Expectation value

$$\langle x \rangle = \frac{1}{N}\sum_{i=1}^{N} x_i$$

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L} \qquad \text{take } \frac{n\pi}{L} = a$$

$$\langle x \rangle = \int_0^L \psi_n^*(x)\, x\, \psi_n(x)\, dx$$

$$= \frac{2}{L}\int_0^L \sin(ax)\, x\, \sin ax \cdot dx = \int_0^L x \sin^2(ax)\, dx$$

$$= \frac{L}{2}$$

This result means that average of many measurements of the position of a particle in an infinite wall would be $x = \frac{L}{2}$'

Notice: Result is independent of 'n'

$\Rightarrow$ Symmetric about $L/2$

$$\langle p \rangle = \int_0^L \psi_n^*(x)\, p\, \psi_n\, dx$$

$$= \int_0^L \psi_n^*(x)\left\{-i\hbar\frac{d}{dx}\right\}\psi_n\, dx = \frac{-2i\hbar}{L}\int_0^L \sin(ax)\frac{d}{dx}\sin ax\, dx$$

$$= \frac{-i\hbar}{L}\left[\sin^2 ax\right]_0^L$$

$$= 0$$

$$\langle E \rangle = \int_0^L \psi_n^* H \psi_n\, dx \qquad H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

$$E = \frac{n^2 h^2}{8mL^2}$$

$\langle x^2 \rangle$, $\langle p^2 \rangle$ — . . . .

Q Using the trial function

$$\psi(x) = A(a^2 - x^2), \quad -a < x < a$$
$$= 0 \quad \text{otherwise}$$

The ground state energy of a one dimensional harmonic oscillator is

(a) $\hbar\omega$ (b) $\sqrt{\frac{5}{14}}\hbar\omega$ (c) $\frac{1}{2}\hbar\omega$ (d) $\sqrt{\frac{5}{7}}\hbar\omega$

Normalise wavefunction A

Obtain $\langle E \rangle$

Minimise $\frac{dE}{da} = 0$, find the value of a^2

Substitute the value of a^2 in $\langle E \rangle$.

$$\langle \psi | \psi \rangle = 1 \Rightarrow \int_{-a}^{a} \psi^* \psi = 1 = \int_{-a}^{a} A^* (a^2 - x^2)^* A (a^2 - x^2)\, dx$$

$$= A^2 \int_{-a}^{a} (a^2 - x^2)^2 dx = 1 \Rightarrow$$

$$\Rightarrow 2A^2 \int_0^a (a^2 - x^2)^2 dx = 1$$

$$\Rightarrow 2A^2 \int_0^a (a^4 + x^4 - 2a^2x^2)\, dx = 1$$

$$\Rightarrow 2A^2 \left[a^4 x + \frac{x^5}{5} - 2a^2 \frac{x^3}{3} \right]_0^a = 1$$

$$\Rightarrow 2A^2 \left[a^5 + \frac{a^5}{5} - \frac{2a^5}{3} \right] = 1$$

$$\Rightarrow 2A^2 a^5 \left[1 + \frac{1}{5} - \frac{2}{3} \right] = 1$$

$$A^2 = \frac{15}{16a^5} \Rightarrow \boxed{A = \sqrt{\frac{15}{16a^5}}}$$

$$\boxed{\psi = \sqrt{\frac{15}{16a^5}}\,(a^2 - x^2)} \quad -a < x < a$$

Energy of Harmonic Oscillator

$$\langle E \rangle = \langle \psi | H | \psi \rangle$$
$$= \langle \psi | T + V | \psi \rangle$$
$$= \langle \psi | T | \psi \rangle + \langle \psi | V | \psi \rangle$$

$$T = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

$$V = \frac{1}{2} m\omega^2 x^2$$

$$\langle E \rangle = \langle \psi | -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} | \psi \rangle + \langle \psi | \frac{1}{2} m\omega^2 x^2 | \psi \rangle$$

$$= -\frac{\hbar^2}{2m} \langle \psi | \frac{d^2}{dx^2} | \psi \rangle + \frac{1}{2} m\omega^2 \langle \psi | x^2 | \psi \rangle$$

Now the ϕ_n depends on variable parameter c_i ($i=1$

in ϕ_n

~~Substitute ϕ_n in~~ $\langle H \rangle = \int \psi_n^* H \psi_n \, d\tau$

Later $E_\phi \Rightarrow \frac{\partial E_\phi}{\partial c_i} = 0$ and ~~obtain~~ variable par

assume ϕ is normalised.

$$-\frac{\hbar^2}{2m}\langle\psi|\frac{d^2}{dx^2}|\psi\rangle$$

$$\langle\psi|\frac{d^2}{dx^2}|\psi\rangle = \int_{-a}^{a}\left(\psi^* \frac{d^2}{dx^2}\psi\right)dx = -\frac{5}{2}a^2$$

$$= \int_{-a}^{a}\sqrt{\frac{15}{16a^5}}(a^2-x^2)\frac{d^2}{dx^2}\sqrt{\frac{15}{16a^5}}(a^2-x^2)\,dx$$

$$= \frac{15}{16a^5}\int_{-a}^{a}(a^2-x^2)\frac{d^2}{dx^2}(a^2-x^2)\,dx$$

$$= \frac{15}{16a^5}\int_{-a}^{a}(a^2-x^2)(-2)\,dx = \frac{-30}{16a^5}\times 2\int_{0}^{a}(a^2-x^2)dx$$

