrt{2E}\ell\right) \quad = -G\sqrt{2(V_0 - E)}e^{\sqrt{(V_0 - E)}\ell}$$

$$\sqrt{(V_0 - E)}C = \sqrt{E}B$$

$$A\cos\left(\sqrt{2E}\ell\right) + B\sin\left(\sqrt{2E}\ell\right) = Ge^{-\sqrt{2(V_0-E)}\ell}$$

$$-\sqrt{2E}A\sin\left(\sqrt{2E}\ell\right) + \sqrt{2E}B\cos\left(\sqrt{2E}\ell\right) = -\sqrt{2(V_0 - E)}Ge^{-\sqrt{2(V_0-E)}\ell}$$

$$\sqrt{2E}\,\frac{\left[-A\sin\left(\sqrt{2E}\ell\right) + B\cos\left(\sqrt{2E}\ell\right)\right]}{A\cos\left(\sqrt{2E}\ell\right) + B\sin\left(\sqrt{2E}\ell\right)} = -\sqrt{2(V_0 - E)}$$

Substitute $B = \frac{\sqrt{V_0 - E}}{\sqrt{E}}A$ From previous slide

$$\frac{\sqrt{2E}\left[-\sin\left(\sqrt{2E}\ell\right) + \frac{\sqrt{V_0 - E}}{\sqrt{E}}\cos\left(\sqrt{2E}\ell\right)\right]}{\cos\left(\sqrt{2E}\ell\right) + \frac{\sqrt{V_0 - E}}{\sqrt{E}}\sin\left(\sqrt{2E}\ell\right)} = -\sqrt{2(V_0 - E)}$$

$$\sqrt{2E}\sin(y)-\sqrt{2E}\frac{\sqrt{V_0-E}}{\sqrt{E}}\cos(y)=\sqrt{2(V_0-E)}\left[\cos(y)+\frac{\sqrt{V_0-E}}{\sqrt{E}}\sin(y)\right]$$

$$y=\sqrt{2E}\ell$$

$$\sqrt{2E}\sin(y)-\sqrt{2}\sqrt{V_0-E}\cos(y)=\sqrt{2(V_0-E)}\cos(y)+\frac{\sqrt{2}(V_0-E)}{\sqrt{E}}\sin(y)$$

$$\left[\sqrt{2E}-\frac{\sqrt{2}(V_0-E)}{\sqrt{E}}\right]\sin(y)=2\sqrt{2(V_0-E)}\cos(y)$$

$$\left[\sqrt{2}E-\sqrt{2}(V_0-E)\right]\sin(y)=\sqrt{2E}\,2\sqrt{(V_0-E)}\cos(y)$$

$$(2E-V_0)\sin(y)=2\sqrt{(V_0-E)}\sqrt{E}\cos(y)$$

$$(2E-V_0)\sin(y)=2\sqrt{V_0E-E^2}\cos(y)$$

$$\tan y=\frac{2\sqrt{V_0E-E^2}}{2E-V_0}=\tan\left(\sqrt{2E}\ell\right)$$

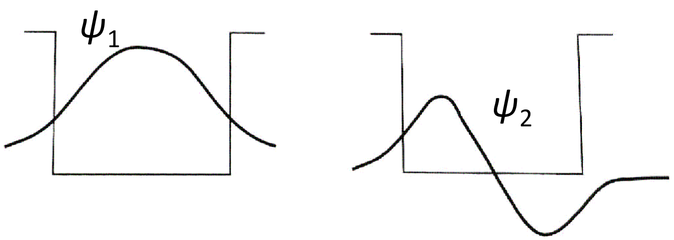
For $V_0\rightarrow\infty$, the energy levels should go over to those of the infinite box case

Show this.

Note that a classical particle with $E < V_0$, the particle would be found only inside the box.

In the QM system there is a probability it is found outside the box (tunneling)

