# *PH 112: Quantum Physics and Applications*

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Week 05 Lecture 1: Particle in a Finite Potential well

D3, Spring 2023

# Second Application: Particle in a box (Recap)

- Energy states of a quantum particle in a box (infinite barrier) are found by solving the time-independent Schrodinger equation.
- Energy states of a particle in a box are quantized and indexed by number *(n)*.

$$E_n = \frac{\hbar^2\pi^2}{2mL^2}n^2 = \frac{h^2}{8mL^2}n^2 \quad \text{where} \quad n = 1, 2, \cdots$$

- Normalized wave-functions are

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) \quad \text{where} \quad n = 1, 2, \cdots$$

- The quantum picture differs significantly from the classical picture when a particle is in a low-energy state of a low quantum number.

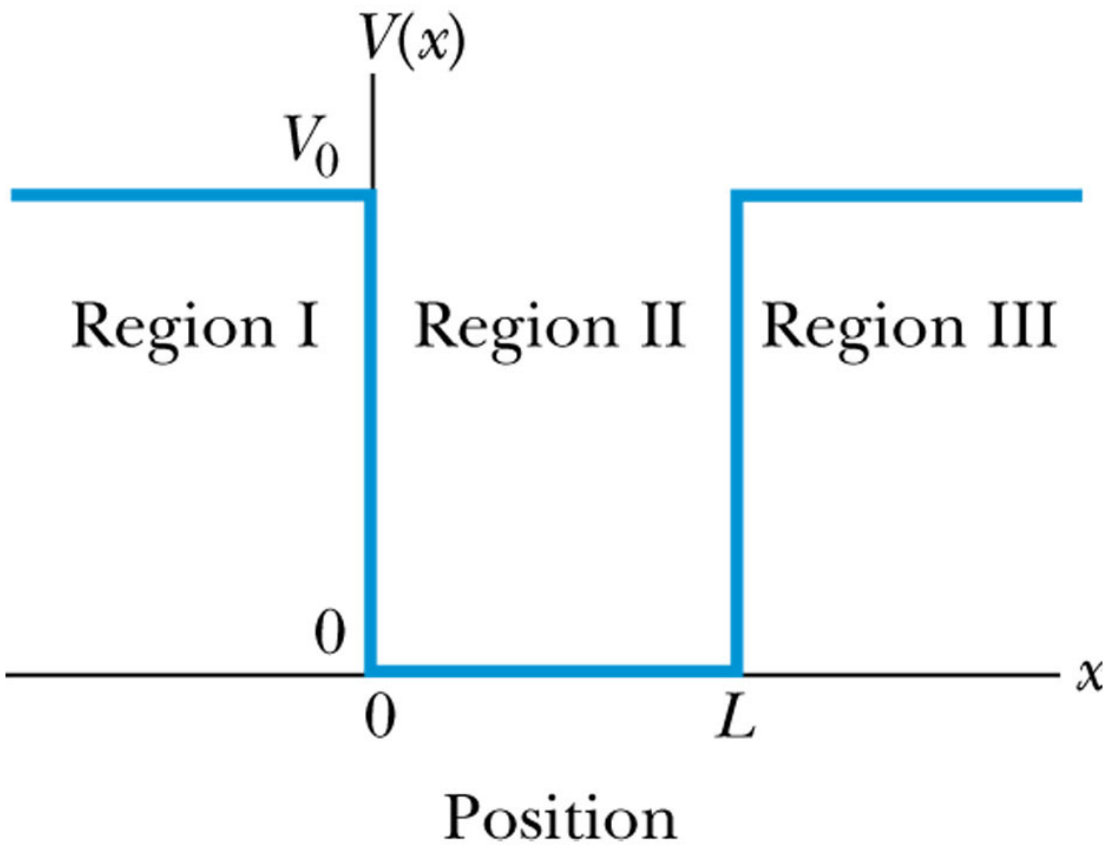
# Third Application: Particle in a finite well

# Finite Square Well

- Infinite potential outside the well is unrealistic, so we relax that assumption.

- A finite potential well is a region where potential energy $V(x)$ is lower than outside the well, but $V(x)$ is *not* infinite outside the well.

- Newtonian mechanics: Particle whose energy $E$ is less than the height of the well ($V_0$) can never escape the well.




$$V(x) = \begin{cases} V_0 & x \le 0 & \text{region I} \\ 0 & 0 < x < L & \text{region II} \\ V_0 & x \ge L & \text{region III} \end{cases}$$

