Approximation Methods

Will discuss
- dimensional analysis
- uncertainty principle
- variational method
- time indpt. perturbation theory

Won't discuss
- WKB approximation
- time dependent pert. theory

in problems w/ single energy scale - unique quantity w/ dims. of energy

$$E_{gnd} = (\text{constant } O(1)) \times (E_{scale})$$

Dim analysis

Mass	M
Length	L
Time	T

1-D SHO

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

params $m \ \omega \ \hbar$

$[\omega] = T^{-1}$

$[m] = M$

$[\hbar] = \underbrace{(M L T^{-1})}_{\vec{p}} \underbrace{(L)}_{\vec{x}} = M L^2 T^{-1}$

$[\text{Energy}] = \underbrace{(M)}_{m} \underbrace{(L^2 T^{-2})}_{c^2}$

$$E_{scale} = m^a \hbar^b \omega^c$$

$$[m^a \hbar^b \omega^c] = (M^a)(M^b L^{2b} T^{-b})(T^{-c}) = M^{a+b} L^{2b} T^{-b-c}$$

$a+b=1 \longrightarrow a=0$

$2b=1 \longrightarrow b=1$

$-b-c=-2 \longrightarrow c=0$

$$E_{scale} = \hbar\omega$$

$$E_{gnd} \sim O(1)\, \hbar\omega$$

H-atom

$$H = \frac{p^2}{2m} - \frac{e^2}{r}$$

$$\left[\frac{e^2}{r}\right] = [e^2] L^{-1} = M L^2 T^{-2}$$

$$\longrightarrow [e^2] = M L^3 T^{-2} \longrightarrow [e] = M^{1/2} L^{3/2} T^{-1}$$

$$[M^a \hbar^b e^c] = M^a (M L^2 T^{-1})^b (M^{1/2} L^{3/2} T^{-1})^c$$

$$= M^{a+b+c/2} L^{2b+3c/2} T^{-b-c}$$

$\rightarrow a = 1 \quad b = -2 \quad c = 4$

$$E_{grnd}^{H\text{-atom}} = O(1) \cdot \left(\frac{-\mu e^4}{\hbar^2} \right)$$

$$E_{grnd}^{true} = \frac{1}{2} \cdot \left(\frac{-\mu e^4}{\hbar^2} \right)$$

$$H = \frac{p^2}{2m} + V(x)$$

$$V(x) = \begin{cases} \infty & x < 0 \\ mgx & x > 0 \end{cases}$$

$m, \hbar, g$

$$E_{grnd} \sim (mg^2\hbar^2)^{1/3}$$

Variational Principle

Focus on using it to get an upperbound/estimate on ground state energy of systems w/ bound states

H - hard to find eigenvalues

$$H | E_n, \alpha \rangle = E_n | E_n, \alpha \rangle$$

α: label for degenerate states

Given a $|\psi\rangle$ or $\langle \vec{x} | \psi \rangle = \psi(\vec{x})$

$$E[|\psi\rangle] = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \quad \text{or} \quad \langle \psi | H | \psi \rangle$$

$\hookrightarrow$ w/ $\langle \psi | \psi \rangle = 1$

$$\text{or} \quad E[\psi(\vec{x})] = \int d^3x \; \psi^*(\vec{x}) \, H \, \psi(\vec{x})$$

$E[\psi(\vec{x})] \leftarrow$ functional

$\psi(\vec{x})$ in $L^2(\mathbb{R}^3)$

$$E[\;] : L^2(\mathbb{R}^3) \rightarrow \mathbb{R}$$

$$E[|\psi\rangle] \geq E_{grnd} \text{ of } H$$

restrict to $\langle\psi|\psi\rangle = 1$

$$|\psi\rangle = \sum_{n,\alpha} c_{n,\alpha} |E_n, \alpha\rangle$$

$$\langle\psi| H |\psi\rangle = \Big(\sum_{m,\beta} c^*_{m,\beta} \langle E_m, \beta|\Big) H \Big(\sum_{n,\alpha} c_{n,\alpha} |E_n, \alpha\rangle\Big)$$

$$= \sum_{m,\beta} \sum_{n,\alpha} c^*_{m,\beta} \, c_{n,\alpha} E_n \underbrace{\langle E_m, \beta | E_n, \alpha\rangle}_{\delta_{mn}\,\delta_{\beta\alpha}}$$

$$= \sum_{m,\alpha} |c_{n,\alpha}|^2 E_n \geq \sum_{n,\alpha} |c_{n,\alpha}|^2 E_{grnd}$$

$$= E_{grnd}$$

Replace the ∞ space of $\psi(\vec{x})$ by finite dimensional subspace

$$\psi(\vec{x}, \underbrace{a_1, a_2, \ldots, a_N}_{N \text{ params}})$$

$$E(\psi(\vec{x}, a_1, \ldots, a_n)) = E(a_1, \ldots, a_n) = \int \psi^*(\vec{x}, a_1, \ldots, a_n) \, H \, \psi(\vec{x}, a_1, \ldots, a_n) \, d^3x$$

$$E_{grnd} \leq \text{minimum}(E(a_1, \ldots, a_n))$$

Art choosing $\psi(\vec{x}, a_1, \ldots, a_n)$

good choice: no nodes. keep KE min as possible
vanish @ large $(\vec{x})$
compatible $L^2(\mathbb{R}^3)$
invariant under any symmetries of H

anharmonic oscillator

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 + \lambda x^4$$

$x \to -x$

width of Gaussian

$$\psi(x, a) = c e^{-ax^2} = \left(\frac{a}{\pi}\right)^{1/4} e^{-ax^2/2}$$

$$E(a) = \int \psi^* H \psi$$

$$= \int_{-\infty}^{\infty} \left(\frac{a}{\pi}\right)^{1/2} e^{-ax^2/2} \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2 + \lambda x^4\right) e^{-ax^2/2}$$

$$= \frac{\hbar^2}{9m} a + \frac{m\omega^2}{a} + \frac{3\lambda}{4a^2} \quad , \quad \frac{dE}{da} = 0 \rightarrow a^3 - \frac{m^2\omega^2 a}{\hbar} - \frac{6\lambda m}{\hbar^2} = 0$$

limiting: $\lambda = 0$ $\qquad$ $\omega = 0$

$$a = \left(\frac{6m\lambda}{\hbar^2}\right)^{1/3}$$

$$E_{grnd} \leq \frac{3}{8}\left(\frac{6m\lambda}{\hbar^2}\right)^{1/3}$$