Lecture # 1

The variational method (Ritz theorem)

- This is another of approximation methods, which has numerous applications.
- Consider an arbitrary physical system with time-independent Hamiltonian. We assume that the energy spectrum is discrete and non-degenerate:

$$H|\varphi_n\rangle = E_n|\varphi_n\rangle \quad , \quad n=0,1,2,\dots$$

Although H is known, E_n and $|\varphi_n\rangle$ are not $\Rightarrow$ we need to diagonalize H in order to find E_n and then determine the eigenstates.

Consider an arbitrary ket $|\Psi\rangle = \sum_{n=0}^{\infty} C_n|\varphi_n\rangle$

Then $\langle\Psi|H|\Psi\rangle = \sum_{n=0}^{\infty} C_n^* \langle\varphi_n|E_n C_n|\varphi_n\rangle =$

$$= \sum_{n=0}^{\infty} |C_n|^2 E_n \geq \underset{\uparrow}{E_0} \sum_{n=0}^{\infty} |C_n|^2 \quad ; \quad \langle\Psi|\Psi\rangle = \sum_{n=0}^{\infty}|C_n|^2$$

the lowest energy

Then, the mean value of the Hamiltonian H in the state $|\Psi\rangle$ is:

$$\langle H \rangle = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \geq \frac{E_0 \sum_n |C_n|^2}{\sum_n |C_n|^2} = E_0$$

For the equality (i.e. $\langle H \rangle = E_0$) $\Rightarrow$ it is necessary that $\underbrace{C_n = 0}_{\text{for all } n\text{'s}}$ except C_0 (i.e. $n=0$)

Then, $|\Psi\rangle$ is an eigenvector of H with the eigenvalue E_0.

This property is the basis for a method of approximate determination of E_0.

We choose kets $|\Psi(\alpha)\rangle$ which depend on a certain number of parameters $\{\alpha\}$, calculate mean value of H, i.e. $\langle H \rangle(\alpha)$ in these states and minimize $\langle H \rangle(\alpha)$ with respect to $\{\alpha\}$ to find (approximately) the energy of the ground state E_0

The kets $|\Psi(\alpha)\rangle$ are called trial kets,

the method $\Rightarrow$ variational method

α – Ritz parameter

Example 1D harmonic oscillator

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

Let's see how close to the exact solution we can get with the variational method.

(a) Try $\psi_\alpha(x) = e^{-\alpha x^2}$, $\alpha > 0$

(that's a very good, completely unbiased :) try)

Then $\langle \psi_\alpha | H | \psi_\alpha \rangle = \int_{-\infty}^{\infty} e^{-\alpha x^2}\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2\right] e^{-\alpha x^2} dx = -\frac{\hbar^2}{2m}(-2\alpha)\int_{-\infty}^{\infty} e^{-2\alpha x^2}\cdot(1 - 2\alpha x^2)\,dx + \frac{1}{2}m\omega^2\int_{-\infty}^{\infty} x^2 e^{-2\alpha x^2} dx = \frac{\hbar^2}{m}\alpha \cdot \underbrace{\int_{-\infty}^{\infty} e^{-2\alpha x^2} dx}_{=\sqrt{\frac{\pi}{2\alpha}}} + \left(-\frac{2\hbar^2\alpha^2}{m} + \frac{1}{2}m\omega^2\right)\underbrace{\int_{-\infty}^{\infty} x^2 e^{-2\alpha x^2} dx}_{} \ominus$

$$\int_{-\infty}^{\infty} x^2 e^{-2\alpha x^2} dx = -\frac{\partial}{\partial(2\alpha)}\int_{-\infty}^{\infty} e^{-2\alpha x^2} dx = -\frac{\partial}{\partial(2\alpha)}\sqrt{\frac{\pi}{2\alpha}} = \frac{\sqrt{\pi}}{2}\frac{1}{(2\alpha)^{3/2}}$$

$$\ominus \left(\frac{\hbar^2}{m}\alpha - \frac{\cancel{2}\hbar^2\alpha^{\cancel{2}}}{2m}\frac{1}{\cancel{2\alpha}} + \frac{1}{2}\frac{m\omega^2}{2}\cdot\frac{1}{2\alpha}\right)\cdot\sqrt{\frac{\pi}{2\alpha}} = \left(\frac{\hbar^2\alpha}{2m} + \frac{m\omega^2}{8\alpha}\right)\sqrt{\frac{\pi}{2\alpha}}$$

So, we get a pretty good agreement with the exact value of E_0 even with an arbitrary trial function.

However, it gets tricky to find an "approximate" eigenstate (which would show a good agreement with a "true" eigenstate) => see pp. 1154–1155 of Cohen-Tannoudji.

