

ECE 162A  
Mat 162A

Lecture #7: 3D, Time Dependence  
Read Chapter 6 of Eisberg, Resnick  
Chapter 5 of French/Taylor

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# Solutions to SE

- Free particle
- Step potential
- Infinite box
- Finite box
- Harmonic oscillator

# Square Well

$$\frac{\hbar^2 k^2}{2m} = E \quad \frac{\hbar^2 \kappa^2}{2m} = V_0 - E$$

For  $|x| < a/2$

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

For  $x < -a/2$

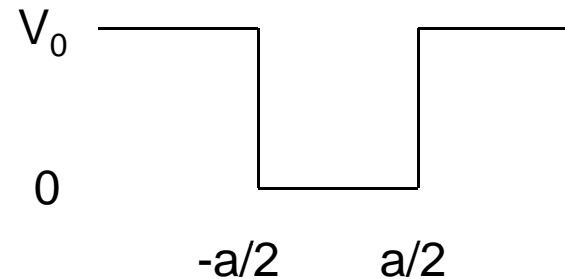
$$\psi(x) = C \exp(\kappa x) + D \exp(-\kappa x)$$

Boundary condition:  $D = 0$

For  $x > a/2$

$$\psi(x) = F \exp(\kappa x) + G \exp(-\kappa x)$$

Boundary condition:  $F = 0$



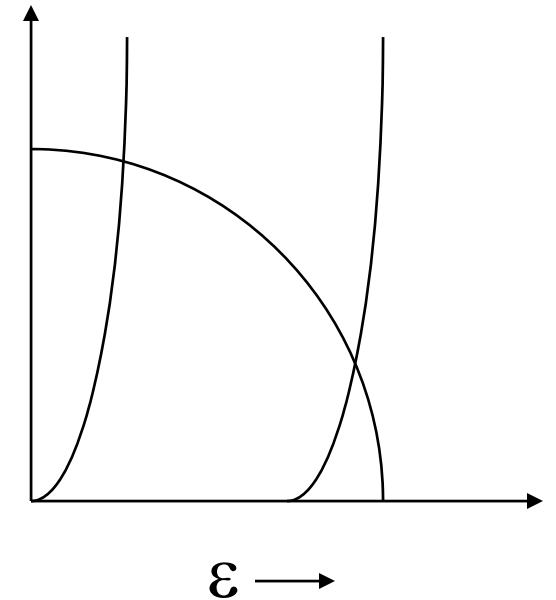
# Solution in Appendix H

- 4 Equations ( $\psi$  and  $d\psi/dx$  at two interfaces)
- 4 Unknowns (A,B,D,G)
- Solution for :

$$\varepsilon \tan \varepsilon = \sqrt{R^2 - \varepsilon^2}$$

where

$$E = \frac{2\hbar^2 \varepsilon^2}{ma^2} \quad R^2 = \frac{mV_0 a^2}{2\hbar^2}$$



# Harmonic Oscillator

- $V(x) = \frac{1}{2} C x^2$
- Very common because it represents any small vibration about a point of stable equilibrium
- Examples
  - Diatomic molecules
  - Atoms vibrating on a lattice.
  - Particle on a string.

# Solution in Appendix I

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

*Solution :*

$$\text{Let } \alpha = \sqrt{\frac{Cm}{\hbar}} \quad \beta = \frac{2mE}{\hbar^2}$$

*Then Schroedinger's Equation becomes*

$$\frac{d^2\psi}{dx^2} + (\beta - \alpha^2 x^2)\psi = 0$$

$$\text{Let } u = \sqrt{\alpha} x$$

$$\frac{d^2\psi}{du^2} + \left(\frac{\beta}{\alpha} - u^2\right)\psi = 0$$

For large  $u$ :

$$\frac{d^2\psi}{du^2} + \left(\frac{\beta}{\alpha} - u^2\right)\psi = 0$$

$$\frac{d^2\psi}{du^2} - u^2\psi \approx 0$$

$$\psi = Ae^{-u^2/2} + Be^{u^2/2}$$

*Finite  $\psi$  means  $B = 0$*

$$\psi \approx Ae^{-u^2/2} \text{ for } u \rightarrow \infty$$

*Try to find  $H(U)$  that satisfies SE:*

$$\psi = AH(u)e^{-u^2/2}$$

# Solutions to Harmonic Oscillator

*Substitute in SE to get the Hermite DE:*

$$\frac{d^2 H}{du^2} - 2u \frac{dH}{du} + \left(\frac{\beta}{\alpha} - 1\right)H = 0$$

