Variational Principle

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Variational Principle

The variational principle gives the upper bound of the ground state for any given Hamiltonian,

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

Since ψ is normalized,

$$\begin{aligned} 1 = \langle \psi | \psi \rangle &= \langle \sum_m c_m \psi_m | \sum_n c_n \psi_n \rangle \\ &= \sum_m \sum_n c_m^* c_n \langle \psi_m | \psi_n \rangle \\ &= \sum_m \sum_n c_m^* c_n \delta_{m,n} = \sum_n |c_n|^2. \end{aligned}$$

Variational Principle

The expectation value of the Hamiltonian of a test wave function ψ is

$$\begin{aligned}\langle H\rangle &= \langle\sum_m c_m\psi_m|H\sum_n c_n\psi_n\rangle \\ &= \sum_m\sum_n c_m^* E_n c_n \langle\psi_m|\psi_n\rangle \\ &= \sum_n E_n|c_n|^2 \geq \sum_n E_{gs}|c_n|^2 = E_{gs}.\end{aligned}$$

Harmonic Oscillator

The Hamiltonian of the harmonic oscillator is

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

The energy eigenvalues are

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right).$$

When we use a Gaussian wave function $\psi(x) = Ae^{-bx^2}$ where $A = (2b/\pi)^{1/4}$, we can find the expectation value of H,

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

Harmonic Oscillator

$$
\begin{aligned}
\langle T \rangle &= -\frac{\hbar^2}{2m}|A|^2 \int e^{-bx^2} \frac{d^2}{dx^2} e^{-bx^2}\, dx \\
&= -\frac{\hbar^2}{2m}|A|^2 \int e^{-bx^2} \frac{d}{dx}(-2bx) e^{-bx^2}\, dx \\
&= -\frac{\hbar^2}{2m}\sqrt{\frac{2b}{\pi}} \int e^{-bx^2} \left(-2be^{-bx^2} + 4b^2x^2e^{-bx^2}\right) dx \\
&= -\frac{\hbar^2}{2m}\sqrt{\frac{2b}{\pi}} \left[-2b\sqrt{\frac{\pi}{2b}} - 2b^2\frac{\partial}{\partial b}\sqrt{\frac{\pi}{2b}}\right] \\
&= -\frac{\hbar^2}{2m}\sqrt{\frac{2b}{\pi}} \left[-2b\sqrt{\frac{\pi}{2b}} + b\sqrt{\frac{\pi}{2b}}\right] \\
&= \frac{\hbar^2 b}{2m}.
\end{aligned}
$$

Harmonic Oscillator

$$\begin{aligned}\langle V\rangle &= \frac{1}{2}m\omega^2|A|^2\int e^{-bx^2}x^2e^{-bx^2}\,dx\\ &= \frac{1}{2}m\omega^2|A|^2\int x^2e^{-2bx^2}\,dx\\ &= -\frac{1}{4}m\omega^2|A|^2\frac{\partial}{\partial b}\left(\sqrt{\frac{\pi}{2m}}\right)\\ &= \frac{m\omega^2}{8b}.\end{aligned}$$

Then,

$$\langle H\rangle = \frac{\hbar^2 b}{2m} + \frac{m\omega^2}{8b}.$$

Harmonic Oscillator

In order to minimize $\langle H \rangle$, we find the stationary value,

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

Therefore,

$$b = \frac{m\omega}{2\hbar}.$$

In conclusion, we find the bound of the ground state energy,

$$\begin{aligned}\langle H \rangle &= \frac{\hbar^2}{2m}\frac{m\omega}{2\hbar} + \frac{1}{8}m\omega^2\frac{2\hbar}{m\omega} \\ &= \frac{1}{2}\hbar\omega.\end{aligned}$$

Since the real wave function of the harmonic oscillator is Gaussian, the variational method gives the exact value.

Delta Function

For the delta function potential,

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

the expectation value for the Gaussian test function is

$$\begin{aligned}\langle V\rangle &= -\alpha|A|^2 \int e^{-bx^2}\delta(x)e^{-bx^2}\,dx \\ &= -\alpha|A|^2 \int e^{-2bx^2}\delta(x) \\ &= -\alpha|A|^2 = -\alpha\sqrt{\frac{2b}{\pi}}.\end{aligned}$$

The expectation of the Hamiltonian is

$$\langle H\rangle = \frac{\hbar^2 b}{2m} - \alpha\sqrt{\frac{2b}{\pi}}.$$

Delta Function

In order to minimize $\langle H \rangle$, we find the stationary value,

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

Therefore,

$$b = \frac{2m^2\alpha^2}{\hbar^2\pi}.$$

In conclusion, we find the bound of the ground state energy,

$$\langle H \rangle = -\frac{m\alpha^2}{\pi\hbar^2}, \tag{1}$$

which is a good approximation to the real energy, $E_{gs} = -\frac{m\alpha}{2\hbar^2}$.