M.Sc. 3rd Semester
Paper: MPHYCC-13 Nuclear and Particle Physics
Topic: Square Well Potential

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OUTLINE

- ❖ Infinite Square Well Potential
- ❖ Finite Square Well Potential

Reference:

1. Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education
2. Shankar, R. (1994), Principles of Quantum Mechanics, Plenum Press.

Infinite Square Well Potential

❖ The simplest such system is that of a particle trapped in a box with infinitely hard walls that the particle cannot penetrate. This potential is called an infinite square well and is given by

$$V(x) = \begin{cases} \infty & x \le 0, x \ge L \\ 0 & 0 < x < L \end{cases}$$

❖ Clearly the wave function must be zero where the potential is infinite.

❖ Where the potential is zero inside the box, the Schrödinger wave equation becomes $\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi$ where $k = \sqrt{2mE/\hbar^2}$.

❖ The general solution is $\psi(x) = A\sin kx + B\cos kx$

Quantization

- Boundary conditions of the potential dictate that the wave function must be zero at $x = 0$ and $x = L$. This yields valid solutions for integer values of n such that $kl = n\pi$.

- The wave function is now $$\psi_n(x) = A\sin\left(\frac{n\pi x}{L}\right)$$

- We normalize the wave function

$$\int_{-\infty}^{\infty} \psi_n^*(x)\psi_n(x)\,dx = 1 \qquad A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right)dx = 1$$

- The normalized wave function becomes

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$

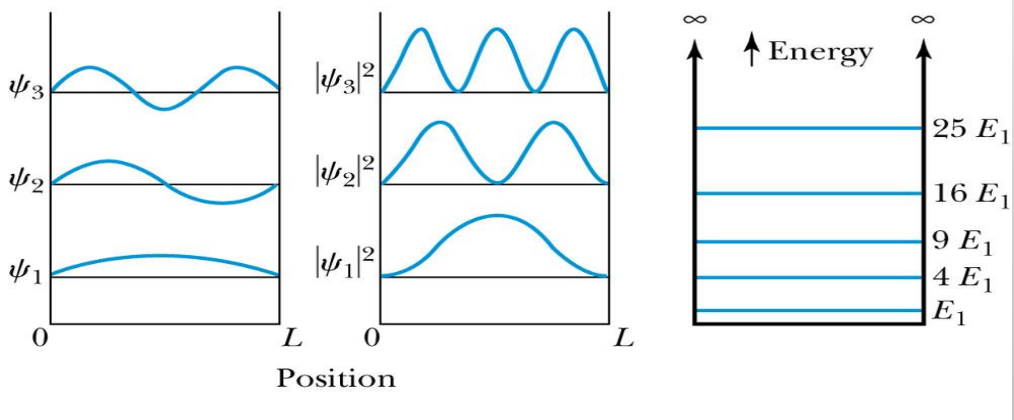
- These functions are identical to those obtained for a vibrating string with fixed ends.

Quantized Energy

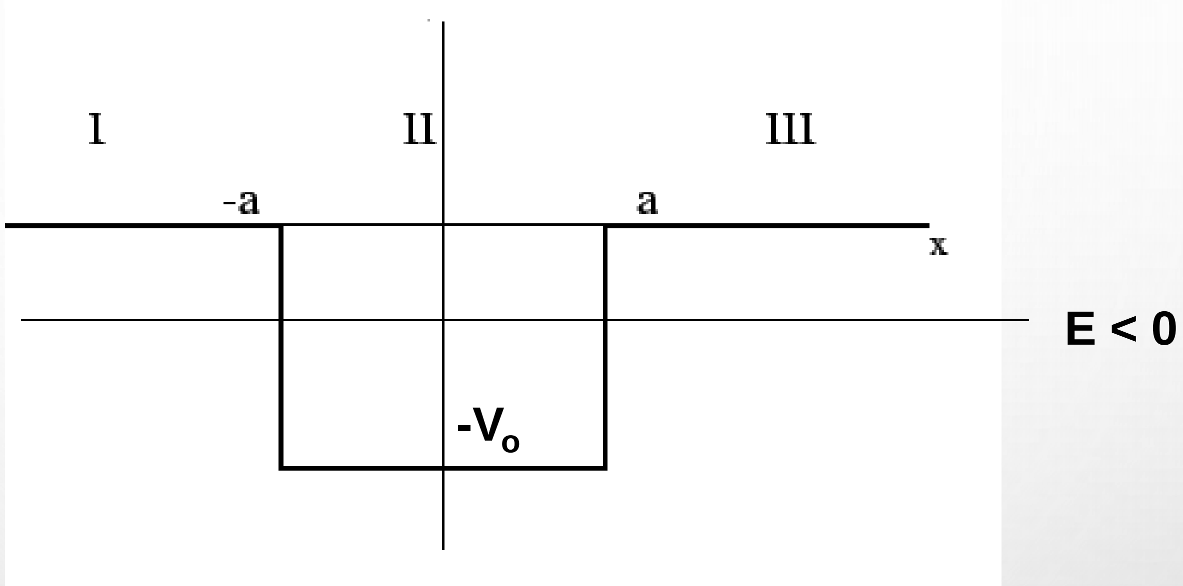
- The quantized wave number now becomes $k_n = \frac{n\pi}{L} = \sqrt{\frac{2mE_n}{\hbar^2}}$
- Solving for the energy yields

