

Chapter 8: The variational principle

This is a common occurrence: Suppose you have a Hamiltonian that (i) cannot be solved exactly and (ii) where perturbation theory cannot be applied because there is no simple H_0 and/or because there is no small H' .

Then, what do we do? 😞

One possibility is to use the **variational principle**: it does not give you the exact answer but gives you an **upper bound to the energy** which is often sufficient.

Select any wave function you wish. Call it Ψ . The claim is that **always**:

$$E_{\text{gs}} \leq \langle \psi | H | \psi \rangle \equiv \langle H \rangle$$

Although we do not know **explicitly** the eigenstates of H , because we cannot solve the problem exactly, we know they exist.

$$H\psi_n = E_n\psi_n$$

Then, in an "abstract" manner we can expand our proposed variational wave function in the **complete basis of eigenstates**:

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

If ψ is normalized, then:

$$1 = \langle \psi | \psi \rangle = \left\langle \sum_m c_m \psi_m \left| \sum_n c_n \psi_n \right. \right\rangle = \sum_m \sum_n c_m^* c_n \langle \psi_m | \psi_n \rangle = \sum_n |c_n|^2$$

Repeating with H included, we find:

$$\langle H \rangle = \left\langle \sum_m c_m \psi_m \left| H \sum_n c_n \psi_n \right. \right\rangle = \sum_m \sum_n c_m^* E_n c_n \langle \psi_m | \psi_n \rangle = \sum_n E_n |c_n|^2$$

But the ground state has the lowest energy by definition:

$E_{\text{gs}} \leq E_n$. Then:

$$\langle H \rangle \geq E_{\text{gs}} \sum_n |c_n|^2 = E_{\text{gs}}$$

The variational principle is powerful, easy to use, and accurate if you have a good intuition on how the wave function should look like. Problem: you do NOT know how close your result is compared to the exact result. You only know you are above.

Example 8.1:

Consider the 1D Harmonic Oscillator with H :

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


Here we know the answer exactly, but we pretend we do not.

As a "trial" wave function we will use a **Gaussian exponential**. Using Gaussians is very common, because the integrals are known.

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

A is the normalization and b is called a "**variational parameter**" that we will optimize by minimizing the energy.

Normalization:

$$1 = |A|^2 \int_{-\infty}^{\infty} e^{-2bx^2} dx = |A|^2 \sqrt{\frac{\pi}{2b}} \Rightarrow A = \left(\frac{2b}{\pi}\right)^{1/4}$$


Next we need the expectation value of the Hamiltonian:

$$\langle H \rangle = \langle T \rangle + \langle V \rangle$$

For the kinetic energy:

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

For the potential energy:

$$\langle V \rangle = \frac{1}{2} m \omega^2 |A|^2 \int_{-\infty}^{\infty} e^{-2bx^2} x^2 dx = \frac{m \omega^2}{8b}$$

Adding kinetic and potential energy: $\langle H \rangle = \frac{\hbar^2 b}{2m} + \frac{m\omega^2}{8b}$

Let us now "optimize" the "variational parameter"

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

If we introduce the "optimal b" into $\langle H \rangle$, we obtain:

$$\langle H \rangle_{\min} = \frac{1}{2} \hbar \omega$$

which is the **exact result**, by chance, in this simple example. **In the vast majority of cases, you will not find the exact result.**

Example 8.2:

Consider now the **attractive delta function**. Here we also know the exact result from QM 411: $E_{\text{gs}} = -m\alpha^2/2\hbar^2$

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - \alpha\delta(x)$$

Here we will use again the Gaussian trial wave function. We know already that **this is not the exact ground state**.

$$\psi(x) = Ae^{-bx^2}$$

The normalization is independent of the Hamiltonian, thus same as Example 8.1:

$$1 = |A|^2 \int_{-\infty}^{\infty} e^{-2bx^2} dx = |A|^2 \sqrt{\frac{\pi}{2b}} \Rightarrow A = \left(\frac{2b}{\pi}\right)^{1/4}$$

$\langle T \rangle$ is the same as well:
$$\langle T \rangle = -\frac{\hbar^2}{2m} |A|^2 \int_{-\infty}^{\infty} e^{-bx^2} \frac{d^2}{dx^2} \left(e^{-bx^2} \right) dx = \frac{\hbar^2 b}{2m}$$

The only difference between Examples 8.1 and 8.2 arises from $\langle V \rangle$:

$$\langle V \rangle = -\alpha |A|^2 \int_{-\infty}^{\infty} e^{-2bx^2} \delta(x) dx = -\alpha \sqrt{\frac{2b}{\pi}}$$

Adding kinetic and potential: $\langle H \rangle = \frac{\hbar^2 b}{2m} - \alpha \sqrt{\frac{2b}{\pi}}$

Optimizing b : $\frac{d}{db} \langle H \rangle = \frac{\hbar^2}{2m} - \frac{\alpha}{\sqrt{2\pi b}} = 0 \Rightarrow b = \frac{2m^2 \alpha^2}{\pi \hbar^4}$

we arrive to $\langle H \rangle_{\min} = -\frac{m\alpha^2}{\pi \hbar^2}$ while exact is $E_{\text{gs}} = -m\alpha^2/2\hbar^2$

Not perfect but close enough i.e. π instead of 2!

