PHYS 2D DISCUSSION SECTION

2012/5/16

- Quiz 3 is graded
- Pick up quiz 3 today, tomorrow, or next Tuesday
- Regrade request: 1 week

Topics

- Probability
- Born interpretation
- Normalization
- Operators
- x & p operators
- Schrodinger's equation
- Free space wave function
- Particle in a box & Finite square well
- Quantum oscillator

Probability

- 2 possible outcomes for a measurement:
- Event 1 has probability p_1 of happening, event 2 has p_2. When taking a measurement, either 1 happens or 2 happens, so $p_1+p_2=1$
- 1 measurement: has a chance p_1 to find result 1, chance p_2 to find result 2
- 100 measurements: find result 1 $100*p_1$ times, result 2 $100*p_2$ times
- N measurements: result in 1 Np_1 times, 2 Np_2 times
- $Np_1+ Np_2 =N(p_1+p_2)=N$

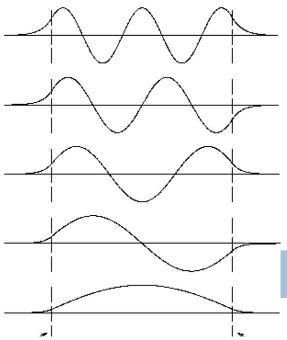
Probability

- M possible outcomes for a measurement:
  - A measurement has chance p_x to return result x, where x goes from 1 to M, and $\Sigma_x p_x = 1$
- If M is infinite:
  - Consider for example x=position of a particle
  - x is now continuous (infinite values of x)
  - If we assign each x a probability, sum over x blows up
  - Define p(x) so that a measurement has chance p(x)dx of finding the particle in an interval dx about x
  - p(x) is now a probability distribution

Probability

- P(x)dx is the probability of finding the particle in a small interval dx around x
- If at each x a function f has value f(x), then the average measured value of f after lots of measurements is $\bar{f} = \int f\,P(x)\,dx$
- Discrete example: Dice
  - x=1 to 6
  - $p_x=1/6$
  - $f_x=x$
  - Average measured value of x = $\Sigma_x f_x p_x=3.5$

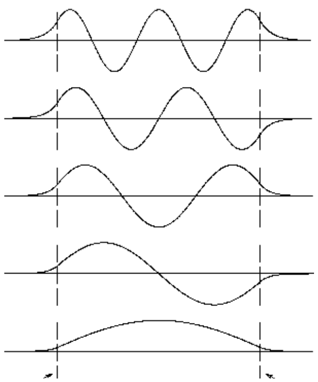
Wave function Ψ



- Wave function $\Psi(x)$ is used to describe a particle
  - It contains all the information about that particle
  - It is a complete description
  - In principle, if we know $\Psi(x)$, we can deduce any physical quantity of the particle we want to know

Born interpretation

- Born interpretation: (the physical meaning of the wave function Ψ(x))
- $|\Psi(x)|^2$ is a probability distribution, which means a measurement (of position x) has a chance $|\Psi(x)|^2 dx$ of returning a value in the interval dx about x, or $$P(x)dx = |\Psi(x,t)|^2 dx$$
- When measuring the position of the particle, the returned value x, which is the position of the particle, can be anywhere from -∞ to ∞ as long as $|\Psi(x)|^2 \neq 0$, but the probability for each x is different



Normalization

- If our $\Psi(x)$ describes 1 particle, then the probability of finding the particle at each x must add up to 1
- For discrete x, $\Sigma_x p_x = 1$
- For continuous x, $\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1$ ($P(x)dx = |\Psi(x,t)|^2 dx$)

- This is the normalization condition, arising from the probabilistic nature of wave functions

Operators

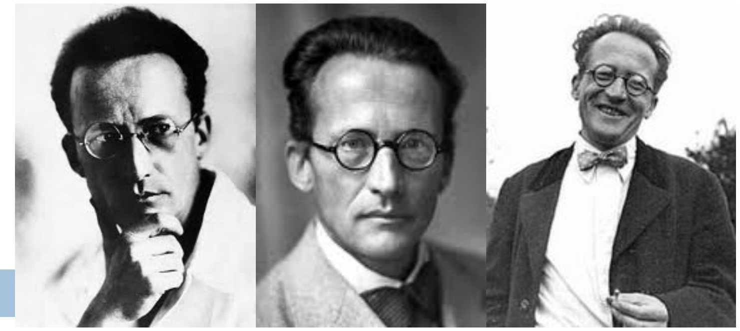
- Wave function contains all physical quantities
  - Position, momentum, energy, etc.
- To extract these information (observables), need to define operators for the corresponding measurable physical quantity f
- Expectation value $\bar{f}$ =average value of f after large number of measurements (of f)
- The operator for f, $\hat{f}$ is defined so that the expectation value is $\bar{f} = \int_{-\infty}^{\infty} \Psi^* (x)\, \hat{f}\, \Psi (x)\, dx$
- $\hat{f}$ can be a number or a differential operator