$$= \frac{-60}{16a^5}\left[a^3-\frac{a^3}{3}\right] = \frac{-60}{16a^5}\times\frac{2a^3}{3}$$

$$= -\frac{20}{8}\frac{1}{a^2} = \boxed{\frac{-5}{2a^2}}$$

$$\Rightarrow \langle\psi|-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}|\psi\rangle = \frac{5\hbar^2}{4ma^2}$$

$$\langle\psi|x^2|\psi\rangle = \frac{15}{16a^5}\int_{-a}^{a}(a^2-x^2)\,x^2\,(a^2-x^2)\,dx$$

$$= \frac{15}{16a^5}\int_{-a}^{a}(a^2-x^2)x^2\,dx$$

$$= \frac{15}{16a^5}\int_{-a}^{a}(a^4x^2+x^6-2a^2x^4)dx$$

$$= \frac{15}{16a^5}\left[2\int_0^a \frac{a^7}{3}+\frac{a^7}{7}-\frac{2a^7}{5}\right]$$

$$= \frac{30}{16a^5}\,\frac{8}{3\times7\times5}\times a^7 = \frac{a^2}{7}$$

$$\therefore \frac{1}{2}m\omega^2\langle\psi|x^2|\psi\rangle = \frac{1}{2\times7}m\omega^2a^2 = \boxed{\frac{1}{14}m\omega^2a^2}$$

$$\langle E\rangle = \langle\psi|-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}|\psi\rangle + \langle\psi|\frac{1}{2}m\omega^2x^2|\psi\rangle$$

$$\langle E\rangle = \frac{5\hbar^2}{4ma^2}+\frac{1}{14}m\omega^2a^2$$

$\frac{dE}{da} = 0$, find a^2

$$\langle E \rangle = \frac{5\hbar^2}{4ma^2} + \frac{1}{14} m\omega^2 a^2$$

$$\frac{dE}{da} = \frac{5\hbar^2}{4m}(-2)a^{-3} + \frac{1}{14} m\omega^2 \, 2a = 0$$

$$= -\frac{10\hbar^2}{4ma^3} + \frac{1}{14} m\omega^2 \times 2a$$

$$\Rightarrow \frac{10\hbar^2}{4ma^3} = \frac{m\omega^2 a}{7}$$

$$= \frac{10 \times 7}{4m^2\omega^2}\hbar^2 = a^4$$

$$\Rightarrow a^4 = \frac{35}{2}\frac{\hbar^2}{m\omega^2}$$

$$\boxed{a^2 = \sqrt{\frac{35}{2}}\,\frac{\hbar}{m\omega}}$$

$$\langle E \rangle = \frac{5}{4}\frac{\hbar^2}{ma^2} + \frac{1}{14} m\omega^2 a^2$$

$$= \frac{5}{4}\frac{\hbar^{\cancel{2}}}{\cancel{m}} \cdot \frac{\cancel{m}\omega}{\cancel{\hbar}}\sqrt{\frac{2}{35}} + \frac{1}{14}\cancel{m}\omega^2\sqrt{\frac{35}{2}} \cdot \frac{\hbar}{\cancel{m}\omega}$$

$$= \frac{5}{4}\sqrt{\frac{2}{35}}\,\hbar\omega + \frac{1}{14}\sqrt{\frac{35}{2}}\Big]$$

$$= \left[\sqrt{\frac{5}{14\times 4}} + \sqrt{\frac{5}{14\times 4}}\right]\hbar\omega$$

$$= 2\sqrt{\frac{5}{14\times 4}}\,\hbar\omega.$$

$$= \sqrt{\frac{5}{14}}\,\hbar\omega$$

The Variational Method

* To evaluate the energy of the ground state.
* Unknown Wavefunctions.

Basic Principle

$\Psi_n =$ Set of Eigen functions of H.

$$H\Psi_n = E\Psi_n$$

$$\Phi = \sum_n a_n \Psi_n \Rightarrow \langle H \rangle = \int \Psi_n^* H \Psi_n \, d\tau = E_n$$

$|\Phi\rangle$

if Ψ_n is normalised.

$$E_\phi = \frac{\int \Phi^* H \phi \, d\tau}{\int \phi^* \phi \, d\tau} = \frac{\langle \phi | H | \Phi \rangle}{\langle \phi | \Phi \rangle}$$

We have to prove that E_ϕ is always greater than E_0 - Ground state energy or the lowest of spectrum E_n.

Scalar Product of with bra $\langle \phi |$ and $H|\phi\rangle$ will be an extremum.

$$E_\phi = \frac{\int \left(\sum a_n^* \Psi_n^* H \sum a_n \Psi_n\right) d\tau}{\int \left(\sum a_n^* \Psi_n^*\right)\left(\sum a_n \Psi_n\right) \cdot d\tau} = \frac{\sum a_n^* a_n E_n}{\sum a_n^* a_n}$$

$$\int \Psi_n^* \Psi_m \, d\tau = \delta_{mn} = 1 \text{ if } m = n \text{ Otherwise zero}$$

$$\therefore E_\phi - E_0 = \frac{\sum |a_n|^2 (E_n - E_0)}{\sum |a_n|^2}$$

Now $E_n \geq E_0$ and $|a_n|^2 \geq 0$ for all n

$$\Rightarrow E_\phi \geq E_0$$