Stationary Solution of Schrodinger Equation

Phys 460, Fall 2009, JP Hu

Schrodinger Equation

- Separation of Variables

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

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

Solving Schrodinger Eq

- Stationary solution:

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

$$-\frac{\hbar^2}{2m}\frac{\partial^2\varphi(x)}{\partial x^2}+V(x)\varphi(x)=E\varphi(x)$$

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

For constant E

$$\hat{H}=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)$$

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

General solution

- Find all of eigenvalues of H

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

$$\hat{H}\varphi_n(x) = E_n\varphi_n(x)$$

$$\psi_n(x,t) = \varphi_n(x)e^{-iE_n t/\hbar}$$

- General solution:

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

$$\psi(x,t) = \sum_n c_n\psi_n(x,t)$$

Examples

- Particle in an infinite square well
- Free Particle
- Particle in a harmonic oscillator

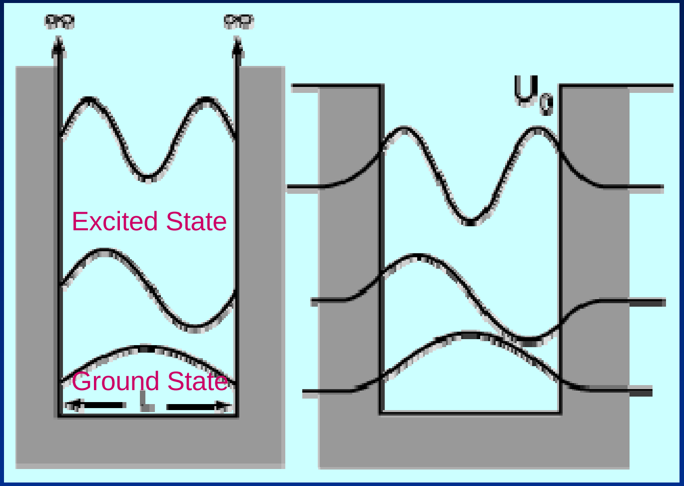
- Particle in a finite square well

- Particle in a delta function potential

Infinite Quantum Well

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

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



General solution:

$$\varphi_n(x) = a_n\cos(nx) + b_n\sin(nx)$$

$$E_n = \frac{\hbar^2 n^2}{2m}$$

Boundary Condition:

$$\varphi_n(L/2) = \varphi_n(-L/2) = 0$$

$$a_n\cos(nL/2) + b_n\sin(nL/2) = a_n\cos(nL/2) - b_n\sin(nL/2) = 0$$

Solution:

$(1) a_n = 0, nL/2 = k\pi, k = 1,2,...$

$(2) b_n = 0, nL/2 = (k+1/2)\pi, k = 1,2...$

Even solution

$$(1)\varphi_k(x) = \sqrt{\frac{2}{L}}\cos(\frac{(2k-1)\pi x}{L}), E_k = \frac{\hbar^2\pi^2(2k-1)^2}{2mL^2}$$

$$(2)\varphi_k(x) = \sqrt{\frac{2}{L}}\sin(\frac{2k\pi x}{L}), E_k = \frac{\hbar^2\pi^2(2k)^2}{2mL^2}$$

$k = 1,2,3...$

Odd solution

Ground state:

$$\varphi_g = \sqrt{\frac{2}{L}}\cos(\frac{\pi x}{L}), E_g = \frac{\hbar^2\pi^2}{2mL^2}$$

Infinite Quantum Well

1. Orthogonal condition: General solution:

$$\int_{-L/2}^{L/2} dx\varphi^{*(e,o)}{}_{k'}(x)\varphi^{(e,o)}{}_{k}(x) = \delta_{kk'}$$

$$\int_{-L/2}^{L/2} dx\varphi^{*(e)}{}_{k'}(x)\varphi^{(o)}{}_{k}(x) = 0$$

$$\delta_{kk'} = \{{}^{0,k\neq k'}_{1,k=k'}$$

$$(1)\varphi^{e}{}_{k}(x) = \sqrt{\frac{2}{L}}\cos(\frac{(2k-1)\pi x}{L}), E_k = \frac{\hbar^2\pi^2(2k-1)^2}{2mL^2}$$

