# Physics 472 Lecture 15

## Variational Principle

A useful theorem for problems that are not amenable to perturbation theory is the following

$$\boxed{E_0 \leq \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \quad \text{for any wave function } \psi.}$$

Proof: write $\psi = \sum_n c_n \psi_n$,

where $H\psi_n = E_n \psi_n$. (We don't know the $E_n$ and $\psi_n$, but we know that such an expansion exists!)

$$\langle\psi|H|\psi\rangle = \sum_n \sum_{n'} c_n^* c_{n'} \langle n|H|n'\rangle$$

$$= \sum_n \sum_{n'} c_n^* c_{n'} E_{n'} \langle n|n'\rangle$$

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

$$\langle\psi|\psi\rangle = \sum_n \sum_{n'} c_n^* c_{n'} \langle n|n'\rangle$$

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

$$\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\sum_n E_n |c_n|^2}{\sum_n |c_n|^2} \geq \frac{\sum_n E_0 |c_n|^2}{\sum_n |c_n|^2} = E_0$$

Q.E.D.

## Examples

### i) Harmonic oscillator

Let $\psi(x) = A e^{-bx^2}$ be a trial wave function.

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

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

$$= |A|^2 \sqrt{\frac{\pi}{2b}}$$

$$\langle\psi|T|\psi\rangle = -\frac{\hbar^2}{2m}|A|^2 \int_{-\infty}^{\infty} e^{-bx^2} \frac{d^2}{dx^2} e^{-bx^2} \, dx$$

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

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

$$\langle\psi|T|\psi\rangle = \frac{\hbar^2}{m}|A|^2 b \int_{-\infty}^{\infty} dx \, (1-2bx^2) e^{-2bx^2}$$

$$= \frac{\hbar^2}{m}|A|^2 b \left( \sqrt{\frac{\pi}{2b}} - \frac{2b}{2}\sqrt{\frac{\pi}{8b^3}} \right)$$

$$= \frac{\hbar^2}{2m}|A|^2 b \sqrt{\frac{\pi}{2b}}$$

$$\langle\psi|V|\psi\rangle = \frac{1}{2} m\omega^2 |A|^2 \int_{-\infty}^{\infty} dx \;\; x^2 e^{-2bx^2}$$

$$= \frac{1}{2} m\omega^2 |A|^2 \frac{1}{2}\sqrt{\frac{\pi}{8b^3}}$$

$$= \frac{m\omega^2 |A|^2}{8b}\sqrt{\frac{\pi}{2b}}$$

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

Minimum:

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

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

$$b^2 = \left(\frac{m\omega}{2\hbar}\right)^2 \Rightarrow b = \frac{m\omega}{2\hbar}$$

$$\Rightarrow \min \langle H \rangle = \frac{\hbar\omega}{4} + \frac{\cancel{m}\omega^{\cancel{2}}\hbar}{4\cancel{m}\cancel{\omega}} = \frac{\hbar\omega}{2}$$

we got lucky, because we guessed the correct functional form of $\psi_0(x)$!

i) <u>Delta-function potential</u>

$$V(x) = -\alpha\,\delta(x)$$

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

(It's easy to calculate everything for a Gaussian!)

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

$$\langle \psi | V | \psi \rangle = -\alpha |\psi(0)|^2 = -\alpha |A|^2$$

$$\langle V \rangle = \frac{\langle \psi | V | \psi \rangle}{\langle \psi | \psi \rangle} = -\alpha \sqrt{\frac{2b}{\pi}}$$

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

minimum:

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

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

$$\min \langle H \rangle = \frac{m\alpha^2}{\pi\hbar^2} - \alpha\left(\frac{4m^2\alpha^2}{\pi^2\hbar^4}\right)^{1/2}$$

$$= -\frac{m\alpha^2}{\pi\hbar^2} > E_0 = -\frac{m\alpha^2}{2\hbar^2}$$

These examples demonstrate how to use the variational principle to estimate the ground state energy. Generally, the more adjustable parameters we include, the lower bound we can achieve. The real utility of the method is for intractable problems, where the exact solution is not known!