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# CHAPTER 6

## Quantum Mechanics II

- 6.1 The Schrödinger Wave Equation
  - 6.2 Expectation Values
  - 6.3 Infinite Square-Well Potential
  - 6.4 Finite Square-Well Potential
  - 6.5 Three-Dimensional Infinite-Potential Well
  - 6.6 Simple Harmonic Oscillator
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# Wave motion

Quantum mechanics is linearly based on wave motion: wave particle duality.

Towards the wave equation:

## Max (particle) velocity

$$y(x, t) = A \sin(\omega t - kx) \quad \text{wave function at fixed location 'x'}$$

$$v_y = \frac{\partial y}{\partial t} = \omega A \cos(\omega t - kx)$$

## Max (particle) acceleration

$$a_y = \frac{\partial^2 y}{\partial t^2} = -\omega^2 A \sin(\omega t - kx) = -\omega^2 y(x, t) \quad \text{SHM } a_y = -\omega y$$

At fixed time  $t$

$$\text{Slope: } \frac{dy}{dx} = -k A \cos(\omega t - kx)$$

$$\frac{\partial^2 y(x, t)}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 y(x, t)}{\partial t^2}$$

$$\text{Curvature: } \frac{\partial^2 y}{\partial x^2} = -k^2 A \sin(\omega t - kx) = -k^2 y(x, t)$$

$$\text{Wave equation } \frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 y}{\partial t^2}$$

$$\frac{\partial^2 y}{\partial t^2} = \frac{-\omega^2 y(x, t)}{-k^2 y(x, t)} = \frac{-\omega^2}{-k^2} = v^2$$

## 5.2: De Broglie Waves = matter waves

- Prince Louis V. de Broglie suggested that mass particles should have wave properties similar to electromagnetic radiation.
- Thus the wavelength of a matter wave is called the de Broglie wavelength:

$$\lambda = \frac{h}{p}$$

- Since for a photon,  $E = pc$  and  $E = hf$ , the energy can be written as

$$hf = pc = p\lambda f$$

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# The Copenhagen Interpretation

- Bohr's interpretation of the wave function consisted of 3 principles:
    - 1) The uncertainty principle of Heisenberg
    - 2) The complementarity principle of Bohr
    - 3) The statistical interpretation of Born, based on probabilities determined by the wave function
  - Together these three concepts form a logical interpretation of the physical meaning of quantum theory. According to the Copenhagen interpretation, physics depends on the outcomes of measurement.
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# Uncertainty principle

When localizing a wave packet over a small region we have

$$\Delta k \cdot \Delta x = 2\pi \rightarrow \Delta k \text{ must be large to have } \Delta x \text{ small (good location)}$$

It is better to use:  $\Delta k \Delta x = \frac{1}{2}$  Gaussian wave packet

Uncertainty principle: It is impossible to measure with no uncertainty the precise values of  $k$  and  $x$  simultaneously for the same particles

Heisenberg

$$k = \frac{2\pi}{\lambda} = \frac{2\pi}{h/p} = p \frac{2\pi}{h} = \frac{p}{\hbar}$$

use Gaussian wave packet

$$\Delta k = \frac{\Delta p}{\hbar}$$

$$\Delta k \Delta x = \frac{1}{2}$$

$$\Delta p \Delta x = \frac{\hbar}{2}$$

This applies to all three directions

$$\Delta p_x \Delta x \geq \frac{\hbar}{2}$$

so we put indices on it

$$\Delta E \cdot \Delta t \geq \frac{\hbar}{2}$$

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# Wave particle duality solution

- The solution to the wave particle duality of an event is given by the following principle.
  - **Bohr's principle of complementarity:** It is not possible to describe physical observables simultaneously in terms of both particles and waves.
  - **Physical observables** are those quantities such as position, velocity, momentum, and energy that can be experimentally measured. In any given instance we must use either the particle description or the wave description.
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## 5.7: Probability, Wave Functions, and the Copenhagen Interpretation

- The wave function determines the likelihood (or probability) of finding a particle at a particular position in space at a given time.

$$P(y) dy = |\Psi(y,t)|^2 dy$$

- The total probability of finding the electron is 1. Forcing this condition on the wave function is called normalization.

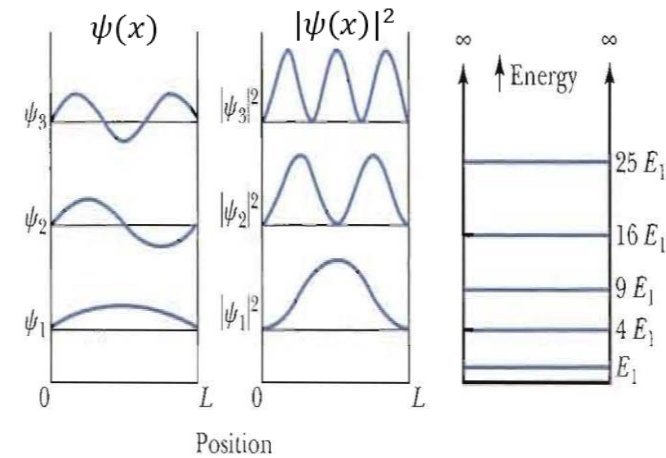
$$\int_{-\infty}^{\infty} P(y) dy = \int_{-\infty}^{\infty} |\Psi(y,t)|^2 dy = 1$$

# Particle in a box (Infinite Square Well)

Consider a particle trapped in a box to have wave behavior;

An integer number of half wavelengths must fit into the box. At the wall's the probability must be zero which means also the wave function must be zero.

$$n \frac{\lambda}{2} = l \quad \text{or} \quad \lambda = \frac{2l}{n} \quad (n = 1, 2, 3 \dots)$$



This condition leads to energy quantization only certain energies are possible

$$E = k = \frac{1}{2}mv^2 = \frac{p^2}{2m} \quad \text{and} \quad pc = hf \quad \text{So; } E = \frac{p^2}{2m} = \frac{h^2}{\lambda^2 2m} = \frac{h^2 n^2}{8ml^2}$$

$$E = \frac{h^2 n^2}{8ml^2} \quad (n = 1, 2, 3 \dots) \quad \text{or} \quad E_n = n^2 \frac{\hbar^2 \pi^2}{2ml^2}$$

Note: Bohr radius  $a_0 = 0.53 \times 10^{-10}$  m and diameter  $2a_0 = 0.1$  nm

**5.13** Calculate the quantized energy levels of an electron in a one-dimensional H-atom ( $l=0.1$ nm)

$$E_n = n^2 \frac{\hbar^2 \pi^2 c^2}{2ml^2 c^2} = n^2 \frac{(4 \times 10^{-16} \text{ eVs})^2 (3 \times 10^8 \frac{\text{m}}{\text{s}})^2 (\frac{10^9 \text{ mm}}{1 \text{ m}})^2}{8(0.5 \times 10^6 \text{ eV})^2 (0.1 \text{ nm})^2} = n^2 38 \text{ eV}$$



# 6.1: The Schrödinger Wave Equation

- The Schrödinger wave equation in its time-dependent form for a particle of energy  $E$  moving in a potential  $V$  in one dimension is

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V\Psi(x,t)$$

- The extension into three dimensions is

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \left( \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right) + V\Psi(x,y,z,t)$$

where  $i = \sqrt{-1}$  is an imaginary number

# The wave function is linear



## EXAMPLE 6.1

The wave equation must be linear so that we can use the superposition principle to form wave packets using two or more waves. Prove that the wave function in Equation (6.1) is linear by showing that it is satisfied for the wave function

$$\Psi(x, t) = a\Psi_1(x, t) + b\Psi_2(x, t)$$

where  $a$  and  $b$  are constants, and  $\Psi_1$  and  $\Psi_2$  describe two waves each satisfying Equation (6.1).

**Strategy** We take the derivatives needed for Equation (6.1) and insert them in a straightforward manner. If Equation (6.1) is satisfied, then the wave equation is linear.