$$H(u) = a_0 + a_1 u + a_2 u^2 + \dots$$

*Calculate the values of  $a_i$ :*

$$\psi_0 = A_0 e^{-u^2/2}$$

$$\psi_1 = A_1 u e^{-u^2/2}$$

$$\psi_2 = A_2 (1 - 2u^2) e^{-u^2/2}$$

*where  $\beta / \alpha = 2n + 1$  causes the series to stop*

Where  $E_n = (n + 1/2)h\nu$  where  $n = 0, 1, 2, \dots$

# Eigenvalues

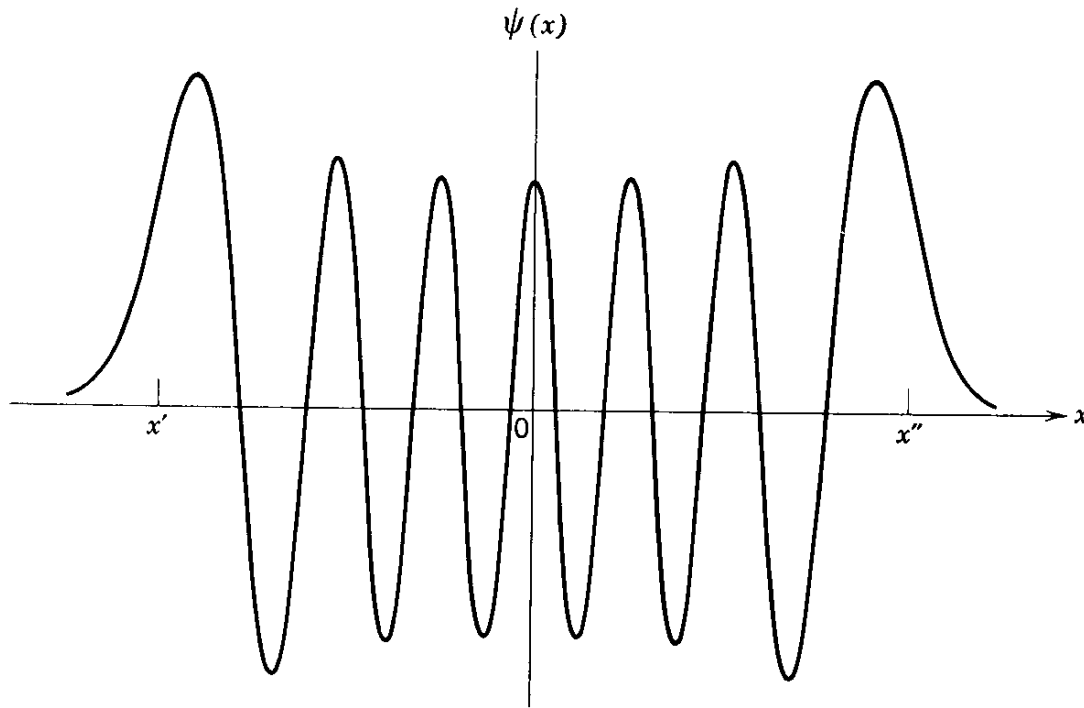
$E_n = (n + 1/2)h\nu$  where  $n = 0, 1, 2, \dots$

And

$$\nu = \frac{1}{2\pi} \sqrt{\frac{C}{m}}$$

- The series  $H(u)$  are called Hermite polynomials.
  
- Page 223,224

# Harmonic oscillator 13<sup>th</sup> mode



**Figure 5-18** The eigenfunction for the thirteenth allowed energy of the simple harmonic oscillator. The classical limits of motion are indicated by  $x'$  and  $x''$ .

