PH 107 :Quantum Physics and Applications

Particle in a finite box potential and Step potential

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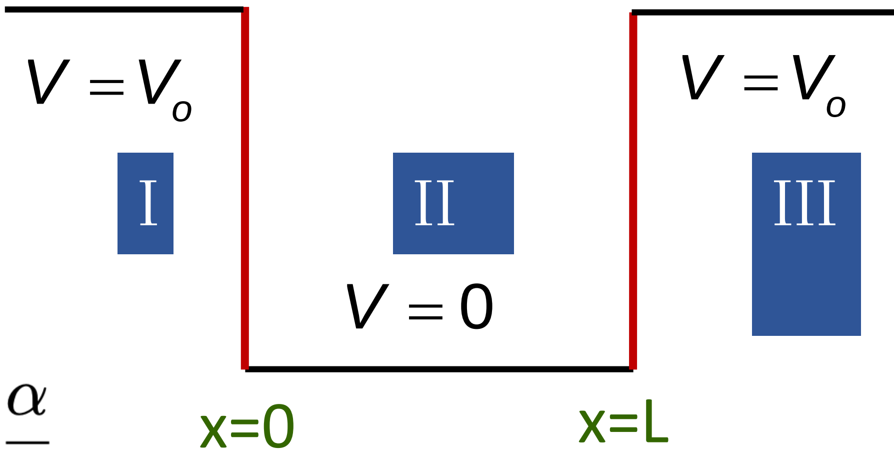
Recap (Finite Potential Well)

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



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

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

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

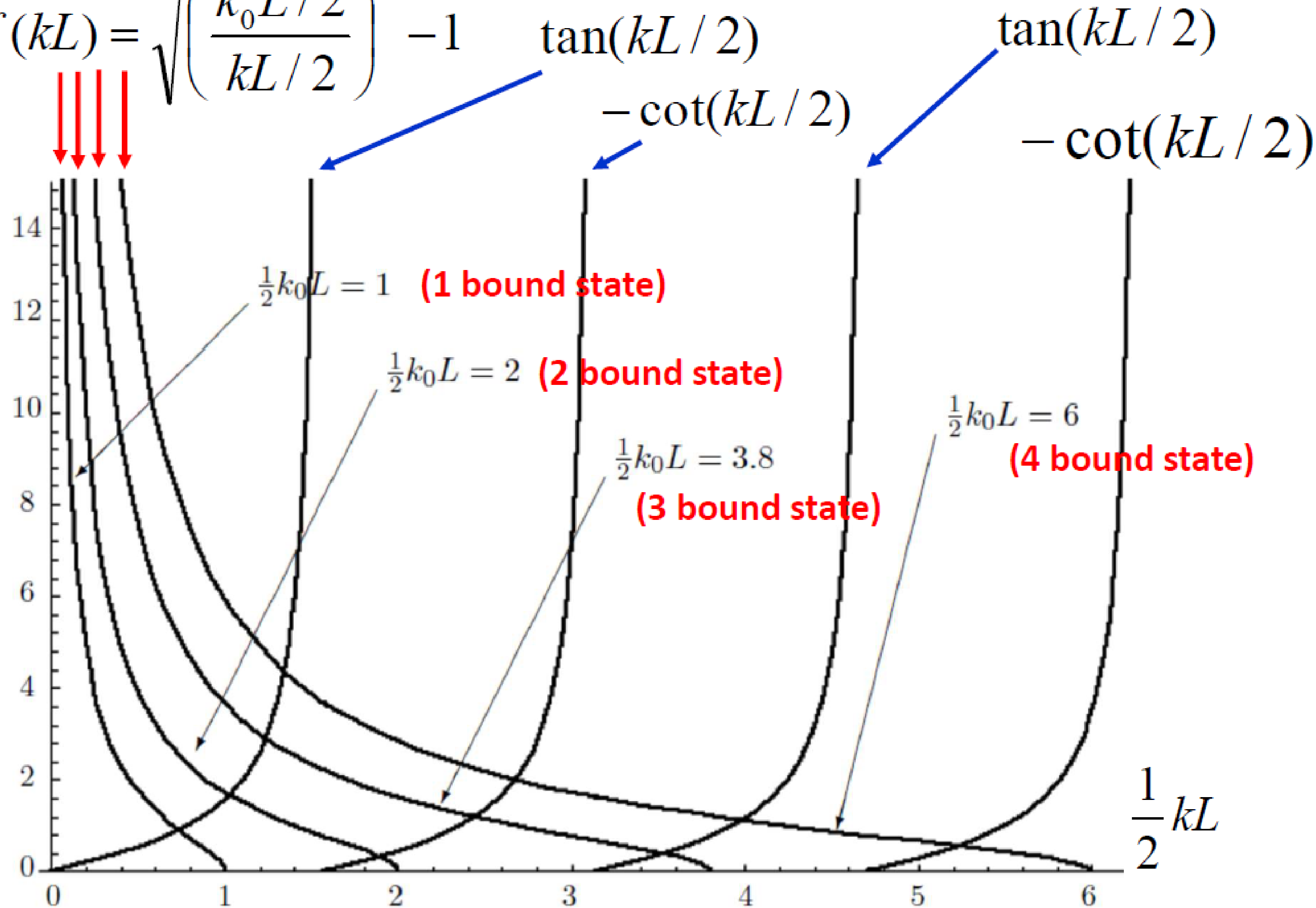
Using $\frac{2m}{\hbar^2}(V_0 - E) = \alpha^2$;

