Lecture 6

Thursday, September 26, 2024 11:30

Last lecture: three-dimensional, many-particle system.

$$\hat{H} = -\sum_{i=1}^{n} \frac{\hbar^2}{2m_i} \nabla_i^2 + V(x_1, y_1, \cdots, z_n)$$

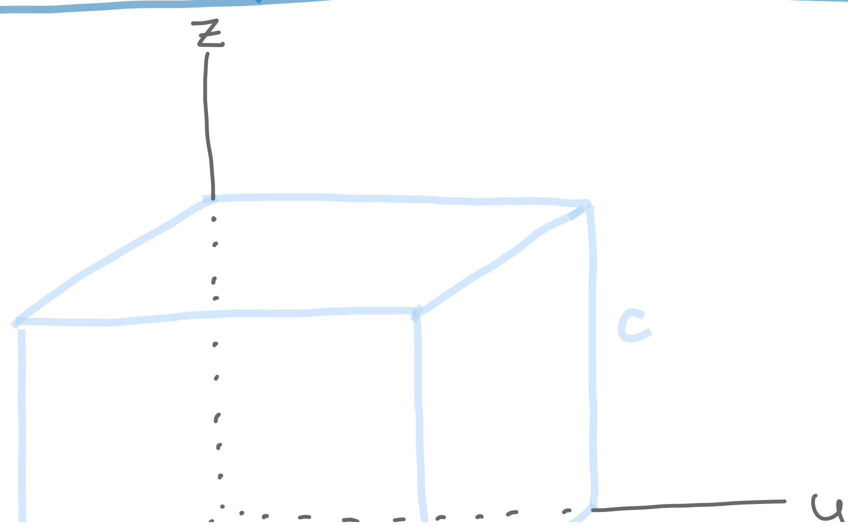
$$\left[-\sum_{i=1}^{n} \frac{\hbar^2}{2m_i} \nabla_i^2 + V(x_1, y_1, \cdots, z_n)\right]\psi = E\psi$$

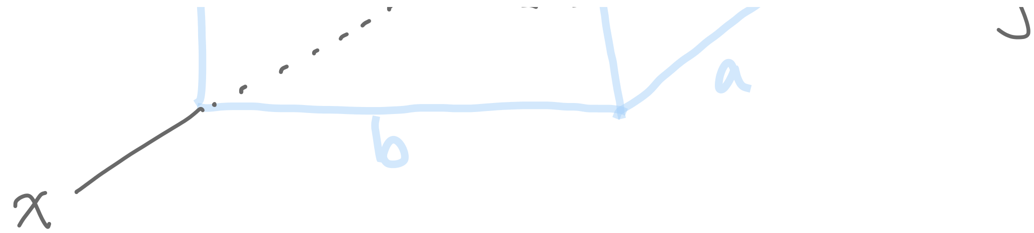
$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |\psi(x_1, y_1, \cdots, z_n)|^2 dx_1 dy_1 \cdots dz_n = 1$$

$$\boxed{\int |\psi|^2 d\tau = 1}$$

shorthand; definite integral

3.5 The Particle in a Three-Dimensional Box





$V(x, y, z) = 0$ in the region $\begin{cases} 0 < x < a \\ 0 < y < b \\ 0 < z < c \end{cases}$

$V = \infty$ elsewhere

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

Separation of variables :

$$\psi(x, y, z) = f(x)g(y)h(z)$$

so

$$\frac{\partial^2\psi}{\partial x^2} = f''(x)g(y)h(z)$$

$$\frac{\partial^2\psi}{\partial y^2} = f(x)g''(y)h(z)$$

$$\frac{\partial^2\psi}{\partial z^2} = f(x)g(y)h''(z)$$

$$-\frac{\hbar^2}{2m}f''gh - \frac{\hbar^2}{2m}fg''h - \frac{\hbar^2}{2m}fgh'' = Efgh$$

$$-\frac{\hbar^2}{2m}f''gh-\frac{\hbar^2}{2m}fg''h-\frac{\hbar^2}{2m}fgh''-Efgh=0$$

divide by fgh

$$\underbrace{\boxed{-\frac{\hbar^2 f''(x)}{2mf(x)}}}_{E_x}\underbrace{\boxed{-\frac{\hbar^2 g''(y)}{2mg(y)}}}_{E_y}\underbrace{\boxed{-\frac{\hbar^2 h''(z)}{2mh(z)}}}_{E_z}-E=0$$

$$\underbrace{-\frac{\hbar^2 f''(x)}{2mf(x)}}_{E_x}=\frac{\hbar^2 g''(y)}{2mg(y)}+\frac{\hbar^2 h''(z)}{2mh(z)}+E$$

$$E_x \equiv -\frac{\hbar^2 f''(x)}{2mf(x)}$$

E_x has to be a constant.

$$E_y \equiv -\frac{\hbar^2 g''(y)}{2mg(y)}$$

$$E_z \equiv -\frac{\hbar^2 h''(z)}{2mh(z)}$$

$$\boxed{E_x+E_y+E_z=E}$$

$$\frac{d^2 f(x)}{dx^2} + \frac{2m}{\hbar^2} E_x f(x) = 0$$

$$\frac{d^2 g(y)}{dy^2} + \frac{2m}{\hbar^2} E_y g(y) = 0$$

$$\frac{d^2 h(z)}{dz^2} + \frac{2m}{\hbar^2} E_z h(z) = 0$$

Use result from 1D PIAB; boundary conditions are slightly different, applied at $x = a$, $y = b$, and $z = c$.

