Lecture 8

Wednesday, October 4, 2023 12:59

Particle in a three-dimensional box

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

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

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |\psi|^2 \, dx\, dy\, dz$$

$$= \int_0^a |f(x)|^2 dx \int_0^b |g(y)|^2 dy \int_0^c |h(z)|^2 dz$$

$$= 1$$

$$\boxed{\begin{aligned} &\iiint F(x)G(y)H(z)\,dx\,dy\,dz \\ &= \int F(x)\,dx \int G(y)\,dy \int H(z)\,dz \end{aligned}}$$

For a cubic box where $a=b=c$,

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

$n_x n_y n_z$	111	211	121	112	221	212	122
$E\,(8ma^2/h^2)$	3	6	6	6	9	9	9
	1		3			3	

degree of degeneracy : number of states with the same energy

3.6 Degeneracy

For an n-fold degenerate energy level, there are n independent wavefunctions $\psi_1, \psi_2, \ldots, \psi_n$, each with the same energy eigenvalue ω:

$$\boxed{\hat{H}\psi_1 = \omega\psi_1}, \quad \hat{H}\psi_2 = \omega\psi_2, \ldots, \hat{H}\psi_n = \omega\psi_n$$

Prove that every linear combination

$$\phi \equiv c_1\psi_1 + c_2\psi_2 + \cdots + c_n\psi_n$$

of ψ for a degenerate level with energy eigenvalue ω is an eigenfunction of the Hamiltonian operator with eigenvalue ω.

$$\hat{H}(c_1\psi_1 + c_2\psi_2 + \dots + c_n\psi_n)$$

$$= \omega(c_1\psi_1 + c_2\psi_2 + \dots + c_n\psi_n)$$

$$\hat{H}(c_1\psi_1 + c_2\psi_2 + \dots + c_n\psi_n)$$

$$= \hat{H}(c_1\psi_1) + \hat{H}(c_2\psi_2) + \dots + \hat{H}(c_n\psi_n)$$

$$= c_1\hat{H}\psi_1 + c_2\hat{H}\psi_2 + \dots + c_n\hat{H}\psi_n$$

$$= c_1\omega\psi_1 + c_2\omega\psi_2 + \dots + c_n\omega\psi_n$$

$$\boxed{\begin{aligned} &\therefore \hat{H}(c_1\psi_1 + c_2\psi_2 + \dots + c_n\psi_n) \\ &= \omega(c_1\psi_1 + c_2\psi_2 + \dots + c_n\psi_n) \end{aligned}}$$

3.7 Average Values

$$\langle B \rangle = \frac{\sum_{j=1}^{N} b_j}{N} \quad \leftarrow \text{needs to be large}$$

↑

average value of B

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

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

$$= 56$$

$$\boxed{\begin{aligned} \frac{1}{N}\sum_b n_b \, b &= \frac{1(0)+2(20)+0(40)+2(60)+3(80)+1(100)}{9} \\ &= 56 \end{aligned}}$$

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

if N is large, $\frac{n_b}{N}$ is the probability of observing b, and

$$\langle B \rangle = \sum_b p_b\, b$$

$$\boxed{\langle B(x,y,z) \rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi^* \hat{B} \psi \, dx\, dy\, dz}$$

In general,

$$B = B(x, y, z, p_x, p_y, p_z)$$

$$\boxed{\langle B \rangle = \int \psi^* \hat{B} \psi \, d\tau}$$

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

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

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

Practice

Find $\langle x \rangle$, $\langle p_x \rangle$, $\langle p_x^2 \rangle$ for the ground state for the particle in a three-dimensional box. $\psi = f(x)g(y)h(z)$

$$\langle x \rangle = \int \psi^* \hat{x} \psi \, d\tau$$

$$\langle x \rangle = \int_0^c \int_0^b \int_0^a f^* g^* h^* \hat{x} \, fgh \, dx\, dy\, dz$$

$$\langle x \rangle = \int_0^a x|f(x)|^2 dx \underbrace{\int_0^b |g(y)|^2 dy}_{1} \underbrace{\int_0^c |h(z)|^2 dz}_{1}$$

$$\langle x \rangle = \int_0^a x\,|f(x)|^2 \, dx$$

$$\langle x \rangle = \frac{2}{a} \int_0^a x \sin^2 \left(\underbrace{\boxed{\frac{\pi x}{a}}}_{b} \right) dx$$