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

and $k_0 = \sqrt{\frac{2mV_0}{\hbar^2}}$

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

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



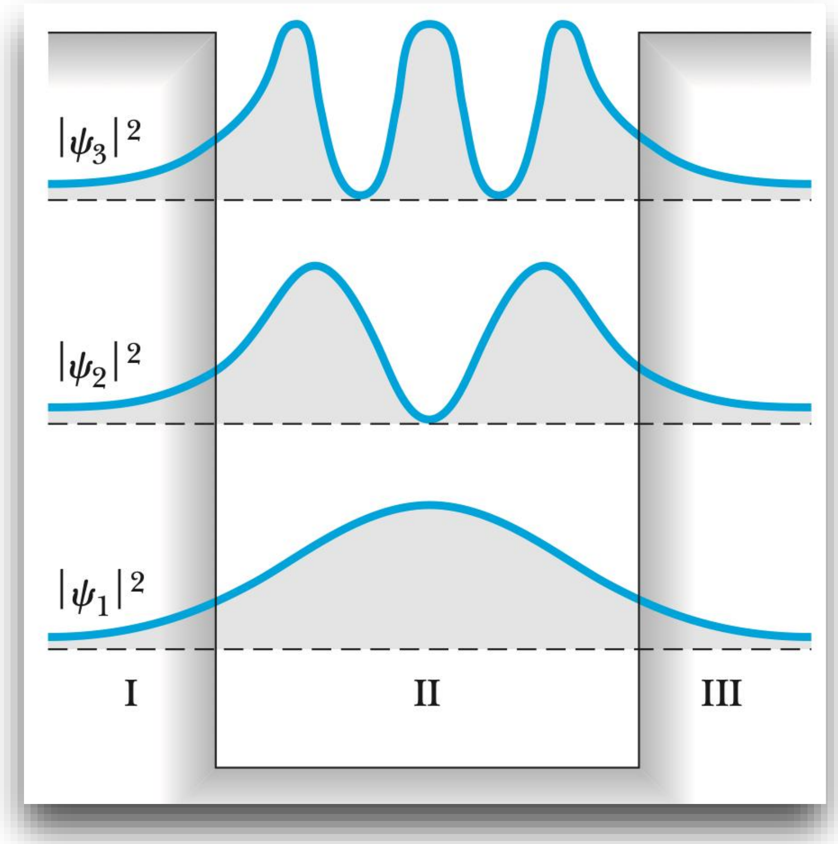
$$k_0 = \sqrt{2mV_0/\hbar^2}$$

As V_o increases, it admits more and more bound states

Wave functions

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

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



Approximate Energy

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

- Bound states with discrete energy eigen values.
- Energy states of finite well is smaller than infinite well.
- Wave functions extends into classically forbidden regions

Case 1: Deep potential well

- We start with a finite square well and increase its depth

  The results should approach the infinite square well!

- Let us consider only the lowest energy states. In that case E *is small and* V_0

$$\tan\left(\frac{kL}{2}\right) = \sqrt{\frac{V_0}{E} - 1} \quad \Longrightarrow \quad \tan\left(\frac{L}{2\hbar}\sqrt{2mE}\right) = \sqrt{\frac{V_0}{E} - 1}$$

$$\tan\left(\frac{L}{2\hbar}\sqrt{2m\ E}\right) = \sqrt{\frac{V_0}{\epsilon} - 1} \qquad \tan\left(\frac{L}{2\hbar}\sqrt{2mE}\right) \to \infty$$

$$\frac{L}{2\hbar}\sqrt{2m\ E} \simeq (2n+1)\frac{\pi}{2} \quad \Longrightarrow \quad E_p \simeq \frac{\hbar^2 p^2 \pi^2}{2mL^2} \quad p = (2n+1)$$

Home work: Work out the condition for cot (kL/2) function.

https://demonstrations.wolfram.com/BoundStatesOfAFinitePotentialWell/

Case 2: Shallow potential well $(V_0 \to 0)$

- $V_0 \longrightarrow 0$ We would expect the situation to tend to that of the free particle

$V_0 = 0$ since, $k_o = 0$, $f_0(E)$ has no values of k which give a real value

If there are no intersections on the graph, thus there are no bound states.

