ECE 162A
Mat 162A

Lecture #9: 3D Solutions.
Expectation Values
Read Chapter 3,8 of French/Taylor

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Midterm Material

- Lecture
- Eisberg/Resnick Chapters 1-6
- French/Taylor 1-5,8,9 (except 5-5)
- Background of quantum theory
  - Wave/particle basis of light:
    - Planck's postulate
    - Planck's constant
  - Wave/particle basis of matter
    - Photoelectric effect, Compton effect, pair production,…
  - Wave/particle duality
  - Uncertainty principle
  - Atom models:
    - Thompson model
    - Rutherford model
    - Bohr model

Midterm Material

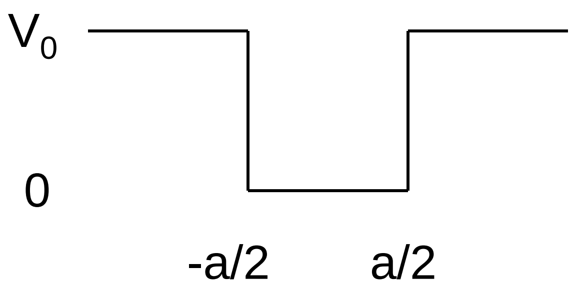
- Time dependent Schroedinger equation
- Time independent Schroedinger equation
- Interpretation of $\Psi(x,t)$, probability
- Requirements on $\Psi(x,t)$
- Understand how to solve SE, apply boundary conditions, initial conditions.
- How to find stationary solutions
- Specific cases (free particle, barrier, infinite square well, finite square well, harmonic oscillator)

Midterm

- Next Thursday. 1 hour, 50 minutes
- One 8.5x11 crib sheet allowed (one side)
- What do you need to know?
  - Given a stationary potential, find a solution to SE (40%)
    - Use separation of variables, find solutions, apply boundary conditions, find eigenvalues, apply initial conditions, find time dependent solution.
  - Given a stationary potential, sketch solutions to SE (30%)
  - Wave-particle duality (15%)
  - Early quantum theory (15%)

Square Well

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



$$For \;\; |x| < a/2$$

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

$$For \;\; x < -a/2$$

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

$$Boundary \;\; condition: \;\; D = 0$$

$$For \;\; x > a/2$$

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

$$Boundary \;\; condition: \;\; F = 0$$

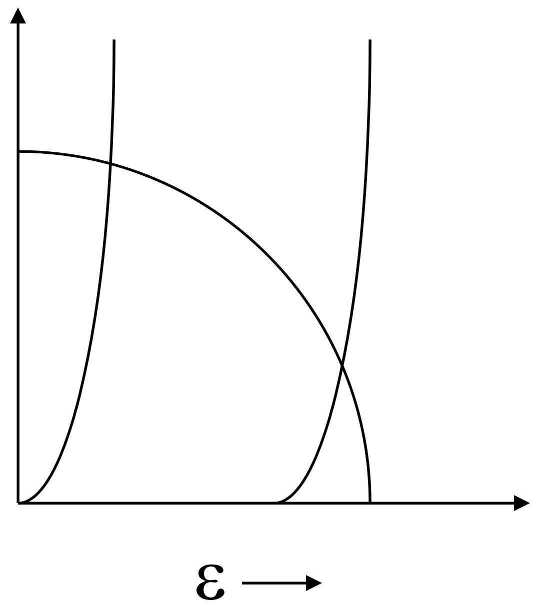
Solution in Appendix H

- 4 Equations (ψ and dψ/dx at two interfaces)
- 4 Unknowns (A,B,D,G)
- Solution for :

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

where

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



3 Dimensional Time Independent Schroedinger Equation

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

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

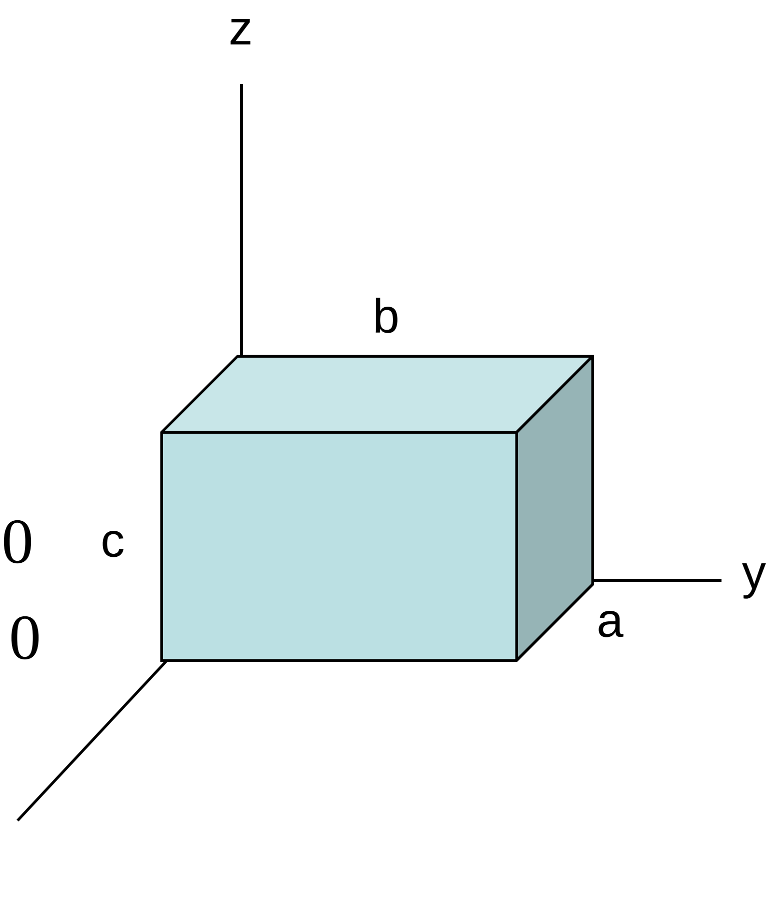
$$-\frac{\hbar^2}{2m}\nabla^2\psi+V\psi=E\psi$$

