* VARIATIONAL PRINCIPLE

→ The variational principle gets to the upper bound for the ground energy state E_{gs} for a system described by the Hamiltonian H

For any normalised function ψ

$$E_{gs} \leq \langle \psi | H | \psi \rangle \equiv \langle H \rangle \quad \cdots \quad (1)$$

→ The expectation value of H in the state ψ is certa[in] to overestimate the ground state energy.

→ Since the unknown eigenfunctions of H form a complete set, ψ can be expressed as.

$$\psi = \sum_n c_n \psi_n \qquad \text{with } H\psi_n = E_n \psi_n .$$

Since ψ is normalised,

$$1 = \langle \psi | \psi \rangle = \left\langle \sum_m c_m \psi_m \middle| \sum_n c_n \psi_n \right\rangle$$

$$= \sum_m \sum_n c_m^* c_n \langle \psi_m | \psi_n \rangle = \sum_n |c_n|^2 .$$

$$\langle H \rangle = \left\langle \sum_m c_m \psi_m \middle| H \sum_n c_n \psi_n \right\rangle = \sum_m \sum_n c_m^* E_n c_n \langle \psi_m | \psi_n \rangle$$

$$= \sum_n E_n |c_n|^2 .$$

But the ground state energy is the smallest eigenvalu[e]
So $E_{gs} \leq E_n$. Hence

$$\boxed{\langle H \rangle \geq E_{gs} \sum_n |c_n|^2 = E_{gs} .}$$

EXAMPLE: Suppose we want to find the ground state energy for the one dimensional harmonic oscillator

$$H = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$$

$$\Psi(x) = Ae^{-bx^2}, \quad b = \text{constant}$$
A = determined by normalization

$$1 = |A|^2 \int_{-\infty}^{+\infty} e^{-2bx^2}\,dx = |A|^2\sqrt{\frac{\pi}{2b}} \Rightarrow A = \left(\frac{2b}{\pi}\right)^{1/4}.$$

Now $\langle H\rangle = \langle T\rangle + \langle V\rangle$.
where
$$\langle T\rangle = \frac{-\hbar^2}{2m}|A|^2 \int_{-\infty}^{+\infty} e^{-bx^2}\frac{d^2}{dx^2}\left(e^{-bx^2}\right)dx$$
$$= \frac{\hbar^2 b}{2m}.$$

$$\langle V\rangle = \frac{1}{2}m\omega^2|A|^2\int_{-\infty}^{+\infty} e^{-2bx^2}x^2\,dx = \frac{m\omega^2}{8b}$$

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

According to equation(1), this exceeds E_{gs} for any b to get the tightest bound.

To minimize $\langle H\rangle$:
$$\frac{d}{db}\langle H\rangle = \frac{\hbar^2}{2m} - \frac{m\omega^2}{8b^2} = 0 \Rightarrow b = \frac{m\omega}{2\hbar}$$

Putting this back into $\langle H\rangle$,
$$\boxed{\langle H\rangle_{min} = \frac{1}{2}\hbar\omega.}$$

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Suppose for the ground state energy of the delta function potential:

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \alpha\,\delta(x).$$

Using a Gaussian trial function,

$$\langle V\rangle = -\alpha|A|^2\int_{-\infty}^{\infty} e^{-2bx^2}\delta(x)\,dx = -\alpha\sqrt{\frac{2b}{\pi}}.$$

$$\langle H\rangle = \frac{\hbar^2 b}{2m} - \alpha\sqrt{\frac{2b}{\pi}}$$ this exceeds E_{gs} for all b.

After minimizing it

$$\frac{d}{db}\langle H\rangle = \frac{\hbar^2}{2m} - \frac{\alpha}{\sqrt{2\pi b}} = 0 \Rightarrow b = \frac{2m^2\alpha^2}{\pi\hbar^4}.$$

So $\langle H\rangle_{min} = \frac{-m\alpha^2}{\pi\hbar^2}$. It higher than E_{gs} since $\pi > 2$.

