Lecture 21

Chapter 7 - Variational Principle

Perturbation theory is one way to handle a system we can't solve exactly

Other main way is variational theory

Idea is very simple:

Suppose Hamiltonian H, ground state energy E_{gs}

Then for any state ψ, have $\langle\psi|H|\psi\rangle \geq E_{gs}$

Proof: Suppose eigenstates ψ_n

write $\psi = \sum_n c_n \psi_n$

Then $\langle\psi|H|\psi\rangle = \sum_n |c_n|^2 E_n \leq E_{gs} \sum_n |c_n|^2 = E_{gs}$

since $E_n \geq E_{gs}$ always

What use is that?

For ψ, use guess for gs. wave function

Let ψ depend on one or more parameters

Vary parameters to make $\langle\psi|H|\psi\rangle$ as low as possible

- makes ψ as close to ψ_{gs} as possible

Easiest to see with examples

Start with one we know:

Try to find ground state of harmonic oscillator

$H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2$

Guess $\psi = A e^{-bx^2}$ (know that's a good guess)

Need to normalize: $\int |\psi|^2 dx = A^2 \int_{-\infty}^{\infty} e^{-2bx^2} dx = |A|^2 \sqrt{\frac{\pi}{2b}} = 1$

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

Then $\langle H \rangle = \int \psi^* \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2 \right] \psi \, dx$

$\frac{d}{dx} \psi = -2bx A e^{-bx^2}$

$\frac{d^2}{dx^2} \psi = -2b A e^{-bx^2} + 4b^2 x^2 A e^{-bx^2}$

$\langle H \rangle = \sqrt{\frac{2b}{\pi}} \int e^{-2bx^2} \left[\frac{\hbar^2}{m} b - 2\frac{\hbar^2}{m} b^2 x^2 + \frac{1}{2} m\omega^2 x^2 \right] dx$

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

Find minimum w/respect to b:

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

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

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

For this b, $\langle H \rangle = \frac{\hbar\omega}{4} + \frac{\hbar\omega}{4} = \frac{1}{2}\hbar\omega$ = correct

Try example that doesn't work out perfectly

$$V(x) = -\alpha\,\delta(x) \qquad \text{Exact } \psi_{gs} = \frac{\sqrt{m\alpha}}{\hbar} e^{-\frac{m\alpha|x|}{\hbar^2}}$$

$$E_{gs} = -\frac{m\alpha^2}{2\hbar^2}$$

But try Gaussian function

$$\psi = \left(\frac{2b}{\pi}\right)^{1/4} e^{-bx^2} \quad \ldots \quad \text{not right form}$$

Already have kinetic energy

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

Need $\langle V \rangle = \sqrt{\frac{2b}{\pi}} \int e^{-bx^2} \left[-\alpha\,\delta(x)\right] e^{-bx^2}\,dx$

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

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

$$\frac{\partial}{\partial b}\langle H \rangle = \frac{\hbar^2}{2m} - \frac{1}{2}\alpha\sqrt{\frac{2}{\pi b}} = 0$$

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

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

and $\langle H \rangle = \frac{1}{\pi}\frac{m\alpha^2}{\hbar^2} - \alpha\frac{2}{\pi}\frac{m\alpha}{\hbar^2} = -\frac{1}{\pi}\frac{m\alpha^2}{\hbar^2}$

Note $-\frac{1}{2} < -\frac{1}{\pi}$, our binding energy is too small by $\frac{2}{\pi} \approx 60\%$

But it is in the right neighborhood...
Our guess wasn't terrible.