PH 107 :Quantum Physics and Applications

Particle in a finite box potential

Lecture 14: 01-02-2022

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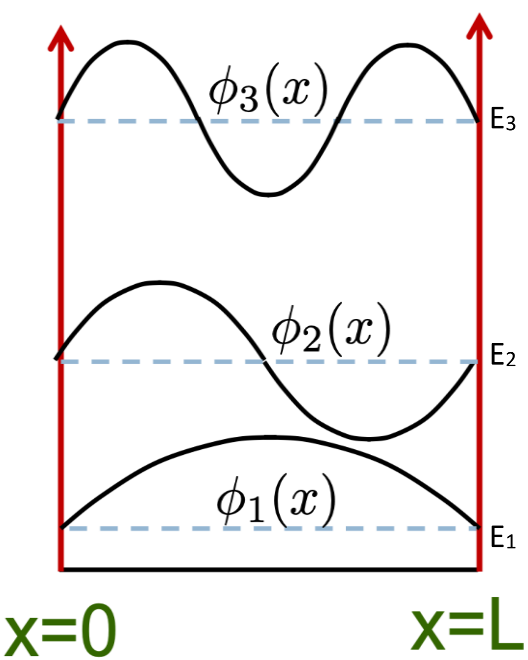
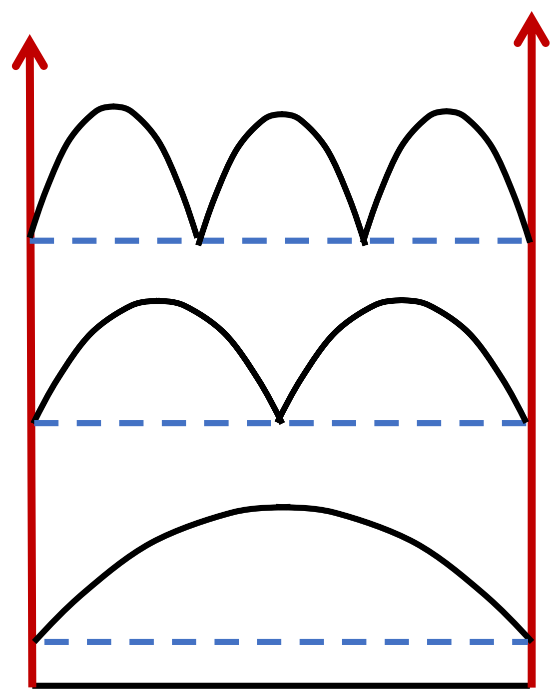
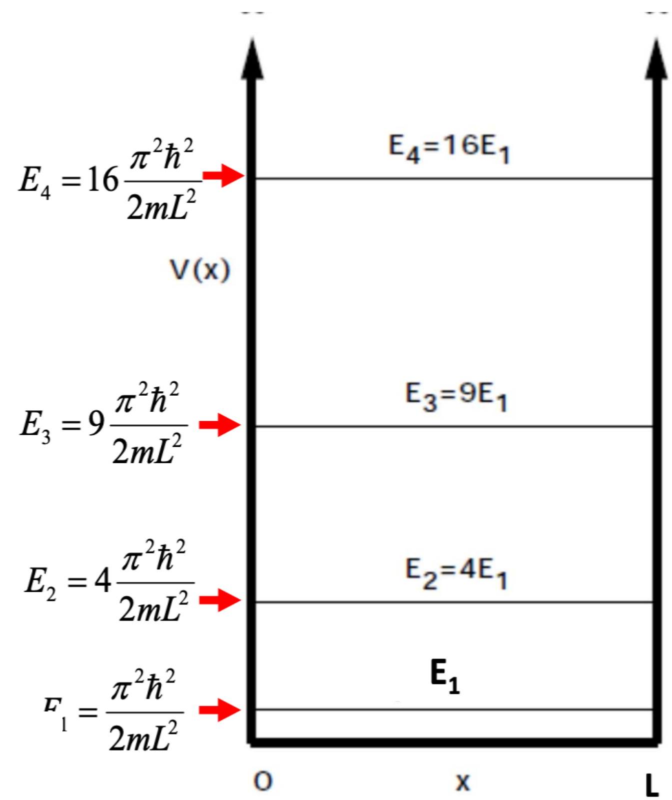
Recap (Infinite box potential)

- Particle in infinite square well has quantized energy. Free particle has continuum energy.
- Quantization is characterization of bound states.
- Zero point energy for confined particle unlike classical system.
- Eigen functions are eigen solutions to momentum operator.
- Probability density of mixed/superposed states (of different energy) oscillates with time.
- Measurement: Concept of collapse of wave function.