$$E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2} \qquad (n = 1, 2, 3, \ldots)$$

- Note that the energy depends on the integer values of *n*. Hence the energy is quantized and nonzero.
- The special case of *n* = 0 is called the ground state energy. $E_1 = \frac{\pi^2 \hbar^2}{2mL^2}$



Bound States Of The Square Well



❖ Consider the potential $V(x)=\begin{cases} -V_o, \ for -a \le x \le a \\ 0, \ for \ |x| > a \end{cases}$

❖ This is a "square" well potential of width 2a and depth V_0.

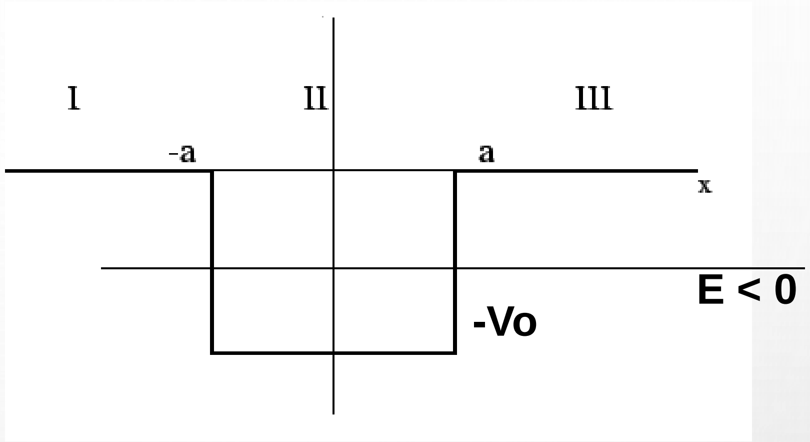
Bound States Of The Square Well

Region I and III:

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

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

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



Region II:

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

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}(V_o - E)\Psi(x)$$

$$l^2 = \frac{2m(V_o - E)}{\hbar^2}$$

The solutions are, in general:

- Region I: $\psi(x) = A\exp(-\kappa x) + B\exp(\kappa x)$, → $\psi(x) = Be^{\kappa x}$, for $x < -a$.
- Region II: $\psi(x) = C\sin(lx) + D\cos(lx)$, for $-a < x < a$,
- Region III: $\psi(x) = F\exp(-\kappa x) + G\exp(\kappa x)$, → $\psi(x) = Fe^{-\kappa x}$, for $x > a$.

In these the A's, B's and C's are constants.

Potential is even function, therefore the solutions can be even or odd. For even solution:

$$\psi(x) = \begin{cases} Fe^{-\kappa x}, & \text{for } x > a, \\ D\cos(lx), & \text{for } 0 < x < a, \\ \psi(-x), & \text{for } x < 0. \end{cases}$$

The continuity of $\psi(x)$, at $x = a$, says

$$Fe^{-\kappa a} = D\cos(la),$$

and the continuity of $d\psi/dx$, says

$$-\kappa Fe^{-\kappa a} = -lD\sin(la).$$

→ $\kappa = l\tan(la)$.