$$(2)\varphi^{o}{}_{k}(x) = \sqrt{\frac{2}{L}}\sin(\frac{2k\pi x}{L}), E_k = \frac{\hbar^2\pi^2(2k)^2}{2mL^2}$$

$$k = 1,2,3...$$

→ Kronecker delta

2. Complete: Any function F(x) with a boundary condition F(L/2)=F(-L/2)=0 can be expanded as:

$$F(x) = \sum_k (c^{e}{}_{k}\varphi^{e}{}_{k}(x) + c^{o}{}_{k}\varphi^{o}{}_{k}(x))$$

$$c_k^{e,o} = \int_{-L/2}^{L/2} dxF(x)\varphi^{*e,o}{}_{k}(x)$$

Dirichlet's Theorem:
Fourier Series

3. General Solution:

$$\psi(x,t) = \sum_k (c^{e}{}_{k}\varphi^{e}{}_{k}(x)e^{-i\frac{\hbar\pi^2(2k-1)^2}{2mL^2}t} + c^{o}{}_{k}\varphi^{o}{}_{k}(x)e^{-i\frac{\hbar\pi^2(2k)^2}{2mL^2}t})$$

$$\sum_k (|c_k^e|^2 + |c_k^o|^2) = 1$$

$$<\hat{H}> = \sum_k (|c_k^e|^2 E^e_k + |c_k^o|^2\ E^o_k)$$

$|C_k|^2$: Describe the probability of the particle in the state k

Example

- A particle in the infinite square Well has the initial wave function,

$$\psi(x,0) = A(x-L/2)(x+L/2)$$

For some constant A. Find $\psi(x,t)$

Solution: $$\psi(x,t) = \sqrt{\frac{30}{L}}\left(\frac{2}{\pi}\right)^3 \sum_k \frac{1}{(2k-1)^3} \cos\left(\frac{(2k-1)\pi x}{L}\right) e^{-i\frac{\hbar\pi^2(2k-1)^2}{2mL^2}t}$$

General Properties of Wavefunction

- In general, eigenvalues of Hamiltonian is real.

- Wavefunctions with diffferent eigenvalues are orthogonal to each other

- Wavefunctions in the space is continous.

$$\rho(x,t)=|\psi(x,t)|^2$$

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

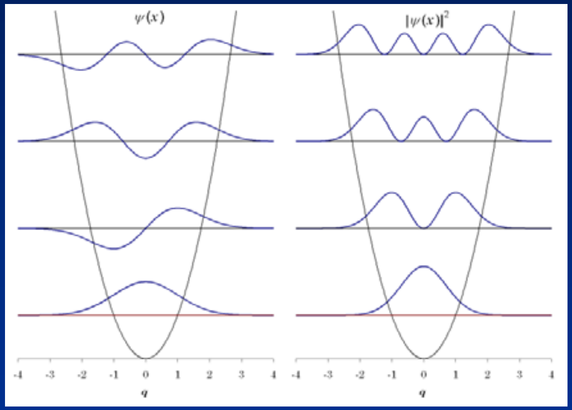
$$\frac{\partial\rho(x,t)}{\partial t}+\frac{\partial}{\partial x}J(x,t)=0$$

- The derivative of wavefunctions with respect to space is continuous if there is no singularity in potential energy.

Harmonic oscillator

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2$$

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



Classical solution:

$$m\omega^2 x = -m\frac{d^2x}{dt^2}$$

$$x(t) = A\sin(\omega t) + B\cos(\omega t)$$

- Most important quantum system
- Exact solvable
- Complex quantum system can be approximated by a combination of multi-Harmonic oscillators

Solution of Harmonic Oscillator

- Algebraic method:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2$$

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

Step1: Raising and Lowering operator:

$$\hat{a} = \frac{1}{\sqrt{2\hbar m\omega}}(i\hat{p} + m\omega\hat{x})$$

$$\hat{a}^{+} = \frac{1}{\sqrt{2\hbar m\omega}}(-i\hat{p} + m\omega\hat{x})$$

$$\Downarrow$$

$$\hat{H} = \hbar\omega(\hat{a}^{+}\hat{a} + 1/2)$$

Step2: if $\Psi(x)$ is an eigenstate with eigenvalue E,

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

$$\Downarrow$$

$$\hat{H}(\hat{a}^{+}\psi(x)) = (E + \hbar\omega)(\hat{a}^{+}\psi(x))$$

$$\hat{H}(\hat{a}\psi(x)) = (E - \hbar\omega)(\hat{a}\psi(x))$$

Step3: let $\Psi_g(x)$ be the ground state with eigenvalue E_g. $E_g>0$.