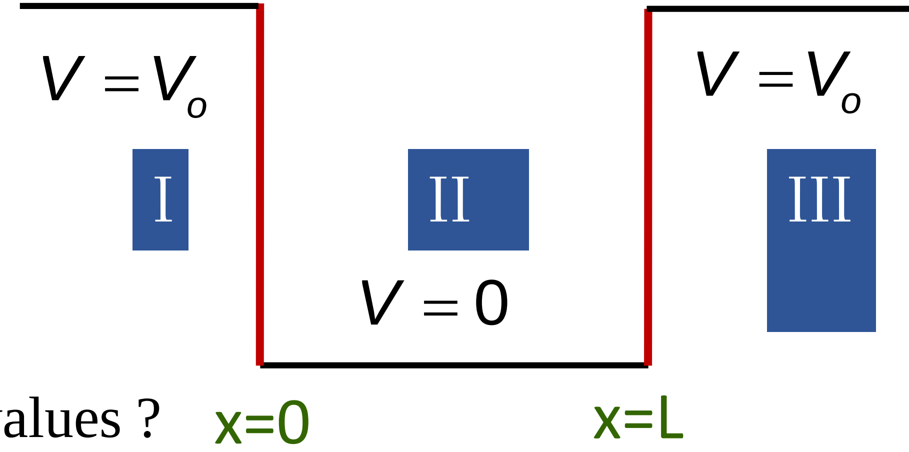






Particle in a one-dimensional finite potential box

$$V(x) = 0 \quad \text{for } 0 < x < L$$
$$= V_o \quad \text{for x} < 0 \text{ or } x > L$$



How to solve the TISE to find the $\phi_n(x)$ values ?

We have two choices here . Either we assume E<V_o or E>V_o. Let's start with E<V_o (bound states)

I

$$-\frac{\hbar^2}{2m}\frac{d^2\phi_1(x)}{dx^2} + V_0\phi_1(x) = E\phi_1(x)$$

$$\frac{d^2\phi_1(x)}{dx^2} + \frac{2m(E - V_0)}{\hbar^2}\phi_1(x) = 0$$

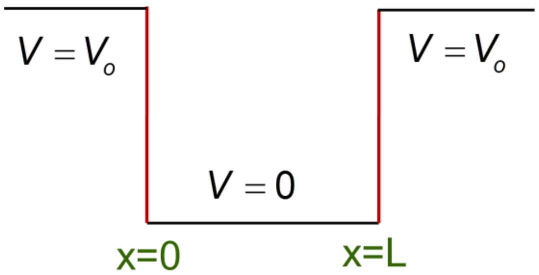
II

$$\frac{d^2\phi_2(x)}{dx^2} + \frac{2mE}{\hbar^2}\phi_2(x) = 0$$

III

$$\frac{d^2\phi_3(x)}{dx^2} + \frac{2m(E - V_0)}{\hbar^2}\phi_3(x) = 0$$

Particle in a one-dimensional finite potential box



For Region I

I

$$\frac{d^2\phi_1(x)}{dx^2} + \frac{2m(E - V_0)}{\hbar^2}\phi_1(x) = 0$$

If we define, $\frac{2m}{\hbar^2}(E - V_0) = \lambda^2$

Then we can write (like before), $\varphi_1(x) = M\sin\lambda x + N\cos\lambda x$

$$\varphi_1(x) = \mathrm{M}\sin\lambda x + \mathrm{N}\cos\lambda x$$

$$= \mathrm{M}\frac{e^{i\lambda x} - e^{-i\lambda x}}{2i} + \mathrm{N}\frac{e^{i\lambda x} + e^{-i\lambda x}}{2}$$