Integral table

$$\int x \sin^2 bx \, dx = \frac{x^2}{4} - \frac{x}{4b} \sin(2bx) - \frac{1}{8b^2} \cos(2bx)$$

$$\langle x \rangle = \frac{2}{a} \left[\frac{x^2}{4} - \cancel{\frac{ax}{4\pi} \sin\left(\frac{2\pi x}{a}\right)} - \frac{a^2}{8\pi^2} \cos\underset{\uparrow\, 1}{\left(\frac{2\pi x}{a}\right)} \right]_0^a$$

$$\langle x \rangle = \frac{2}{a} \left[\frac{a^2}{4} - \cancel{\frac{a^2}{8\pi^2}} - \left(- \cancel{\frac{a^2}{8\pi^2}} \right) \right]$$

$$\boxed{\langle x \rangle = \frac{a}{2}}$$

$$\langle p_x \rangle = \int \psi^* \hat{p}_x \psi \, d\tau$$

$$= \int_0^c \int_0^b \int_0^a f^* g^* h^* \boxed{\frac{\hbar}{i} \frac{\partial}{\partial x}} f g h \, dx \, dy \, dz$$

$$= \frac{\hbar}{i} \int_0^a f(x) \frac{d}{dx} f(x) \, dx \underbrace{\int_0^b |g(y)|^2 dy}_{1} \underbrace{\int_0^c |h(z)|^2 dz}_{1}$$

$$\boxed{= \frac{\hbar}{i} \int_0^a f(x) f'(x) \, dx}$$

$$= \frac{\hbar}{i} \int_0^a \frac{d}{dx} \boxed{\frac{1}{2} \left[f(x) \right]^2} dx$$

$$= \frac{\hbar}{2i} f^2(x) \Big|^a \qquad \boxed{\frac{d}{dx} \frac{1}{2} f(x)^2}$$

0

$$\boxed{\begin{aligned} &= 2 \cdot \tfrac{1}{2} f(x) \cdot f'(x) \\ &= f(x) \cdot f'(x) \end{aligned}}$$

boundary conditions:

$$f(0) = 0$$

$$f(a) = 0$$

$$\boxed{\langle p_x \rangle = 0}$$

$$\langle p_x{}^2 \rangle = \int_0^c \int_0^b \int_0^a f^* g^* h^* \left(-\hbar^2 \frac{\partial^2}{\partial x^2}\right) fgh \, dx\, dy\, dz$$

$$\langle p_x{}^2 \rangle = -\hbar^2 \int_0^a f(x) \frac{d^2}{dx^2} f(x)\, dx$$

$$\boxed{\langle p_x{}^2 \rangle = -\hbar^2 \int_0^a f(x) f''(x)\, dx}$$

$$f(x) = \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{\pi x}{a}\right)$$

$$f'(x) = \left(\frac{2}{a}\right)^{1/2} \left(\frac{\pi}{a}\right) \cos\left(\frac{\pi x}{a}\right)$$

$$f''(x) = \left(\frac{2}{a}\right)^{1/2} \left(\frac{\pi^2}{a^2}\right) - \sin\left(\frac{\pi x}{a}\right)$$

a

$$\langle p_x^2 \rangle = \hbar^2 \left(\frac{2}{a}\right)\left(\frac{\pi^2}{a^2}\right) \int_0 \sin^2\left(\underbrace{\frac{\pi x}{a}}_{b}\right) dx$$

Integral table

$$\int \sin^2 bx \, dx = \frac{x}{2} - \frac{1}{4b}\sin(2bx)$$

$$\langle p_x^2 \rangle = \frac{2\pi^2\hbar^2}{a^3}\left[\frac{x}{2} - \frac{a}{4\pi}\sin\left(\frac{2\pi x}{a}\right)\right]_0^a$$

$$= \frac{2\pi^2\hbar^2}{a^3}\,\frac{a}{2}$$

$$\hbar = \frac{h}{2\pi}$$

$$= \frac{\cancel{2}\cancel{\pi^2} h^2 / 4\cancel{\pi^2}}{\cancel{2}a^2}$$

$$\hbar^2 = \frac{h^2}{4\pi^2}$$

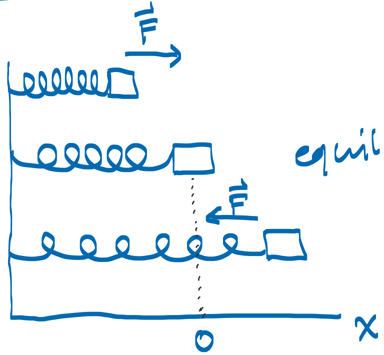
$$\boxed{\langle p_x^2 \rangle = \frac{h^2}{4a^2}}$$