Free Particle in a 3D Box

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

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

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



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

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

$$Divide \quad by \quad XYZ$$

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

$$FunctionofX \;\; FunctionofY \;\; FunctionofZ = Const.$$

$$E_x + E_y + E_z = E$$

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

$$X = e^{ikx}$$

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

Simplest to use Sines and Cosines to match boundary conditions

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

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

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

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

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

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 intial conditions.

Motion of a Particle in a Box

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

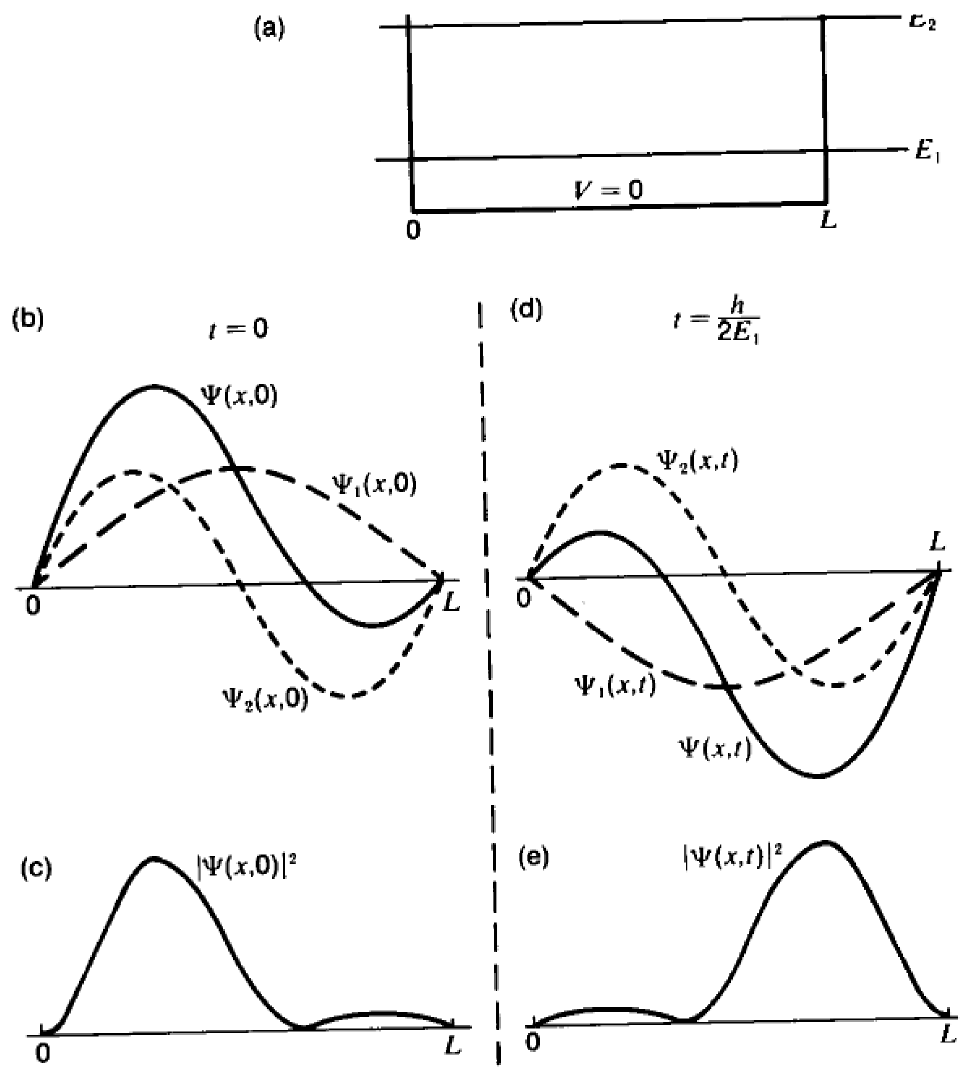
$$E_n = E_0 n^2$$

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

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

Wave functic evolut

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)