- However, if there is any potential well at all, no matter how shallow, there will be at least one bound state with non-zero energy.

Consequence of Heisenberg's Uncertainty principle!

The broader and deeper potential well will have greater number of bound states

Quantum Tunneling

For X < 0, $\varphi_1(x) = Ae^{\alpha x}$

For X > L, $\varphi_1(x) = Ae^{-\alpha x}$

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

Note,

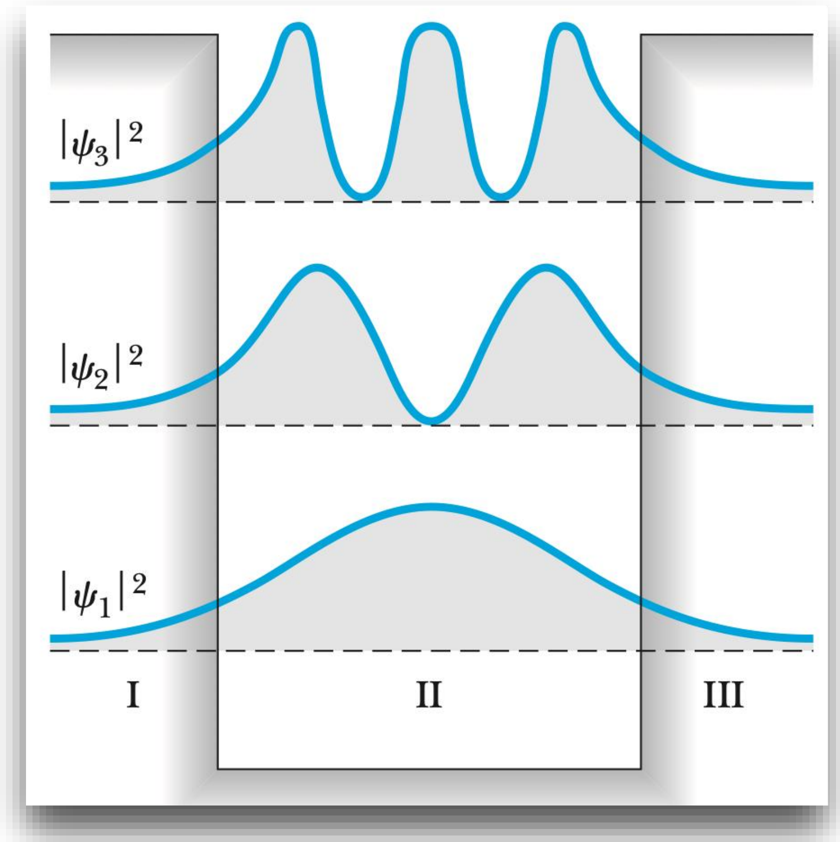
$$V_0 \rightarrow \infty \Longrightarrow \alpha \rightarrow \infty$$