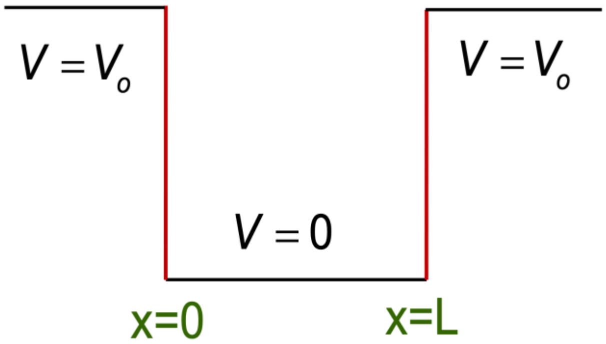
$$= \frac{N - i\mathrm{M}}{2}e^{i\lambda x} + \frac{N + i\mathrm{M}}{2}e^{-i\lambda x}$$

$$\varphi_1(x) = Ae^{i\lambda x} + Be^{-i\lambda x}$$

Instead let us define $\frac{2m}{\hbar^2}(V_0 - E) = \alpha^2$

Here the LHS is a positive quantity. This implies $\lambda = \pm i\alpha$

In terms of α , $\varphi_1(x) = Ae^{i\lambda x} + Be^{-i\lambda x}$ becomes



$$\varphi_1(x) = Ae^{\alpha x} + Be^{-\alpha x}$$

II

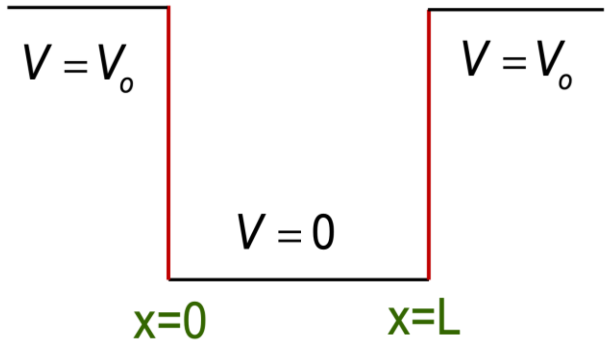
$$\frac{d^2\phi_2(x)}{dx^2} + \frac{2mE}{\hbar^2}\phi_2(x) = 0$$

$$\Rightarrow \phi_2(x) = C\sin kx + D\cos kx \text{ , where } k^2 = \frac{2mE}{\hbar^2}$$

III

$$\frac{d^2\phi_3(x)}{dx^2} + \frac{2m(E - V_0)}{\hbar^2}\phi_3(x) = 0$$

$$\Rightarrow \varphi_3(x) = Ge^{\alpha x} + He^{-\alpha x}$$



Now, we recall that the wave function needs to be finite, i.e. $\phi(x) \to 0$ as $x \to \infty$

So, for region I, $B = 0$ (since $x < 0$), i.e. , $\varphi_1(x) = Ae^{\alpha x}$

For region III, $G = 0$ (since $x > 0$), i.e. $\varphi_3(x) = He^{-\alpha x}$

Finally, for region II, we need to satisfy the boundary conditions:

$$\varphi_1(0) = \varphi_2(0); \varphi_2(L) = \varphi_3(L);$$

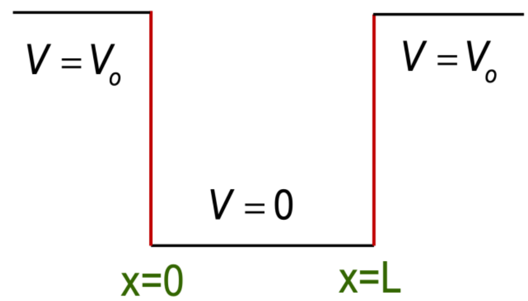
$$\varphi_1'(0) = \varphi_2'(0); \varphi_2'(L) = \varphi_3'(L);$$

At x = 0, $\varphi_1(0) = \varphi_2(0) \Longrightarrow Ae^0 = C\sin(0) + D\cos(0)$