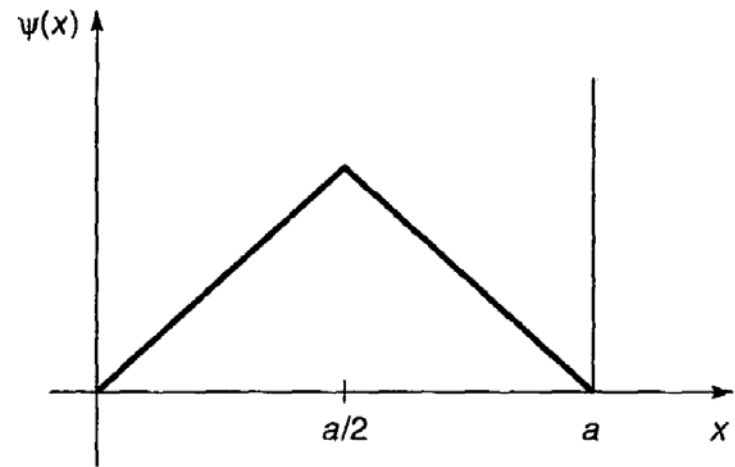
Note: If variational state is known to be orthogonal to ground state (e.g. even vs odd), then the upper bound found is for the **first excited state** (see HW problem).

Example 8.3:

As wave function you can use anything, including a function with discontinuous first derivatives:

Consider as potential the infinite square well between 0 and a .

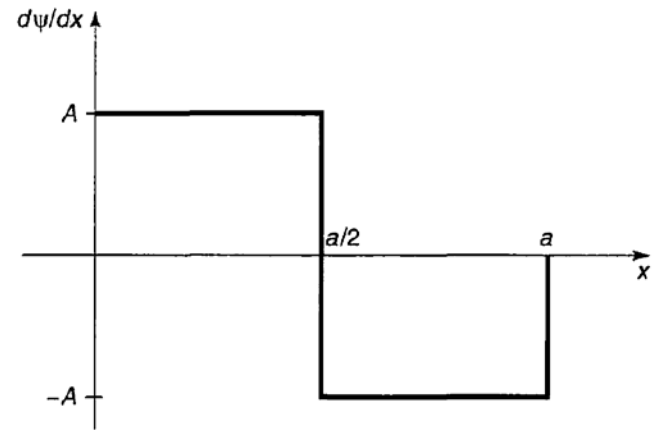
$$\psi(x) = \begin{cases} Ax, & \text{if } 0 \leq x \leq a/2, \\ A(a-x), & \text{if } a/2 \leq x \leq a, \\ 0, & \text{otherwise,} \end{cases}$$



$$1 = |A|^2 \left[\int_0^{a/2} x^2 dx + \int_{a/2}^a (a-x)^2 dx \right] = |A|^2 \frac{a^3}{12} \Rightarrow A = \frac{2}{a} \sqrt{\frac{3}{a}}$$

The challenge is how to handle $\langle T \rangle$ that contains a second derivative!

$$\frac{d\psi}{dx} = \begin{cases} A, & \text{if } 0 < x < a/2, \\ -A, & \text{if } a/2 < x < a, \\ 0, & \text{otherwise,} \end{cases}$$



The derivative of a step function is a Dirac delta. Number in front is the jump:

$$\frac{d^2\psi}{dx^2} = A\delta(x) - 2A\delta(x - a/2) + A\delta(x - a)$$

$$\langle H \rangle = -\frac{\hbar^2 A}{2m} \int [\delta(x) - 2\delta(x - a/2) + \delta(x - a)]\psi(x) dx$$

$$= -\frac{\hbar^2 A}{2m} [\psi(0) - 2\psi(a/2) + \psi(a)] = \frac{\hbar^2 A^2 a}{2m} = \boxed{\frac{12\hbar^2}{2ma^2}}$$

The exact result is:

$$E_{\text{gs}} = \pi^2 \hbar^2 / 2ma^2$$

Variational theorem holds because $12 > \pi^2$