# Finite Square Well: Differences

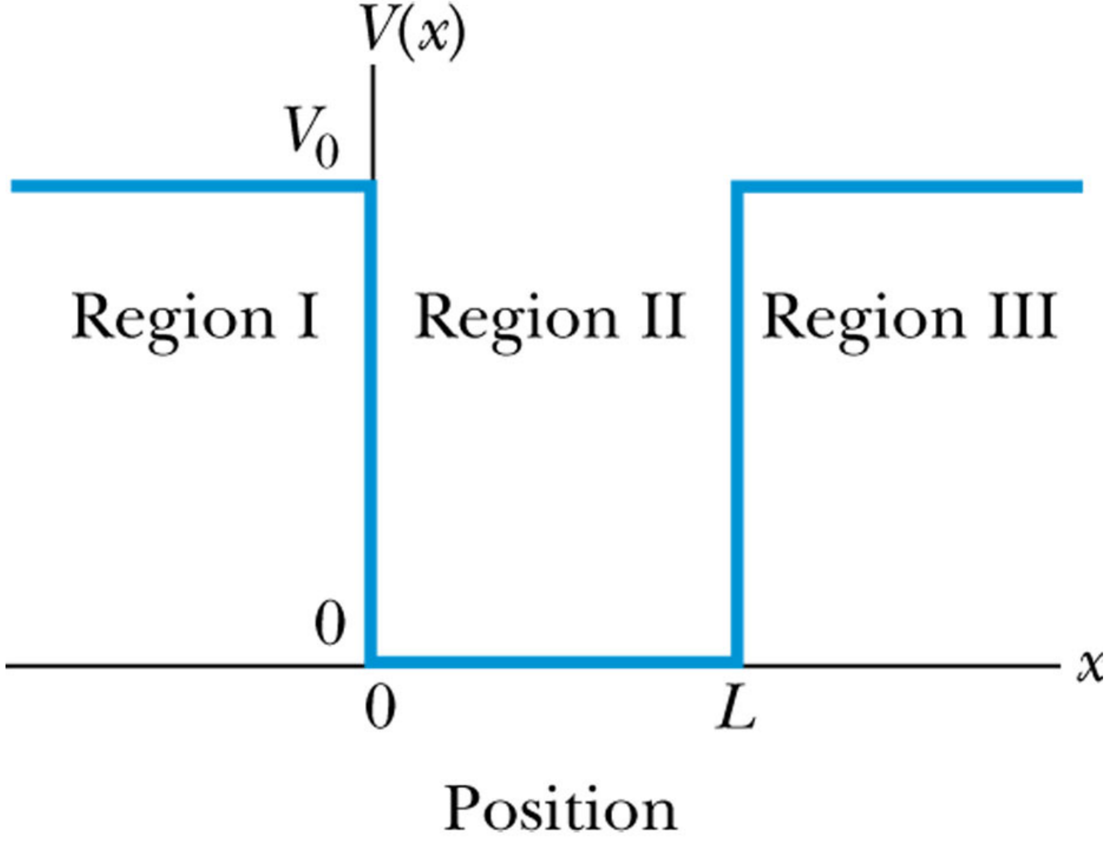
- In quantum mechanics such a trapped state is referred to as *a bound state*.

- For infinite well: All states are bound states.

- Finite well:

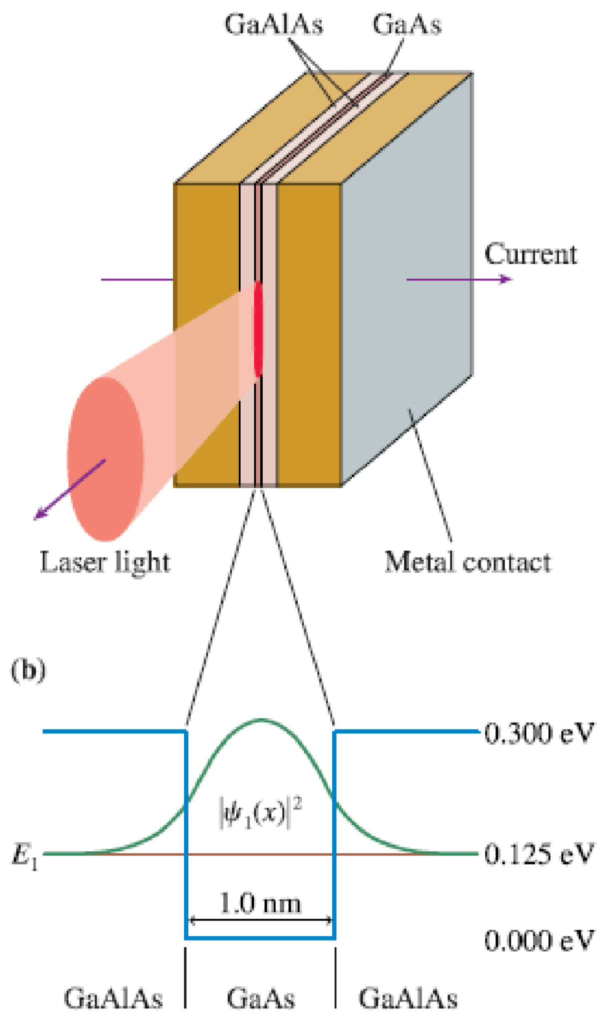
  1. $E > V_0$: Particle energy can be greater than potential ($V_0$); particle is not bound.

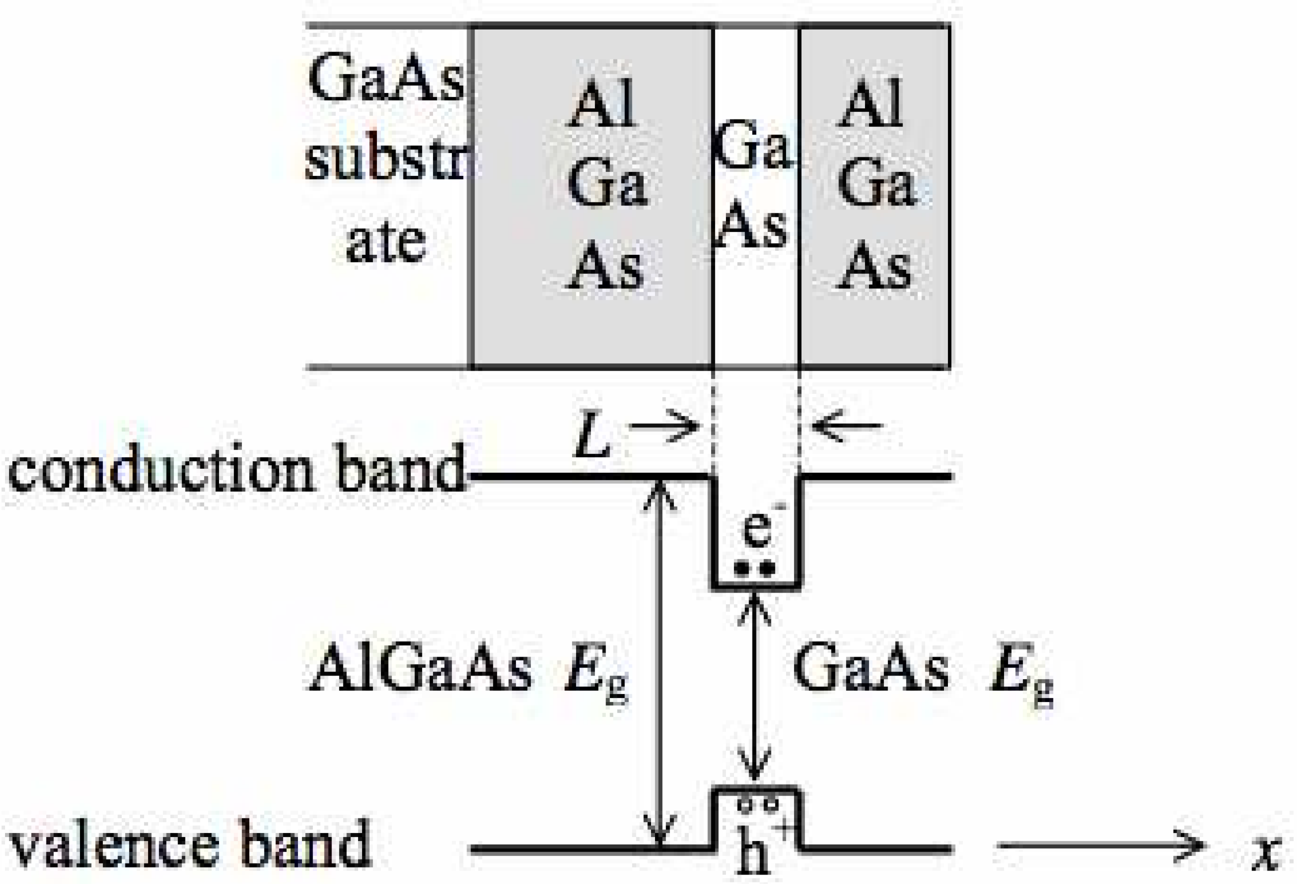
  2. $E < V_0$: Bound states for a finite well are subtly different from infinite well.