$\Longrightarrow A = D$

At x = 0, $\varphi_1'(0) = \varphi_1'(0) \Longrightarrow A\alpha e^0 = Ck\cos(0) - Dk\sin(0)$

$\Longrightarrow A\alpha = Ck$



We know

$$\phi_2(x) = C\sin(kx) + D\cos(kx)$$

$$\phi_3(x) = He^{-\alpha x}$$

At x= L, $\varphi_2(L) = \varphi_3(L) \Longrightarrow C\sin kL + D\cos kL = He^{-\alpha L}$

At x= L,$\varphi_2'(L) = \varphi_2'(L) \Longrightarrow Ck\cos(kL) - Dk\sin(kL) = -\alpha He^{-\alpha L}$

We get , (1) $A = D$

(2) $A\alpha = Ck$

(3) $C \sin kL + D \cos kL = He^{-\alpha L}$

(4) $Ck \cos(kL) - Dk \sin(kL) = -\alpha He^{-\alpha L}$

Four Equations & Four Unknowns (actually five including Energy)

Express all constants in terms of A.

$$D = A$$
$$C = \frac{\alpha}{k} A$$
$$\frac{\alpha}{k} A \sin kL + A \cos kL = He^{-\alpha L}$$
$$\frac{\alpha}{k} Ak \cos(kL) - Ak \sin(kL) = -\alpha He^{-\alpha L}$$

Divide last eqn by second last.

$$\frac{\alpha \cos(kL) - k \sin(kL)}{\alpha \sin(kL) + k \cos(kL)} = -\frac{\alpha}{k}$$

$$\frac{\alpha \ \cos(kL) - k \ \sin(kL)}{\alpha \ \sin(kL) + k \ \cos(kL)} = -\frac{\alpha}{k} = -f(k) = f(E)$$

Similarly, LHS is also another function of *k* or equivalently *E*, say $g(k)$

If we plot *g(k)* and *f(k)* versus *k* in the same graph, then the points of intersection satisfy the equation *g(k)* = *f(k)*.

All points k_n, for which $f(k_n) = g(k_n)$, gives the allowed values of *k*, or equivalently the allowed values of *E*, i.e., E_n.

$$\frac{\alpha\ \cos(kL) - k\ \sin(kL)}{\alpha\ \sin(kL) + k\ \cos(kL)} = -\frac{\alpha}{k} = f(E)$$

$$\Longrightarrow \frac{\left(\frac{\alpha}{k}\right) - \tan(kL)}{\left(\frac{\alpha}{k}\right)\tan(kL) + 1} = -\frac{\alpha}{k}$$

$$\Longrightarrow \left(\frac{\alpha}{k}\right) - \tan(kL) = -\left(\frac{\alpha}{k}\right)^2 \tan(kL) - \left(\frac{\alpha}{k}\right)$$

$$\Longrightarrow \left[1 - \left(\frac{\alpha}{k}\right)^2\right]\tan(kL) = 2\left(\frac{\alpha}{k}\right)$$

$$\Longrightarrow \tan(kL) = \frac{2\left(\frac{\alpha}{k}\right)}{\left[1 - \left(\frac{\alpha}{k}\right)^2\right]}$$

$$\Longrightarrow \tan(kL) = \frac{2\tan\left(\frac{kL}{2}\right)}{1 - \tan^2\left(\frac{kL}{2}\right)} = \frac{2\left(\frac{\alpha}{k}\right)}{\left[1 - \left(\frac{\alpha}{k}\right)^2\right]}$$

Energy Eigen Values

$$\tan(kL) = \frac{2\tan\left(\frac{kL}{2}\right)}{1-\tan^2\left(\frac{kL}{2}\right)} = \frac{2\left(\frac{\alpha}{k}\right)}{\left[1-\left(\frac{\alpha}{k}\right)^2\right]}$$

$$\implies \tan\left(\frac{kL}{2}\right) = \frac{\alpha}{k}$$

Also, we know

$$\tan(2\theta) = \frac{2\cot(\theta)}{\cot^2(\theta)-1} = \frac{2\cot(-\theta)}{1-\cot^2(-\theta)}$$

$$\cot\left(-\frac{kL}{2}\right) = -\cot\left(\frac{kL}{2}\right) = \frac{\alpha}{k}$$

