PHYS 3313 – Section 001
Lecture #20

Monday, April 10, 2017
Dr. Amir Farbin

- Infinite Square-well Potential
- Finite Square Well Potential
- Penetration Depth
- Degeneracy
- Simple Harmonic Oscillator

Announcements

- Reminder: Homework #4
  - End of chapter problems on CH5: 8, 10, 16, 24, 26, 36 and 47
  - Due this Wednesday, Apr. 12
- Quiz 3 results
  - Class average: 25.1
    - Equivalent to: 50.2/100
    - Previous quizzes: 21/100 and 57.6/100
  - Top score: 47/50
- Reminder: Quadruple extra credit
  - Colloquium on April 19, 2017
  - Speaker: Dr. Nigel Lockyer, Director of Fermilab
  - Make your arrangements to take advantage of this opportunity

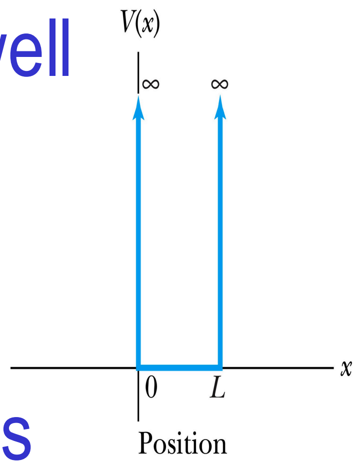
Reminder: Special project #6

- Show that the Schrodinger equation becomes Newton's second law in the classical limit. (15 points)
- Deadline Monday, Apr. 17, 2017
- You MUST have your own answers!

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

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



- The wave function must be zero where the potential is infinite.
- Where the potential is zero inside the box, the time independent Schrödinger wave equation $-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$ becomes $\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi \quad = -k^2\psi$ where $k = \sqrt{2mE/\hbar^2}$.
- The general solution is $\psi(x) = A\sin kx + B\cos kx$.

Quantization

- Since the wave function must be continuous, the boundary conditions of the potential dictate that the wave function must be zero at $x = 0$ and $x = L$. These yield valid solutions for B=0, and for **integer values** of n such that $kL = n\pi$ ➔ $k=n\pi/L$
- The wave function now becomes $\psi_n(x) = A\sin\left(\frac{n\pi x}{L}\right)$
- We normalize the wave function $\int_{-\infty}^{+\infty}\psi_n^*(x)\psi_n(x)dx = 1$

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

- 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

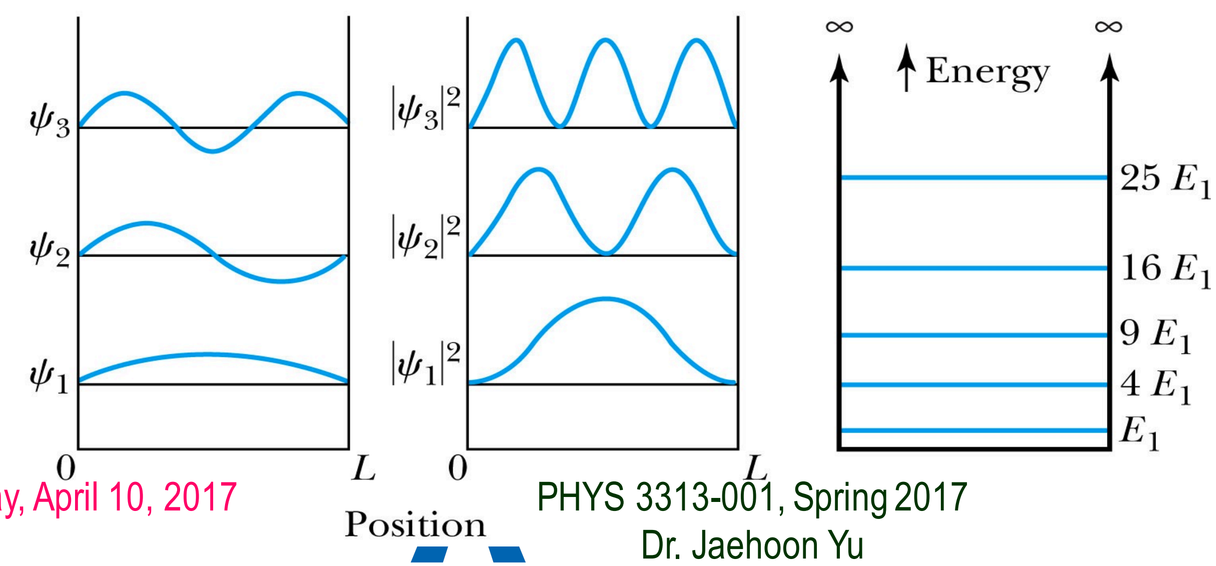
- The quantized wave number now becomes $k_n(x) = \frac{n\pi}{L} = \sqrt{\frac{2mE_n}{\hbar^2}}$
- Solving for the energy yields

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

- Note that the energy depends on the integer values of *n*. Hence the energy is quantized and nonzero.
- The special case of *n* = 1 is called the **ground state energy**.