$$V(x) = \begin{cases} V_0 & x \le 0 & \text{region I} \\ 0 & 0 < x < L & \text{region II} \\ V_0 & x \ge L & \text{region III} \end{cases}$$

# Real-life potential well: Quantum-well LASER




Constrained motion along the x-axis; free motion in the y – z plane.

# Finding the solutions

# Finite Square Well: Approach

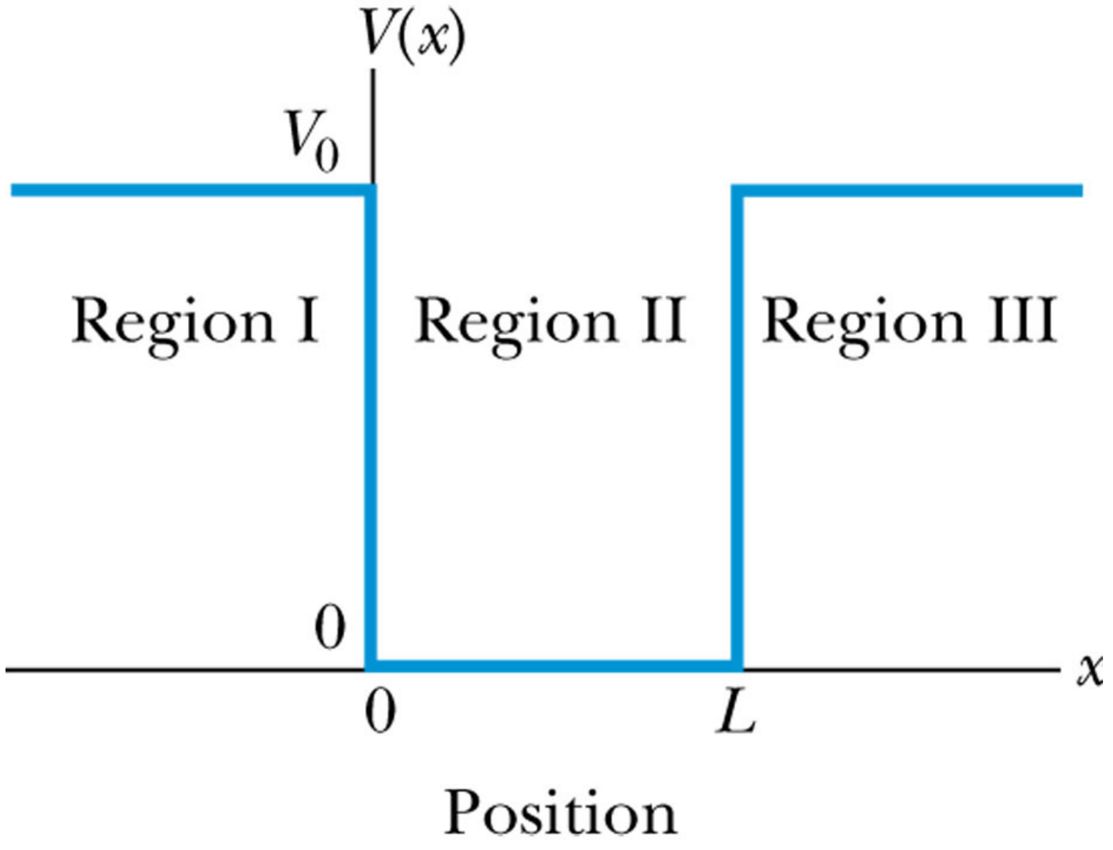
- We need to obtain a solution of TISE

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

everywhere ($-\infty < x < \infty$).