$$T = \frac{p^2}{2m}$$

$$\frac{h^2}{8ma^2}$$

Chapter 4

4.2 The One-Dimensional Harmonic Osillator



$$F_x = -kx$$

k: force constant of spring

$$-kx = m\frac{d^2x}{dt^2} \qquad (F = ma)$$

$$\boxed{x = A\sin(2\pi\nu t + b)}$$

A: amplitude of the vibration

ν: vibration frequency

$$\boxed{\nu = \frac{1}{2\pi}\left(\frac{k}{m}\right)^{1/2}}$$

$$F_x = -\frac{\partial V}{\partial x}, \quad F_y = -\frac{\partial V}{\partial y}, \quad F_z = -\frac{\partial V}{\partial z}$$

$$F_x = -\frac{dV}{dx} = -kx$$

$$\frac{dV}{dx} = kx$$

$$\int dV = \int kx\,dx$$

$$V = \frac{1}{2}kx^2 + \underset{\underset{0}{\uparrow}}{C}$$

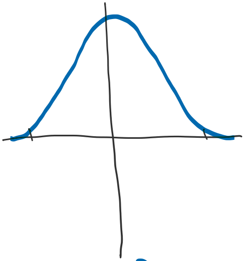
$$\boxed{V = \frac{1}{2}kx^2}$$

$$\boxed{V = 2\pi^2\nu^2 m x^2}$$

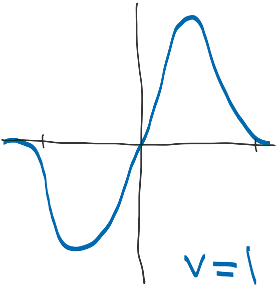
$$T = \frac{1}{2}m\left(\frac{dx}{dt}\right)^2$$

$$E = T + V = \frac{1}{2}kA^2 = 2\pi^2\nu^2 m A^2$$

Harmonic Oscillator Wavefunctions



v=0



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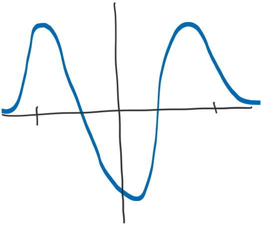
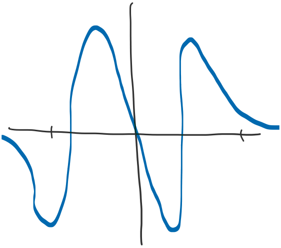


v=2



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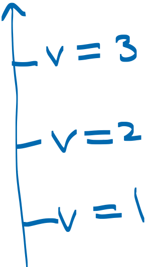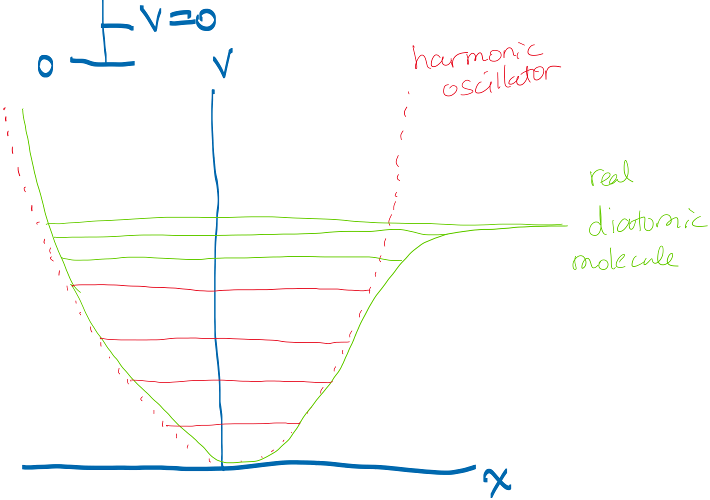$$\boxed{E=\left(v+\tfrac{1}{2}\right)h\nu\,,\quad v=0,1,2,\ldots}$$