**Solution** We take each of the derivatives needed for Equation (6.1).

$$\frac{\partial \Psi}{\partial t} = a \frac{\partial \Psi_1}{\partial t} + b \frac{\partial \Psi_2}{\partial t}$$

$$\frac{\partial \Psi}{\partial x} = a \frac{\partial \Psi_1}{\partial x} + b \frac{\partial \Psi_2}{\partial x}$$

$$\frac{\partial^2 \Psi}{\partial x^2} = a \frac{\partial^2 \Psi_1}{\partial x^2} + b \frac{\partial^2 \Psi_2}{\partial x^2}$$

We insert these derivatives into Equation (6.1) to yield

$$i\hbar \left( a \frac{\partial \Psi_1}{\partial t} + b \frac{\partial \Psi_2}{\partial t} \right) = -\frac{\hbar^2}{2m} \left( a \frac{\partial^2 \Psi_1}{\partial x^2} + b \frac{\partial^2 \Psi_2}{\partial x^2} \right) + V(a\Psi_1 + b\Psi_2)$$

Rearrangement of this equation gives

$$a \left( i\hbar \frac{\partial \Psi_1}{\partial t} + \frac{\hbar^2}{2m} \frac{\partial^2 \Psi_1}{\partial x^2} - V\Psi_1 \right) = -b \left( i\hbar \frac{\partial \Psi_2}{\partial t} + \frac{\hbar^2}{2m} \frac{\partial^2 \Psi_2}{\partial x^2} - V\Psi_2 \right)$$

Because  $\Psi_1$  and  $\Psi_2$  each satisfy Equation (6.1), the quantities in parentheses are identically zero, and therefore  $\Psi$  is also a solution.

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# General Solution of the Schrödinger Wave Equation

- The **general form** of the **solution of the Schrödinger wave equation is given by:**

$$\Psi(x,t) = Ae^{i(kx-\omega t)} = A[\cos(kx - \omega t) + i \sin(kx - \omega t)]$$

which also describes a wave moving in the x direction. In general the amplitude may also be complex. *This is called the wave function of the particle.*

- The wave function is also **not** restricted to being real. Notice that the sin term has an imaginary number. Only the physically measurable quantities must be real. These include the probability, momentum and energy.
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## EXAMPLE 6.2

Show that  $Ae^{i(kx-\omega t)}$  satisfies the time-dependent Schrödinger wave equation.

**Strategy** We take appropriate derivatives needed for Equation (6.1) and insert them into Equation (6.1) to see whether it is satisfied.

### Solution

$$\frac{\partial \Psi}{\partial t} = -i\omega Ae^{i(kx-\omega t)} = -i\omega \Psi$$

$$\frac{\partial \Psi}{\partial x} = ik\Psi$$

$$\frac{\partial^2 \Psi}{\partial x^2} = i^2 k^2 \Psi = -k^2 \Psi$$

We insert these results into Equation (6.1) to yield

$$i\hbar(-i\omega\Psi) = -\frac{\hbar^2}{2m}(-k^2\Psi) + V\Psi$$

$$\left(\hbar\omega - \frac{\hbar^2 k^2}{2m} - V\right)\Psi = 0$$

If we use  $E = hf = \hbar\omega$  and  $p = \hbar k$ , we obtain

$$\left(E - \frac{p^2}{2m} - V\right)\Psi = 0$$

which is zero in our nonrelativistic formulation, because  $E = K + V = p^2/2m + V$ . Thus  $e^{i(kx-\omega t)}$  appears to be an acceptable solution at this point.

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**Beware: Appears to be an acceptable solution at this point**



### EXAMPLE 6.3

Determine whether  $\Psi(x, t) = A \sin(kx - \omega t)$  is an acceptable solution to the time-dependent Schrödinger wave equation.

**Strategy** We again take the derivatives needed for Equation (6.1) and insert them into the equation to see whether it is satisfied.

#### Solution

$$\frac{\partial \Psi}{\partial t} = -\omega A \cos(kx - \omega t)$$

$$\frac{\partial \Psi}{\partial x} = kA \cos(kx - \omega t)$$

$$\frac{\partial^2 \Psi}{\partial x^2} = -k^2 A \sin(kx - \omega t) = -k^2 \Psi$$

After we insert these relations into Equation (6.1), we have

$$\begin{aligned} -i\hbar \omega \cos(kx - \omega t) &= \left( \frac{\hbar^2 k^2}{2m} + V \right) \Psi \\ &= \left( \frac{\hbar^2 k^2}{2m} + V \right) A \sin(kx - \omega t) \end{aligned} \quad (6.5)$$

(not true)

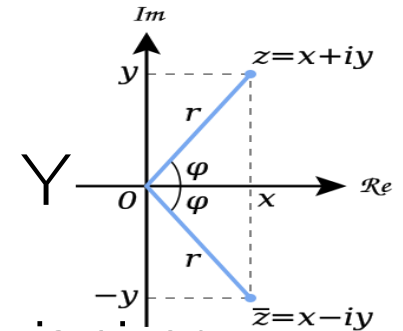
This equation is generally *not* satisfied for all  $x$  and  $t$ , and  $A \sin(kx - \omega t)$  is, therefore, not an acceptable wave function. This function is, however, a solution to the classical wave equation [Equation (6.3)].

## Normalization and Probability

- The probability  $P(x) dx$  of a particle being between  $x$  and  $X + dx$  was given in the equation

$$P(x) dx = \Psi^*(x,t) \Psi(x,t) dx$$

here  $\Psi^*$  denotes the complex conjugate of  $\Psi$



- The probability of the particle being between  $x_1$  and  $x_2$  is given by

$$P = \int_{x_1}^{x_2} \Psi^* \Psi dx$$

- The wave function must also be normalized so that the probability of the particle being somewhere on the  $x$  axis is 1.

$$\int_{-\infty}^{\infty} \Psi^*(x,t) \Psi(x,t) dx = 1$$

Normalize the wave function below (useful integrals are in Appendix 3) and at Wolframalpha.com

5.  $\Psi^* \Psi = A^2 r^2 \exp\left(\frac{-2r}{\alpha}\right)$ . The condition for normalization becomes

$$\int_0^{\infty} \Psi^* \Psi dr = A^2 \int_0^{\infty} r^2 \exp\left(\frac{-2r}{\alpha}\right) dr = A^2 \left[ \frac{2}{(2/\alpha)^3} \right] = \frac{A^2 \alpha^3}{4} = 1. \text{ Therefore}$$

$$A = \sqrt{\frac{4}{\alpha^3}} = 2\alpha^{-3/2}.$$

## Problem 6.10

A wave function  $\Psi$  is  $A(e^{ix} + e^{-ix})$  in the region  $-\pi < x < \pi$  and zero elsewhere. Normalize the wave function and find the probability that the particle is (a) between  $x=0$  and  $x=\pi/4$  and (b) between  $x=0$  and  $x=\pi/8$ .

1. Using the Euler relations between exponential and trig functions, we find

$$\psi = A(e^{ix} + e^{-ix}) = 2A \cos(x).$$

Normalization:  $\int_{-\pi}^{\pi} \psi^* \psi dx = 4A^2 \int_{-\pi}^{\pi} \cos^2(x) dx = 4A^2 \pi = 1$ . Thus  $A = \frac{1}{2\sqrt{\pi}}$ .

The probability of being in the interval  $[0, \pi/8]$  is

$$P = \int_0^{\pi/8} \psi^* \psi dx = \frac{1}{\pi} \int_0^{\pi/8} \cos^2(x) dx = \frac{1}{\pi} \left( \frac{x}{2} + \frac{1}{4} \sin(2x) \right) \Big|_0^{\pi/8}$$
$$= \frac{1}{16} + \frac{1}{4\pi\sqrt{2}} = 0.119.$$

(a) The probability of being in the interval  $[0, \pi/4]$  is

$$P = \int_0^{\pi/4} \psi^* \psi dx = \frac{1}{\pi} \int_0^{\pi/4} \cos^2(x) dx = \frac{1}{\pi} \left( \frac{x}{2} + \frac{1}{4} \sin(2x) \right) \Big|_0^{\pi/4}$$
$$= \frac{1}{8} + \frac{1}{4\pi} = 0.205.$$



# Properties of Valid Wave Functions

## Boundary conditions

- 1) In order to avoid infinite probabilities, the wave function must be finite everywhere.
- 2) In order to avoid multiple values of the probability, the wave function must be single valued.
- 3) For finite potentials, the wave function and its derivative must be continuous. This is required because the second-order derivative term in the wave equation must be single valued. (There are exceptions to this rule when  $V$  is infinite.)
- 4) In order to normalize the wave functions, they must approach zero as  $x$  approaches infinity.

