2/26/01

Lecture 20 Review

(1) The state of a particle is represented by a normalized vector $|\Psi\rangle$ in the Hilbert space $L_2(-\infty, \infty)$.

(2) The time developement of $|\Psi\rangle$ is given by

$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \hat{H} |\Psi\rangle$$

(3) Observable quantities $Q(x, p, t)$ are represented by Hermitian operators $\hat{Q}(\hat{x}, \hat{p}, t)$ with $[\hat{x}, \hat{p}] = i\hbar$

Expectation value of Q is $\langle \Psi | \hat{Q} \Psi \rangle$

(4) A measurement of an observable Q is certian to give one of the eigenvalues of $\hat{Q}$. The prob. of geting λ is

$$P_\lambda = |\langle e_\lambda | \Psi \rangle|^2$$

with $\hat{Q} |e_\lambda\rangle = \lambda |e_\lambda\rangle$

Solutions of Schrodinger eq. (Chap. 2)

Find set of eigenvectors (eigenfunctions) and eigenvalues for

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

$$\hat{H} |\Psi_n\rangle = E_n |\Psi_n\rangle$$

Solve Schrodinger eq

$$\frac{\partial \psi^2}{\partial x^2} = -k^2(x)\, \psi(x)$$

$$k^2(x) = 2m\left[E - V(x)\right]/\hbar^2$$

and adjust E to satisfy b.c.

Example $\psi \to 0$ as $x \to \pm\infty$
so wave function is normalizable.

Numerical solution of S. eq.
(See Computational Physics by S. Koonin
for example)

$$\frac{\partial \psi^2}{\partial x^2} \approx \frac{\psi(x+a) + \psi(x-a) - 2\psi(x)}{a^2}$$

For some small distance a

Note $\frac{\partial \psi}{\partial x} \approx \frac{\psi(x+a) - \psi(x)}{a}$

Chose symmetric difference

$$\left.\frac{\partial \psi}{\partial x}\right|_{x=x_0} \approx \frac{\psi(x_0+a) - \psi(x_0-a)}{2a}$$

$$\left.\frac{\partial^2 \psi}{\partial x^2}\right|_{x=x_0} \approx \left(\left.\frac{\partial \psi}{\partial x}\right|_{x_0+\frac{a}{2}} - \left.\frac{\partial \psi}{\partial x}\right|_{x_0-\frac{a}{2}}\right)\frac{1}{a}$$

$$= \frac{\psi(x_0+a) - \psi(x_0) - \left[\psi(x_0) - \psi(x_0-a)\right]}{a^2}$$

$$\frac{\partial^2 \psi}{\partial x^2} = \left[\psi(x_0+a) + \psi(x_0-a) - 2\psi(x_0)\right]/a^2$$

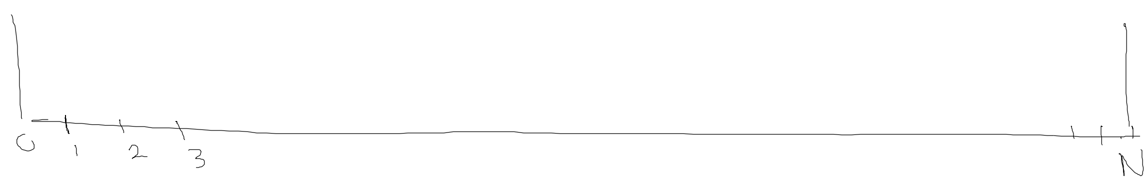
Chose a grid

$x_n = n a$ $\qquad$ $k_n^2 = 2m\left[E - V(x_n)\right]/\hbar^2$

$$\psi_{n+1} + \psi_{n-1} - 2\psi_n = -a^2 k_n \psi_n$$

Solve for ψ_{n+1}

$$\psi_{n+1} = \left[2 - a^2 k_n^2\right]\psi_n - \psi_{n-1}$$



$x_0 = 0$ $\qquad$ $x \longrightarrow$ $\qquad$ $x_N = Na$

Measure E and $V(x)$ in units of V_0

$$a^2 k_n^2 = \left(\frac{2 m a^2}{\hbar^2} V_0\right)\left[\frac{E}{V_0} - \frac{V(x_n)}{V_0}\right]$$

$$a^2 k_n^2 = \gamma\left(\frac{E}{V_0} - \frac{V(x_n)}{V_0}\right)$$

$\gamma \equiv \dfrac{2 m a^2}{\hbar^2} V_0$ $\qquad$ big γ small $\hbar$ classical like behavior

small γ (large $\hbar$) pronounced quantum behavior

Start at $x=0$ $\quad \psi_0 = 0 \quad \psi_1 = \epsilon$ any small #

Guess E

Integrate to find ψ_N

adjust E untill $\psi_N \approx 0$