Variational Method

Another approximate calculations

When to use...

Perturbation theory?

When the system can be well-described by a solvable Hamiltonian, and the deviations can be treated as small perturbation.

Variational Method?

When we cannot find even approximate eigenvalues and eigenfunctions (usually the case for strongly-interacting systems), so we would be happy even with a reasonable guess of the ground state energy

Main goal: place as tight as possible bound on the ground-state energy E_g of the Hamiltonian $\hat{H}$.

Basic statement: for <u>any</u> normalized wavefunction ψ: $E_g \leq \langle \psi | \hat{H} | \psi \rangle = \langle \hat{H} \rangle_\psi$ average value of $\hat{H}$ in this state.

Proof: if $\{|\psi_n\rangle\}$ is the eigenfunction basis of $\hat{H}$ (even though we don't know it, then

$$\psi = \sum_n c_n \psi_n$$

$$\hat{H}\psi = \sum_n c_n \hat{H}\psi_n = \sum_n c_n E_n \psi_n$$

$$\langle \psi | \hat{H} | \psi \rangle = \sum_{n,m} c_m^* \langle \psi_m | \hat{H} | \psi_n \rangle c_n =$$

$$= \sum_{n,m} c_n c_m^* E_n \delta_{nm} = \sum_n |c_n|^2 E_n$$

Since $E_n \geq E_{ground}$ $\quad \langle\psi|\hat{H}|\psi\rangle \geq E_{ground} \sum_n |C_n|^2 = E_{ground}$

The real trick is to find the best trial wave function (or ansatz) to obtain the tightest upper limit.

How to obtain the optimal ansatz?

- Use physical intuition regarding the shape of the wave function
- Minimize the calculated estimated energy values by varying any introduced parameters

For example: $\psi(\lambda_1, \lambda_2 ..)$ $\quad \lambda_1, \lambda_2$ - introduced parameters.

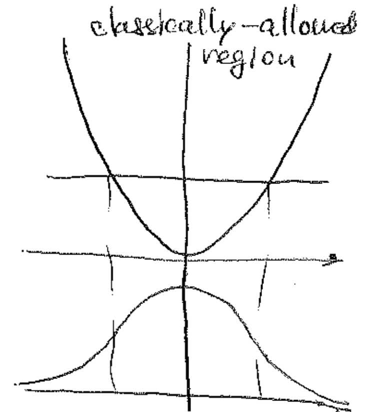
$\langle\hat{H}\rangle(\lambda_1, \lambda_2) = \langle\psi(\lambda_1, \lambda_2 ..)|\hat{H}|\psi(\lambda_1, \lambda_2 ..)\rangle$

How can we check that $\langle\hat{H}\rangle_{\lambda_1, \lambda_2}$ is the closest to the ground state, i.e, has a minimum value?

$$\frac{\partial\langle H\rangle}{\partial\lambda_1} = 0 \qquad \frac{\partial\langle H\rangle}{\partial\lambda_2} = 0$$

One can vary the parameters for each ansatz to find the minimum $\langle H\rangle$ value for this ansatz. Then one need to compare the estimates for several ansatzs $\rightarrow$ the lowest bound corresponds to the most precise approximation of the true ground state wave function

Simple examples:



1D harmonic oscillator

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

Reasonable guesses

$$\psi_1(x) = A e^{-x^2/b^2} \qquad \int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 1 \quad \Rightarrow \quad A = \sqrt[4]{\frac{2b\hbar}{\pi}}$$

$$\psi_2(x) = \frac{A}{x^2+b^2} \qquad \text{Normalization!} \quad A = \sqrt{2b^3/\pi}$$

$$\psi_3(x) = \begin{cases} A\cos\frac{\pi x}{a} & |x| < a/2 \\ 0 & |x| \geq a/2 \end{cases} \qquad \text{Normalization} \quad A = \sqrt{\frac{2}{a}}$$