- For the potential well, we have three regions

| | | |
|---|---|---|
| Region I | $x \leq 0$ | $V(x) = V_0$ |
| Region II | $0 < x < L$ | $V(x) = 0$ |
| Region III | $x \geq L$ | $V(x) = V_0$ |




$$V(x) = \begin{cases} V_0 & x \leq 0 & \text{region I} \\ 0 & 0 < x < L & \text{region II} \\ V_0 & x \geq L & \text{region III} \end{cases}$$

# Finite Square Well: Differential equations

- In regions I and III

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_I}{dx^2}+V\psi_I=E\psi_I$$

$$\frac{d^2\psi_I}{dx^2}-k_I^2\psi_I=0 \text{ where } k_I=k_{III}=\frac{\sqrt{2m(V_0-E)}}{\hbar}$$

- In region II

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2}=E\psi_{II}$$

$$\frac{d^2\psi_{II}}{dx^2}+k_{II}^2\psi_{II}=0 \text{ where } k_{II}=k=\frac{\sqrt{2mE}}{\hbar}$$

# Finite Square Well: General solutions

- Solutions in Region I and III

  - Region I: Second term grows to infinity, we must have $B = 0$.

  - Region III: First term grows to infinity, we must have $E = 0$.

$$Ae^{k_I x} + Be^{-k_I x} \rightarrow Ae^{k_I x}$$

$$Ee^{k_{III} x} + Fe^{-k_{III} x} \rightarrow Fe^{-k_{III} x}$$

- Solutions in Region II

$$Ce^{ikx} + De^{-ikx} \text{ or}$$

$$C \sin kx + D \cos kx$$

We need to find the values of *A, C, D* and *F using the fact that* both $\psi(x)$ and $\frac{d\psi(x)}{dx}$ are continuous everywhere.

# Finite Square Well: Boundary conditions

- *At x = 0:* Match $\psi(x)$ and $\dfrac{d\psi(x)}{dx}$ from solutions in Region I and II

$$\psi_I(x=0) = \psi_{II}(x=0) \quad \Longrightarrow \quad A = D$$

$$\left.\frac{d\psi_I(x)}{dx}\right|_{x=0} = \left.\frac{d\psi_{II}(x)}{dx}\right|_{x=0} \quad \Longrightarrow \quad k_I\, A = k\, C$$

- *At x = L:* Match $\psi(x)$ and $\dfrac{d\psi(x)}{dx}$ from solutions in Region II and III

$$\psi_{II}(x=L) = \psi_{III}(x=L) \quad \Longrightarrow \quad F\, e^{-k_I L} = C\sin(kL) + D\cos(kL)$$

$$\left.\frac{d\psi_{II}(x)}{dx}\right|_{x=L} = \left.\frac{d\psi_{III}(x)}{dx}\right|_{x=L} \quad \Longrightarrow \quad -k_I F\, e^{-k_I L} = C\, k\, \cos(kL) - D\, k\, \sin(kL)$$

# Solving the equations

- We have four linear equations and 4 constants

$$A = D \quad \text{and} \quad F\, e^{-k_I L} = C \sin(kL) + D \cos(kL)$$

$$k_I\, A = k\, C \quad \text{and} \quad -k_I F\, e^{-k_I L} = C\, k\, \cos(kL) - D\, k\, \sin(kL)$$

- Express all constants in terms of *A*:

$$D = A \quad \text{and} \quad F = A\, e^{k_I L} \left[ \frac{k_I}{k} \sin(kL) + \cos(kL) \right]$$

$$C = \frac{k_I}{k} A \quad \text{and} \quad F = A\, e^{k_I L} \left[ -\cos(kL) + \frac{k}{k_I} \sin(kL) \right]$$

# Energy Eigenvalues

- Equating RHS of two equations relating F:

$$\frac{k_I}{k}\sin(kL)+\cos(kL)=-\cos(kL)+\frac{k}{k_I}\sin(kL)\quad\Longrightarrow\quad\tan(kL)=2\frac{f_0(E)}{1-f_0^2(E)}$$

$$\hbar k_I=\sqrt{2m(V_0-E)}\,;\quad \hbar k=\sqrt{2mE}\,;\quad \frac{k_I}{k}=\sqrt{\frac{V_0}{E}-1}=f_0(E)$$

$$\text{Using}\quad \tan(2\theta)=\frac{2\tan\theta}{1-\tan^2\theta}\quad\text{we have}\quad \tan\theta=f_0(E)\quad\Longrightarrow\quad \tan\left(\frac{kL}{2}\right)=f_0(E)$$

# Properties of the solutions

# Energy Eigenvalues

$$\tan\left(\frac{kL}{2}\right) = f_0(E) = \sqrt{\frac{V_0}{E} - 1}$$

- The above equation governs the allowed energy levels for a particle in a finite potential!

- This is a transcendental equation. If we expand tan as a series, then it is an infinite series in *k.*

- The equation cannot be solved analytically, thus both sides are plotted for the given parameters $(m, L, V_0)$.

- The intersections then lead to the allowed values of E

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

# Graphical solution

We will introduce new (dimensionless) variables $z, z_0$ to simplify the calculation

$$z := \frac{kL}{2} = \frac{L}{2}\sqrt{\frac{2mE}{\hbar^2}} \quad , \quad z_0 := \frac{L}{2\hbar}\sqrt{2mV_0}$$

To relate our old variables $k$ and $k_l$ to the new ones, we first look at

$$k^2 + k_l^2 = \frac{2mE}{\hbar^2} + \frac{2m(V_0 - E)}{\hbar^2} = \frac{2mV_0}{\hbar^2} \quad \Longrightarrow \quad k_l^2 = k^2\left(\frac{2mV_0}{\hbar^2 k^2} - 1\right)$$

