Lecture 16

The variational principle

The variational principle let you get un upper bound for the ground state energy when you can not directly solve the Schrödinger's equation.

How does it work?

(1) Pick any normalized function ψ .

(2) The ground state energy E_{gs} is

$$\boxed{E_{gs} \leq \langle \psi | H | \psi \rangle \equiv \langle H \rangle}$$

3) Some choices of the trial function ψ will get your E_{gs} that is close to actual value.

Proof

$H\psi_n = E_n \psi_n$ but you don't know how to get ψ_n

Still, your can expand your function ψ as

$$\psi = \sum_n c_n \psi_n .$$

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

$$= \sum_m \sum_n c_m^* c_n \delta_{mn} = \sum_n |c_n|^2$$

$$\langle H \rangle = \Big\langle \underbrace{\sum_m c_m \psi_m}_{\psi} \Big| H \underbrace{\sum_n c_n \psi_n}_{\psi} \Big\rangle =$$

$$= \sum_m \sum_n \langle c_m \psi_m | c_n \underbrace{E_n \psi_n} \rangle = \sum_m \sum_n c_m^* c_n E_n \langle \psi_m | \psi_n \rangle$$

since $H\psi_n = E_n \psi_n$

$$= \sum_m \sum_n c_m^* c_n E_n \delta_{mn} = \sum_n E_n |c_n|^2$$

But $E_{gs} \leq E_n$ since the ground state has the lowest eigenvalue.

Therefore,

$$\langle \psi | H | \psi \rangle = \sum_n E_n |c_n|^2 \geqslant E_{gs} \underbrace{\sum_n |c_n|^2}_{=1} \Rightarrow$$

$$\boxed{\langle \psi | H | \psi \rangle \geqslant E_{gs}}$$

QED

Example 1

Get an upper bound for the ground state energy of the 1D harmonic oscillator

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

using a trial function

$$\psi(x) = A e^{-bx^2} \quad \text{(Gaussian)},$$

where b is a constant and A is determined from normalization condition.

Solution:

First, let's normalize our trial function:

$$\boxed{\int_0^\infty x^{2n} e^{-x^2/a^2} dx = \sqrt{\pi}\frac{(2n)!}{n!}\left(\frac{a}{2}\right)^{2n+1}}$$

Class exercise (normalize the trial function):

$$\langle\psi|\psi\rangle = 1 = |A|^2 \int_{-\infty}^{\infty} e^{-2bx^2} dx = 2|A|^2 \int_0^\infty e^{-2bx^2} dx$$

$$[n=0, \; a = \sqrt{1/2b}\,]$$

$$\langle\psi|\psi\rangle = \cancel{2}|A|^2 \sqrt{\pi}\frac{1}{\sqrt{2b}}\frac{1}{\cancel{2}} = \left(\frac{\pi}{2b}\right)^{1/2}|A|^2 = 1$$

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

Next, we need to calculate

$$\langle\psi|H|\psi\rangle$$

to get upper bound for E_{gs}.

$$\langle H \rangle = \langle T \rangle + \langle V \rangle$$

$$\langle T \rangle = -\frac{\hbar^2}{2m}|A|^2 \int_{-\infty}^{\infty} e^{-bx^2} \frac{d^2}{dx^2}\left(e^{-bx^2}\right) dx$$

$$= -\frac{\hbar^2}{2m}|A|^2 \int_{-\infty}^{\infty} e^{-bx^2} (-b)\cdot 2 \; \frac{d}{dx}\left(e^{-bx^2} x\right) dx$$

$$= 2b\frac{\hbar^2}{2m}\left(\frac{2b}{\pi}\right)^{1/2} \int_{-\infty}^{\infty} e^{-bx^2} \left\{ e^{-bx^2}(-2bx^2) + e^{-bx^2} \right\} dx$$