$$\Longrightarrow \delta_n = \frac{1}{\alpha_n} \rightarrow 0$$

$$E \rightarrow V_0 \Longrightarrow \alpha \rightarrow 0$$

$$\Longrightarrow \delta_n = \frac{1}{\alpha_n} \rightarrow \infty$$

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



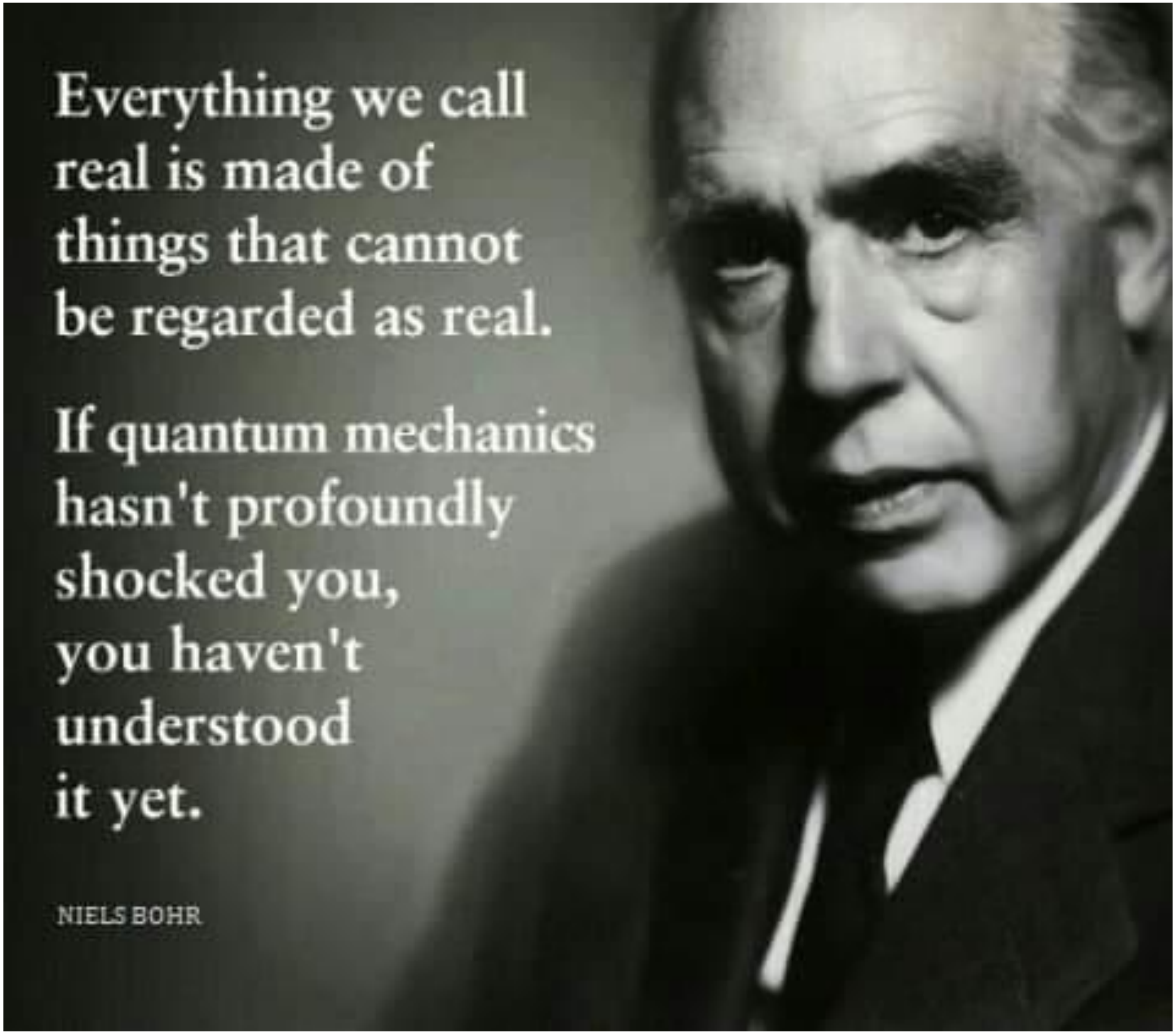
The penetration depth/leakage of the wave function is depends on estimate of α.

Quantum Tunneling

- Non-zero wavefunction in classically forbidden regions (KE < 0!) is a purely quantum mechanical effect.

- Quantum mechanics allows tunnelling between classically allowed regions.

- It follows from requiring that both $\boldsymbol{\psi}(x)$ and $\frac{\boldsymbol{\psi}(x)}{dx}$ are continuous.


Everything we call real is made of things that cannot be regarded as real.
If quantum mechanics hasn't profoundly shocked you, you haven't understood it yet.
NIELS BOHR

General properties of quantum states

1. Quantum (discrete) energy states are a typical property of any well-type potential.

2. The corresponding wavefunctions (and probability) are mostly confined inside the potential but exhibit non-zero "tails" in the classically forbidden regions of KE < 0!

   (Except when V (x) → ∞ where the tails are not allowed.)

   Both properties result from requiring the wavefunction $\boldsymbol{\psi}(x) and \ \frac{\boldsymbol{\psi}(x)}{dx}$ to be continuous everywhere.

   (Except when V (x) → ∞ where $\psi'(x)$ is not continuous.)

General properties of quantum states

1. Lowest energy (ground) state is always above the bottom of the potential and is symmetric. [Consequence of Uncertainty Principle.]

2. Wider and/or more shallow the potential, the lower the energies of the quantum states. [Consequence of Uncertainty Principle.]