**Solutions that do not satisfy these properties do not generally correspond to physically realizable circumstances.**

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$$\Psi(x,t) = Ae^{i(kx-\omega t)} = A[\cos(kx - \omega t) + i \sin(kx - \omega t)] \quad \text{Not normalizable}$$

## *Glicker - Questions*

15) Consider to normalize the wave function  $e^{i(kx-\omega t)}$ ?

- a) It can not be normalized
- b) It can be normalized
- c) It can be normalized by a constant factor
- d) It can not be normalized because it is a complex function

# Time-Independent Schrödinger Wave Equation

- The potential in many cases will not depend explicitly on time.
- The dependence on time and position can then be separated in the Schrödinger wave equation. Let  $\Psi(x,t) = \psi(x)f(t)$ ,

which yields: 
$$i\hbar \psi(x) \frac{\partial f(t)}{\partial t} = -\frac{\hbar^2 f(t)}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x)f(t)$$

Now divide by the wave function: 
$$i\hbar \frac{1}{f(t)} \frac{df(t)}{dt} = -\frac{\hbar^2}{2m} \frac{1}{\psi(x)} \frac{d^2 \psi(x)}{dx^2} + V(x)$$

- The *left side* of this last equation depends only on **time**, and the *right side* depends only on **spatial coordinates**. Hence each side must be equal to a constant. The time dependent side is

$$i\hbar \frac{1}{f} \frac{df}{dt} = B$$

# Time-Independent Schrödinger Wave Equation (con' t)

- We integrate both sides and find:  $i\hbar \int \frac{df}{f} = \int B dt \quad i\hbar \ln f = Bt + C$

where  $C$  is an integration constant that we may choose to be 0. Therefore

$$\ln f = \frac{Bt}{i\hbar}$$

This determines  $f$  to be  $f(t) = e^{Bt/i\hbar} = e^{-iEt/\hbar}$  here  $B = E$  for a free particle wave function :

$$i\hbar \frac{1}{f(t)} \frac{df(t)}{dt} = E$$

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

- This is known as the **time-independent Schrödinger wave equation**, and it is a fundamental equation in quantum mechanics.

# Stationary State

- Recalling the separation of variables:  $\Psi(x,t) = \psi(x)f(t)$   
and with  $f(t) = e^{-i\omega t}$  the wave function can be written as:

$$\Psi(x,t) = \psi(x)e^{-i\omega t}$$

- The probability density becomes:

$$\Psi^* \Psi = \psi^2(x)(e^{i\omega t} e^{-i\omega t})$$

$$\Psi^* \Psi = \psi^2(x)$$

- The probability distributions are constant in time. This is a standing wave phenomena that is called the stationary state.

# Comparison of Classical and Quantum Mechanics

- Newton's second law and Schrödinger's wave equation are both differential equations.
- Newton's second law can be derived from the Schrödinger wave equation, so the latter is the more fundamental.
- Classical mechanics only appears to be more precise because it deals with macroscopic phenomena. The underlying uncertainties in macroscopic measurements are just too small to be significant.
- Ray optics is characteristic of particle-like behavior and is a good approximation in a classical description as long as the wavelength of the radiation is smaller than the obstacles (apertures etc) it passes.
- **The only correct theory is quantum mechanics.**

## 6.2: Expectation Values

- The **expectation value** is the expected result of the average of many measurements of a given quantity. The expectation value of  $x$  is denoted by  $\langle x \rangle$
- Any measurable quantity for which we can calculate the expectation value is called a **physical observable**. The expectation values of physical observables (for example, position, linear momentum, angular momentum, and energy) must be real, because the experimental results of measurements are real.
- The average value of  $x$  is

$$\bar{x} = \frac{N_1x_1 + N_2x_2 + N_2x_2 + N_2x_2 + \dots}{N_1 + N_2 + N_3 + N_4 + \dots} = \frac{\sum_i N_i x_i}{\sum_i N_i}$$

# Continuous Expectation Values

- We can change from discrete to continuous variables by using the probability  $P(x,t)$  of observing the particle at a particular  $x$ .

$$\overline{x} = \frac{\int_{-\infty}^{\infty} xP(x) dx}{\int_{-\infty}^{\infty} P(x) dx}$$

- Using the wave function, the expectation value is of **position**:

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

- The expectation value of **any function  $g(x)$**  for a normalized wave function:

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



# Momentum Operator

An operator transforms one function into another

- To find the expectation value of  $p$ , we first need to represent  $p$  in terms of  $x$  and  $t$ . Consider the derivative of the wave function of a free particle with respect to  $x$ :

$$\frac{\partial \Psi}{\partial x} = \frac{\partial}{\partial x} [e^{i(kx - \omega t)}] = ike^{i(kx - \omega t)} = ik\Psi$$

With  $k = p / \hbar$  we have  $\frac{\partial \Psi}{\partial x} = i \frac{p}{\hbar} \Psi$

This yields  $p[\Psi(x, t)] = -i\hbar \frac{\partial \Psi(x, t)}{\partial x}$

- This suggests we define the momentum operator as

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

$$\langle Q \rangle = \int_{-\infty}^{\infty} \Psi^* Q \Psi dx$$

- The expectation  $\langle p \rangle = -i\hbar \int_{-\infty}^{\infty} \Psi^*(x, t) \frac{\partial \Psi(x, t)}{\partial x} dx$

# Position and Energy Operators

- The position  $x$  is its own operator as seen above.
- The time derivative of the free-particle wave function is

$$\frac{\partial \Psi}{\partial t} = \frac{\partial}{\partial t} \left[ e^{i(kx - \omega t)} \right] = -i\omega e^{i(kx - \omega t)} = -i\omega \Psi$$

Substituting  $\omega = E / \hbar$  yields  $E[\Psi(x,t)] = i\hbar \frac{\partial \Psi(x,t)}{\partial t}$

- The energy operator is  $\hat{E} = i\hbar \frac{\partial}{\partial t}$
- The expectation value of the energy is

$$\langle E \rangle = i\hbar \int_{-\infty}^{\infty} \Psi^*(x,t) \frac{\partial \Psi(x,t)}{\partial t} dx$$



## EXAMPLE 6.6

Use the momentum and energy operators with the conservation of energy to produce the Schrödinger wave equation.

**Strategy** We first find the energy  $E$  as the sum of the kinetic and potential energies. Our treatment is entirely non-relativistic. We want to use the operator functions, so we write the kinetic energy in terms of momentum.

**Solution** The energy is

$$E = K + V = \frac{p^2}{2m} + V \quad (6.27)$$

We allow the operators of both sides of this equation to act on the wave function. The left side gives

$$\hat{E}\Psi = i\hbar \frac{\partial \Psi}{\partial t} \quad (6.28)$$

The application of the operators on the right side of Equation (6.27) on  $\Psi$  gives

$$\begin{aligned} \left[ \frac{1}{2m} (\hat{p})^2 + V \right] \Psi &= \frac{1}{2m} \left( -i\hbar \frac{\partial}{\partial x} \right)^2 \Psi + V\Psi \\ &= -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi \end{aligned}$$

Notice that the operator  $(\hat{p})^2$  implies two successive applications of the  $\hat{p}$  operator, not the algebraic square of one  $\hat{p}$  operator. Now we set the previous equation equal to Equation (6.28) and obtain

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi \quad (6.29)$$

which is the time-dependent Schrödinger wave equation, Equation (6.1). It should be noted that this example is not a determination of the Schrödinger wave equation, but rather a verification of the consistency of the definitions.