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

$$\left. + \underbrace{\int_0^{\infty} e^{-2bx^2} dx}_{\frac{1}{2}\sqrt{\frac{\pi}{2b}}} \right\} = 4b\frac{\hbar^2}{2m}\frac{\cancel{\sqrt{2b}}}{\cancel{\sqrt{\pi}}}\left\{ -\cancel{2b}\,\frac{1}{4}\,\frac{1}{\cancel{2b}}\sqrt{\frac{\cancel{\pi}}{\cancel{2b}}} + \frac{1}{2}\sqrt{\frac{\cancel{\pi}}{\cancel{2b}}} \right\}$$

$$= 4b\frac{\hbar^2}{2m}\left\{ -\frac{1}{4} + \frac{1}{2} \right\} = \boxed{\frac{\hbar^2 b}{2m}}$$

$$\int_0^{\infty} x^2 e^{-2bx^2} dx = \sqrt{\pi}\;\frac{2}{1}\left(\frac{1}{\sqrt{2b}}\,\frac{1}{2}\right)^3 = \frac{1}{4}\,\frac{1}{2b}\sqrt{\frac{\pi}{2b}} \qquad n = 1 \quad a = \frac{1}{\sqrt{2b}}$$

$$\int_0^{\infty} x^{2n} e^{-x^2/a^2} dx = \sqrt{\pi}\,\frac{(2n)!}{n!}\left(\frac{a}{2}\right)^{2n+1}$$

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

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

$$= \frac{1}{2} m\omega^2 \cancel{\sqrt{\frac{2b}{\pi}}} \frac{1}{4b} \cancel{\sqrt{\frac{\pi}{2b}}} = \frac{m\omega^2}{8b} \Rightarrow$$

$$\langle H \rangle = \langle T \rangle + \langle V \rangle$$

Eq. (1) $\quad \langle H \rangle = \frac{\hbar^2 b}{2m} + \frac{m\omega^2}{8b} \geq E_{gs}$ for <u>any</u> $b \Rightarrow$

We can get lowest bound by minimizing this expression:

$$\frac{d}{db}\langle H \rangle = \frac{d}{db}\left\{ \frac{\hbar^2 b}{2m} + \frac{m\omega^2}{8b} \right\}$$

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

$$\frac{\hbar^2}{2m} = \frac{m\omega^2}{8b^2} \qquad b^2 = \frac{m^2\omega^2}{4\hbar^2} \qquad \boxed{b = \frac{m\omega}{2\hbar}}$$

We now plug $\quad b = \frac{m\omega}{2b} \quad$ into our Eq. (1) to get

$$\langle H \rangle = \frac{\hbar^2 b}{2m} + \frac{m\omega^2}{8b} = \frac{\hbar^{\cancel{2}}\, \cancel{m}\omega}{2\cancel{\hbar}\cdot 2\cancel{m}} + \frac{\cancel{m}\,\omega^{\cancel{2}}\, \cancel{2}\hbar}{4\,\cancel{8}\,\cancel{m}\cancel{\omega}} = \boxed{\frac{\hbar\omega}{2}}$$

Class exercise:

Find the best upper bound for the ground state energy of the delta-function potential

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

using gaussian function:

$$\psi(x) = \left(\frac{2b}{\pi}\right)^{1/4} e^{-bx^2}.$$

Solution:

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

$$\langle V \rangle = -\alpha\left(\frac{2b}{\pi}\right)^{1/2}\int_{-\infty}^{\infty} e^{-2bx^2}\,\delta(x)\,dx$$

$$= -\alpha\sqrt{\frac{2b}{\pi}}$$

$$\langle H \rangle = \frac{\hbar^2 b}{2m} - \alpha\sqrt{\frac{2b}{\pi}}$$

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

$$\frac{\hbar^4}{4m^2} = \frac{\alpha^2}{2b\pi} \qquad b = \frac{\alpha^2}{2\pi}\frac{4m^2}{\hbar^4} = \frac{2m^2\alpha^2}{\pi\hbar^4}$$

$$\langle H \rangle = \frac{\cancel{\hbar^2}\,\cancel{2}m^{\cancel{2}}\alpha^2}{\pi\hbar^{\cancel{4}\,2}\,\cancel{2m}} - \alpha\sqrt{\frac{2\cdot 2m^2\alpha^2}{\pi^2\hbar^4}} = \frac{\alpha^2 m}{\pi\hbar^2} - \frac{\alpha^2 2m^2}{\pi\hbar^2}$$

$$\langle H \rangle_{min} = -\frac{m\alpha^2}{\pi\hbar^2} \geq E_{gs}$$