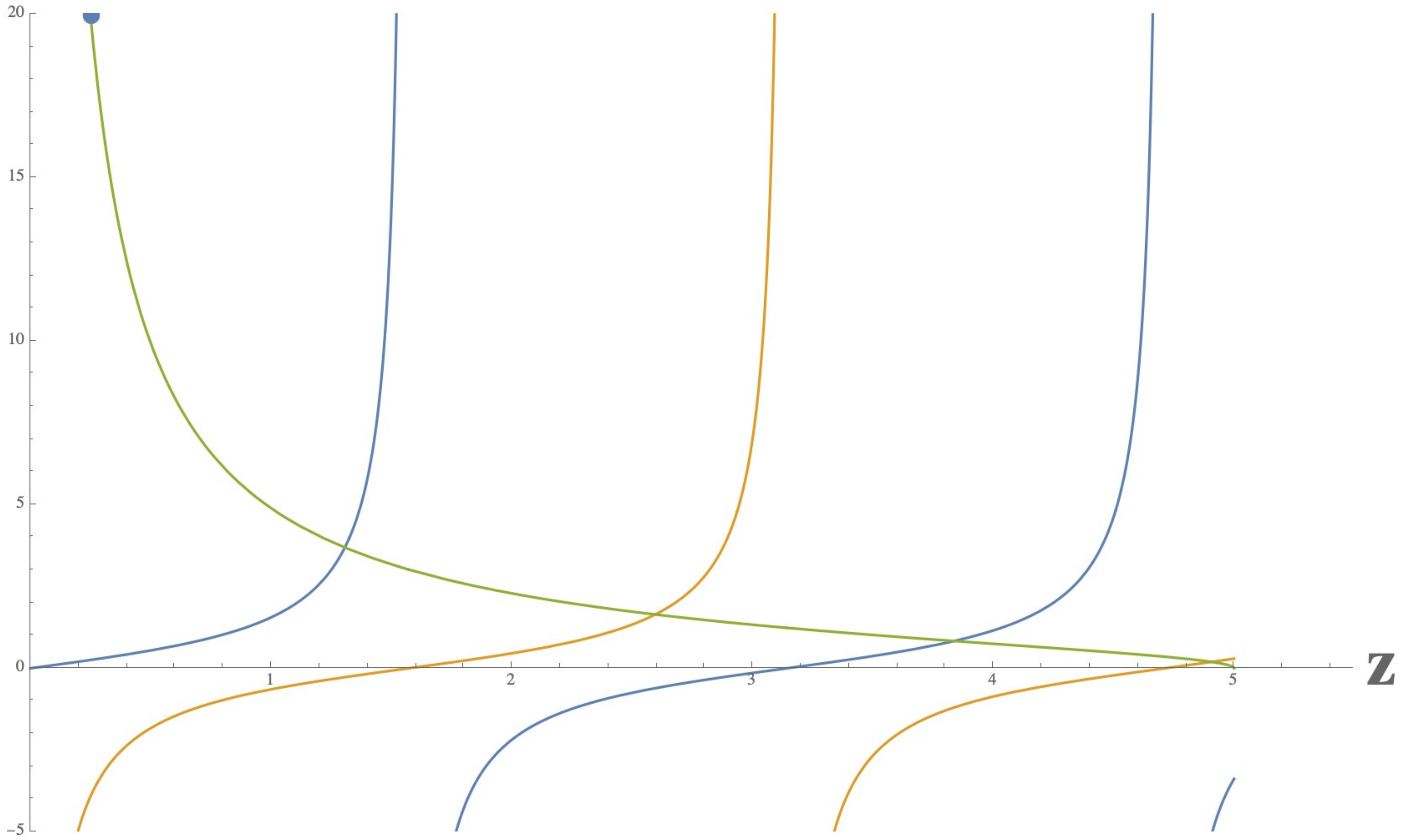
Rewriting $V_0$ in terms of $z_0$, we have

$$k_l^2 = k^2\left(\frac{4z_0^2}{k^2L^2} - 1\right) = k^2\left(\frac{z_0^2}{z^2} - 1\right) \Longrightarrow \frac{k_l}{k} = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1} \Rightarrow \text{insert in Eq. 1}$$

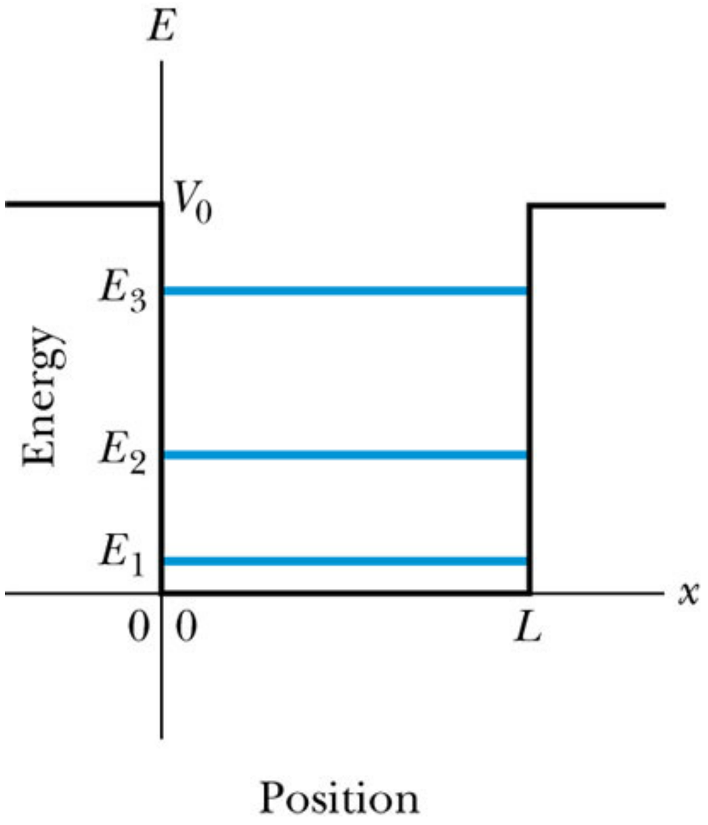
$$\tan z = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$$