x & p operators

- For example, if f is the position x
  - By definition, $\bar{x} = \int_{-\infty}^{\infty} \Psi^*(x)\, \hat{x}\, \Psi(x)\, dx$
  - But $\bar{x} = \int_{-\infty}^{\infty} x\, P(x)\, dx = \int_{-\infty}^{\infty} x\, |\Psi(x)|^2\, dx$

    $= \int_{-\infty}^{\infty} x\, \Psi^*(x)\, \Psi(x)\, dx = \int_{-\infty}^{\infty} \Psi^*(x)\, x\, \Psi(x)\, dx$
  - So $\hat{x} = x$
- For momentum p, $\hat{p}$ is a differential operator
  - It can be derived: $\hat{p} = \frac{\hbar}{i} \frac{d}{dx}$
  - So $\bar{p} = \int_{-\infty}^{\infty} \Psi^*(x)\, \hat{p}\, \Psi(x)\, dx = \int_{-\infty}^{\infty} \Psi^*(x)\, \frac{\hbar}{i} \frac{d}{dx}\, \Psi(x)\, dx$
  - $\hat{p} = \frac{\hbar}{i} \frac{d}{dx}$ acts on the wave function $\Psi(x)$ to the right

Schrodinger's equation



- Relates the wave function of a particle to the environment (U(x)) of the particle

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = \hat{H} \Psi(x, t)$$

- The equation that determines the wave function
- Total energy $E=p^2/2m+U(x)$
- Convert p to $\hat{p}$ and x to $\hat{x}$ to get $\hat{H}$
- $\hat{H} = \frac{\hat{p}^2}{2m} + U(\hat{x}) = \frac{\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2}{2m} + U(\hat{x}) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(\hat{x})$

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

Schrodinger's equation

- Time-dependent Schrodinger's equation:

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = \hat{H} \Psi(x, t)$$

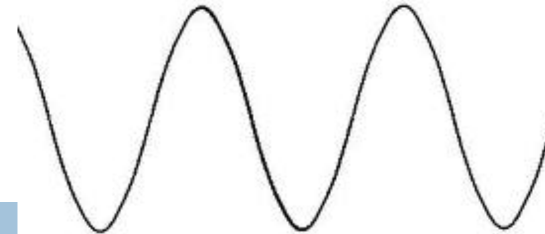
where $\hat{H}$ is the total energy operator (Hamiltonian)

- If we assume that Ψ(x,t) can be separated

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

- Then we have the time-independent Schrodinger's equation $\hat{H}\psi(x) = E\psi(x)$, where E is the total energy
- Also $i\hbar \frac{\partial}{\partial t} \phi(t) = E\phi(t)$

