Variational method

This is another tool we sometimes use to tackle problems / Hamiltonians that we don't have an exact solution for.

This can only be used to get upper-bounds on the energy but could still be really powerful.

* $\forall |\psi\rangle \in \mathcal{H}$ we can see that

$$\langle \psi | H | \psi \rangle \geq E_{gs} \rightsquigarrow \text{The ground state energy.}$$

$$|\psi\rangle = \sum_i \alpha_i |\psi_i\rangle \rightsquigarrow$$

$$\langle H \rangle = \sum_i |\alpha_i|^2 E_i \geq \sum_i |\alpha_i|^2 E_{gs} = E_{gs} \times 1.$$

So, any guess for the ground state, over estimates the energy.

Assignment: Use this to prove that first order perturbation of energy upto the first order overestimates the energy.

So, here's what we do.

We make a guess but involve some parameters and then minimize the energy based on those parameters.

Example:

① H.O. $\psi(x)$: $\lim_{x \to \pm\infty} |\psi(x)| = 0$

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

$$E_{(A,\alpha)} = \langle \psi(x) | H | \psi(x) \rangle = |A|^2 \int_{-\infty}^{+\infty} e^{-\alpha x^2} \left(\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{m\omega^2 x^2}{2} \right) e^{-\alpha x^2}\, dx$$

$$= |A|^2 \int_{-\infty}^{+\infty} e^{-\alpha x^2} \left(\frac{-\hbar^2}{2m} \left(-2\alpha\, e^{-\alpha x^2} + 4\alpha^2 x^2 e^{-\alpha x^2} \right) + \frac{m\omega^2 x^2 e^{-\alpha x^2}}{2} \right) dx$$

$$= \underbrace{|A|^2 \left(\frac{-\hbar^2}{2m} \right) (-2\alpha) \int_{-\infty}^{+\infty} \left(e^{-\alpha x^2} \right)^2 dx}_{\Downarrow} + \left(\frac{m\omega^2}{2} - \frac{4\alpha^2 \hbar^2}{2m} \right) |A|^2 \int_{-\infty}^{+\infty} e^{-2\alpha x^2} x^2\, dx$$

Normalization $\leftarrow 1$

$$\frac{\hbar^2}{m} \alpha + \left(\frac{m\omega^2}{2} - \frac{2\alpha^2 \hbar^2}{m} \right) \frac{1}{4\alpha} = \frac{\hbar^2}{m} (1 - 1/2) \alpha + \frac{m\omega^2}{8} \frac{1}{\alpha}$$

$$E_\alpha = \frac{\hbar^2}{2m} \alpha + \frac{m\omega^2}{8} 1/\alpha$$

$$\text{Min} \Rightarrow \frac{dE_\alpha}{d\alpha} = 0 \Rightarrow \frac{\hbar^2}{2m} = \frac{m\omega^2}{8\alpha^2} \Rightarrow \alpha = \sqrt{\frac{m^2 w^2}{2\hbar^2}} = \frac{m\omega}{2\hbar}$$

$$\Rightarrow E_{min} = \hbar\omega/2 \quad , \quad \psi_{min}(x) = A\, e^{-\frac{m\omega}{2\hbar} x^2}$$

$\psi_{n=2}$ We can do the same for excited states.

$\forall \psi$: $\langle \psi | \psi_{gs} \rangle = 0$

$\langle \psi | H | \psi \rangle \geq E_2$ $\Rightarrow$ gives an upper-bound for the first excited state.

H.O.

We know that $\psi_1(x)$ is odd, has only one node and is orthogonal to $\psi_0(x)$ and $\lim_{x \to \pm\infty} \psi(x) = 0$

Guess : $\psi_1(x) = (\alpha x + \beta)\, e^{-\gamma x^2}$

Normalization Odd $\beta = 0$ Need to optimize this.

$$\ldots \Rightarrow E_1(\gamma) = \frac{3\hbar^2}{2m}\gamma + \frac{3m\omega^2}{8\gamma}$$

$$\gamma_{min} = \frac{m\omega}{2\hbar} \Rightarrow E_1(\gamma_{min}) = \frac{3\hbar\omega}{2}$$

Radial Schrödinger's eq. for the Hydrogen atom:

* $\psi(r) = ?$ Make a guess.

* Assignment : Take $\psi(r) = A e^{-\alpha r^2}$.