3. Inside "Finite Potential Well" potentials the number of quantum states is finite. When the total energy E is larger than the height of the potential, the energy becomes continuous,

4. When V = V (x), both bound and continuous states are stationary, i.e, the time-dependent wavefunctions are $\boldsymbol{\psi}(x,t) = \boldsymbol{\varphi}(x)\exp(-iEt/\hbar)$

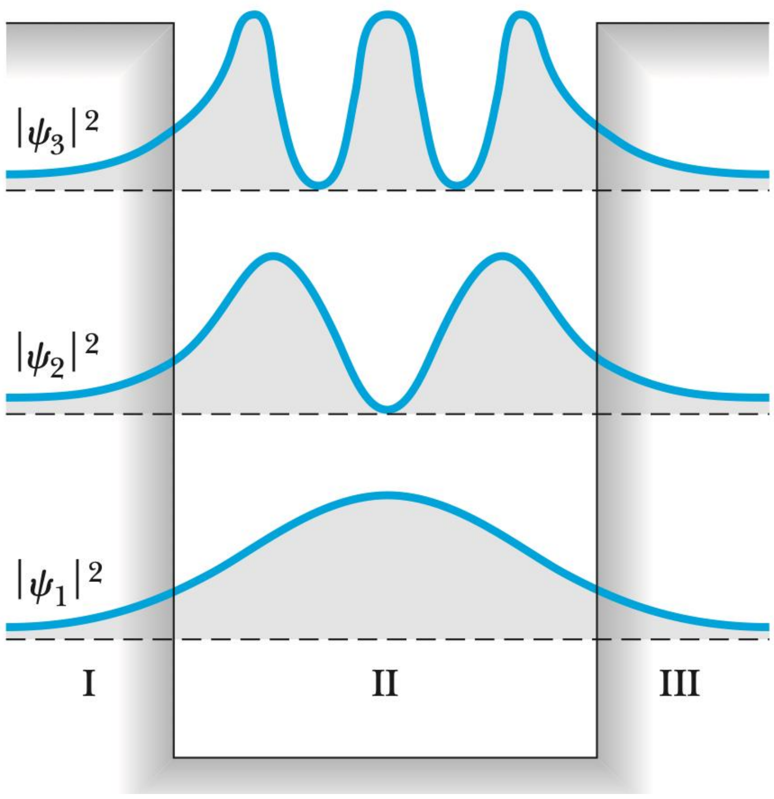
Doubt 1

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

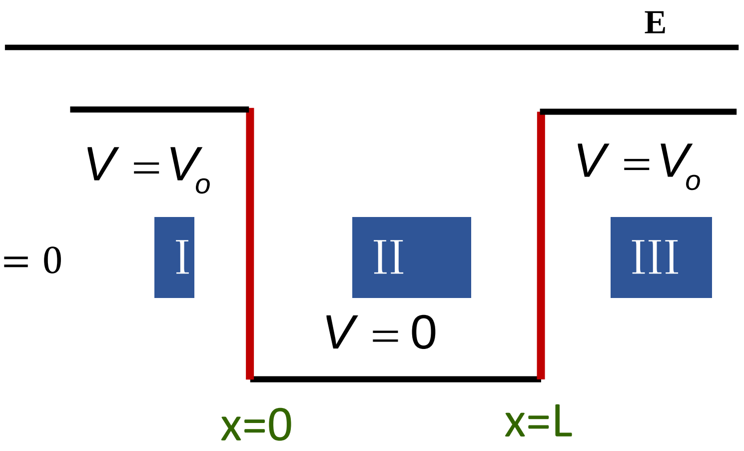


$$\alpha^2 = \frac{2m}{\hbar^2}(V_0 - E)$$

$$\delta_n \sim \sqrt{\frac{\hbar^2}{2m(V_0 - E)}} \sim \hbar$$

The phenomena of wave function leakage is visible for quantum systems

Case E > V_o



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

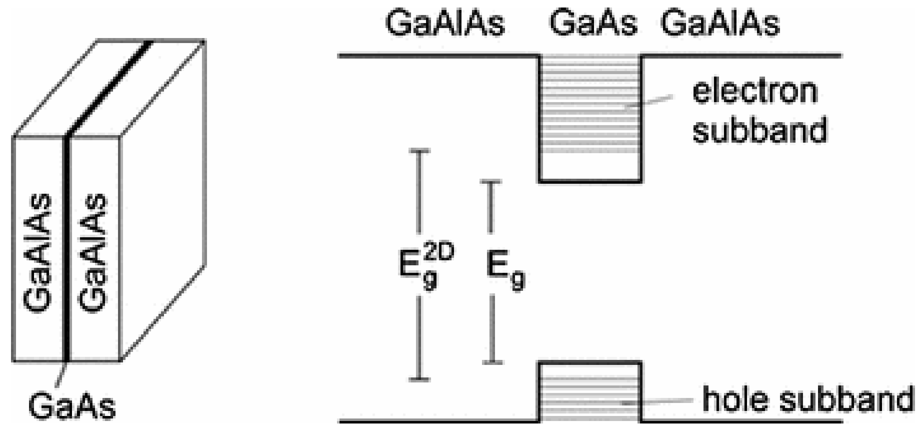
II $$\frac{d^2\phi_2(x)}{dx^2} + \frac{2mE}{\hbar^2}\phi_2(x) = 0$$