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

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



$$E_3 = \frac{9\pi^2\hbar^2}{2mL^2} = 9E_1$$

$$E_2 = \frac{2\pi^2\hbar^2}{mL^2} = 4E_1$$

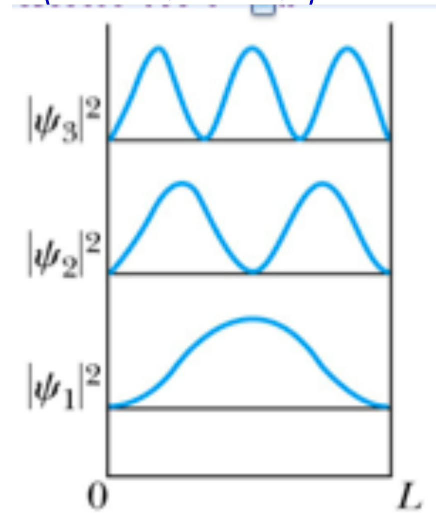
$$E_1 = \frac{\pi^2\hbar^2}{2mL^2}$$

How does this correspond to Classical Mech.?

- What is the probability of finding a particle in a box of length L? $\frac{1}{L}$
- Bohr's **correspondence principle** says that QM and CM must correspond to each other! When?
  - When n becomes large, the QM approaches to CM
- So when n→∞, the probability of finding a particle in a box of length L is

$$P(x) = \psi_n^*(x)\psi_n(x) = |\psi_n(x)|^2 = \frac{2}{L}\lim_{n\to\infty}\sin^2\left(\frac{n\pi x}{L}\right) \approx \frac{2}{L}\left\langle \sin^2\left(\frac{n\pi x}{L}\right)\right\rangle = \frac{2}{L}\cdot\frac{1}{2} = \frac{1}{L}$$

- Which is identical to the CM probability!!
- One can also see this from the plot of P!



Expectation Values & Operators

- Expectation value for any function g(x)

$$\langle g(x) \rangle = \int_{-\infty}^{+\infty} \Psi(x,t)^* g(x) \Psi(x,t) dx$$

- Position operator is the same as itself, x
- Momentum Operator

$$\hat{p} = -i\hbar \frac{\partial}{\partial x}$$

- Energy Operator

$$\hat{E} = i\hbar \frac{\partial}{\partial t}$$

Ex 6.8: Expectation values inside a box

Determine the expectation values for x, x^2, p and p^2 of a particle in an infinite square well for the first excited state.

What is the wave function of the first excited state? n=? 2

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

$$\langle x\rangle_{n=2}=\int_{-\infty}^{+\infty}\psi^*_{n=2}(x)\,x\,\psi_{n=2}(x)=\frac{2}{L}\int_0^L x\sin^2\left(\frac{2\pi x}{L}\right)dx=\frac{L}{2}$$

$$\langle x^2\rangle_{n=2}=\frac{2}{L}\int_0^L x^2\sin^2\left(\frac{2\pi x}{L}\right)dx=0.32L^2$$

$$\langle p\rangle_{n=2}=\frac{2}{L}\int_0^L \sin\left(\frac{2\pi x}{L}\right)(-i\hbar)\frac{\partial}{\partial x}\left[\sin\left(\frac{n\pi x}{L}\right)\right]dx=-i\hbar\frac{2}{L}\frac{2\pi}{L}\int_0^L\sin\left(\frac{2\pi x}{L}\right)\cos\left(\frac{2\pi x}{L}\right)dx=0$$

$$\langle p^2\rangle_{n=2}=\frac{2}{L}\int_0^L \sin\left(\frac{2\pi x}{L}\right)(-i\hbar)^2\frac{\partial^2}{\partial x^2}\left[\sin\left(\frac{2\pi x}{L}\right)\right]dx=\hbar^2\frac{2}{L}\left(\frac{2\pi}{L}\right)^2\int_0^L\sin^2\left(\frac{2\pi x}{L}\right)dx=\frac{4\pi^2\hbar^2}{L^2}$$

$$E_2=\frac{4\pi^2\hbar^2}{2mL^2}=\frac{\langle p^2\rangle_{n=2}}{2m}$$

Ex 6.9: Proton Transition Energy

A typical diameter of a nucleus is about 10^{-14}m. Use the infinite square-well potential to calculate the transition energy from the first excited state to the ground state for a proton confined to the nucleus.