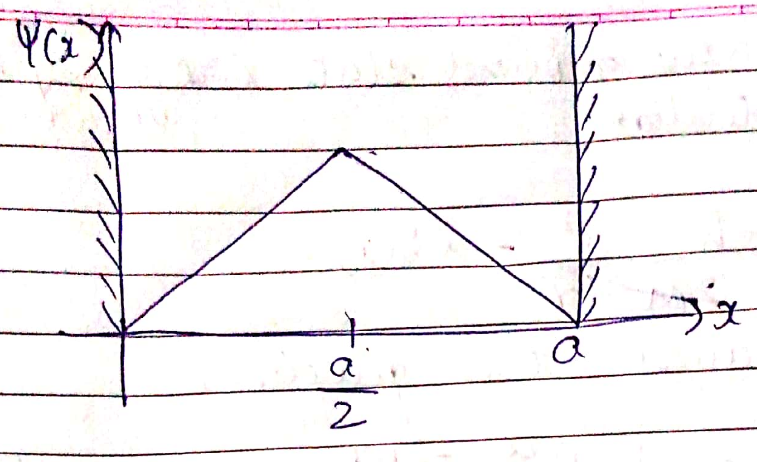
EXAMPLE: Find an upper bound on the ground state energy of the one-dimensional infinite square well using "triangular" trial wave function.

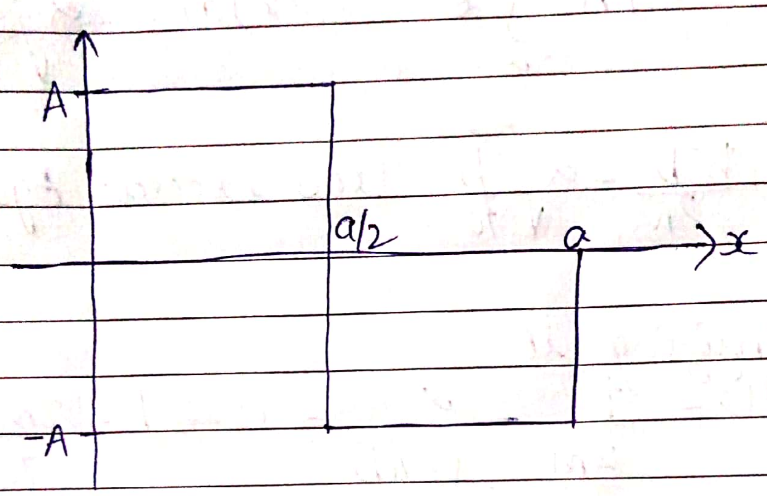
$$\psi(x) = \begin{cases} Ax & \text{if } 0 \le x \le a/2. \\ A(a-x) & \text{if } a/2 \le x \le a. \\ 0 & \text{otherwise.} \end{cases}$$

where A is determined by normalisation.

$$1 = |A|^2\left[\int_0^{a/2} x^2\,dx + \int_{a/2}^{a}(a-x)^2\,dx\right]$$

$$= |A|^2\frac{a^3}{12} \Rightarrow A = \frac{2}{a}\sqrt{\frac{3}{a}}$$





In this case $\frac{d\psi}{dx} = \begin{cases} A & \text{if } 0 < x < a/2 \\ -A & \text{if } a/2 < x < a \\ 0 & \text{otherwise.} \end{cases}$

The derivative of a step function is

$$\frac{d^2\psi}{dx^2} = A\delta(x) - 2A\delta(x - a/2) + \delta(x-a)\,\psi(x)dx.$$

and hence

$$\langle H \rangle = -\frac{\hbar^2 A}{2m}\int [\delta(x) - 2\delta(x-a/2) + \delta(x-a)]\,\psi(x)dx.$$

$$= \frac{-\hbar^2 A}{2m}\left[\psi(0) - 2\psi(a/2)\right] = \frac{\hbar^2 A^2 a}{2m}$$

$$= \frac{12\hbar^2}{2ma^2}.$$

The exact ground state energy is $E_{gs} = \frac{\pi^2\hbar^2}{2ma^2}$, so the theorem works