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

Easy to check the solution in all three regime are oscillatory wave function with varying amplitude.

https://demonstrations.wolfram.com/BoundStatesOfAFinitePotentialWell/

Application: quantum well structure is in LASER technology



Summary Finite box potential

- Energy is quantized same as infinite box potential and non-zero ground state energy.
- Non-zero probability in the classically forbidden region.
- At least one bound state exits for any small Vo.
- In the limit of large Vo , eigen solutions tends towards infinite box potential.
- The energies for same "n" are lower as compared to infinite box potential (due to leaking of the wave function).
- Wave functions are exponentially decaying for particle with E< V, in case region of finite potential.
- In case of E> V, the wave functions are oscillatory in nature. The wave number, k, are different in regions depending on the value of V.

Doubt 2

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

- 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.

Reference "Quantum Mechanics Concepts and applications"
By N. Zettili Page 234-239

Energy Eigen Values

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

In General, $\beta_n tan\,\beta_n = \sqrt{(R)^2 - (\beta_n)^2}$ *For even states*

$$-\beta_n Cot\,\beta_n = \sqrt{(R)^2 - (\beta_n)^2} \quad \textit{For odd states}$$

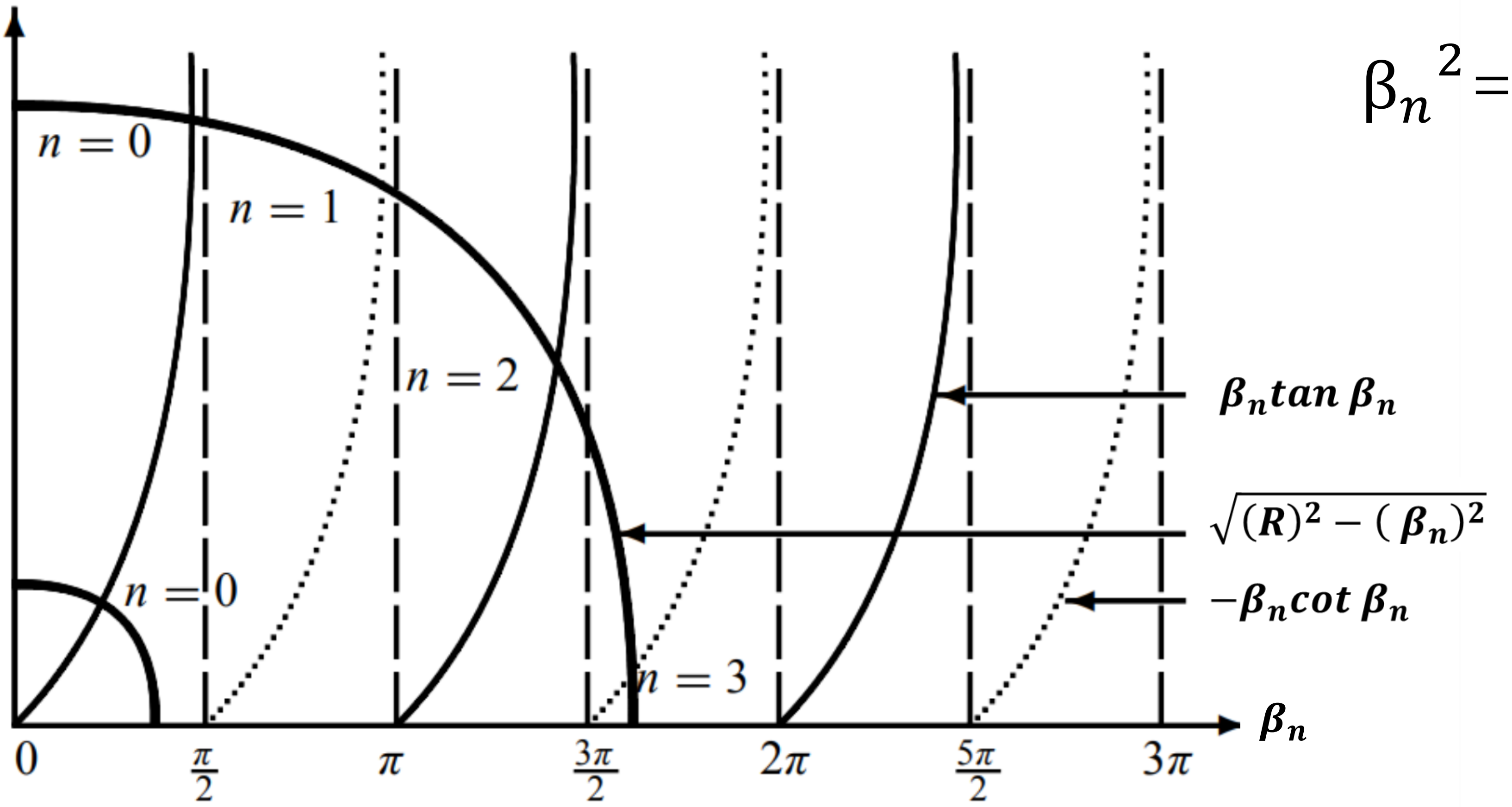
Where $\beta_n{}^2 = \frac{k_n^2 L^2}{4} = \frac{mE_nL^2}{2\hbar^2}$ *and* $R^2 = \frac{k_o^2 L^2}{4} = \frac{mV_oL^2}{2\hbar^2}$