The energy of the state n is $E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2}$

What is n for the ground state? n=1

$$E_1 = \frac{\pi^2 \hbar^2}{2mL^2} = \frac{\pi^2 \hbar^2 c^2}{2mc^2 L^2} = \frac{1}{mc^2} \frac{\pi^2 \cdot (197.3 eV \cdot nm)^2}{2 \cdot (10^{-5} nm)} = \frac{1.92 \times 10^{15} eV^2}{938.3 \times 10^6 eV} = 2.0 MeV$$

What is n for the 1st excited state? n=2

$$E_2 = 2^2 \frac{\pi^2 \hbar^2}{2mL^2} = 8.0 MeV$$

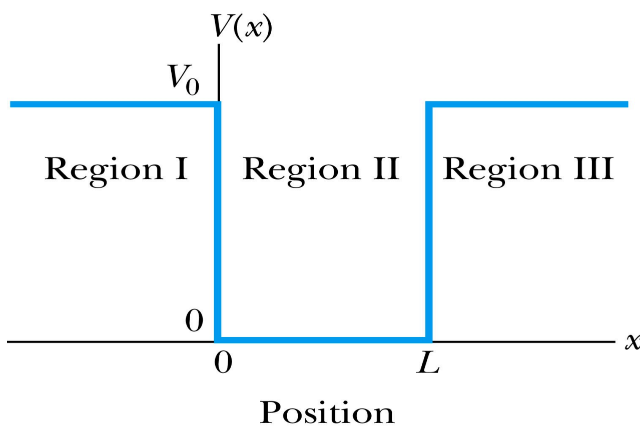
So the proton transition energy is

$$\Delta E = E_2 - E_1 = 6.0 MeV$$

Finite Square-Well Potential

- The finite square-well potential is $V(x) = \begin{cases} V_0 & x \le 0, \\ 0 & 0 < x < L \\ V_0 & x \ge L \end{cases}$

- The Schrödinger equation outside the finite well in regions I and III is $-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} = (E - V_0)$ for regions I and III, or using $\alpha^2 = 2m(V_0 - E)/\hbar^2$ yields $\frac{d^2\psi}{dx^2} = \alpha^2\psi$. The solution to this differential has exponentials of the form $e^{\alpha x}$ and $e^{-\alpha x}$. In the region x > L, we reject the positive exponential and in the region x < 0, we reject the negative exponential. Why?



$$\psi_I(x) = Ae^{\alpha x} \quad \text{region I}, x < 0$$

$$\psi_{III}(x) = Ae^{-\alpha x} \quad \text{region III}, x > L$$

This is because the wave function should be 0 as x→±infinity.

Finite Square-Well Solution

- Inside the square well, where the potential *V* is zero and the particle is free, the wave equation becomes $\frac{d^2\psi}{dx^2} = -k^2\psi$ where $k = \sqrt{2mE/\hbar^2}$
- Instead of a sinusoidal solution we can write

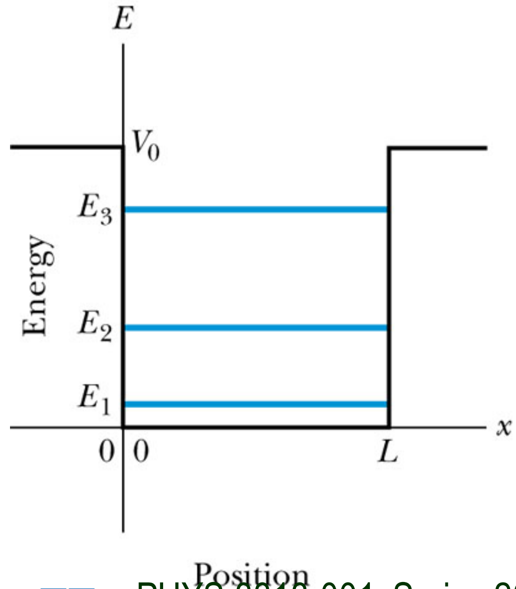
$$\psi_{II}(x) = Ce^{ikx} + De^{-ikx} \quad \text{region II, } 0 < x < L$$

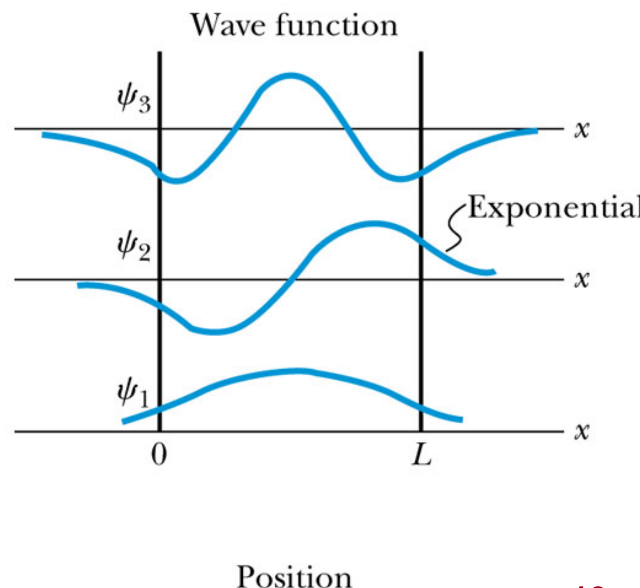
- The boundary conditions require that

$$\psi_I = \psi_{II} \text{ at } x = 0 \text{ and } \psi_{II} = \psi_{III} \text{ at } x = L$$

and the wave function must be smooth where the regions meet.

- Note that the wave function is nonzero outside of the box.
- Non-zero at the boundary either..
- What would the energy look like?





