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## Variational method of Approximation →

By this we estimate ground state energy for systems for which $\hat{H}$ is known but wave function are unknown.

$$\boxed{E_{gs} \simeq \langle H_{min} \rangle}$$

$E_g \le \langle H \rangle$ ↳ Principle

Here

$$\langle H \rangle = \langle \psi | \hat{H} | \psi \rangle$$

$|\psi\rangle$ = Normalized trial wave function

- $|\psi\rangle$ trial wave function should be acceptable quantum mechanically.
  Means $|\psi\rangle$ & its first order derivative should be finite, continious and differentiable everywhere
- $|\psi\rangle$ should be square integrable and it should vanish as $x \to \pm\infty$
- In trial wave function there is a parameter (adjustable parameter)

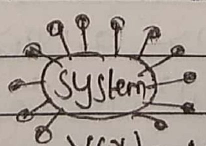
$\psi(x) = A e^{-bx^2}$ → trial wave function → Not exact.

$A$ = Normalization constant

$b$ = Adjustable parameter

→ The best value of adjustabe parameter will give an approximate ground state wave function.

Story :) behind —




$V(x)$ → given

$\hat{H} = \hat{T} + \hat{V}$ → known

$E_{gs} = ?$ → SE solve XXXXX

Best way —

✓ $E_{gs} \simeq \langle \psi | \hat{H} | \psi \rangle_{min}$

$|\psi\rangle$ → arbitrary → make it exact

$\boxed{|\psi\rangle = A e^{-bx^2}}$ ⇒ $b$ = adjustable par. ↳ Best value.

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## Format of Problem Asked in CSIR Net & Working Procedure :—

Variational method of approximation — $E_{gs} \approx \langle \hat{H} \rangle_{min}$

Question ⇒ $V(x)$ = given also, $\hat{H} = \hat{T} + \hat{V}$ → given

trial wave function ⇒ given ⇒ $|\psi\rangle$

$E_{gs} = ?$ → Best value of parameter = ?

1stly finding ⟶ $\langle \hat{H} \rangle = \langle \psi | \hat{H} | \psi \rangle$

$$\langle \hat{H} \rangle = \langle \hat{T} \rangle + \langle \hat{V} \rangle$$

Step-1. Normalized trial wave function

eg:— $\psi(x) = A e^{-bx^2}$ $\langle \psi | \psi \rangle = 1$

$A = \left(\frac{2b}{\pi}\right)^{1/4}$ → After calculation

Step:-2 find expectation value of $\hat{H}$ ie $\langle \hat{H} \rangle$

- $\langle \hat{T} \rangle$
- $\langle \hat{V} \rangle$
- $\langle \hat{H} \rangle = \langle \hat{T} \rangle + \langle \hat{V} \rangle$

Step-3

minimise $\langle \hat{H} \rangle$ wrt adjustable parameter (b)

⟶ $\frac{d\langle \hat{H} \rangle}{db} = 0$ $b = b_1, b_2$

⟶ $\left.\frac{d^2 \langle \hat{H} \rangle}{db^2}\right|_{b=b_1} = (+)ve$

⟶ $b = b_1$ best value of adjustable parameter

⇒ $E_{gs} \approx \langle \hat{H} \rangle \big|_{b=b_1} = \langle H \rangle_{min}.$

Que: Estimate ground state energy for a particle moving under potential $V(x) = \frac{1}{2}m\omega^2x^2$ using gaussian wave function as trial wavefunction and find best value of adjustable parameter.

Soln:

Concept :- Gaussian trial wavefunction (1-D) :-

$$\psi(x) = A e^{-bx^2}$$

$$A = \left(\frac{2b}{\pi}\right)^{1/4}$$

$$\langle \hat{T} \rangle = \frac{\hbar^2 b}{2m}$$

Remember it

Gaussian trial wave.function (3D) :-

$$\psi(r) = A e^{-br^2}$$

$$A = \left[\frac{2b}{\pi}\right]^{3/4}$$

$$\langle \hat{T} \rangle = \frac{3\hbar^2 b}{2m}$$

Remember it

Solution: given that — $V(x) = \frac{1}{2}m\omega^2x^2$ also

$$\psi(x) = A.e^{-bx^2}$$

$$A = \left(\frac{2b}{\pi}\right)^{1/4} \text{ (याद रखो)}$$

$$\langle \hat{H} \rangle = \langle \hat{T} \rangle + \langle \hat{V} \rangle$$

$$\langle \hat{T} \rangle = \frac{\hbar^2 b}{2m} \text{ (याद रखो)}$$

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$$\langle \hat{V} \rangle = \langle \psi | V | \psi \rangle$$