## 6.3: 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

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

- 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  $\psi(x) = A \sin kx + B \cos kx$ .
-

# Infinite Square well

Divide the problem into 3 parts: two are outside the well and one is inside the well.

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

**OUTSIDE:**  $x < 0$  and  $x > L$ ;  $\psi = 0$

**INSIDE:**  $V = 0$  and  $-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi$  with boundary condition  $\psi = 0$  at  $x = 0, L$

$$\frac{d^2\psi}{dx^2} = -k^2\psi; \quad \text{and} \quad k^2 = \frac{2mE}{\hbar^2} \quad \psi = A\sin kx + B\cos kx$$

At  $x = 0$ ;

$$0 = A\sin 0 + B\cos 0 \quad \text{So; } B = 0$$

At  $x = L$ ;

$$0 = A\sin kL \quad (n = 1, 2, 3 \dots)$$

$$kL = n\pi \quad (n = 1, 2, 3 \dots)$$

$$\text{So; } k = \frac{\pi n}{L}$$

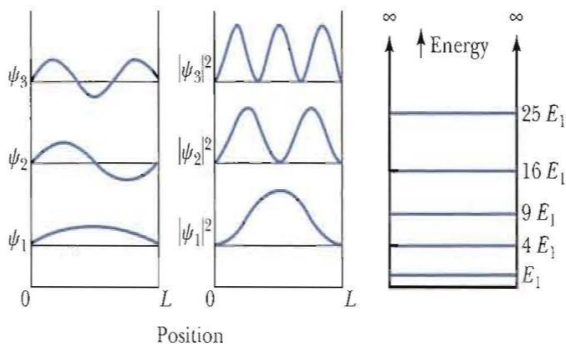
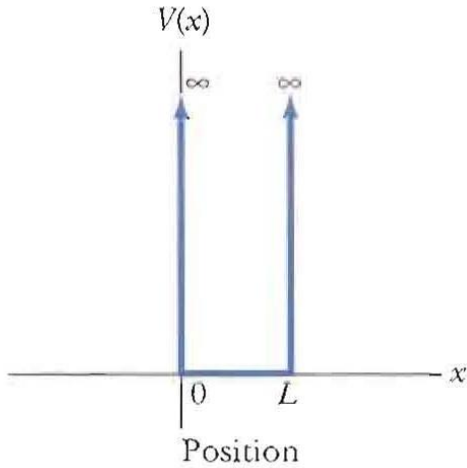
$$\psi = A\sin kx = A\sin \frac{\pi n}{L} x$$

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$$

Determine the only constant  $A$ :  $\int_0^L A^2 \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$

$$A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx \Big|_{=1} \quad A^2 \frac{L}{2} = 1 \rightarrow A = \sqrt{\frac{2}{L}}$$

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



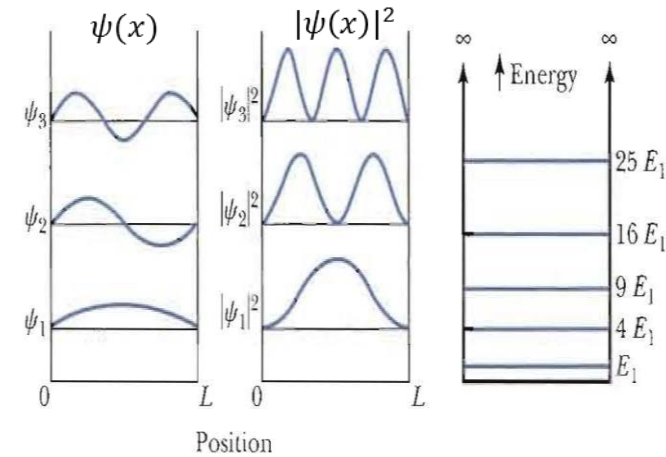
## Quantized Energy

# Particle in a box

Consider a particle trapped in a box to have wave behavior;

An integer number of half wavelengths must fit into the box. At the wall's the probability must be zero which means also the wave function must be zero.

$$n \frac{\lambda}{2} = l \quad \text{or} \quad \lambda = \frac{2l}{n} \quad (n = 1, 2, 3 \dots \dots)$$



This condition leads to energy quantization only certain energies are possible

$$E = k = \frac{1}{2}mv^2 = \frac{p^2}{2m} \quad \text{and} \quad pc = hf \quad \text{So; } E = \frac{p^2}{2m} = \frac{h^2}{\lambda^2 2m} = \frac{h^2 n^2}{8ml^2}$$

$$E = \frac{h^2 n^2}{8ml^2} \quad (n = 1, 2, 3 \dots \dots) \quad \text{or} \quad E_n = n^2 \frac{\hbar^2 \pi^2}{2ml^2}$$

Note: Bohr radius  $a_0 = 0.53 \times 10^{-10}$  m and diameter  $2a_0 = 0.1$  nm

**5.13** Calculate the quantized energy levels of an electron in a one-dimensional H-atom ( $l=0.1$ nm)

$$E_n = n^2 \frac{\hbar^2 \pi^2 c^2}{2ml^2 c^2} = n^2 \frac{(4 \times 10^{-16} \text{ eVs})^2 (3 \times 10^8 \frac{\text{m}}{\text{s}})^2 (\frac{10^9 \text{ mm}}{1 \text{ m}})^2}{8(0.5 \times 10^6 \text{ eV})^2 (0.1 \text{ nm})^2} = n^2 38 \text{ eV}$$



## EXAMPLE 6.9

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. Of course, this is only a rough calculation for a proton in a nucleus.

**Strategy** To find the transition energy between the ground and first excited energy states, we use Equation (6.35) to find  $E_1$  and  $E_2$ .

**Solution** The energy of the ground state, from Equation (6.35), is

$$\begin{aligned} E_1 &= \frac{\pi^2 \hbar^2 c^2}{2mc^2 L^2} = \frac{1}{mc^2} \frac{\pi^2 (197.3 \text{ eV} \cdot \text{nm})^2}{2(10^{-5} \text{ nm})^2} \\ &= \frac{1}{mc^2} (1.92 \times 10^{15} \text{ eV}^2) \end{aligned}$$

The mass of the proton is  $938.3 \text{ MeV}/c^2$ , which gives

$$E_1 = \frac{1.92 \times 10^{15} \text{ eV}^2}{938.3 \times 10^6 \text{ eV}} = 2.0 \text{ MeV}$$

The first excited state energy is found [again from Equation (6.35)] to be  $E_2 = 4E_1 = 8 \text{ MeV}$ , and the transition energy is  $\Delta E = E_2 - E_1 = 6 \text{ MeV}$ . This is a reasonable value for protons in the nucleus.

### Example 6.8

work out expectation value by using the recipe  $\langle A \rangle = \int_{-\infty}^{+\infty} \psi^* A \psi dx$   
 for particle in an infinite box with  $\psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$

$$\langle x \rangle_{n=2} = \frac{2}{L} \int_{-\infty}^{+\infty} x \sin^2\left(\frac{2\pi x}{L}\right) dx = L/2$$

This is a reasonable result since the average position is in the middle of the box. Even though the wave function in the second excited state is zero in the middle.

$$\begin{aligned} \langle p \rangle_{n=2} &= -i\hbar \frac{2}{L} \int_{-\infty}^{+\infty} \sin\left(\frac{2\pi x}{L}\right) \frac{d}{dx} \sin\left(\frac{2\pi x}{L}\right) dx \\ &= i\hbar \frac{2}{L} \int_{-\infty}^{+\infty} \sin\left(\frac{2\pi x}{L}\right) \cos\left(\frac{2\pi x}{L}\right) dx = 0 \end{aligned}$$

This is reasonable since the particle is moving as often to the right as it is moving to the left and so  $\langle p \rangle = 0$

### Example 6.9

use the infinite square well as model for the transition of a proton from the first excited state to the groundstate in a nucleus with  $r_N = 10^{-14} \text{ m}$

$$E_1 = \frac{\pi^2 \hbar^2 c^2}{2mc^2 L^2} = \frac{1}{mc^2} \frac{\hbar^2 (157.3 \text{ eV} \cdot \text{nm})^2}{(2 \times 10^{-5} \text{ nm})^2} = \frac{11.92 \times 10^{15} \text{ eV}^2}{938 \frac{\text{MeV} \cdot c^2}{c^2}} = 2.0 \text{ MeV}$$

$$E_2 = 4E_1 = 8 \text{ MeV}$$

$$\Delta E = (8 - 2) \text{ MeV} = \underline{\underline{6 \text{ MeV}}}$$

close to observation  
same order of magnitude



## Problem 6.12

A particle in an infinite square-well potential has ground-state energy 4.3 eV. (a) Calculate and sketch the energies of the next three levels, and (b) sketch the wave functions on top of the energy levels.