- 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.

Energy Eigen Values

$$R^2 = \frac{mV_oL^2}{2\hbar^2}$$

$$\beta_n{}^2 = \frac{mE_nL^2}{2\hbar^2}$$

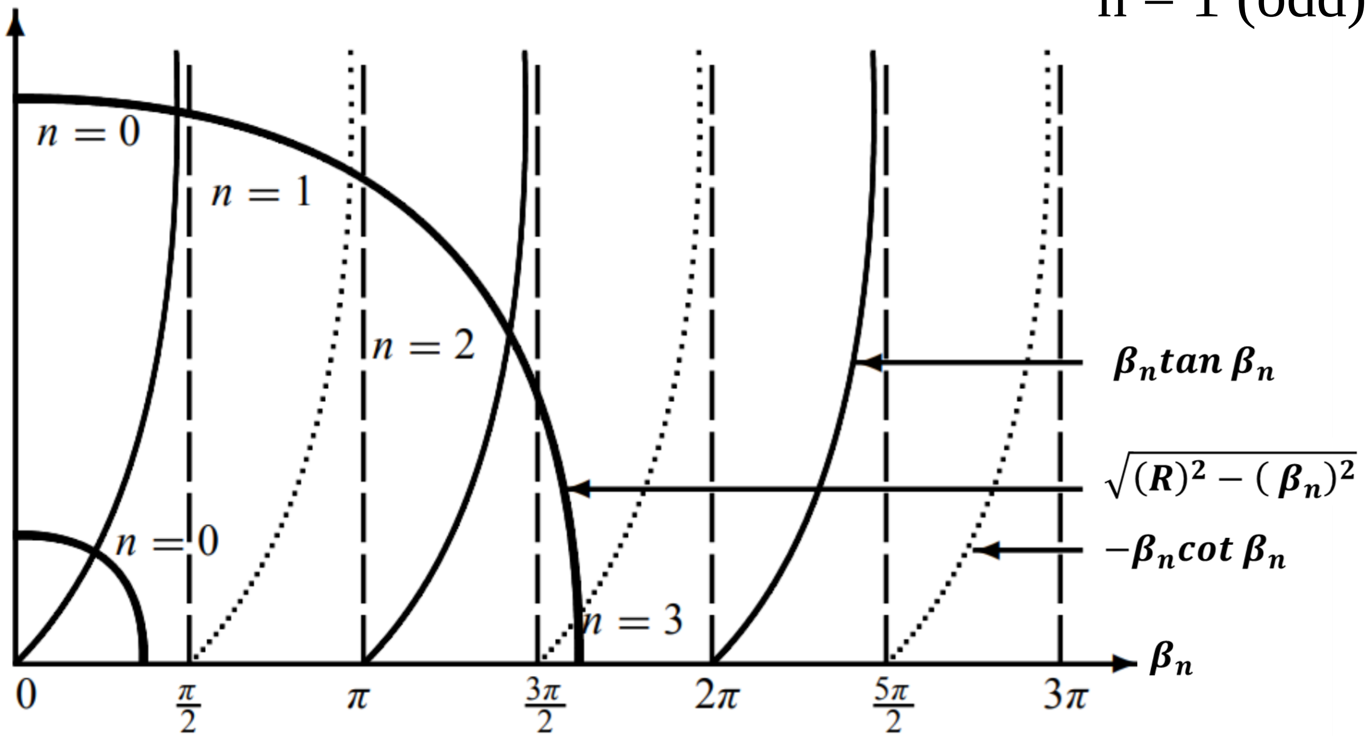


- **At least one bound state will be present no matter howsoever small V_o .**
- **The deeper and broader the well, the larger the value of R, and hence the greater the number of bound states.**