Energy Eigen Values

Using $\frac{2m}{\hbar^2}(V_0 - E) = \alpha^2$; $\frac{2mE}{\hbar^2} = k^2$ and $k_0 = \sqrt{\frac{2mV_0}{\hbar^2}}$

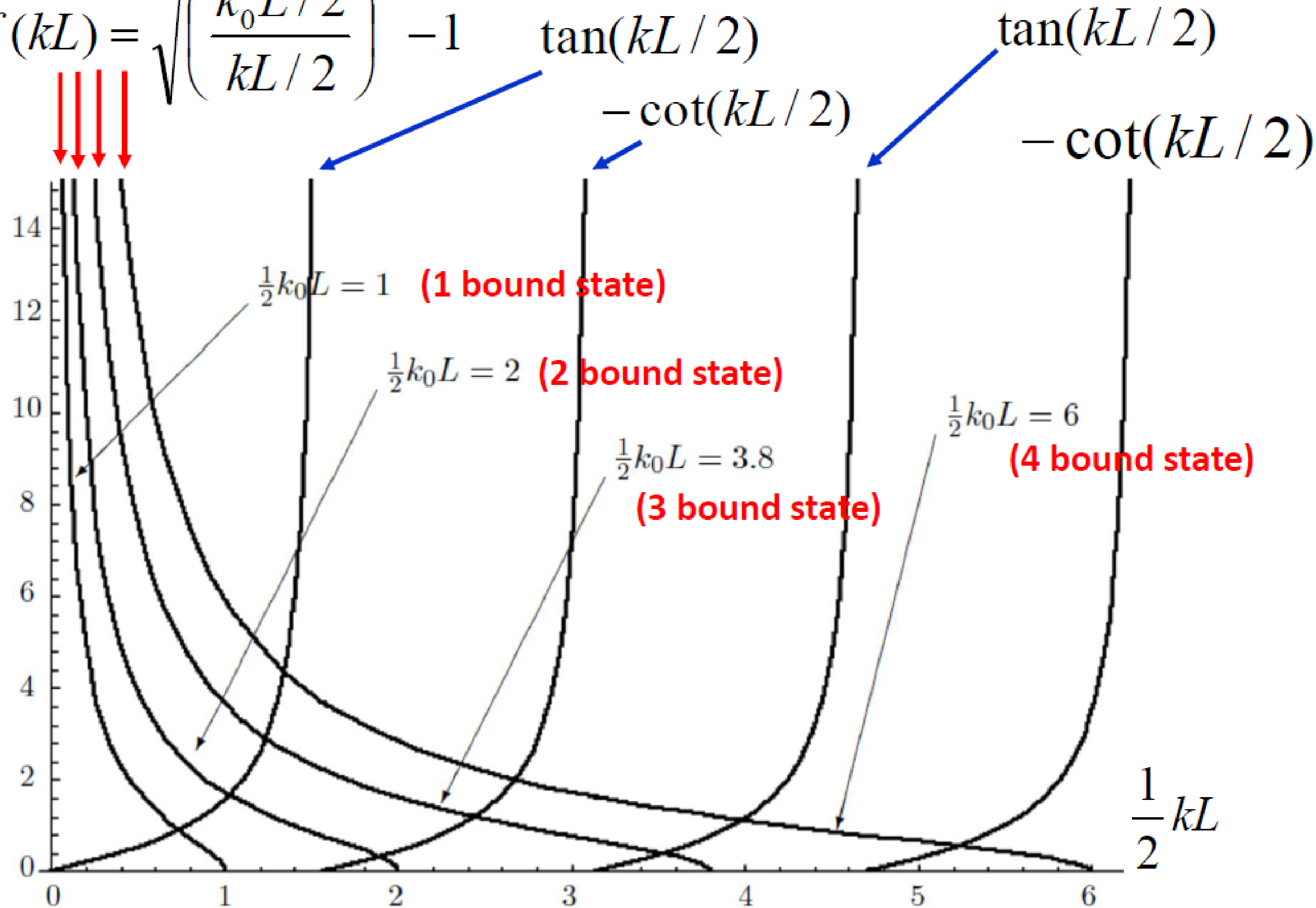
$$\frac{\alpha}{k} = \sqrt{\frac{V_0 - E}{E}} = \sqrt{\frac{V_0}{E} - 1} = \sqrt{\left(\frac{k_0}{k}\right)^2 - 1} = \sqrt{\left(\frac{k_0 L/2}{kL/2}\right)^2 - 1}$$