K and *l are functions of E, so* $\kappa = l\tan(la)$. *is formula for allowed energies.*

Bound States Of The Square Well

$$\kappa = l\tan(la).$$

$$z = la, \quad \text{and} \quad z_0 \equiv \frac{a}{\hbar}\sqrt{2mV_0}.$$

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

$$l^2 = \frac{2m\left(V_o - E\right)}{\hbar^2}$$

$$\kappa^2 - \ell^2 = \frac{2mV_o}{\hbar^2}$$

$$\kappa a = \sqrt{z_o^2 + z^2}$$

$$\tan z = \sqrt{\frac{z_o^2}{z^2} + 1}$$

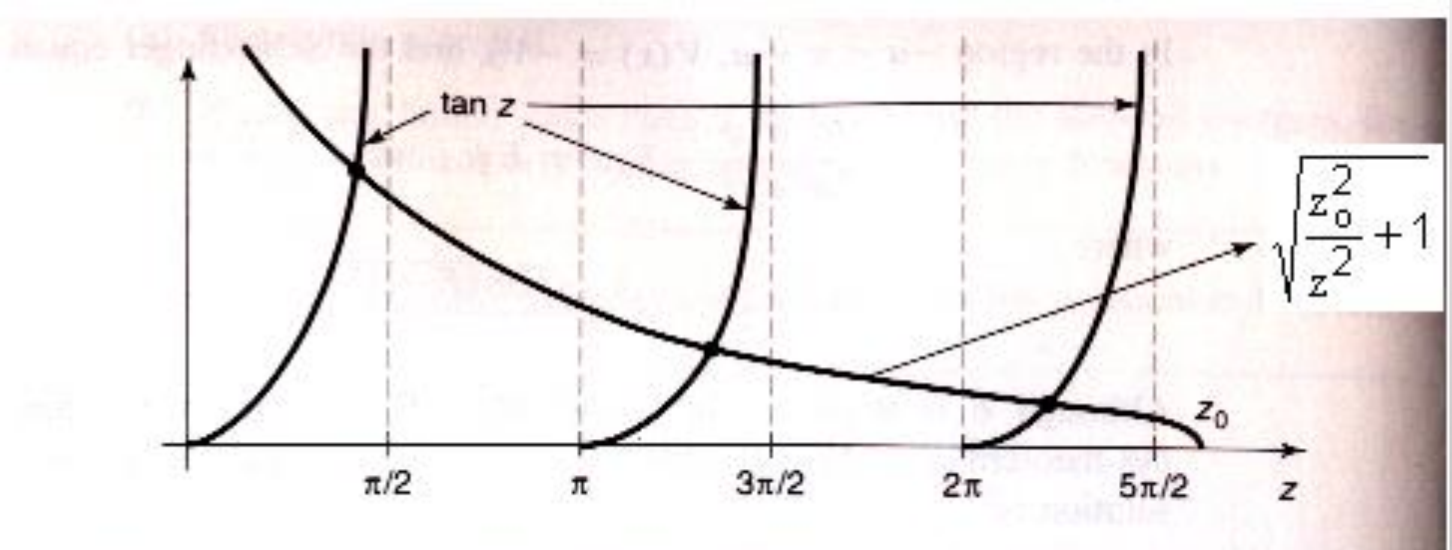


FIGURE 2.18: Graphical solution to Equation 2.156, for $z_0 = 8$ (*even* states).