$$\hat{a}\psi_g(x) = 0$$

Step4: Solve:

$$\frac{1}{\sqrt{2\hbar m\omega}}(i\hbar\frac{\partial}{\partial x} + m\omega x)\psi_g(x) = 0$$

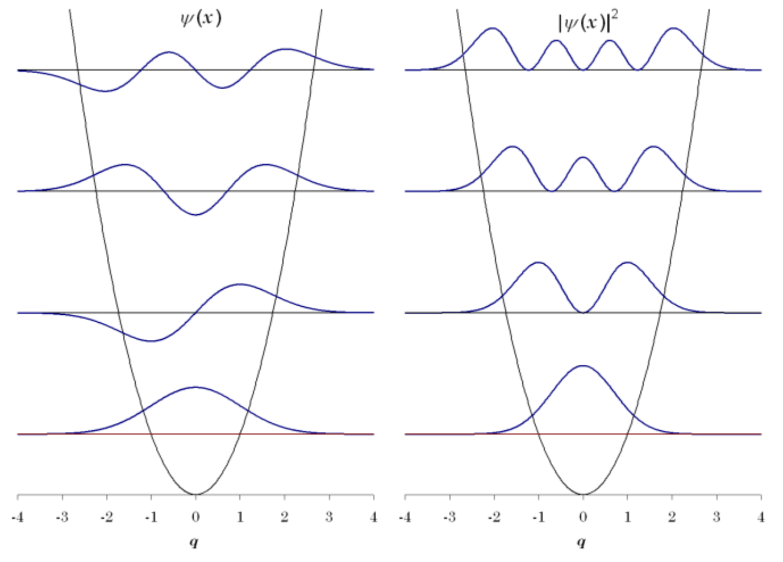
$$\psi_g(x) = (\frac{m\omega}{\hbar\pi})^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$$

$$\hat{H}\psi_g(x) = \frac{\hbar\omega}{2}\psi_g(x)$$

$$E_g = \frac{\hbar\omega}{2}$$

Solution of Harmonic Oscillator

- Step 5: Excited states:



$$\psi_g(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$$

$$\hat{H}\psi_g(x) = \frac{\hbar\omega}{2}\psi_g(x)$$

$$E_g = \frac{\hbar\omega}{2}$$

$$\hat{H}\psi_n(x) = \left(n + \frac{1}{2}\right)\hbar\omega\psi_n(x)$$

$$\psi_n(x) = \frac{1}{\sqrt{n!}}(\hat{a}^+)^n\psi_g(x)$$

$$\hat{a}\psi_n(x) = \sqrt{n}\psi_{n-1}(x)$$

$$\hat{a}^+\psi_n(x) = \sqrt{n+1}\psi_{n+1}(x)$$

Solution of Harmonic Oscillator (differenatial equations)

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2$$

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

- Define dimensionless variables:

$$\frac{\partial^2 \psi}{\partial \xi^2} = (\xi^2 - K)\psi$$

$$\xi = \sqrt{\frac{m\omega}{\hbar}}x$$

$$K = \frac{2E}{\hbar\omega}$$

- Consider the boundary condition (vanish at infinite)

$$\frac{\partial^2 \phi}{\partial \xi^2} - 2\xi\frac{d\phi}{d\xi} + (K-1)\phi = 0$$

$$\psi(\xi) = e^{-\xi^2/2}\phi(\xi)$$

$$\phi(\xi) = \sum_{j=0} c_j \xi^j$$

$$\psi_n(x) = (\frac{m\omega}{\hbar\pi})^{1/4}\frac{1}{\sqrt{2^n n!}}H_n(\xi)e^{-\frac{m\omega}{2\hbar}x^2}$$

$$H_0(x) = 1$$

$$H_1(x) = 2x$$

$$H_2(x) = 4x^2 - 2$$

$H_n(x)$: Hermite Polynomials