$$tan\left(\frac{kL}{2}\right) = \sqrt{\left(\frac{k_o L/2}{kL/2}\right)^2 - 1}$$

and $-cot\left(\frac{kL}{2}\right) = \sqrt{\left(\frac{k_o L/2}{kL/2}\right)^2 - 1}$

Graphical intersection of LHS and RHS is the estimate of the allowed energy states.

$$f(kL) = \sqrt{\left(\frac{k_0 L/2}{kL/2}\right)^2 - 1}$$



$$k_0 = \sqrt{2mV_0/\hbar^2}$$

As V_o increases, it admits more and more bound states

Energy Eigen Values

$$tan\left(\frac{kL}{2}\right) = \sqrt{\left(\frac{k_oL/2}{kL/2}\right)^2 - 1} \quad \text{and } -cot\left(\frac{kL}{2}\right) = \sqrt{\left(\frac{k_oL/2}{kL/2}\right)^2 - 1}$$

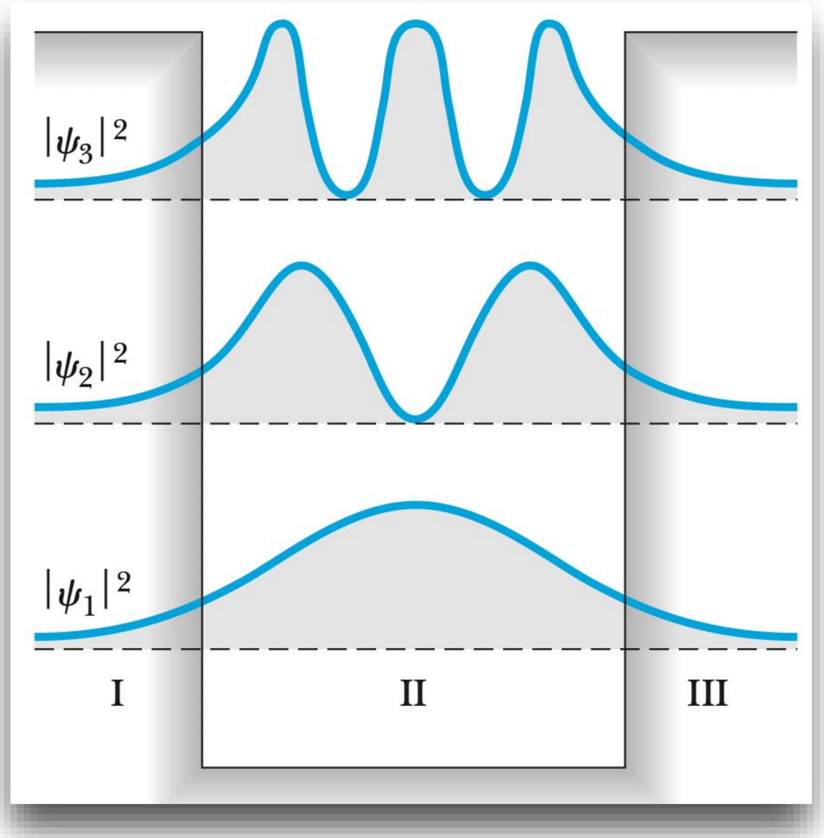
- LHS is a trigonometric function and RHS consists of a circle of radius R.
- Solutions are given by points where circle intersects the trigonometric function.
- Solution form a discrete set.
- The number of solutions depends of R and hence on V_o.

- At least one bound state will be present no matter howsoever small $\boldsymbol{V_o}$.
- The deeper and broader the well, the larger the value of R, and hence the greater the number of bound states.