(a) We know the energy values from Equation (6.35). The energy value  $E_n$  is proportional to  $n^2$  where  $n$  is the quantum number. If the ground state energy is 4.3 eV ,

1. then the next three levels correspond to:  $4E_1 = 17.2$  eV for  $n = 2$ ;  $9E_1 = 38.7$  eV for  $n = 3$ ; and  $16E_1 = 68.8$  eV for  $n = 4$ .

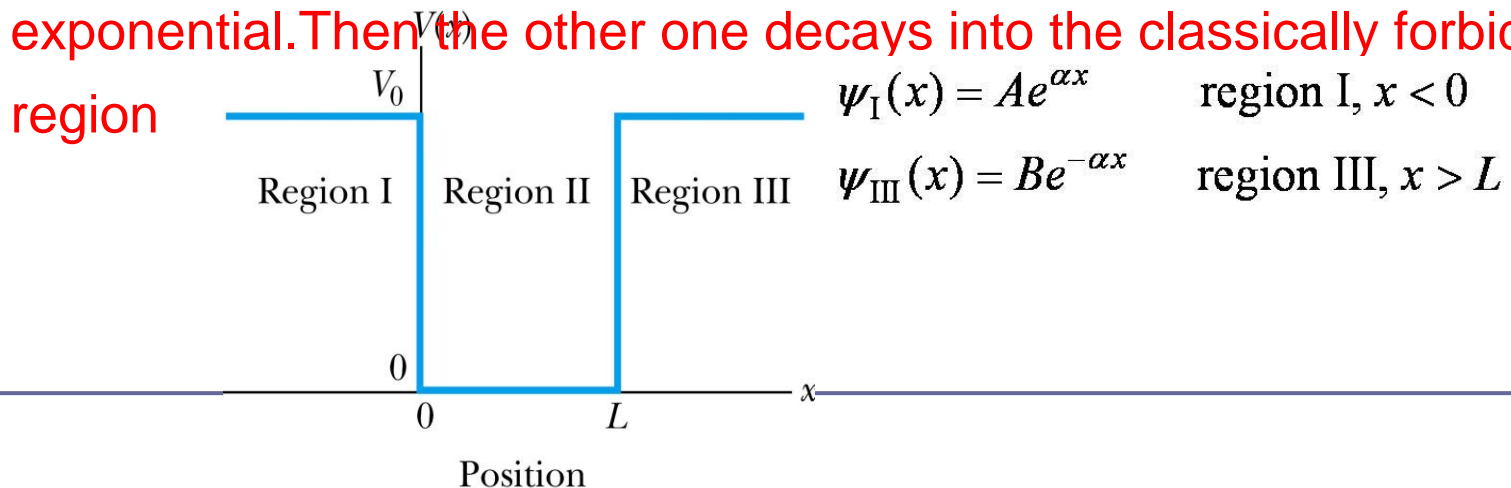
(a) The wave functions and energy levels will be like those shown in Figure 6.3.

# 6.4: Finite Square-Well Potential

- The finite square-well potential is  $V(x) = \begin{cases} V_0 & x \leq 0 & \text{region I} \\ 0 & 0 < x < L & \text{region II} \\ V_0 & x \geq L & \text{region III} \end{cases}$
- The Schrödinger equation outside the finite well in regions I and III is

$$-\frac{\hbar^2}{2m} \frac{1}{\psi} \frac{d^2\psi}{dx^2} = E - V_0 \quad \text{regions I, III or using } \alpha^2 = 2m(V_0 - E)/\hbar^2$$

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. Then the other one decays into the classically forbidden region



# Finite Square-Well Solution

- Inside the square well, where the potential  $V$  is zero, 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 have

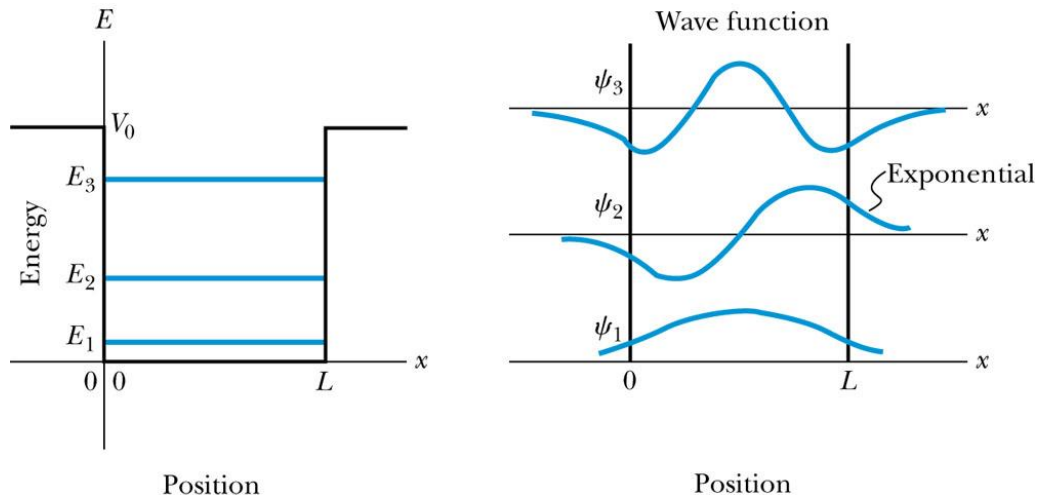
$$\psi_{\text{II}} = Ce^{ikx} + De^{-ikx} \quad \text{region II, } 0 < x < L$$

- The boundary conditions require that

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

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

- Note that the wave function is nonzero outside of the box.



We will skip the tedious procedure of fulfilling the above boundary conditions, but discuss the results

## *Clicker - Questions*

13) Compare the results of the finite and infinite square well potential?

- a) The wavelengths are longer for the finite square well.
- b) The wavelengths are shorter for the finite square well.
- c) The wavelengths are the same.

## *Glicker - Questions*

13) Compare the finite and infinite square well potentials and chose the correct statement.

- a) There is a finite number of bound energy states for the finite potential.
- b) There is an infinite number of bound energy states for the finite potential.
- c) There are bound states which fulfill the condition  $E > V_0$ .

## 6.5: 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

$$\frac{p^2}{2m}\psi + V\psi = E\psi$$

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

Given:

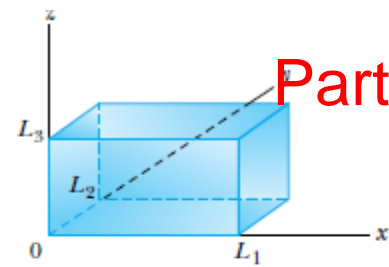
$$p^2 = p_x^2 + p_y^2 + p_z^2, \text{ and } \hat{p}_x\psi = -i\hbar\frac{\partial\psi}{\partial x} \quad \hat{p}_y\psi = -i\hbar\frac{\partial\psi}{\partial y} \quad \hat{p}_z\psi = -i\hbar\frac{\partial\psi}{\partial z}$$

- The three dimensional Schrödinger wave equation is

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

Laplace operator

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 6.6. The particle is constrained to be inside the box. Find the wave functions and energies. Then find the ground-state energy and wave function and the energy of the first excited state for a cube of sides  $L$ .