# 3 Dimensional Time Independent Schroedinger Equation

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

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

# Free Particle in a 3D Box

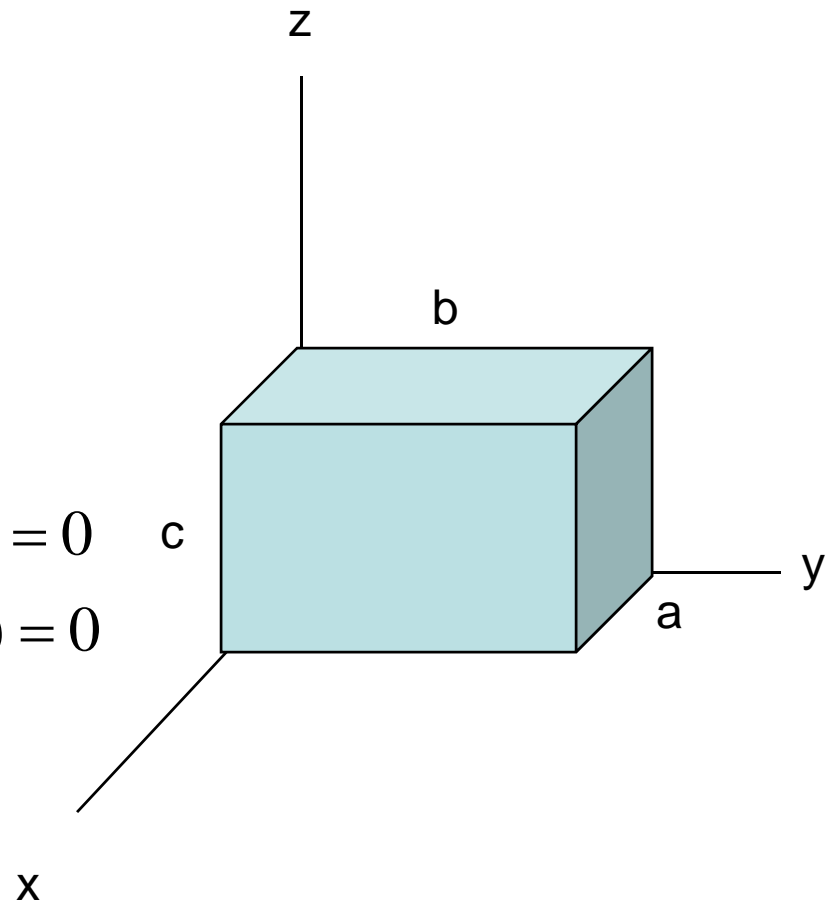
$$-\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi(x, y, z) + V(x, y, z) \psi(x, y, z) = E \psi(x, y, z)$$

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

*Boundary Conditions :*

$$\psi(0, y, z) = \psi(x, 0, z) = \psi(x, y, 0) = 0$$

$$\psi(a, y, z) = \psi(x, b, z) = \psi(x, y, c) = 0$$



# Separation of Variables

- Voltage is separable
- Boundary conditions are separable

So try:

$$\psi(x, y, z) = X(x)Y(y)Z(z)$$

# 3D Particle in a Box

$$-\frac{\hbar^2 YZ}{2m} \frac{d^2 X}{dx^2} - \frac{\hbar^2 XZ}{2m} \frac{d^2 Y}{dy^2} - \frac{\hbar^2 XY}{2m} \frac{d^2 Z}{dz^2} = EXYZ$$

Divide by XYZ

$$-\frac{\hbar^2}{2mX} \frac{d^2 X}{dx^2} - \frac{\hbar^2}{2mY} \frac{d^2 Y}{dy^2} - \frac{\hbar^2}{2mZ} \frac{d^2 Z}{dz^2} = E$$

Function of X    Function of Y    Function of Z = Const.

$$E_x + E_y + E_z = E$$

$$-\frac{\hbar^2}{2m} \frac{d^2 X}{dx^2} = E_x X$$

$$X = e^{ikx}$$

$$\psi = e^{ikx} e^{iky} e^{ikz} = e^{ikx+iky+ikz}$$

# Simpler to use Sines and Cosines to match boundary conditions

$$X(x) = \sin \frac{n_x \pi x}{a} \quad n_x = 1, 2, 3, \dots$$

$$Y(y) = \sin \frac{n_y \pi y}{b} \quad n_y = 1, 2, 3, \dots$$

$$Z(z) = \sin \frac{n_z \pi z}{c} \quad n_z = 1, 2, 3, \dots$$

$$E = \frac{\hbar^2}{2m} \left( \left( \frac{n_x \pi}{a} \right)^2 + \left( \frac{n_y \pi}{b} \right)^2 + \left( \frac{n_z \pi}{c} \right)^2 \right)$$

$$E = \frac{h^2}{8m} \left( \frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2} \right)$$

# Time Dependence of Solution

- Solve for stationary solutions  $\psi_n(x)$  with energies  $E_n$

$$\Psi(x, t) = \sum_n A_n \psi_n(x) e^{-i\omega_n t}$$

$$\omega_n = E_n / \hbar$$

- Find the values for  $A_n$  that satisfy the initial conditions.