First ansatz:

$$\langle \hat{H} \rangle_1 = \langle \psi_1 | \hat{H} | \psi_1 \rangle = \int_{-\infty}^{+\infty} \psi_1^* \hat{H} \psi_1 dx = A^2 \int_{-\infty}^{+\infty} e^{-x^2/b^2} \left[-\frac{\hbar^2}{2m}\frac{d^2 e^{-x^2/b^2}}{dx^2} + \right.$$

$$\left. + \frac{1}{2}m\omega^2 x^2 e^{-x^2/b^2} \right] dx =$$

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

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

Minimize: $\frac{d\langle \hat{H} \rangle_1}{db} = 0 = \frac{\hbar^2}{2m} - \frac{m\omega^2}{8b^2} \quad \Rightarrow \quad b = \frac{m\omega}{2\hbar}$

$$\langle \hat{H}_1 \rangle = \frac{\hbar^2}{2m}\left(\frac{m\omega}{2\hbar}\right) + \frac{m\omega^2}{8}\left(\frac{2\hbar}{m\omega}\right) = \hbar\omega/2$$

$$E_g \leq \langle \hat{H} \rangle_1 = \frac{1}{2}\hbar\omega$$

$$\langle \hat{H} \rangle_2 = A^2 \int_{-\infty}^{+\infty} \frac{1}{x^2+b^2} \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \left(\frac{1}{x^2+b^2} \right) + \frac{1}{2} m\omega^2 \frac{x^2}{x^2+b^2} \right] dx$$

$$= -\frac{A^2\hbar^2}{2m} \int_{-\infty}^{+\infty} \frac{1}{(x^2+b^2)} \frac{2A(3x^2-b^2)}{(x^2+b^2)^3} dx + \frac{A^2}{2} m\omega^2 \int_{-\infty}^{+\infty} \frac{x^2}{(x^2+b^2)^2} dx =$$

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

Let's adjust b to minimize this value

$$\frac{d\langle \hat{H} \rangle_2}{db} = 0 = -\frac{\hbar^2}{2mb^3} + m\omega^2 b \qquad b =$$

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

$$E_{ground} \leq \langle \hat{H}_2 \rangle = \frac{\hbar^2}{4\cancel{m}} \frac{\sqrt{2}\cancel{m\omega}}{\hbar} + \frac{\cancel{m\omega^2}}{2} \frac{\hbar^2}{\sqrt{2}\cancel{m\omega}} = \frac{1}{\sqrt{2}} \hbar\omega \approx 0.7\hbar\omega$$

What about our third ansatz?

$$\psi(x) = \begin{cases} A\cos \pi x/a & |x| < a/2 \\ 0 & |x| \geq a/2 \end{cases}$$

$$\psi'(x) = \begin{cases} -A\pi/a \sin \pi x/a & |x| < a/2 \\ 0 & |x| \geq a/2 \end{cases}$$

$$\psi''(x) = \begin{cases} -\frac{A\pi^2}{a^2} \cos\frac{\pi x}{a} & |x| < a/2 \\ A\,\delta(x \pm a/2) & |x| = a/2 \\ 0 & |x| > a/2 \end{cases}$$

Thus

$$\langle H \rangle_3 = \int_{-a/2}^{a/2} A\cos\frac{\pi x}{a} \left[-\frac{\hbar^2}{2m} \overbrace{\left(-\frac{A\pi^2}{a^2}\cos\frac{\pi x}{a} + A\,\delta(x + a/2) + A\,\delta(x - a/2) \right)}^{\psi''(x)} + \frac{1}{2} m\omega^2 x^2 \cos \pi x/a \right] dx$$

$$= A^2 \int_{-a/2}^{a/2} \left(-\frac{\hbar^2}{2m} \right) \cos^2\frac{\pi x}{a}\, dx + \underbrace{\cancel{A^2 \cos \pi/2}}_{=0} + \underbrace{\cancel{A^2 \cos(-\pi/2)}}_{=0} +$$

$$+ \frac{A^2}{2} m\omega^2 \int_{-a/2}^{a/2} x^2 \cos^2\frac{\pi x}{a}\, dx = \frac{\pi^2 - 6}{24\pi^2} m\omega^2 a^2 + \frac{\pi^2\hbar^2}{2ma^2}$$

Minimize $\langle \hat{H} \rangle_3$:

$$\frac{d\langle \hat{H} \rangle_3}{da} = \frac{\pi^2-6}{24\pi^2} m\omega^2 (2a) + \frac{\hbar^2\pi^2}{2m}\left(-\frac{2}{a^3}\right) = 0$$

$$a^4 = \frac{12\pi^2}{\pi^2-6}\,\frac{\hbar^2\pi^2}{m^2\omega^2} \Rightarrow a^2 = \sqrt{\frac{12\pi^2}{\pi^2-6}}\,\frac{\pi\hbar}{m\omega}$$

$$E_{ground} \leq \sqrt{\frac{\pi^2-6}{12}}\,\hbar\omega = 0.5678\,\hbar\omega$$

From the three proposed functions the first one is the closest to the true state (in fact it is the ~~best~~ true ground state) The third ansatz would be the second best guess.