## Particle in 3-D box

**Strategy** We employ some of the same strategies to solve this problem as we used for the one-dimensional case. First, because we are considering the walls of the box to be absolutely closed, they are infinite potential barriers, and the wave function  $\psi$  must be zero at the walls and beyond. We expect to see standing waves similar to Equation (6.31).

But how should we write the wave function so as to properly include the  $x$ ,  $y$ , and  $z$  dependence of the wave function? In this case the mathematics will follow from the physics. The particle is free within the box. Therefore, the  $x$ -,  $y$ -, and  $z$ -dependent parts of the wave function must be independent of each other. Inside the box  $V = 0$ , so the wave equation we must solve is

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi \quad (6.46)$$

It is therefore reasonable to try a wave function of the form

$$\psi(x, y, z) = A \sin(k_1x)\sin(k_2y)\sin(k_3z) \quad (6.47)$$

where  $A$  is a normalization constant. The quantities  $k_i$  ( $i = 1, 2, 3$ ) are determined by applying the appropriate boundary conditions. To find the energies, we substitute the wave function into the Schrödinger equation and solve for  $E$ .

**Solution** The condition that  $\psi = 0$  at  $x = L_1$  requires that  $k_1L_1 = n_1\pi$  or  $k_1 = n_1\pi/L_1$ . The values for the  $k_i$  are

$$k_1 = \frac{n_1\pi}{L_1} \quad k_2 = \frac{n_2\pi}{L_2} \quad k_3 = \frac{n_3\pi}{L_3} \quad (6.48)$$

where  $n_1$ ,  $n_2$ , and  $n_3$  are integers. Not surprisingly, we have found that in three dimensions, it is necessary to use *three* quantum numbers to describe the physical state.

**Figure 6.6** A three-dimensional box that contains a free particle. The potential is infinite outside the box, so the particle is constrained to be inside the box.

In order to find the energies using Equation (6.43), we first need to take the appropriate derivatives of the wave function. We do this first for the variable  $x$ .

$$\begin{aligned} \frac{\partial\psi}{\partial x} &= \frac{\partial}{\partial x}[A \sin(k_1x)\sin(k_2y)\sin(k_3z)] \\ &= k_1A \cos(k_1x)\sin(k_2y)\sin(k_3z) \\ \frac{\partial^2\psi}{\partial x^2} &= \frac{\partial}{\partial x}[k_1A \cos(k_1x)\sin(k_2y)\sin(k_3z)] \\ &= -(k_1)^2A \sin(k_1x)\sin(k_2y)\sin(k_3z) \\ &= -k_1^2\psi \end{aligned}$$

The derivatives for  $y$  and  $z$  are similar, and Equation (6.43) becomes

$$\frac{\hbar^2}{2m}(k_1^2 + k_2^2 + k_3^2)\psi = E\psi$$

This gives

$$E = \frac{\hbar^2}{2m}(k_1^2 + k_2^2 + k_3^2)$$

We substitute the values of  $k_i$  from Equation (6.48) in this equation to obtain

$$E = \frac{\pi^2\hbar^2}{2m}\left(\frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2} + \frac{n_3^2}{L_3^2}\right) \quad (6.49)$$

## Problem 6.26

Find the energies of the second, third, fourth, and fifth levels for the three dimensional cubical box. Which energy levels are degenerate?

A given state is **degenerate** when there is more than one wave function for a given energy

$E = \frac{\pi^2 \hbar^2}{2mL^2} (n_1^2 + n_2^2 + n_3^2) = E_0 (n_1^2 + n_2^2 + n_3^2)$  where  $E_0 = \frac{\pi^2 \hbar^2}{2mL^2}$ . Then the second, third, fourth, and fifth levels are

1. :

$$E_2 = (2^2 + 1^2 + 1^2) E_0 = 6E_0 \quad (\text{degenerate})$$

$$E_3 = (2^2 + 2^2 + 1^2) E_0 = 9E_0 \quad (\text{degenerate})$$

$$E_4 = (3^2 + 1^2 + 1^2) E_0 = 11E_0 \quad (\text{degenerate})$$

$$E_5 = (2^2 + 2^2 + 2^2) E_0 = 12E_0 \quad (\text{not degenerate})$$



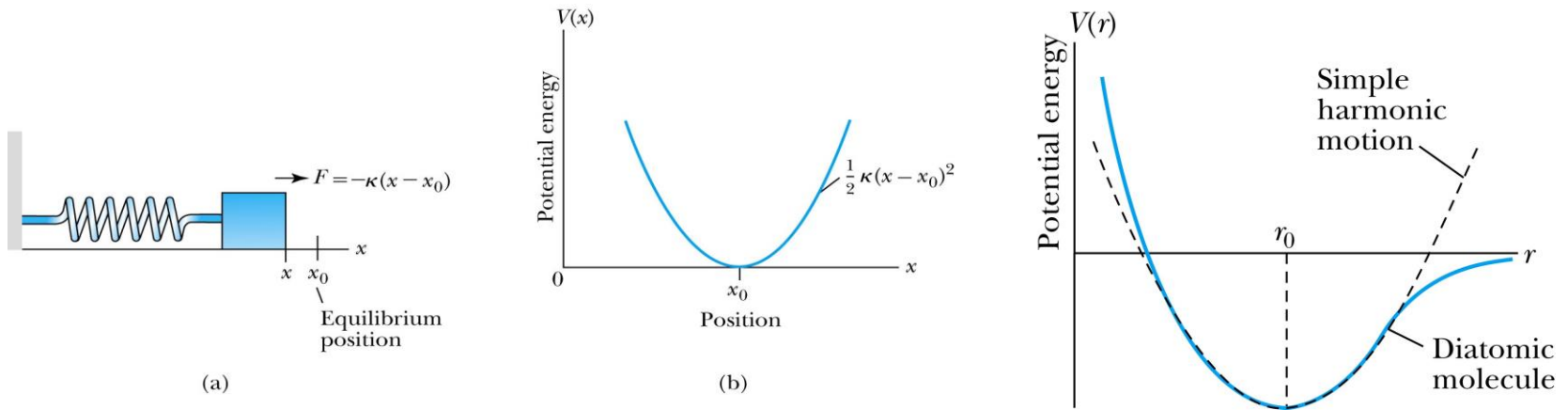
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# Degeneracy

- 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 can remove the degeneracy.
-

# 6.6: Simple Harmonic Oscillator

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



- Consider the Taylor expansion of a potential function:

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

Redefining the minimum potential and the zero potential, we have

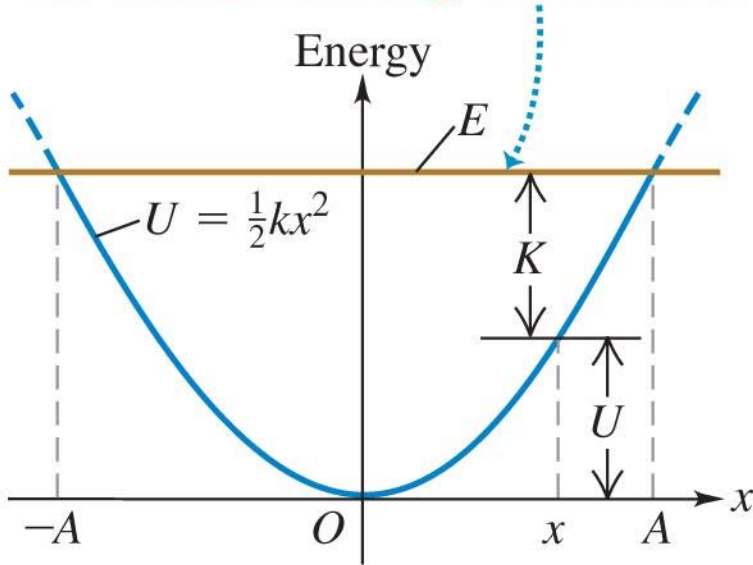
$$V(x) = \frac{1}{2}V_2(x - x_0)^2$$

Substituting this into the wave equation:

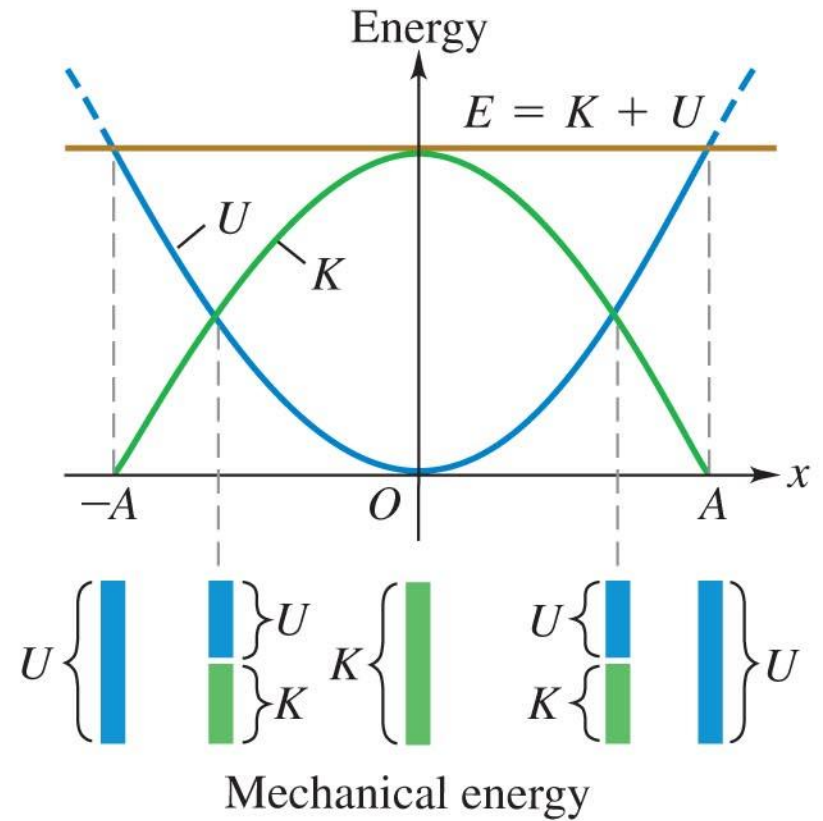
$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2} \left( E - \frac{\kappa x^2}{2} \right) \psi = \left( -\frac{2mE}{\hbar^2} + \frac{m\kappa x^2}{\hbar^2} \right) \psi$$

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

The mechanical energy  $E$  is constant.

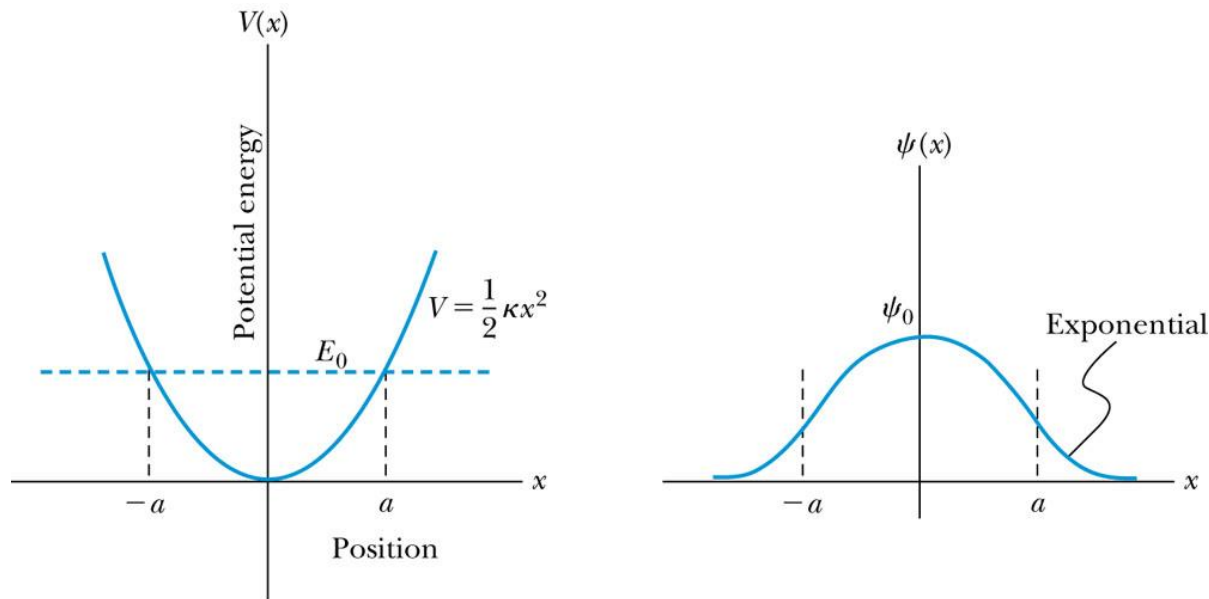


(a) The potential energy  $U$  and total energy  $E$  of an object in SHM as a function of  $x$  position



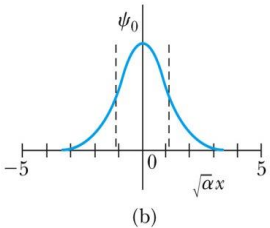
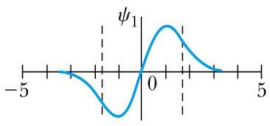
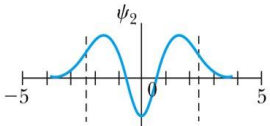
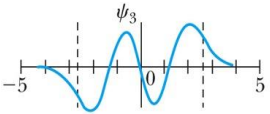
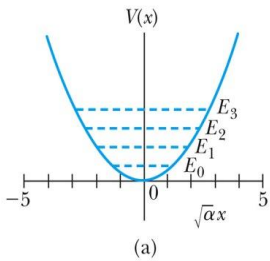
(b) The same graph as in (a), showing kinetic energy  $K$  as well

# 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 polynomials 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



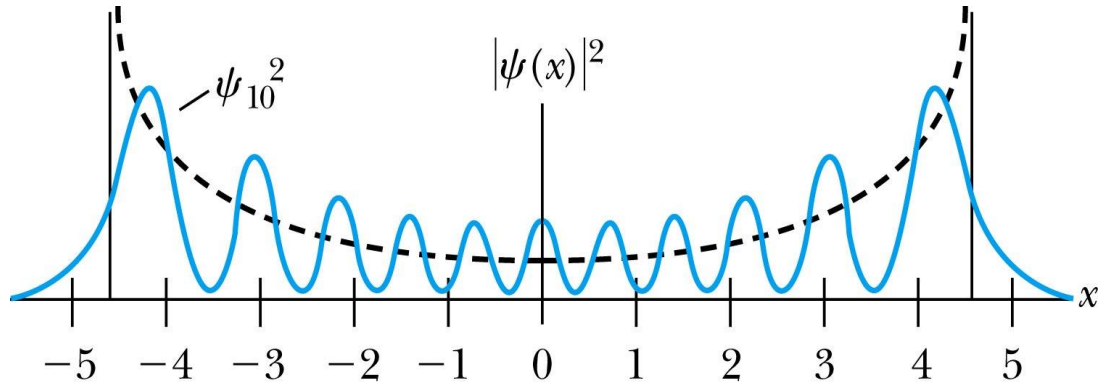
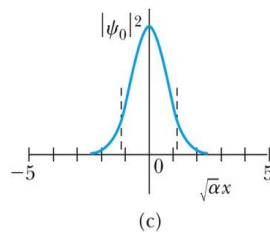
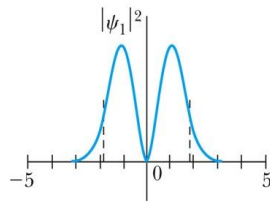
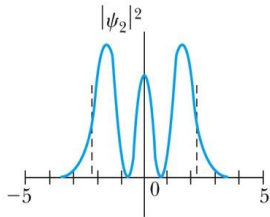
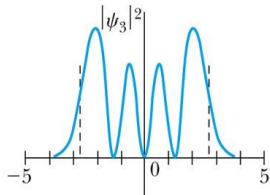
Wave functions

$$\psi_3(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{3}} (\sqrt{\alpha}x)(2\alpha x^2 - 3)e^{-\alpha x^2/2}$$

$$\psi_2(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{2}} (2\alpha x^2 - 1)e^{-\alpha x^2/2}$$

$$\psi_1(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \sqrt{2\alpha} x e^{-\alpha x^2/2}$$

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



- 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 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.