Penetration Depth

- The penetration depth is the distance outside the potential well where the probability significantly decreases. It is given by

$$\delta x \approx \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m\left(V_0 - E\right)}}$$

- It should not be surprising to find that the penetration distance that violates classical physics is proportional to Planck's constant.

Three-Dimensional Infinite-Potential Well

- The wave function must be a function of all three spatial coordinates.
- We begin with the conservation of energy $E = K + V = \frac{p^2}{2m} + V$
- Multiply this by the wave function to get

$$E\psi = \left(\frac{p^2}{2m} + V\right)\psi = \frac{p^2}{2m}\psi + V\psi$$

- Now consider momentum as an operator acting on the wave function. In this case, the operator must act twice on each dimension. Given:

$$p^2 = p_x^2 + p_y^2 + p_z^2 \qquad \hat{p}_x\psi = -i\hbar\frac{\partial\psi}{\partial x} \quad \hat{p}_y\psi = -i\hbar\frac{\partial\psi}{\partial y} \quad \hat{p}_z\psi = -i\hbar\frac{\partial\psi}{\partial z}$$

- The three dimensional Schrödinger wave equation is

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) + V\psi = E\psi \xrightarrow{\text{Rewrite}} -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

Ex 6.10: Expectation values inside a box

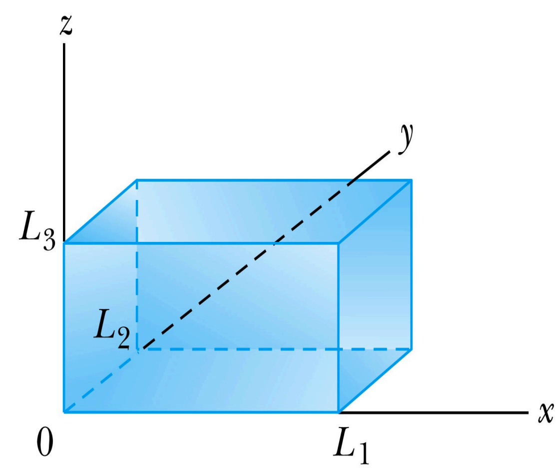
Consider a free particle inside a box with lengths L_1, L_2 and L_3 along the x, y, and z axes, respectively, as shown in the figure. The particle is constrained to be inside the box. Find the wave functions and energies. Then find the ground energy and wave function and the energy of the first excited state for a cube of sides L.

What are the boundary conditions for this situation?

Particle is free, so x, y and z wave functions are independent from each other!

Each wave function must be 0 at the wall! Inside the box, potential V is 0.

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \Rightarrow -\frac{\hbar^2}{2m}\nabla^2\psi = E\psi$$



A reasonable solution is

$$\psi(x,y,z) = A\sin(k_1 x)\sin(k_2 y)\sin(k_3 z)$$

Using the boundary condition

$$\psi = 0 \text{ at } x = L_1 \Rightarrow k_1 L_1 = n_1\pi \Rightarrow k_1 = n_1\pi / L_1$$

So the wave numbers are $k_1 = \frac{n_1\pi}{L_1}$ $k_2 = \frac{n_2\pi}{L_2}$ $k_3 = \frac{n_3\pi}{L_3}$

Ex 6.10: Expectation values inside a box

Consider a free particle inside a box with lengths L_1, L_2 and L_3 along the x, y, and z axes, respectively, as shown in figure. The particle is constrained to be inside the box. Find the wave functions and energies. Then find the round energy and wave function and the energy of the first excited state for a cube of sides L.

The energy can be obtained through the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi = E\psi$$

$$\frac{\partial\psi}{\partial x} = \frac{\partial}{\partial x}\left(A\sin(k_1x)\sin(k_2y)\sin(k_3z)\right) = k_1A\cos(k_1x)\sin(k_2y)\sin(k_3z)$$

$$\frac{\partial^2\psi}{\partial x^2} = \frac{\partial^2}{\partial x^2}\left(A\sin(k_1x)\sin(k_2y)\sin(k_3z)\right) = -k_1^2A\sin(k_1x)\sin(k_2y)\sin(k_3z) = -k_1^2\psi$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi = \frac{\hbar^2}{2m}\left(k_1^2+k_2^2+k_3^2\right)\psi = E\psi$$

$$E = \frac{\hbar^2}{2m}\left(k_1^2+k_2^2+k_3^2\right) = \frac{\pi^2\hbar^2}{2m}\left(\frac{n_1^2}{L_1^2}+\frac{n_2^2}{L_2^2}+\frac{n_3^2}{L_3^2}\right)$$

What is the ground state energy?

$E_{1,1,1}$ when $n_1=n_2=n_3=1$, how much?

When are the energies the same for different combinations of n_i?