Wave functions

$$\phi_2(x) = C\sin kx + D\cos kx$$

$$\boldsymbol{\varphi_1(x) = Ae^{\alpha x}} \qquad \boldsymbol{\varphi_3(x) = He^{-\alpha x}}$$



- There is a non zero probability of finding the particle in Region I and III

- The probability decays exponentially but it is non- zero.

- **Classically, this is forbidden.**

Penetration of the wave function in the classically forbidden region has immense practical consequences (NSOM, near field scanning optical microscopy).

Wave functions

The exponential "tails" of the wave function

$$\phi_n(x) = A\ e^{\alpha_n x} \quad \forall\ x < 0$$

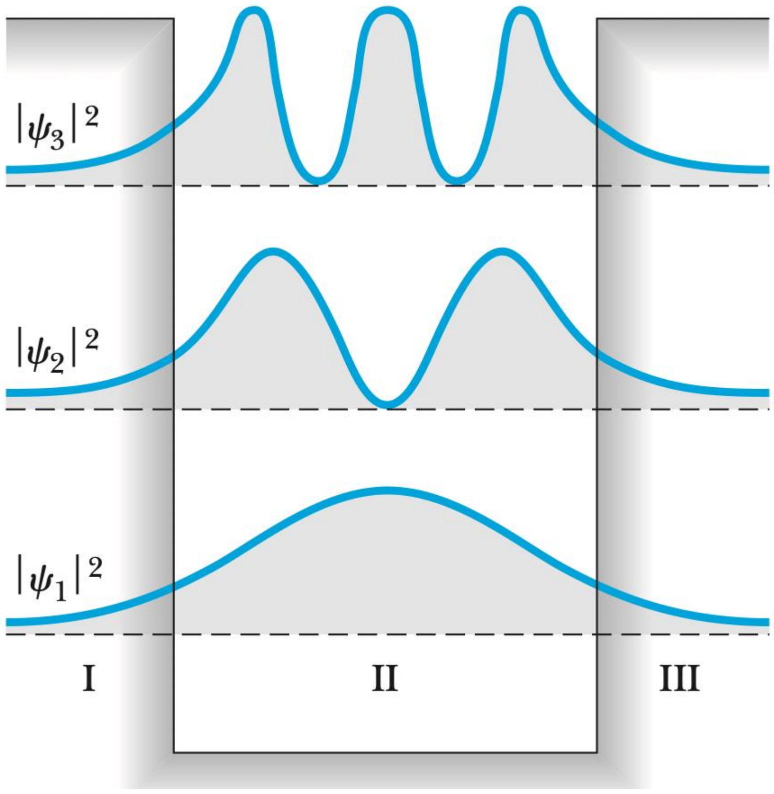
Penetration length $\delta_n = \dfrac{1}{\alpha_n}$