Energy Eigen Values

1. $0 < R < \frac{\pi}{2}$ or $0 < V_o < \left(\frac{\pi}{2}\right)^2 \frac{2\hbar^2}{mL^2}$ ➡ One (even) bound state for n = 0

2. $\frac{\pi}{2} < R < \pi$ or $\left(\frac{\pi}{2}\right)^2 \frac{2\hbar^2}{mL^2} < V_o < \pi^2 \frac{2\hbar^2}{2mL^2}$ ➡ Two bound states for n = 0 (even), n = 1 (odd)



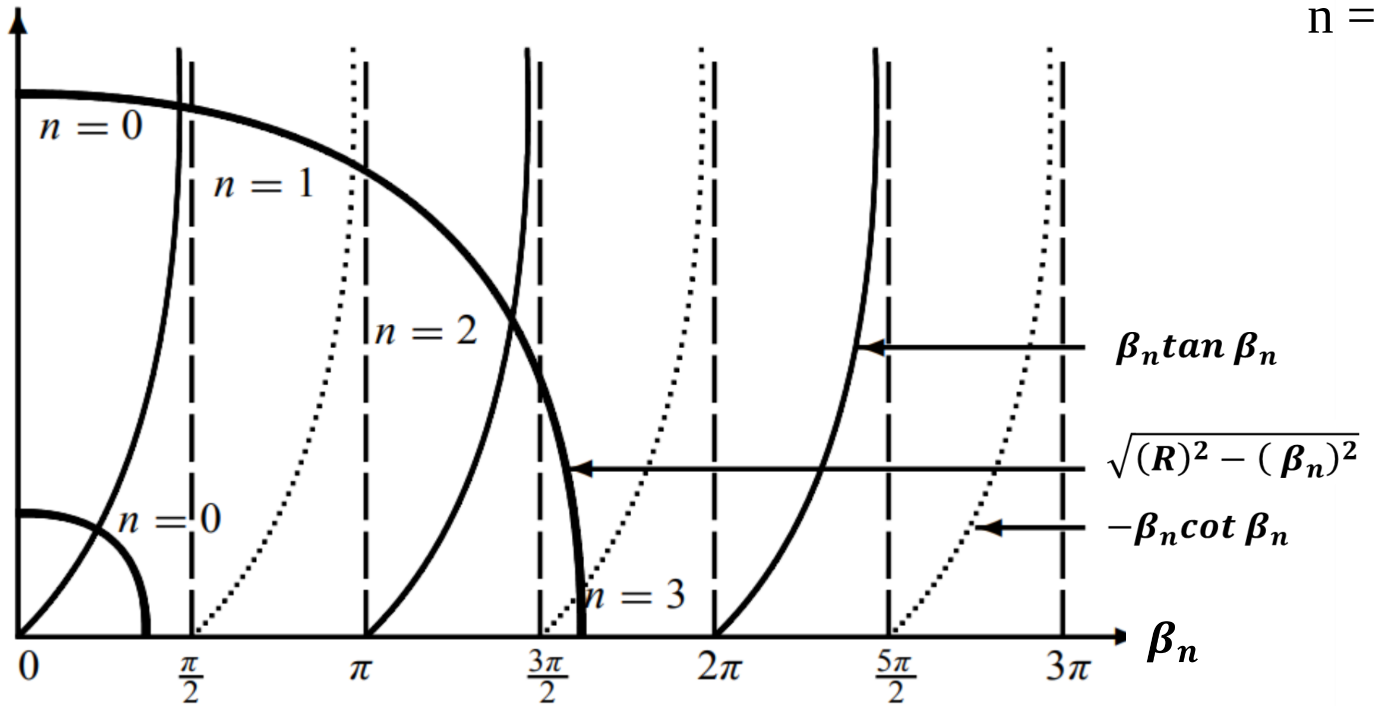
The states consists of a set of alternating even and odd states.

Energy Eigen Values

3. For "n" allowed states ➡ $R = \frac{n\pi}{2}$ and $V_o = \left(\frac{\pi}{2}\right)^2 \frac{2\hbar^2}{mL^2} n^2$

4. For limiting case V_o ➡ ∞; $\beta_n = \frac{n\pi}{2}$ ➡ $E_n = \frac{\pi^2\hbar^2}{2mL^2} n^2$

n = 1, 2, 3…



At large V_o , energy expression is similar to that for the infinite potential well.