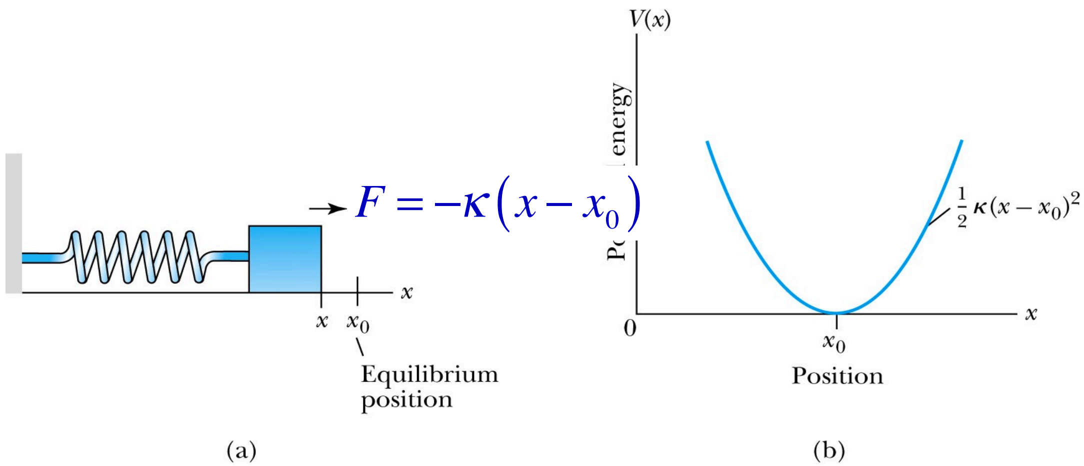
Degeneracy*

- Analysis of the Schrödinger wave equation in three dimensions introduces three quantum numbers that quantize the energy.
- A quantum state is degenerate when there is more than one wave function for a given energy.
- Degeneracy results from particular properties of the potential energy function that describes the system. A perturbation of the potential energy, such as the spin under a B field, can remove the degeneracy.

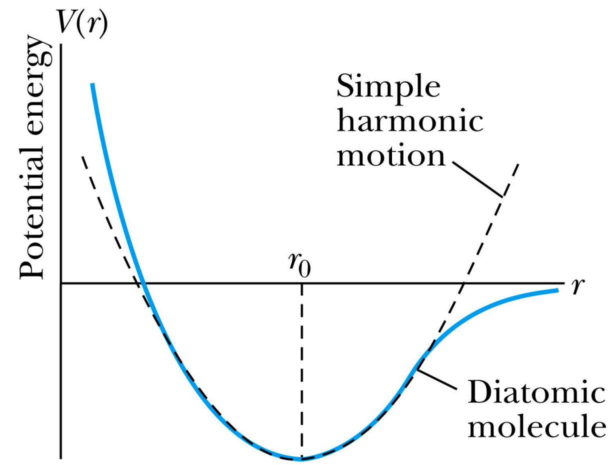
***Mirriam-webster: having two or more states or subdivisions**

The Simple Harmonic Oscillator

- Simple harmonic oscillators describe many physical situations: springs, diatomic molecules and atomic lattices.



$$F = -\kappa\left(x - x_0\right)$$



- Consider the Taylor expansion of a potential function:

$$V\left(x\right) = V_0 + V_1\left(x - x_0\right) + \frac{1}{2}V_2\left(x - x_0\right)^2 + \cdots$$

The minimum potential at $x=x_0$, so $dV/dx=0$ and $V_1=0$; and the zero potential $V_0=0$, we have

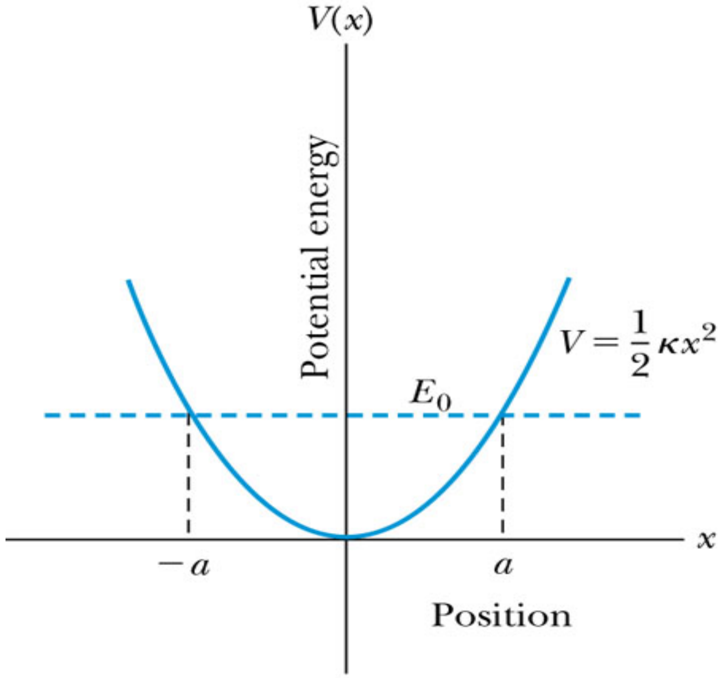
$$V\left(x\right) = \frac{1}{2}V_2\left(x - x_0\right)^2$$