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

Therefore,

Time Evolution

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

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

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

Expectation Values

$$\langle x \rangle = \int x \left|\psi(x)\right|^2 dx = \int \psi^*(x) x \psi(x) dx$$

$$\left\langle x^2 \right\rangle = \int \psi^*(x) x^2 \psi(x) dx$$

$$\langle p \rangle = \int \psi^*(x) (-i\hbar \frac{d}{dx}) \psi(x) dx$$

$$\langle V \rangle = \int \psi^*(x) V(x) \psi(x) dx$$

Expectation Values

$$\langle x \rangle = \int x|\psi(x)|^2 dx = \int \psi^*(x) x \psi(x) dx$$

$$\langle x^2 \rangle = \int \psi^*(x) x^2 \psi(x) dx$$

$$\langle p \rangle = \int \psi^*(x)(-i\hbar \frac{d}{dx})\psi(x) dx$$

$$\langle V \rangle = \int \psi^*(x) V(x) \psi(x) dx$$

Calculate these for the lowest order solution for an infinite square well

Expectation Values

$$\langle x \rangle = \int x |\psi(x)|^2 dx$$

$$1D \ \textit{Infinite Square Well}$$

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

$$\langle x \rangle = \int x |\psi(x)|^2 dx = \frac{2}{L} \int_0^L x \sin^2(\frac{n\pi x}{L}) dx$$

$$\langle x \rangle = \frac{1}{L} \int_0^L x(1 - \cos(\frac{2n\pi x}{L}) dx$$

$$\langle x \rangle = \frac{1}{L} (\frac{x^2}{2} - \frac{x^2}{2} \cos(\frac{2n\pi x}{L}) + \frac{xL}{2n\pi} \sin(\frac{2n\pi x}{L}))\Big|_0^L$$

$$\langle x \rangle = \frac{1}{L} (\frac{L^2}{2}) = \frac{L}{2}$$

Hyrdrogen like solutions 3 Dimensional Time Independent Schroedinger Equation

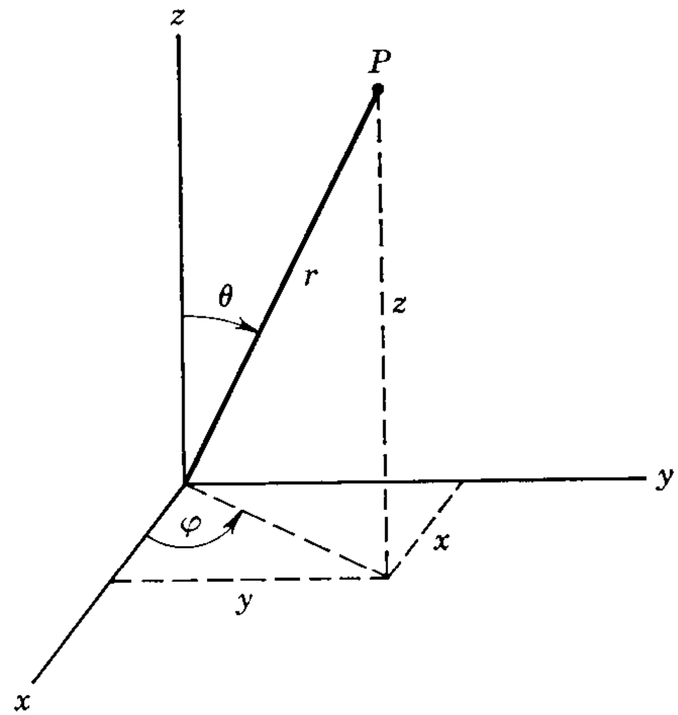
$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(x,y,z)+V(x,y,z)\psi(x,y,z)$$
$$=E\psi(x,y,z)$$

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

$$If\ \ V(x,y,x)=V(r)$$

$$Switch\ \ coordinate\ \ systems$$

Spherical Coordinates



$$r = \sqrt{x^2 + y^2 + z^2}$$

$$x = r \sin\theta \cos\phi$$

$$y = r \sin\theta \sin\phi$$

$$z = r \cos\theta$$

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 \frac{\partial}{\partial r}) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}(\sin\theta \frac{\partial}{\partial\theta}) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial^2\phi}$$

Transform

$$r = \sqrt{x^2 + y^2 + z^2}$$

$$x = r\sin\theta\cos\phi$$

$$y = r\sin\theta\sin\phi$$

$$z = r\cos\theta$$

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial x}\frac{\partial}{\partial\theta} + \frac{\partial\phi}{\partial x}\frac{\partial}{\partial\phi}$$

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial^2\phi}$$

Solution to SE in Spherical Coordinates

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

$$If\ \ V(r,\theta,\phi) = V(r) = -\frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r}$$

$$Then\ try\ separation\ of\ \ \text{variables}$$

$$\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)$$

$$Substitute\ and\ divide\ by\ R\Theta\Phi$$

$$-\frac{\hbar^2}{2mR}\left(\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)\right) + \frac{1}{\Theta r^2\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \frac{1}{\Phi r^2\sin^2\theta}\frac{d^2\Phi}{d^2\phi} + V(r) = E$$