Summary:

There is no infallible method for knowing to what energy level the variational method gives an approximate value. In practice, one chooses trial functions with a simple analytical form and a very limited number of oscillations. Therefore, there is a good chance that we get the energy of the ground state or, more precisely, an upper limit of the energy. Unfortunately, there is no reliable method for evaluating the order of magnitude of the error.

$$\langle \Psi_\alpha | \Psi_\alpha \rangle = \int_{-\infty}^{\infty} e^{-2\alpha x^2} dx = \sqrt{\frac{\pi}{2\alpha}}$$

Then, $\langle H \rangle(\alpha) = \dfrac{\langle \Psi_\alpha | H | \Psi_\alpha \rangle}{\langle \Psi_\alpha | \Psi_\alpha \rangle} = \dfrac{\hbar^2 \alpha}{2m} + \dfrac{m\omega^2}{8\alpha}$

Now let's find the minimum of $\langle H \rangle(\alpha)$:

$$\left.\frac{\partial \langle H \rangle(\alpha)}{\partial \alpha}\right|_{\alpha=\alpha_0} = 0 \Rightarrow \frac{\hbar^2}{2m} - \frac{m\omega^2}{8\alpha_0^2} = 0 \Rightarrow$$

$\alpha_0 = \dfrac{m\omega}{2\hbar}$ (since we specified before that $\alpha > 0$) $\Rightarrow$

$$\langle H \rangle(\alpha_0) = \frac{\hbar^2}{2m} \cdot \frac{m\omega}{2\hbar} + \frac{m\omega^2}{8} \cdot \frac{2\hbar}{m\omega} = \frac{\hbar\omega}{4} + \frac{\hbar\omega}{4} = \frac{\hbar\omega}{2}$$

So, an "approximate" value of the lowest energy $E_0 = \dfrac{\hbar\omega}{2}$ is actually an <u>exact result</u>.

What if our choice of the "trial" function is not as good? $\Rightarrow$ Let's try $\Psi_a(x) = \dfrac{1}{x^2+a}$, $a > 0$

$$\langle \Psi_a | H | \Psi_a \rangle (a) = \int_{-\infty}^{\infty} \frac{1}{x^2+a} \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2 \right) \frac{1}{x^2+a} dx =$$

$$= -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \left(\frac{-2}{(x^2+a)^2} + \frac{16x^2}{2(x^2+a)^3} \right) \frac{dx}{x^2+a} + \frac{1}{2} m\omega^2 \underbrace{\int_{-\infty}^{\infty} \frac{x^2 dx}{(x^2+a)^2}}_{=\frac{\pi}{2\sqrt{a}}} =$$

$$= -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \left(\frac{6}{(x^2+a)^3} - \frac{16a}{2(x^2+a)^4} \right) dx + \frac{1}{2} m\omega^2 \left(\int_{-\infty}^{\infty} \frac{dx}{x^2+a} - a \int_{-\infty}^{\infty} \frac{dx}{(x^2+a)^2} \right) =$$

5

$$= -\frac{\hbar}{2m}\left(-\cancel{2}\cdot\frac{3\pi}{\cancel{8}_{4}a^{5/2}} + \frac{\pi}{2a^{5/2}}\right) + \frac{1}{2}m\omega^2\cdot\frac{\pi}{2\sqrt{a}} =$$

$$= -\frac{\hbar^2}{2m}\frac{\pi}{a^{5/2}}\left(-\frac{1}{4}\right) + \frac{m\omega^2\pi}{4\sqrt{a}}$$

$$\langle \psi_a | \psi_a \rangle = \int_{-\infty}^{\infty}\frac{dx}{(x^2+a)^2} = \frac{\pi}{2a\sqrt{a}}$$

$$\langle H \rangle = \frac{\langle \psi_a | H | \psi_a \rangle}{\langle \psi_a | \psi_a \rangle} = \frac{\frac{\hbar^2}{8m}\frac{\pi}{a^{5/2}} + \frac{m\omega^2\pi}{4\sqrt{a}}}{\frac{\pi}{2a\sqrt{a}}} =$$

$$= \frac{\hbar^2}{4ma} + \frac{m\omega^2 a}{2}$$

$$\frac{\partial\langle H\rangle}{\partial a} = -\frac{\hbar^2}{4ma^2} + \frac{m\omega^2}{2}\bigg|_{a=a_0} = 0 \Rightarrow a_0 = \frac{\hbar}{\sqrt{2}m\omega}$$

Then $\langle H\rangle(a_0) = \frac{\hbar^2}{4m}\frac{\sqrt{2}m\omega}{\hbar} + \frac{m\omega^2}{2}\cdot\frac{\hbar}{\sqrt{2}m\omega} = \hbar\omega\left(\frac{\sqrt{2}}{4}+\frac{1}{2\sqrt{2}}\right)$

$$= \hbar\omega\,\frac{\sqrt{2}\cdot\sqrt{2}+2}{4\sqrt{2}} = \hbar\omega\cdot\frac{4}{4\sqrt{2}} = \frac{\hbar\omega}{\sqrt{2}}$$

So, the minimal value of ground state energy obtained using the trial function $\psi_a = \frac{1}{x^2+a}$ is $\frac{\hbar\omega}{\sqrt{2}}$, while the exact value is $\frac{\hbar\omega}{2}$ $\Rightarrow$ so the error (per quantum) is $\frac{\hbar\omega}{\hbar\omega}\left(\frac{1}{\sqrt{2}}-\frac{1}{2}\right)$

$$= \frac{2-\sqrt{2}}{2\sqrt{2}} \approx \frac{2-1.4}{2\cdot 1.4} = \frac{0.6}{2.8} \approx 21\%$$