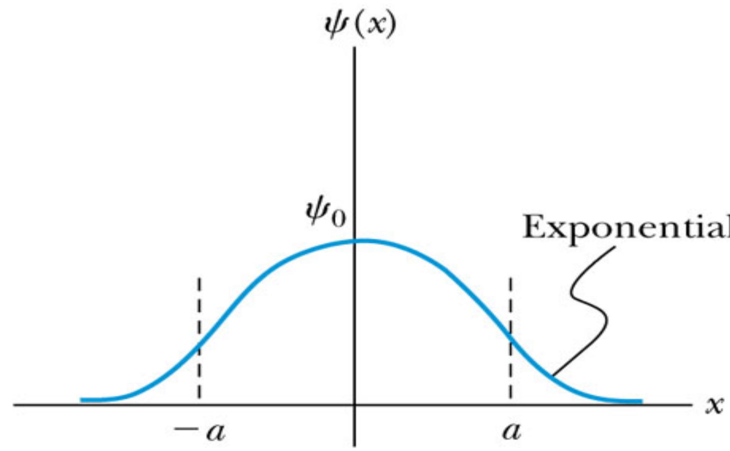
Substituting this into the wave equation:

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

Let $\alpha^2 = \frac{m\kappa}{\hbar^2}$ and $\beta = \frac{2mE}{\hbar^2}$ which yields $\frac{d^2\psi}{dx^2} = \left(\alpha^2 x^2 - \beta\right)\psi$.