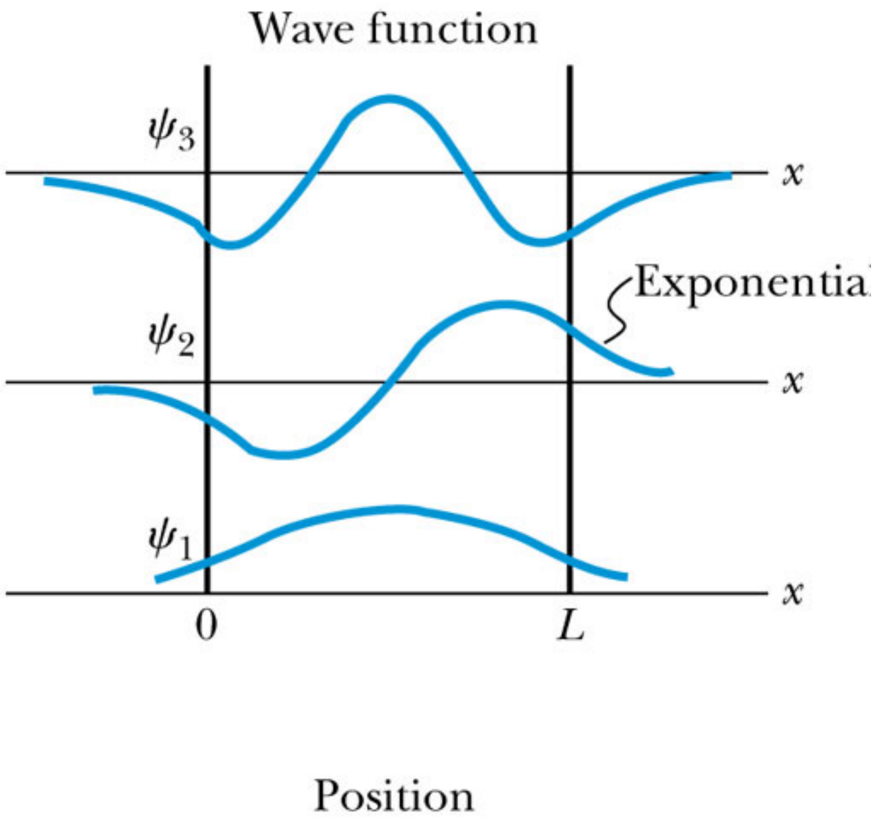
We can now study this graphically by plotting both the left hand and the right hand function for given values of $z_0$, e.g. for $L$, $m$ and $V_0$

$$\frac{\sqrt{z_0^2 - z^2}}{z}, \tan(z), -\cot(z)$$



# Energy Eigenvalues and wavefunctions

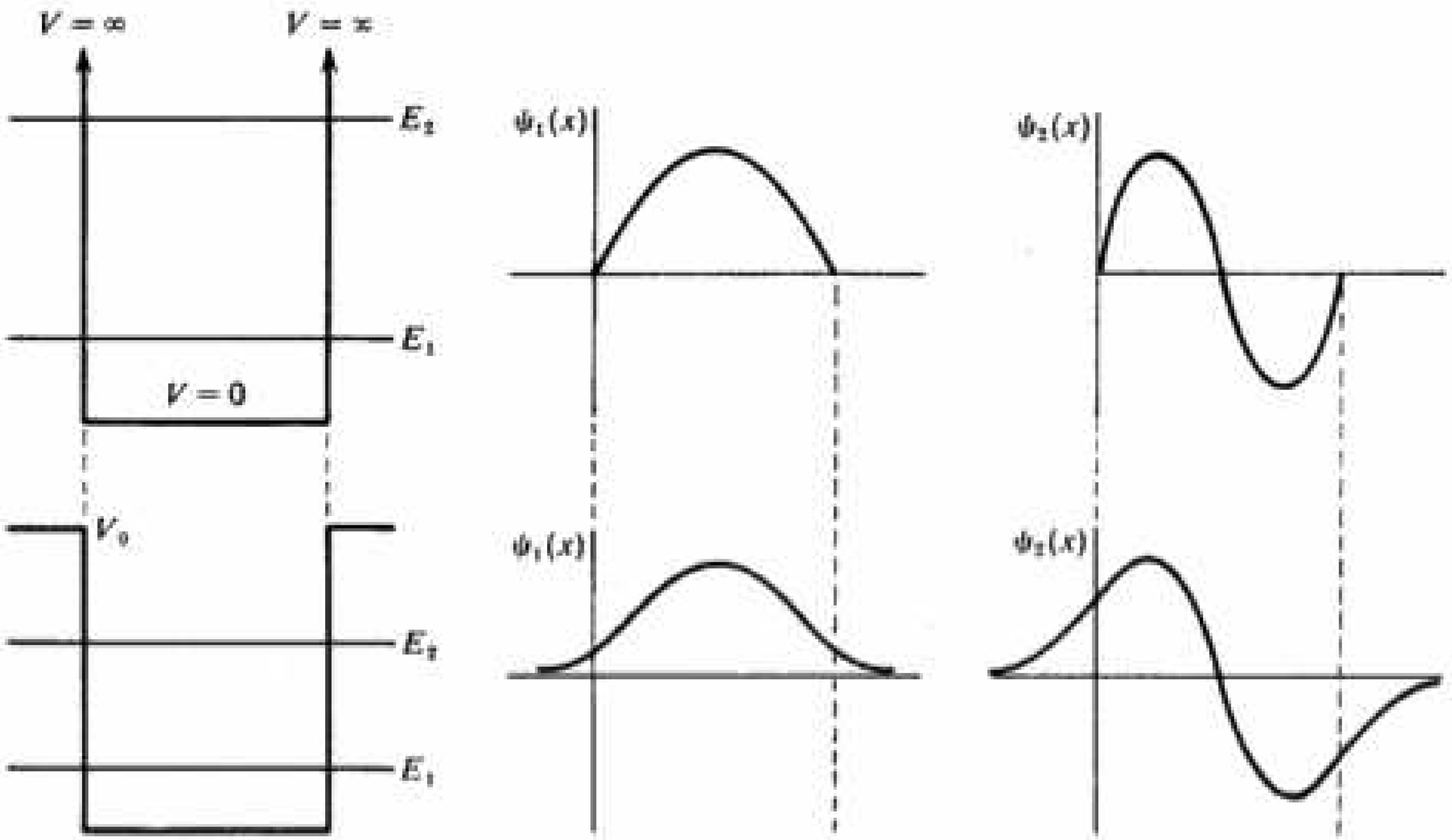



- There is a non zero probability of finding the particle in the classically forbidden region.

