ECE 162A
Mat 162A

Lecture #5: Schroedinger Theory of Quantum Mechanics
Read Chapter 5,6 of Eisberg,Resnick

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Makeup class: 1 pm Friday, Oct. 17

Schroedinger's Equation (1926)

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

– Kinetic energy + potential energy = total energy

Free particle (V=0)

- Schroedinger's equation:

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

- Sin or cosine alone do not work
- Exponential does work:

$$\psi(x,t) = A\exp(i(kx-\omega t))$$

$$\frac{\hbar^2k^2}{2m} = \hbar\omega$$

$$\frac{\hbar^2k^2}{2m} = E$$

Schroedinger's equation is linear

- No terms in ψ^2 (except in voltage term)
- Hence, if ψ_1 and ψ_2 are solutions, then

□ $\psi = a\psi_1 + b\psi_2$ is a solution.

Schroedinger's equation is in the nonrelativistic limit.

- Instead of

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

Use (following Dirac) to suggest the form of the equation:

$$E = \sqrt{c^2 p^2 + (m_0 c^2)^2}$$

Probability

- If, at instant t, a measurement is made to locate the particle associated with the wave function $\psi(x,t)$, then the probability that the particle will be found at a coordinate between x and x+dx is

$$\psi(x,t)\ \psi^*(x,t)dx$$

Where * means complex conjugate.

- It does not tell us that a particle in a given energy state will be found in a precise location at a certain time, but only the relative probabilities that the particle will be found in various locations at that time.
- The prediction is statistical!

- What is the probability function for a free particle?
- Is it real and positive?
- Draw the probability function for the free particle solution.

Quantum Mechanical Problem Solution

- Solve Schroedinger's equation. Determine eigenfunctions. $\psi_i(x,t,\ldots)$. Normalize eigenfunctions.
- Apply boundary conditions and determine solutions (eigenvalues). E_i
- The complete solution is

$$\psi(x,t) = \sum_i A_i \psi_i(x,t)$$

- Apply initial condition to determine the coefficients. A_i
- The instantaneous state of the system is exactly known for all time, but particle positions are only determined by measurement and the average of many measurements is given by

$$\left|\psi(\mathrm{x},\mathrm{t})\right|^2$$

The probability is real and positive:

$$|\psi(\mathrm{x,t})|^2 = \psi(\mathrm{x,t})\,\psi^*(\mathrm{x,t})$$

$$\psi(\mathrm{x,t}) = \mathrm{R}(\mathrm{x,t}) + \mathrm{iI}(\mathrm{x,t}) \quad \text{where R and I are real}$$

so

$$|\psi(\mathrm{x,t})|^2 = (R+iI)(R-iI) = R^2 + I^2 \geq 0$$

Normalize eigenfunctions

$$\int_{-\infty}^{\infty} P dx = 1$$

$$\int_{-\infty}^{\infty} \Psi^* \Psi dx = 1$$

$$\Psi = \sum_i A_i \psi_i$$

$$Normalize$$

$$\int_{-\infty}^{\infty} \psi_i^* \psi_i dx = 1$$

The solutions are orthogonal

$$\int_{-\infty}^{\infty} \psi_i * \psi_j dx = 0 \quad if \;\; i \neq j$$

If the wavefunctions are normalized

$$\int_{-\infty}^{\infty} \psi_i * \psi_j dx = \delta_{ij}$$

Orthonormal eigenfunctions

where

$$\delta_{ij} = \; 1 \; if \;\; i = j$$

$$0 \;\; if \;\; i \neq j$$

Expectation Values

- We may not know the position without making a measurement, but we can calculation the average value for the position (the expectation value).

$$\langle x \rangle = \overline{x} = \int_{-\infty}^{\infty} xP(x,t)dx$$

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

- This is true for any variable (energy, momentum, …)
- The order doesn’t matter here, but will later when we calculate the expectation value of operators.

Operators

- Use operators to represent mathematical operations. For example:

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

- Momentum
- Energy

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

- Note that

$$\hat{p}^2 \leftrightarrow -\hbar^2 \frac{\partial^2}{\partial x^2}$$

- So Schroedinger's equation becomes in operator form

$$\frac{\hat{p}^2}{2m} + V = \hat{E} \qquad \frac{\hat{p}^2}{2m}\Psi + V\Psi = \hat{E}\Psi$$

Momentum Expectation Value

$$\overline{p} = \int \Psi^* \hat{p} \Psi dx$$

The expectation value for the dynamic quantity f(x,p,t) is

$$\overline{\mathrm{f(x,p,t)}} = \int_{-\infty}^{\infty} dx \Psi^* \hat{f}(x, -i\hbar \frac{\partial}{\partial x}, t) \Psi$$