Wide, Deep Well

If z is very large,

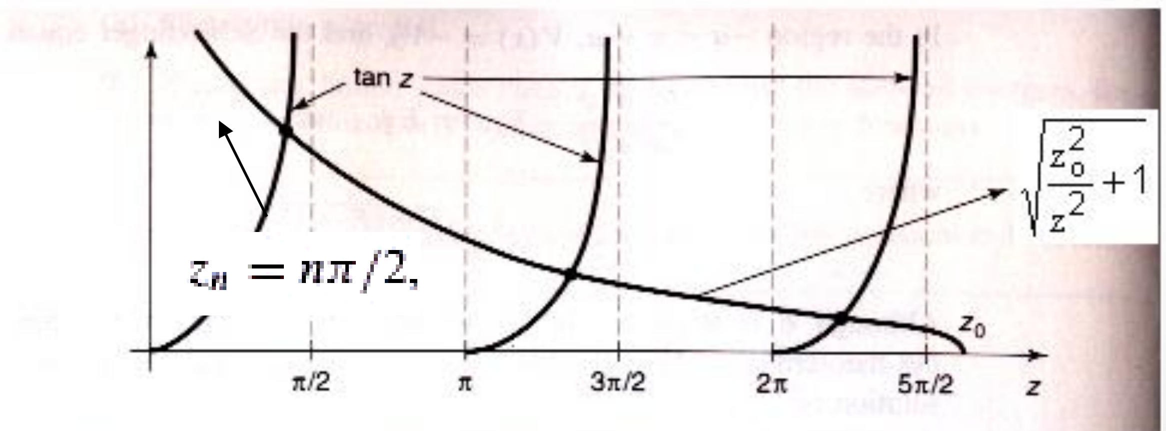


FIGURE 2.18: Graphical solution to Equation 2.156, for $z_0 = 8$ (*even* states).

$z \equiv la,$

$$\tan z = \sqrt{\frac{z_o^2}{z^2}+1}$$

$$E_n + V_0 \cong \frac{n^2\pi^2\hbar^2}{2m(2a)^2}.$$

Infinite square well energies for well width of 2a.

This is half the energy, the others come from the odd wave functions.

SHALLOW NARROW WELL

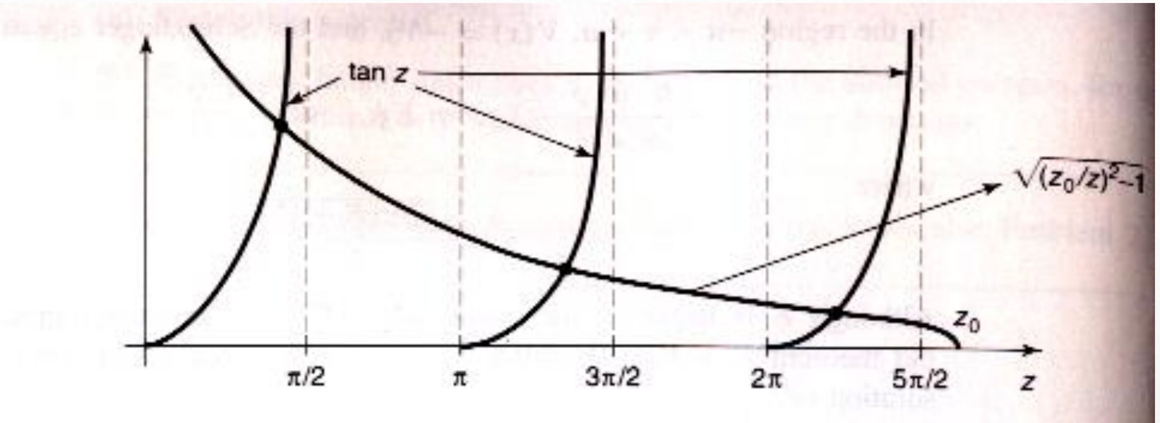


FIGURE 2.18: Graphical solution to Equation 2.156, for $z_0 = 8$ (*even* states).