- Probability decreases exponentially as we move away from the box.

# Comparing Infinite and Finite Potential well




## Infinite well

1. $\psi(x)$ confined to the well.
2. Infinite tower of states.
3. NO unbound states

## Finite well

1. $\psi(x)$ spreads out beyond the well.
2. Finite tower of states
3. Unbound states for $E > V_0$

# Special cases

# Case 1: Deep potential well $(V_0 \gg 1)$

- 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 $E \equiv \epsilon \ll V_0$

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

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

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

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

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

  $V_0 = 0$ since, $z_0 = 0$, $f_0(E)$ has no values of $z$ which give a real value

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

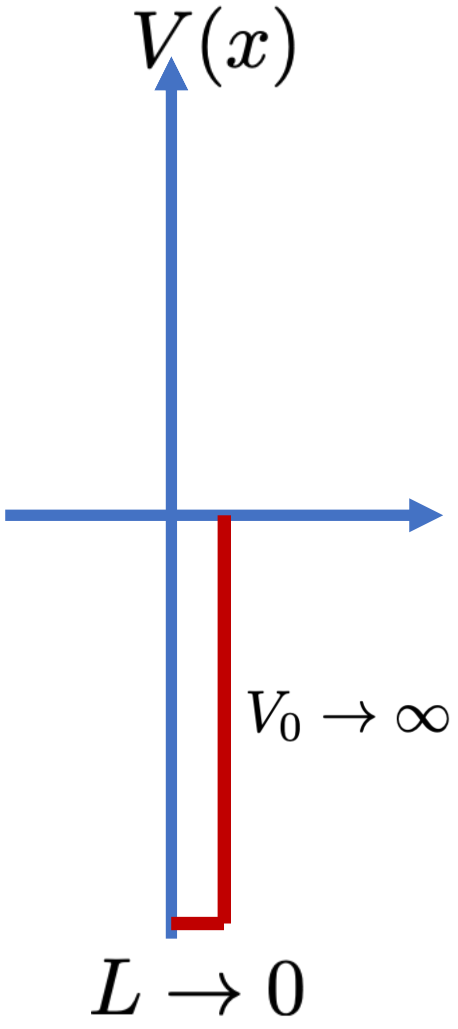
- However, if there is any potential well at all, no matter how shallow, there will be at least one bound state with non-zero energy.

  Consequence of Heisenberg's Uncertainty principle!

# Case 3: Deep and Narrow potential well

- $V_0 \to \infty, L \to 0$ such that $V_0 L = g =$ constant
- We then have $$z_0 = \frac{L}{2\hbar}\sqrt{2mV_0} \implies z_0 \propto \frac{g}{\sqrt{V_0}} \to 0$$
- Like in the previous case, $z_0 \to 0$ and NOT zero.
- Hence, no matter how small $z_0$ there will be at least one bound state with non-zero energy.

Consequence of Heisenberg's Uncertainty principle!



# Quantum Tunnelling

# Quantum Tunneling: Basic idea

$$\text{For } x < 0, \qquad \psi(x) \propto e^{k_I\, x}$$
$$\text{For } x > L, \qquad \psi(x) \propto e^{-k_I\, x}$$

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

- Notice the following behavior

$$V_0 \to \infty \implies k_I \to \infty \implies \frac{1}{k_I} \to 0$$
$$E \to V_0 \implies k_I \to 0 \implies \frac{1}{k_I} \to \infty$$

- $k_I$ determines depth of tunneling is determined by.

Note $\delta \propto \hbar$. Very tiny for macroscopic particles!

$$\delta = \frac{1}{k_I} = \frac{\hbar}{\sqrt{2m(V_0 - E)}}$$

# Quantum Tunneling: Basic idea

$$\text{For } x < 0, \qquad \psi(x) \propto e^{k_I x}$$

$$\text{For } x > L, \qquad \psi(x) \propto e^{-k_I x}$$

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

Note $\delta \propto \hbar$. Very tiny for macroscopic particles!

$$\delta = \frac{1}{k_I} = \frac{\hbar}{\sqrt{2m(V_0 - E)}}$$

Electron in a box $V_0 - E \sim 1$ ev

$$\delta = \frac{1.05 \times 10^{-34}}{(9.1 \times 10^{-31} \times 1.6 \times 10^{-19})^{\frac{1}{2}}} \sim 2.7 \text{Å}$$

An Iron ball of mass of 1 gm $V_0 - E \sim 1\, ev$

$$\delta = \frac{1.05 \times 10^{-34}}{(1 \times 1.6 \times 10^{-19})^{\frac{1}{2}}} \sim 10^{-25}\, m$$

# Quantum Tunneling: Basic idea

We notice the following interesting behavior

$$V_0 \to \infty \implies k_I \to \infty \implies \frac{1}{k_I} \to 0$$

$$E \to V_0 \implies k_I \to 0 \implies \frac{1}{k_I} \to \infty$$

- Non-zero wavefunction in classically forbidden regions (KE < 0!) is a purely quantum mechanical effect.
- Quantum mechanics allows tunnelling between classically allowed regions. (We will discuss more in the next application.)
- It follows from requiring that both $\psi(x)$ and $\frac{d\psi(x)}{dx}$ are continuous.

# Summary: Quantum States in potential wells

# 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 $\psi(x) \text{ and } \dfrac{d\psi(x)}{dx}$ to be continuous everywhere.