A hydrogen molecule can be approximated a simple harmonic oscillator with force constant  $k=1.1 \times 10^3$  N/m

39. The classical frequency for a two-particle oscillator is [see Chapter 10, Equation (10.4)]

$\omega = \sqrt{k/\mu} = \sqrt{k(m_1 + m_2)/m_1 m_2} = \sqrt{2k/m}$  since the masses are equal in this case. The energies of the ground state ( $E_0$ ) and the first three excited states are given by

$E_n = \left(n + \frac{1}{2}\right) \hbar \omega$  so the possible transitions (from  $E_3$  to  $E_2$ ,  $E_3$  to  $E_1$ , etc. are  $\Delta E = \hbar \omega$ ,

$2\hbar \omega$ , and  $3\hbar \omega$ . Specifically these calculations give:

$$\hbar \omega = \hbar \sqrt{\frac{2k}{m}} = (6.582 \times 10^{-16} \text{ eV} \cdot \text{s}) \sqrt{\frac{2(1.1 \times 10^3 \text{ N/m})}{1.673 \times 10^{-27} \text{ kg}}} = 0.755 \text{ eV with a wavelength,}$$

$$\lambda = \frac{hc}{E} = \frac{1240 \text{ eV} \cdot \text{nm}}{0.755 \text{ eV}} = 1640 \text{ nm}.$$

$$2\hbar \omega = 2(6.582 \times 10^{-16} \text{ eV} \cdot \text{s}) \sqrt{\frac{2(1.1 \times 10^3 \text{ N/m})}{1.673 \times 10^{-27} \text{ kg}}} = 1.51 \text{ eV}$$

$$\lambda = \frac{hc}{E} = \frac{1240 \text{ eV} \cdot \text{nm}}{1.51 \text{ eV}} = 821 \text{ nm}$$

See Appendix 3 Mathematical Relations

$$\int \sin^2 x dx = \frac{1}{2}x - \frac{1}{4}\sin 2x$$

11. A wave function has the value  $A \sin x$  between  $x = 0$  and  $\pi$  but zero elsewhere. Normalize the wave function and find the probability that the particle is (a) between  $x = 0$  and  $x = \pi/4$  and (b) between  $x = 0$  and  $\pi/2$ .

normalize:  $\int_0^{\pi} \psi^* \psi dx = A^2 \int_0^{\pi} \sin^2 x dx = A^2 \left( \frac{1}{2}x - \frac{1}{4}\sin 2x \right) \Big|_0^{\pi} = \frac{\pi}{2} A^2 = 1 \rightarrow A = \sqrt{\frac{2}{\pi}}$

(a)  $P = \int_0^{\pi/4} \psi^* \psi dx = \frac{2}{\pi} \left( \frac{x}{2} - \frac{1}{4}\sin 2x \right) \Big|_0^{\pi/4} = \frac{2}{\pi} \left( \frac{\pi}{8} - \frac{1}{4} \right) = \frac{1}{4} - \frac{1}{2\pi} = 0.091$

(b)  $P = \frac{2}{\pi} \left( \frac{x}{2} - \frac{1}{4}\sin 2x \right) \Big|_0^{\pi/2} = \frac{2}{\pi} \left( \frac{\pi}{4} - 0 \right) = \frac{1}{2} = 0.5$

# Deuteron in a nucleus

22. Consider a finite square-well potential well of width  $3.00 \times 10^{-15}$  m that contains a particle of mass  $1.88 \text{ GeV}/c^2$ . How deep does this potential well need to be to contain three energy levels? (This situation approximates a deuteron inside a nucleus.)

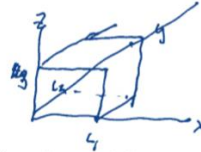
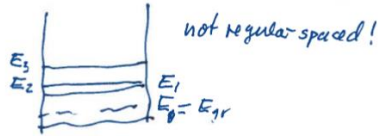
We approximate with the infinite square well energy

$$E = \frac{\hbar^2 k^2}{8mL^2} = \frac{9 \hbar^2 c^2}{8mc^2 L^2} = \frac{9 (1240 \text{ eV}\cdot\text{nm})^2}{8 (1.88 \times 10^9 \text{ eV}) \cdot (3 \times 10^{-6} \text{ nm})^2}$$

$E = 102 \text{ MeV}$



# Rectangular box



31. A particle is trapped in a rectangular box having sides  $L$ ,  $2L$ , and  $4L$ . Find the energy of the ground state and first three excited states. Are any of these states degenerate?

$$E = \frac{\hbar^2 k^2}{2m} \left( \frac{n_1^2}{L^2} + \frac{n_2^2}{4L^2} + \frac{n_3^2}{16L^2} \right)$$

for groundstate  $n_1 = n_2 = n_3 = 1$

$$E_{gr} = \frac{\hbar^2 k^2}{2mL^2} \left( 1 + \frac{1}{4} + \frac{1}{16} \right) = \frac{21}{32} \frac{\hbar^2 k^2}{mL^2}$$

for smallest additional energy = first excited state, make  $n_2 = 2$

$$E_1 = \frac{\hbar^2 k^2}{2mL^2} \left( 1 + \frac{1}{4} + \frac{1}{4} \right) = \frac{3}{4} \frac{\hbar^2 k^2}{mL^2} \quad (\text{not degenerate})$$

second excited state  $n_1 = 1, n_2 = 2, n_3 = 2$

$$E_2 = \frac{\hbar^2 k^2}{2mL^2} \left( 1 + \frac{1}{4} + \frac{9}{16} \right) = \frac{29}{32} \frac{\hbar^2 k^2}{mL^2} \quad (\text{not degenerate}), \quad E_3 = \frac{33}{32} \frac{\hbar^2 k^2}{mL^2}$$

wave function  $\Psi(x, y, z) = A \sin \frac{n_1 \pi}{L} \sin \frac{n_2 \pi}{L_2} \sin \frac{n_3 \pi}{L_3}$

$$V = \frac{kx^2}{2} \quad \alpha^2 = \frac{mk}{\hbar^2} \quad \beta = \frac{2mE}{\hbar^2}$$

38. Show that the energy of a simple harmonic oscillator in the  $n = 1$  state is  $3\hbar\omega/2$  by substituting the wave function  $\psi_1 = Axe^{-\alpha x^2/2}$  directly into the Schrödinger equation.

$$\frac{d\psi}{dx} = Ae^{-\alpha x^2/2} - A\alpha x e^{-\alpha x^2/2}$$

$$\frac{d^2\psi}{dx^2} = -3A\alpha x e^{-\alpha x^2/2} + A\alpha^2 x^3 e^{-\alpha x^2/2} = (\alpha^2 x^2 - 3\alpha)\psi$$

$$\frac{d^2\psi}{dx^2} = (\alpha^2 x^2 - \beta)\psi = (\alpha^2 x^2 - 3\alpha)\psi \rightarrow \beta = 3\alpha \text{ or } \frac{2mE}{\hbar^2} = 3\sqrt{\frac{mk}{\hbar^2}}$$

$$E = \frac{3}{2} \sqrt{\frac{\hbar^2}{m}} = \frac{3}{2} \hbar\omega$$