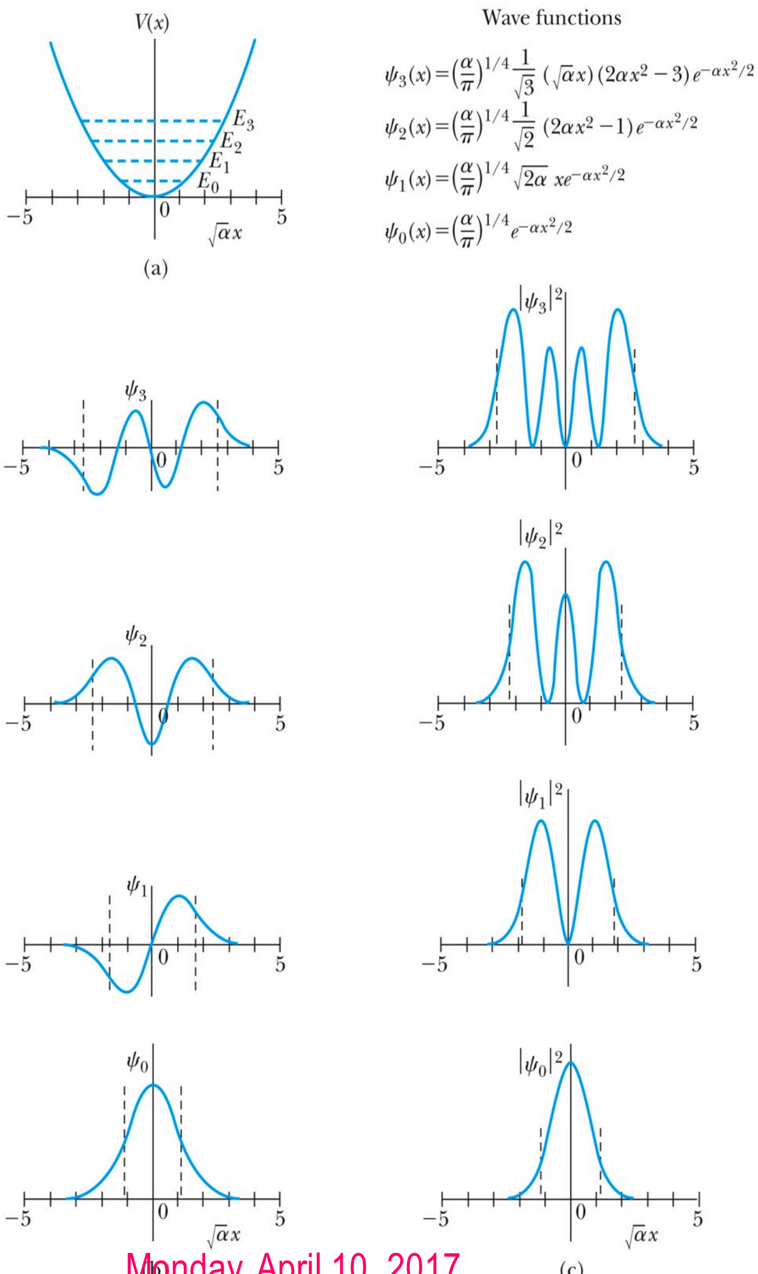
Parabolic Potential Well

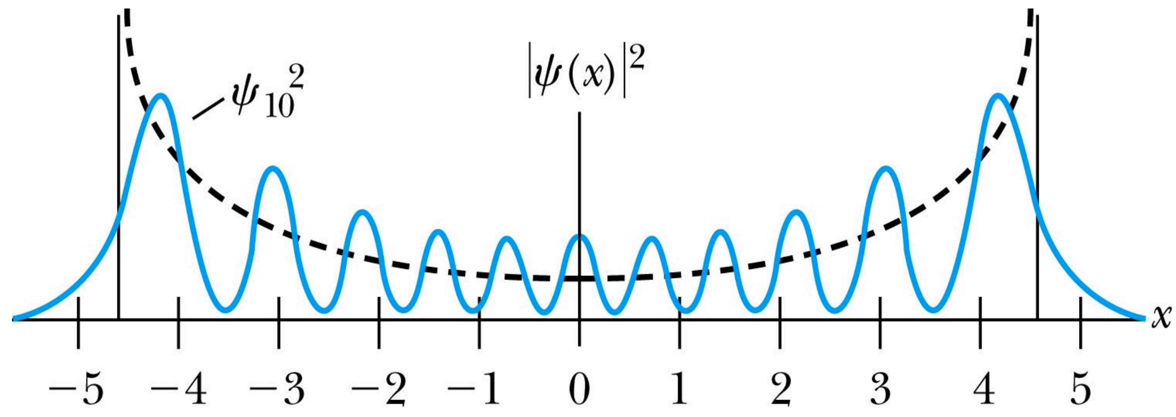




- If the lowest energy level is zero, this violates the uncertainty principle.
- The wave function solutions are $\psi_n = H_n(x) e^{-\alpha x^2/2}$ where $H_n(x)$ are Hermite polynomial function of order *n*.
- In contrast to the particle in a box, where the oscillatory wave function is a sinusoidal curve, in this case the oscillatory behavior is due to the polynomial, which dominates at small *x*. The exponential tail is provided by the Gaussian function, which dominates at large *x*.

Analysis of the Parabolic Potential Well





- The energy levels are given by

$$E_n = \left(n + \frac{1}{2}\right)\hbar\sqrt{\kappa/m} = \left(n + \frac{1}{2}\right)\hbar\omega$$

- The zero point energy is called the Heisenberg limit:

$$E_0 = \frac{1}{2}\hbar\omega$$

- Classically, the probability of finding the mass is greatest at the ends of motion's range and smallest at the center (that is, proportional to the amount of time the mass spends at each position).
- Contrary to the classical one, the largest probability for this lowest energy state is for the particle to be at the center.

Ex. 6.12: Harmonic Oscillator stuff

- Normalize the ground state wave function ψ_0 for the simple harmonic oscillator and find the expectation values <x> and <x^2>.

$$\psi_n(x) = H_n(x)e^{-\alpha x^2/2} \Rightarrow \psi_0(x) = H_0(x)e^{-\alpha x^2/2} = Ae^{-\alpha x^2/2}$$

$$\int_{-\infty}^{+\infty}\psi_0^*\psi_0\,dx = \int_{-\infty}^{+\infty}A^2e^{-\alpha x^2}\,dx = 2A^2\int_0^{+\infty}e^{-\alpha x^2}\,dx = 2A^2\left(\frac{1}{2}\sqrt{\frac{\pi}{\alpha}}\right) = 1$$

$$A^2 = \sqrt{\frac{\alpha}{\pi}} \Rightarrow A = \left(\frac{\alpha}{\pi}\right)^{1/4} \Rightarrow H_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \Rightarrow \psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4}e^{-\alpha x^2/2}$$

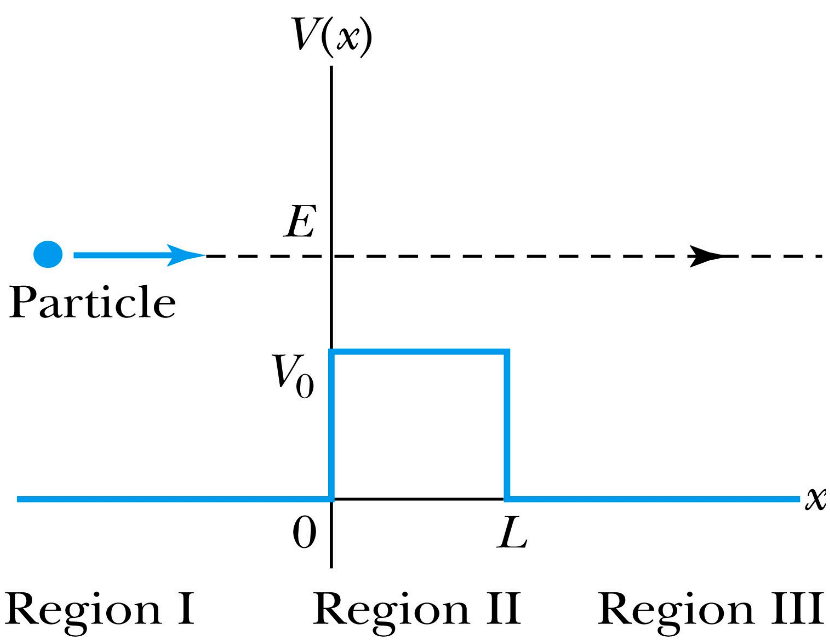
$$\langle x\rangle = \int_{-\infty}^{+\infty}\psi_0^*x\psi_0\,dx = \sqrt{\frac{\alpha}{\pi}}\int_{-\infty}^{+\infty}xe^{-\alpha x^2}\,dx = 0$$