Free space wave function



- Putting Schrodinger's equation to use
- Free space: U(x)=0

$$\hat{H}\psi(x) = E\psi(x)$$

$$i\hbar \frac{\partial}{\partial t}\phi(t) = E\phi(t)$$

$$\hat{H} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

$$\frac{d^2}{dx^2}\cos(x) = -\cos(x)$$

$$\frac{d^2}{dx^2}\sin(x) = -\sin(x)$$

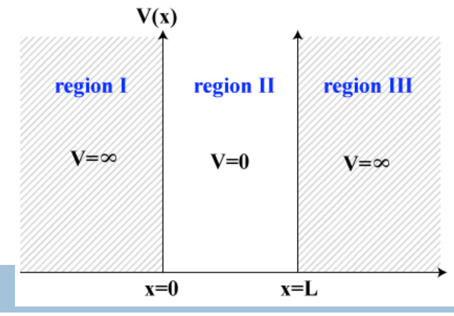
$$e^{ix} = \cos(x) + i\sin(x)$$

- So, $\psi(x) = Ae^{\pm ikx}, \quad E = \frac{\hbar^2 k^2}{2m}$

$$\phi(t) = Be^{-i\omega t}, \quad E = \hbar\omega$$

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

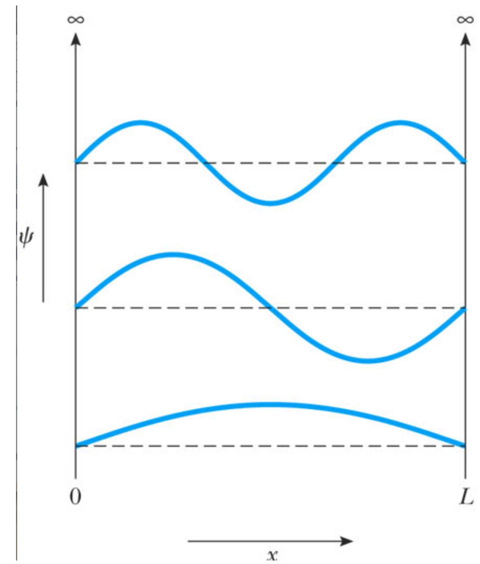
Particle in a box



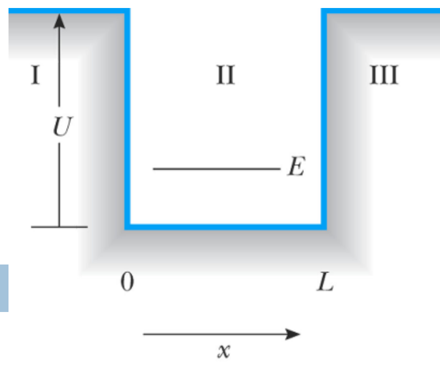
- Not so trivial application of Schrodinger's equation
- $\phi(t) = Be^{-i\omega t}$ doesn't affect observables
- 1-D box, particle is restricted so $x \in [0, L]$
- To prevent particle from moving beyond $[0, L]$, we let V= ∞ outside the box
- When V= ∞, ψ(x)=0, the wall is infinitely high
- To find ψ(x) in region II, consider the time-independent Schrodinger's equation and require ψ(x) be continuous (ψ(0)=ψ(L)=0)

Particle in a box

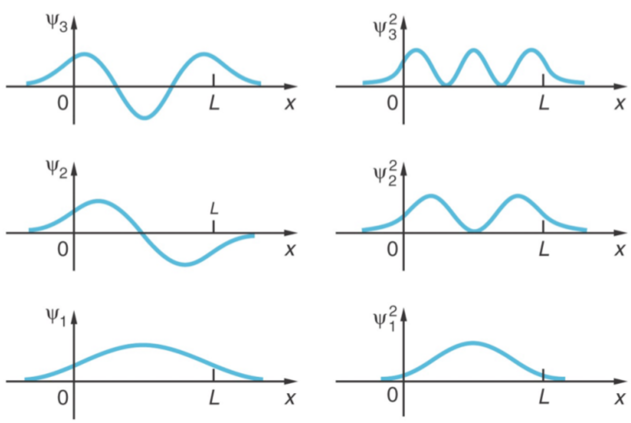
- $\psi(x)=A\sin kx=A\sin[(n\pi/L)x]$
- $$E = \frac{n^2\pi^2\hbar^2}{2mL}$$
- n=1, 2, 3, …
- Integer n (quantization) comes from boundary conditions



Finite square well

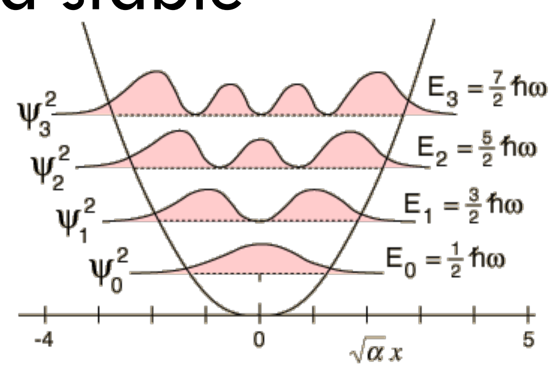


- The potential outside II is now V=U, not ∞
- Wave function similar to particle in a box
- Significant difference at the boundary (x=0 or L)
- Wave function is non-zero outside II, for a small distance (penetration depth)
- To find ψ(x), require ψ and dψ/dx be continuous at x=0 & x=L



Quantum oscillator

- Classical oscillator: $E=p^2/2m+U(x)$, $U(x)=m\omega^2x^2/2$
- Ex. Spring
- Quantum version: $$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)+\frac{m\omega^2 x^2}{2}\psi(x)=E\psi(x)$$
- $E=(n+1/2)\hbar\omega$, $n=0, 1, 2, \ldots$
- $n=0$ correspond to zero classical amplitude, but $E=\hbar\omega/2\neq 0$
- Can model small oscillations around stable equilibrium points



- Questions?