$$= \frac{1}{2} m\omega^2 \times |A|^2 \int_{-\infty}^{+\infty} e^{-2bx^2} \cdot x^2 \cdot dx$$

$$= \frac{1}{\cancel{2}} m\omega^2 \times \left(\frac{2b}{\pi}\right)^{1/2} \cdot \cancel{2} \int_0^{\infty} e^{-2bx^2} \cdot x^2 \cdot dx$$

<u>Note</u> — $\int_0^{\infty} x^m \cdot e^{-\alpha x^n} \cdot dx = \frac{1}{n} \frac{\Gamma\frac{m+1}{n}}{(\alpha)^{\frac{m+1}{n}}}$

$$\Rightarrow (m\omega^2)\left(\frac{2b}{\pi}\right)^{1/2} \times \frac{1}{2} \frac{\Gamma 3/2}{(2b)^{3/2}}$$

$\Gamma 3/2 = \frac{1}{2} \Gamma 1/2$
$\Rightarrow \frac{1}{2}\sqrt{\pi}$

$$\Rightarrow (m\omega^2) \times \frac{(2b)^{1/2}}{\cancel{\sqrt{\pi}}} \times \frac{\frac{1}{2} \times \cancel{\sqrt{\pi}}}{(2b)^{3/2}}$$

$$\langle \hat{V} \rangle = \frac{m\omega^2}{4(2b)} = \frac{m\omega^2}{8b}$$

$$\Rightarrow \langle \hat{H} \rangle = \frac{\hbar^2 b}{2m} + \frac{m\omega^2}{8b}$$

<u>Now</u>

$$\frac{d\langle \hat{H} \rangle}{db} = \frac{\hbar^2}{2m} + \frac{m\omega^2}{8}\left(\frac{-1}{b^2}\right) = 0$$

$$\frac{\hbar^2}{2m} - \frac{m\omega^2}{8b^2} = 0$$

$$\Rightarrow \frac{m\omega^2}{\cancel{4}8b^2} = \frac{\hbar^2}{\cancel{2}m}$$

$$b^2 = \frac{m^2\omega^2}{4\hbar^2}$$

$$b = \pm \frac{m\omega}{2\hbar}$$

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$$\psi(x) = \frac{1}{\sqrt{2^n n! \pi x_0}} \times e^{-\frac{x^2}{x_0^2}} H_n\left(\frac{x}{x_0}\right)$$



$$b = \pm \frac{m\omega}{2\hbar}$$

$$b_1 = \frac{m\omega}{2\hbar} \qquad b_2 = -\frac{m\omega}{2\hbar}$$

$$\frac{d^2\langle \hat{H} \rangle}{db^2} = -\frac{m\omega^2}{8}\left(\frac{-2}{b^3}\right) = \frac{m\omega^2}{4b^3}$$

$$\left\langle \frac{d^2\langle H\rangle}{db^2} \right|_{b=b_1} = (+)ve$$

$$\left.\frac{d^2\langle H\rangle}{db^2}\right|_{b=b_2} = (-ve)$$

At $b = b_1$ $\langle H \rangle$ is minimum

$\Rightarrow$ Best value of adjustabe parameter $(b_1) \Rightarrow$

$$b_1 = \frac{m\omega}{2\hbar}$$

$$\Rightarrow \quad E_{gs} = \langle H \rangle \Big|_{b=b_1}$$

$$E_{gs} = \langle H \rangle_{min} = \frac{\hbar^2 b}{2m} + \frac{m\omega^2}{8b} \qquad b = \frac{m\omega}{2\hbar}$$

$$\Rightarrow E_{gs} = \frac{\hbar^2}{2m}\left(\frac{m\omega}{2\hbar}\right) + \frac{m\omega^2 \times 2\hbar}{8 \times m\omega}$$

$$E_{gs} = \frac{\hbar\omega}{4} + \frac{\hbar\omega}{4} = \frac{1}{2}\hbar\omega$$

$$\boxed{E_{gs} \simeq 1/2\, \hbar\omega}$$ also we know for H.O.

$E = 1/2\, \hbar\omega$.

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