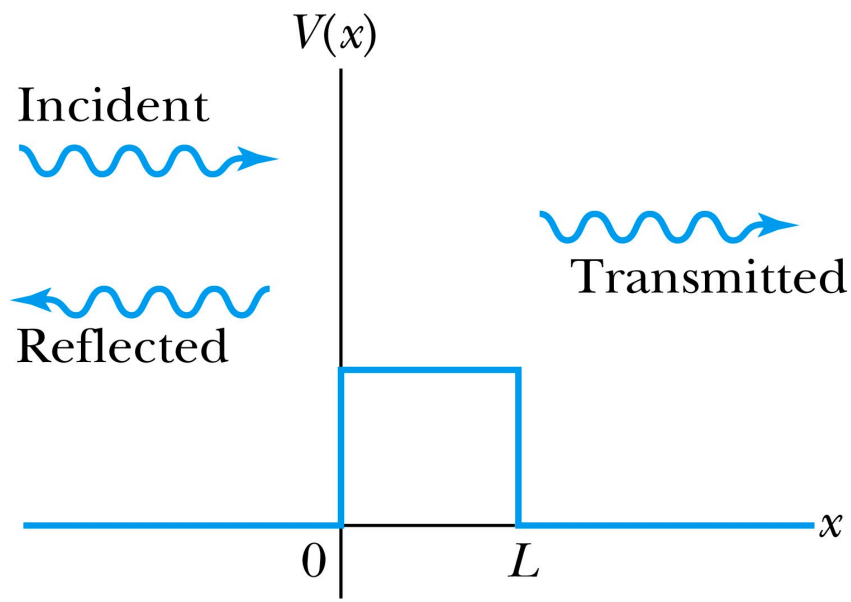
$$\langle x^2\rangle = \int_{-\infty}^{+\infty}\psi_0^*x^2\psi_0\,dx = \sqrt{\frac{\alpha}{\pi}}\int_{-\infty}^{+\infty}x^2e^{-\alpha x^2}\,dx = 2\sqrt{\frac{\alpha}{\pi}}\int_0^{+\infty}x^2e^{-\alpha x^2}\,dx = 2\sqrt{\frac{\alpha}{\pi}}\left(\frac{\sqrt{\pi}}{4\alpha^{3/2}}\right) = \frac{1}{2\alpha}$$

$$\langle x^2\rangle = \frac{\hbar}{2\sqrt{m\kappa}} \Rightarrow \omega = \sqrt{\kappa/m} \Rightarrow \langle x^2\rangle = \frac{\hbar}{2m\omega}$$

Barriers and Tunneling

- Consider a particle of energy E approaching a potential barrier of height V_0 and the potential everywhere else is zero.
- We will first consider the case when the energy is greater than the potential barrier.
- In regions I and III the wave numbers are: $k_I = k_{III} = \frac{\sqrt{2mE}}{\hbar}$
- In the barrier region we have $k_{II} = \frac{\sqrt{2m(E - V_0)}}{\hbar}$ where $V = V_0$





Reflection and Transmission

- The wave function will consist of an incident wave, a reflected wave, and a transmitted wave.
- The potentials and the Schrödinger wave equation for the three regions are as follows:

$$\text{Region I } (x<0) \qquad V=0 \qquad \frac{d^2\psi_I}{dx^2}+\frac{2m}{\hbar^2}E\psi_I=0$$

$$\text{Region II } (0<x<L) \qquad V=V_0 \qquad \frac{d^2\psi_{II}}{dx^2}+\frac{2m}{\hbar^2}(E-V_0)\psi_{II}=0$$

$$\text{Region III} (x>L) \qquad V=0 \qquad \frac{d^2\psi_{III}}{dx^2}+\frac{2m}{\hbar^2}E\psi_{III}=0$$

- The corresponding solutions are:

$$\text{Region I } (x<0) \qquad \psi_I=Ae^{ik_Ix}+Be^{-ik_Ix}$$

$$\text{Region II } (0<x<L) \qquad \psi_{II}=Ce^{ik_{II}x}+De^{-ik_{II}x}$$

$$\text{Region III} (x>L) \qquad \psi_{III}=Fe^{ik_Ix}+Ge^{-ik_Ix}$$

- As the wave moves from left to right, we can simplify the wave functions to:

$$\text{Incident wave} \qquad \psi_I(\text{incident})=Ae^{ik_Ix}$$

$$\text{Reflected wave} \qquad \psi_I(\text{reflected})=Be^{-ik_Ix}$$

$$\text{Transmitted wave} \qquad \psi_{III}(\text{transmitted})=Fe^{ik_Ix}$$