Note: The wave function contains information not just on the probability density versus time, but also the momentum, energy, or f(x,p,t)

Solve Time Dependent Schroedinger Equation when V(x) is a function of x only

Derive the time Independent Schroedinger Equation

Solve Time Dependent Schroedinger Equation when V(x) is a function of x only

Try separation of variables

$$\Psi(x,t) = \psi(x)\varphi(t)$$

$$-\frac{\hbar^2 \varphi(t)}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x)\phi(t) = -i\hbar\,\psi(x)\frac{d\phi(t)}{dt}$$

$$-\frac{\hbar^2}{2m\psi}\frac{d^2\psi(x)}{dx^2} + V(x) = \frac{-i\hbar}{\varphi(t)}\frac{d\phi(t)}{dt}$$

LHS is a function of x only and RHS is a function of t only, so both sides must equal a constant.

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

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

Time Independent Schroedinger Equation

Time Independent Schroedinger Equation

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

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$$

Requirements on Solution

- $\psi(x)$, $d\psi(x)/dx$ must be finite. (or at least the integral of $\psi^*\psi$ must be finite).
- $\psi(x)$, $d\psi(x)/dx$ must be single valued.
- $\psi(x)$, $d\psi(x)/dx$ must be continuous.
- Note: If $V(x)$ is not continuous, then $d^2\psi(x)/dx^2$ is not continuous.

Qualitative Plots

- Lowest energy solution has no nodes.
- Successively higher energy solutions have additional nodes.
- Curvature related to E-V
- Decay rate related to V-E.
- For constant V:
  - sinusoid for E>V (k constant)
  - Exponential decay for E<V (κ constant)
- Amplitudes larger in smaller curvature regions.
  - (Classically, lower P means slower velocity, more likely to find there.)

$$\frac{\hbar^2 k^2}{2m} = E - V$$

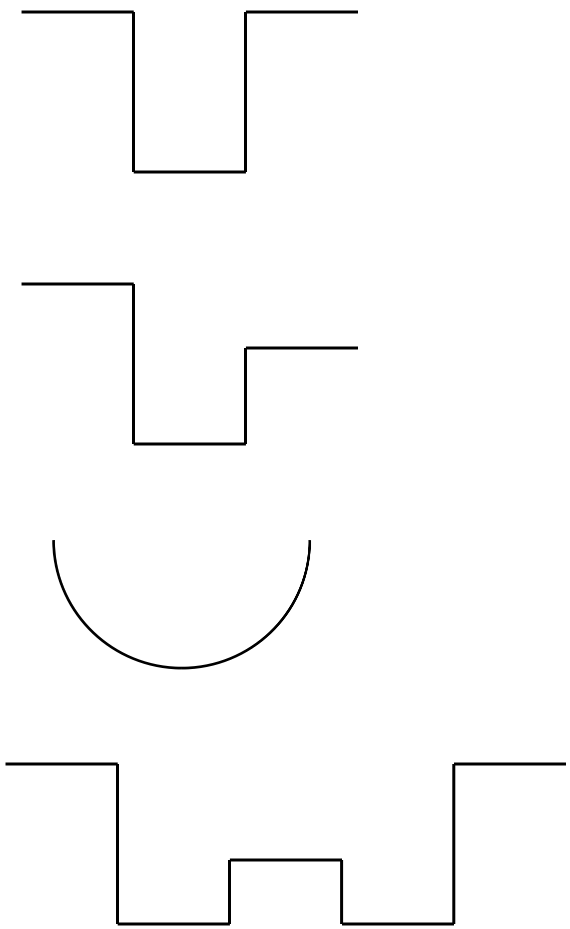
$$\frac{\hbar^2 \kappa^2}{2m} = V - E$$

Symmetry

- If $V(x)$ is symmetric, then all solutions are either
  - Symmetric (even parity)
  - Antisymmetric (odd parity)

Sketch the solutions

How do they differ from infinite square well?



Eigenvalue Equation

- Using operators, Schroedinger's equation can be expressed as an eigenvalue equation

$$E_{op}\psi = E\psi$$

where

$$E_{op} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V$$

- The solution of the equation involves finding the particular solutions $\psi_{n,}$ called eigenfunctions and E_n called eigenvalues.

Solutions to SE

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

Free particle (V=0)

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

$$Solution: \quad \psi(x) = \exp(ikx)$$

$$where \quad \frac{\hbar^2 k^2}{2m} = E$$

The complete solution is

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar} = e^{ikz-i(E/\hbar)t}$$

There are no constraints on E, any value is allowed at this point. This corresponds to a wave moving to the right. -k solutions are also valid.