# Motion of a Particle in a Box

$$\psi(x) = A_1 \sin\left(\frac{\pi x}{L}\right) + A_2 \sin\left(\frac{2\pi x}{L}\right) + \dots$$

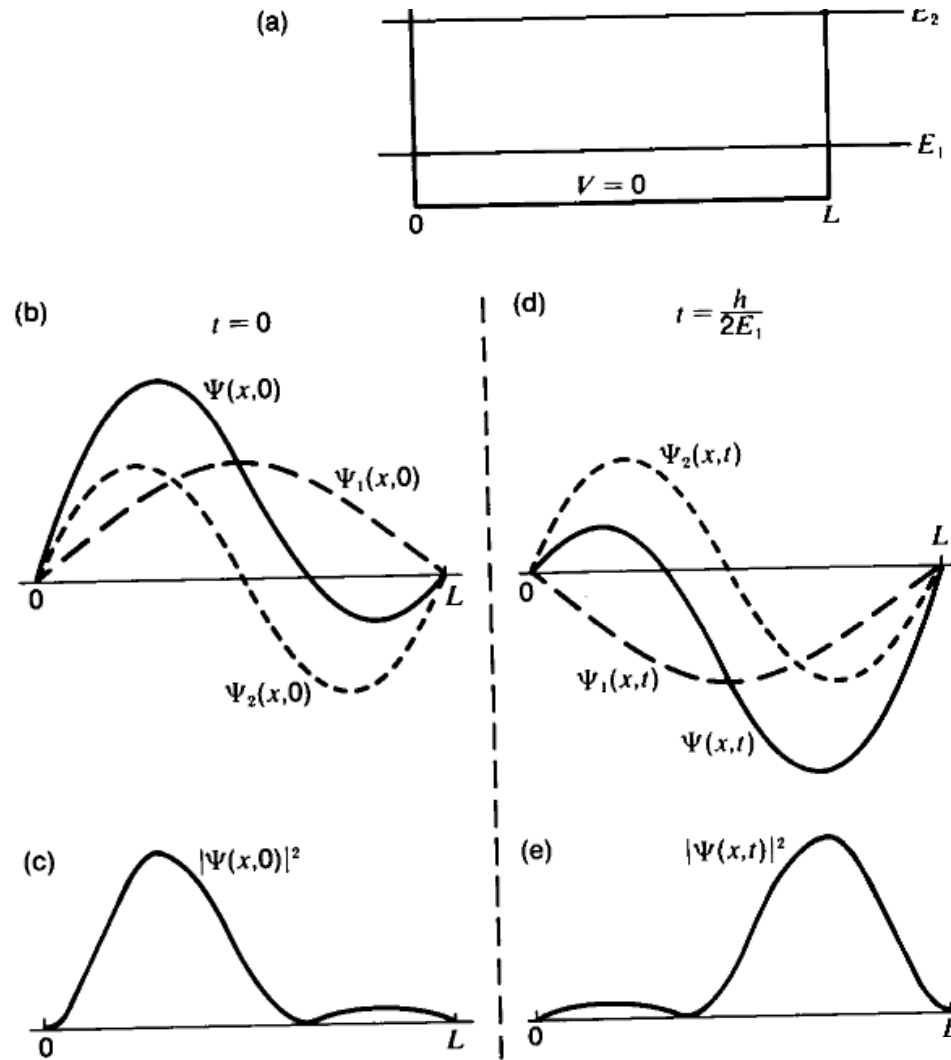
$$E_n = E_0 n^2$$

*Special case*  $A_1 = A_2 = 1$ ; others 0

$$\Psi(x, t) = \sin\left(\frac{\pi x}{L}\right)e^{i\omega t} + \sin\left(\frac{2\pi x}{L}\right)e^{4i\omega t}$$

# Wave function evolution

Fig. 8-1 Superposition of the lowest stationary states of an infinite square well. (a) Potential energy function for the well, with the two lowest energy eigenvalues shown. (b) Eigenfunctions for the two lowest energy states (broken lines) and the superposition of these functions (solid line), at  $t = 0$ . (c) Probability density function at  $t = 0$  for the superposition shown in (b). (d) and (e) Plots corresponding to (b) and (c) for the later time  $t = h/(2E_1)$ .



ing  $E = 0$  at the bottom of the well)

$$E_n = \frac{n^2 h^2}{8mL^2}$$

Therefore,

# Time Evolution

$$\psi(x) = \sin\left(\frac{\pi x}{L}\right) + \sin\left(\frac{2\pi x}{L}\right) = f_1 + f_2$$

$$\Psi(x, t) = f_1 e^{i\omega t} + f_2 e^{4i\omega t}$$

$$|\Psi(x, t)|^2 = f_1^2 + f_2^2 + 2f_1 f_2 \cos((E_2 - E_1)t / \hbar)$$