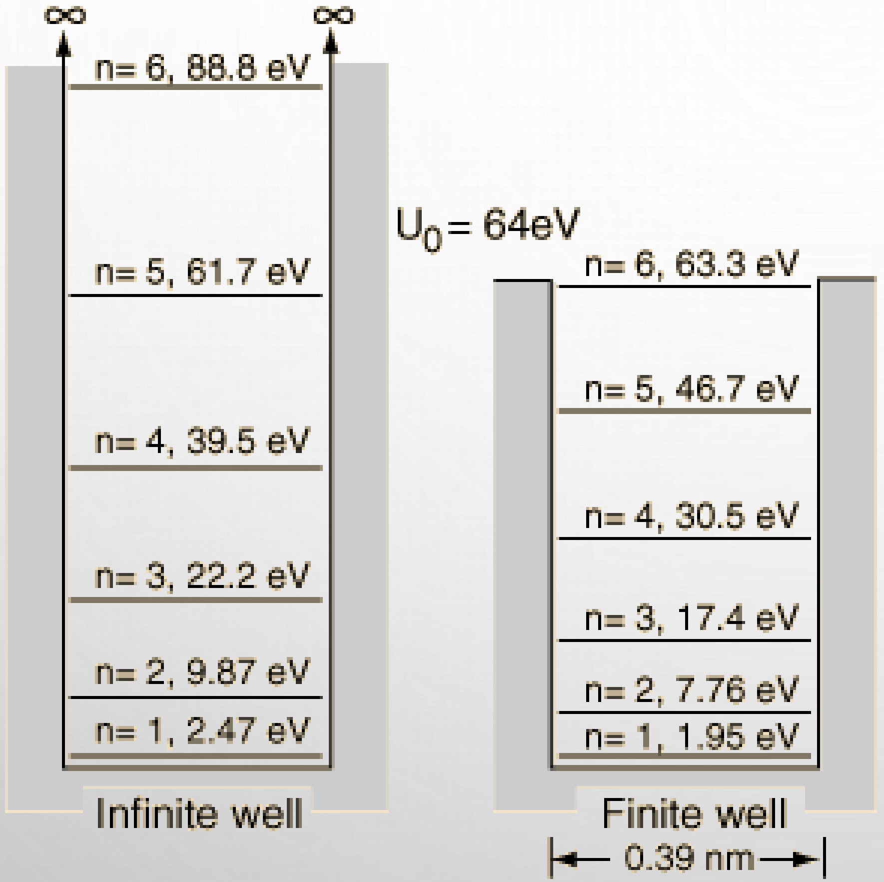
$$\tan z = \sqrt{\frac{z_o^2}{z^2} + 1}$$

$$z \equiv la, \quad \text{and} \quad z_0 \equiv \frac{a}{\hbar}\sqrt{2mV_0}.$$

As z_o decreases, fewer bound states, until finally,)for zo < $\pi/2$, the lowest odd state disappears) only one bound state remains.

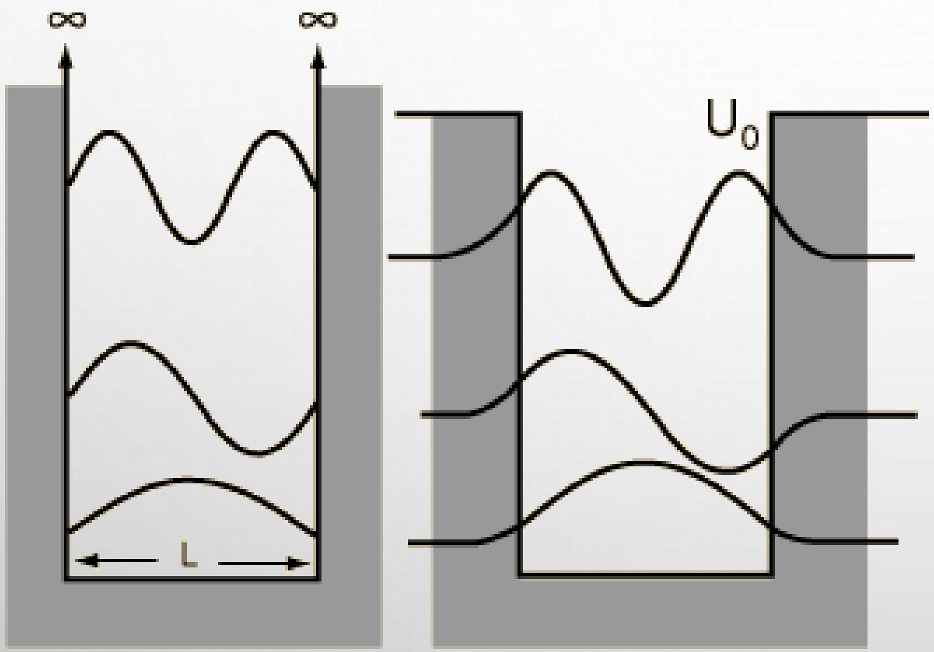
There is one bound state no matter how weak the well becomes.

Finite Well Energy Levels



The energy levels for an electron in a potential well of depth 64 eV and width 0.39 nm are shown in comparison with the energy levels of an infinite well of the same size.

Particle In Finite Walled Box



For the finite potential well, the solution to the Schrodinger equation gives a wavefunction with an exponentially decaying penetration into the classically forbidden region. Confining a particle to a smaller space requires a larger confinement energy. Since the wavefunction penetration effectively "enlarges the box", the finite well energy levels are lower than those for the infinite well.

THANK YOU