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

# General properties of quantum states

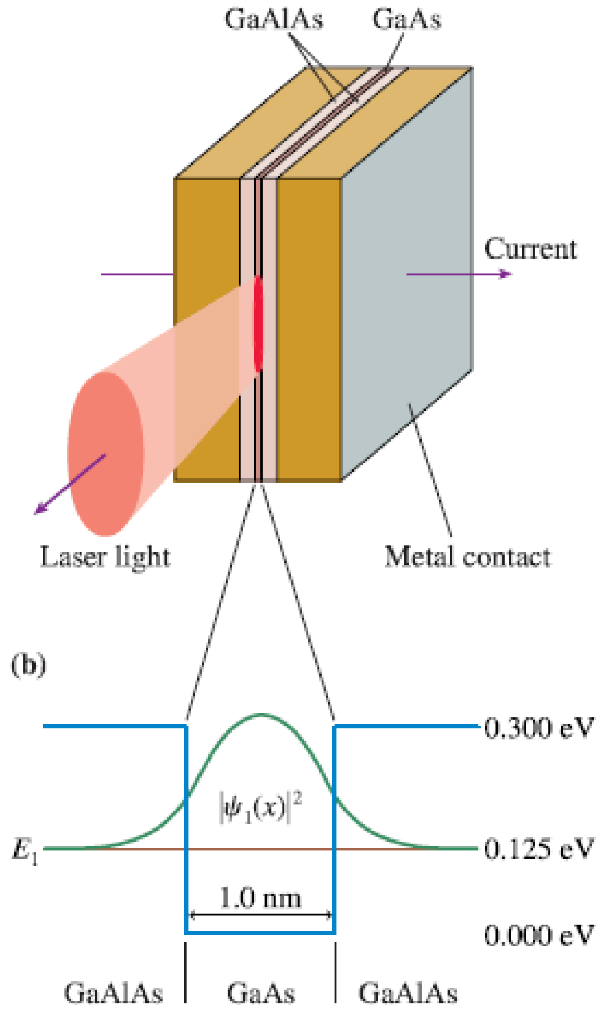
1. Lowest energy (ground) state is always above the bottom of the potential and is symmetric. [Consequence of Uncertainty Principle.]

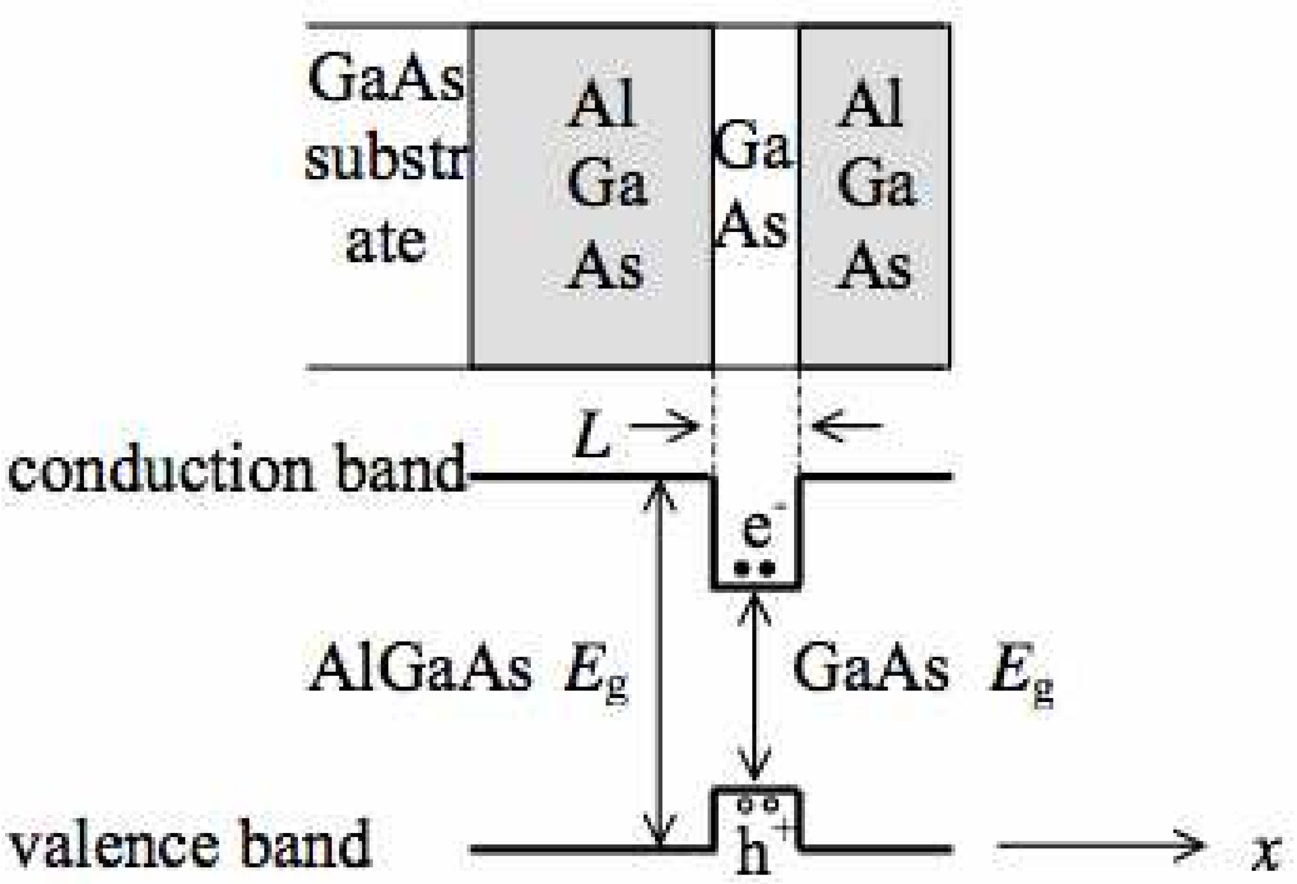
2. Wider and/or more shallow the potential, the lower the energies of the quantum states. [Consequence of Uncertainty Principle.]

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 states are continuous.

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

# Real-life potential well: Quantum-well LASER




Constrained motion along the x-axis; free motion in the y – z plane.

# Recommended Reading

Finite square well section 6.5