Lets examine in more detail the wave function in the region x > ℓ

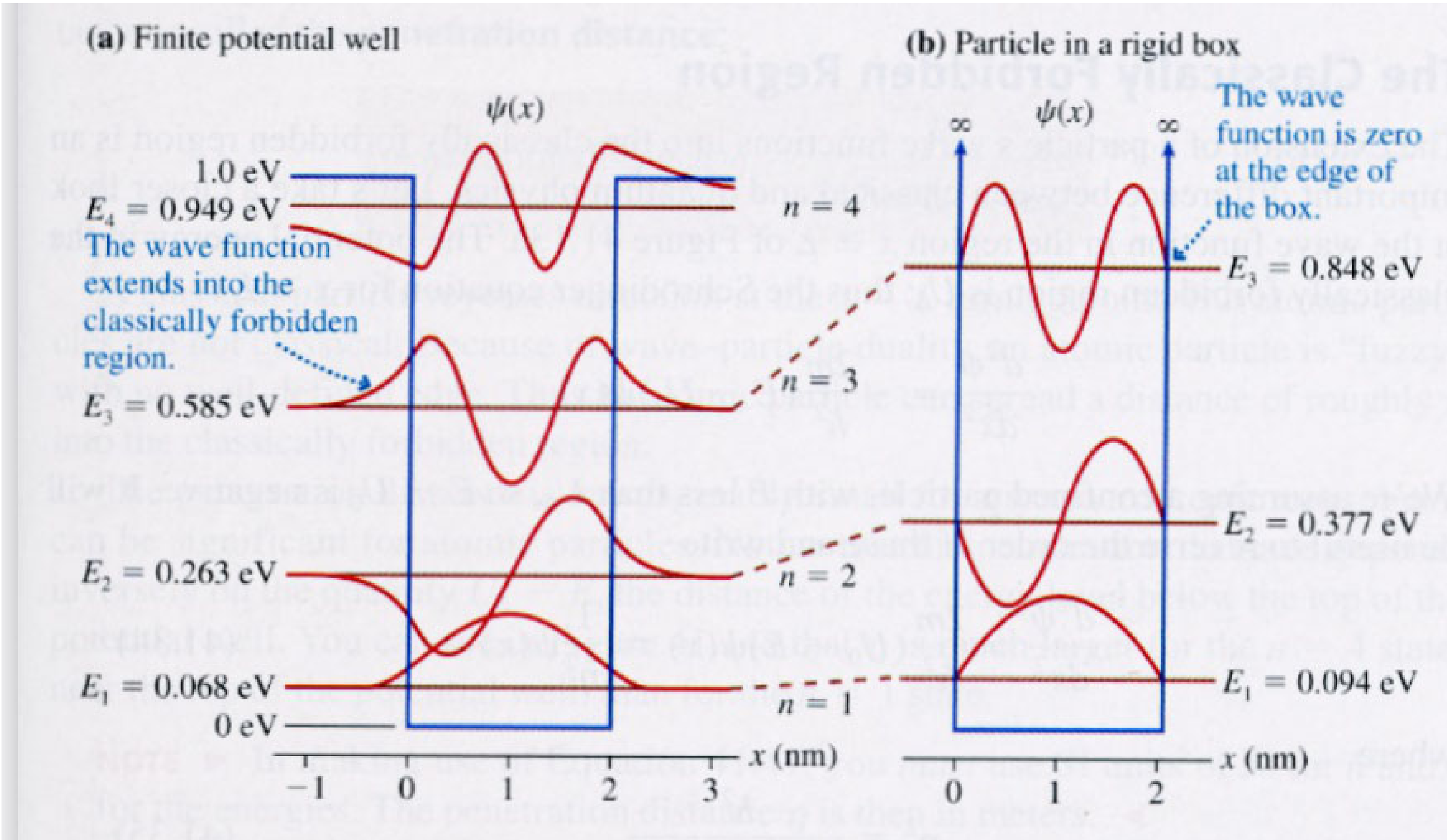


$$\psi_{\mathrm{III}} = G e^{-\sqrt{\frac{2m(V_0 - E)}{\hbar^2}}x}$$

Tunneling is more important

when m is small

the energy is near the top of the top of the potential



Taken from: http://cs.westminstercollege.edu/~ccline/courses/phys301/Knight

Now consider $E > V_0$

$$\psi_I = Ae^{-i\sqrt{2(E-V_0)}x} + Be^{i\sqrt{2(E-V_0)}x} = Ae^{-iKx} + Be^{iKx}$$

$$\psi_{II} = C\cos\left(\sqrt{2E}x\right) + D\sin\left(\sqrt{2E}x\right) = C\cos(kx) + D\sin(kx)$$

$$\psi_{III} = Ge^{-i\sqrt{2(E-V_0)}x} + Fe^{i\sqrt{2(E-V_0)}x} = Ge^{-iKx} + Fe^{iKx}$$

Suppose the particle starts at x = -∞ and heads toward the right $\Rightarrow G = 0$

But both *A* and *B* can be nonzero as the particle can be reflected by the potential

expect reflection $\propto \left|A/B\right|^2$

expect transmission $\propto \left|F/B\right|^2$

How do you expect transmission to behave as a function of E?

For a detailed treatment of the scattering states see https://www.youtube.com/watch?v=Ex-gF7FQm5o

The figure below is reproduced from that video