$$f(x) = \left(\frac{2}{a}\right)^{\frac{1}{2}} \sin\left(\frac{n_x \pi x}{a}\right), \quad E_x = \frac{n_x^2 h^2}{8ma^2}$$

$$g(y) = \left(\frac{2}{b}\right)^{\frac{1}{2}} \sin\left(\frac{n_y \pi y}{b}\right), \quad E_y = \frac{n_y^2 h^2}{8mb^2}$$

$$h(z) = \left(\frac{2}{c}\right)^{\frac{1}{2}} \sin\left(\frac{n_z \pi z}{c}\right), \quad E_z = \frac{n_z^2 h^2}{8mc^2}$$

$n_x, n_y, n_z = 1, 2, 3, \ldots$

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

$$\Psi(x,y,z) = \left(\frac{8}{abc}\right)^{\frac{1}{2}} \sin\left(\frac{n_x \pi x}{a}\right) \sin\left(\frac{n_y \pi y}{b}\right) \sin\left(\frac{n_z \pi z}{c}\right)$$

$$\int_{-\infty}\int_{-\infty}\int_{-\infty} |\Psi|^2 \, dx\,dy\,dz = \int_0 |f(x)|^2 dx \int_0 |g(y)|^2 dy \cdot \int_0^c |h(z)|^2 dz = 1$$

Suppose we have a cubic box, so $a = b = c$. Then,

$$E = \frac{h^2}{8ma^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

$n_x n_y n_z$	111	211	121	112	122	212
$E(8ma^2/h^2)$	3	6	6	6	9	9

Degree of degeneracy: the number of states at a particular energy level.

Usually an effect of symmetry.

Average Values

$$\langle B \rangle = \frac{\sum_{j=1}^{N} b_j}{N}$$

$\langle B \rangle$: average value of B

$b_1, b_2, \ldots, b_N$: observed values

N : the number of systems

$$\langle B \rangle = \frac{\sum_{b} n_b b}{N}$$

1st expression :

$$\frac{1}{N}\sum_{j=1}^{N} b_j = \frac{0+20+20+60+60+80+80+100}{9}$$

$$= 56$$

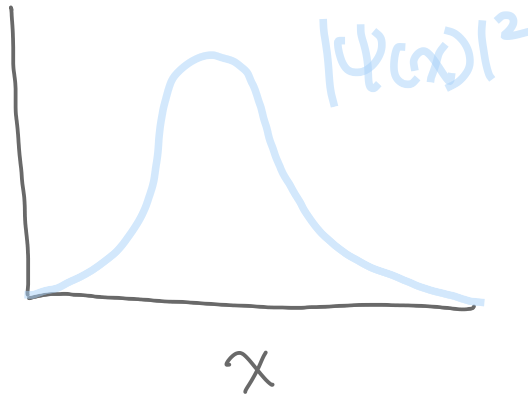
2nd expression :

$$\frac{1}{N}\sum_{b} n_b b = \frac{1(0)+2(20)+0(40)+2(60)+2(80)+1(100)}{9}$$

$$= 56$$

$$\langle B \rangle = \sum_b \left(\frac{n_b}{N}\right) b = \boxed{\sum_b P_b\, b}$$

probability of observing b



$$\langle x \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{x} \Psi \, dx$$

expected value for the x-coordinate of the particle

$$\langle B \rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \Psi^* \hat{B} \Psi \, dx\,dy\,dz$$

$$\boxed{\langle B \rangle = \int \Psi^* \hat{B} \Psi \, dZ}$$

expected value for $\hat{B}$

$$\langle A + B \rangle = \langle A \rangle + \langle B \rangle$$

$$\langle cB \rangle = c\langle B \rangle$$

$\langle AB \rangle \neq \langle A \rangle \langle B \rangle$

Chapter 4: The Harmonic Oscillator

$$\underbrace{y''(x)} + \underbrace{c^2 y(x)} = 0 \quad , \quad c^2 > 0$$

$$a^2 + c^2 = 0 \quad , \quad a = \pm ic$$

$$y = A\cos cx + B\sin cx$$

Power-Series Solution of Differential Equations

$$\boxed{y(x)} = \sum_{n=0}^{\infty} a_n x^n = a_0 + a_1 x + a_2 x^2 + \cdots$$

Differentiate term-by-term:

$$y'(x) = a_1 + 2a_2 x + 3a_3 x^2 + \cdots$$

$$= \sum_{n=1}^{\infty} n a_n x^{n-1}$$

$$\boxed{y''(x)} = 2a_2 + 3(2)a_3 x + (4)(3)a_4 x^2 + \cdots$$

$$= \sum_{n=2}^{\infty} n(n-1)a_n x^{n-2}$$

$$\boxed{\sum_{n=2}^{\infty} n(n-1)a_n x^{n-2} + \sum_{n=0}^{\infty} c^2 a_n x^n = 0}$$