Penetration length is proportional to Planck's constant

$$\phi_n(\delta_n) = \frac{\phi_n(0)}{e}$$

Effective dimension of the potential well $L + 2\delta_n$

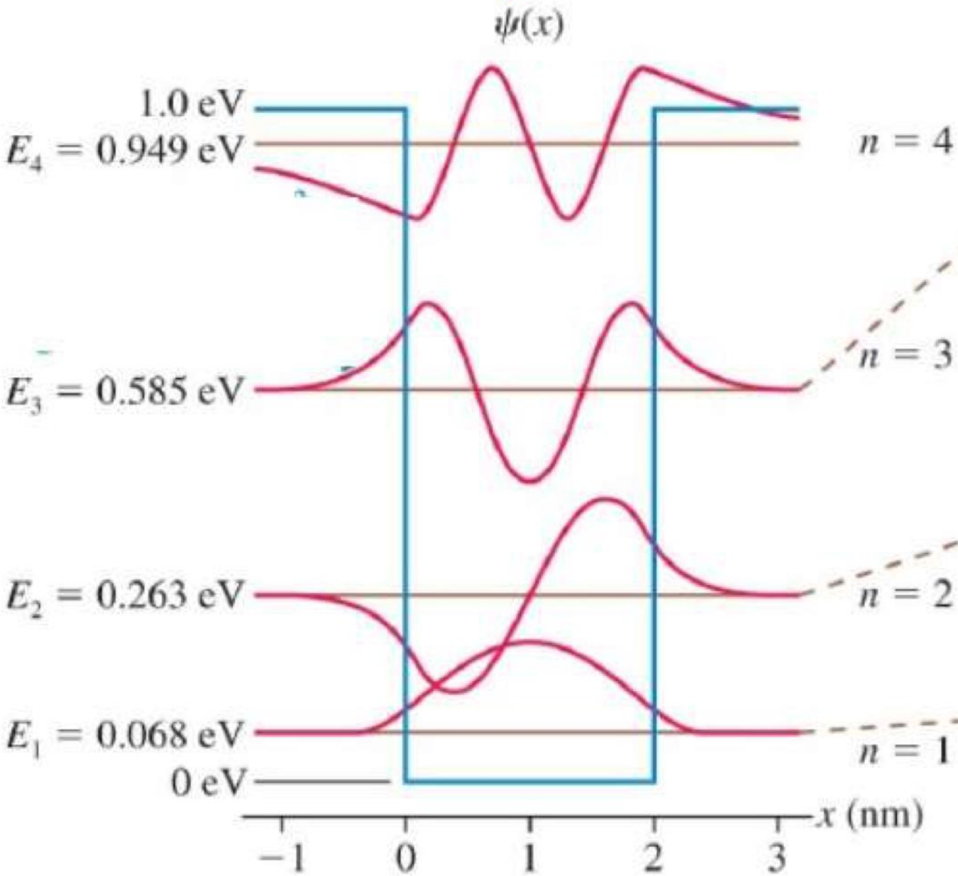
Approximate Energy $E_n \approx \dfrac{n^2\pi^2\hbar^2}{2m(L+2\delta_n)^2}$



Energy states of finite well is smaller than infinite well.

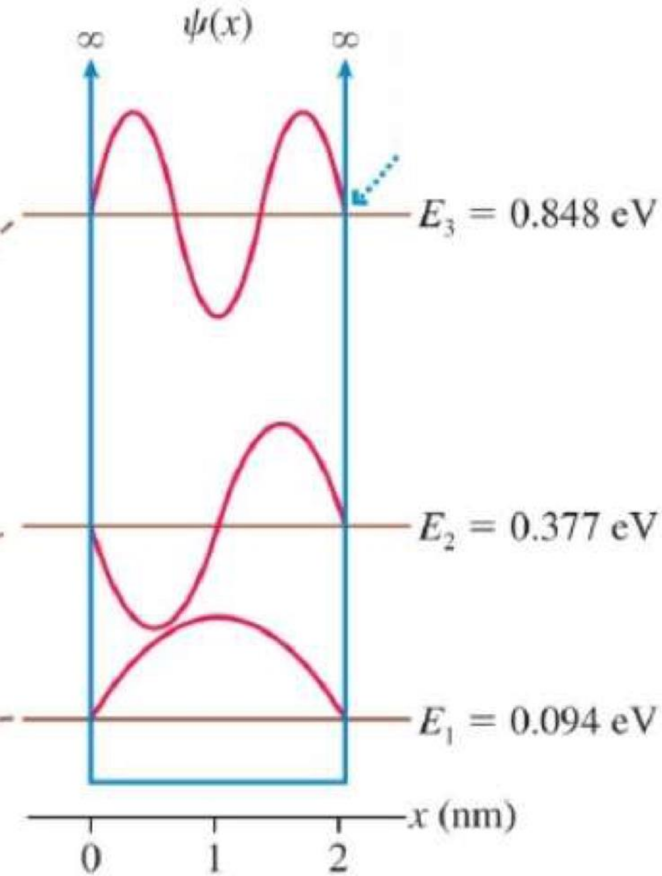
Comparison of finite and infinite potential wells

Electron in a finite well with
L=2 nm and V_0=1 eV



Wave functions extend into classically forbidden region

Electron in an infinite well with L=2 nm and V_0= ∞



Wave functions are zero at the wall