Variational Principle and the First Excited State

A corollary to the variational principle goes like this:

Corollary. If $\langle \psi | \psi_0 \rangle = 0$ where $\psi$ is the trial function and $\psi_0$ is the ground state wave function, then $\langle H \rangle = \langle \psi | H | \psi \rangle \geq E_1$ where $E_1$ is the energy of the first excited state.

We can expand $\psi$ in terms of the eigenfunctions of $H$ in the usual way:

$$\psi = \sum_{n=0}^{\infty} c_n \psi_n$$

(1)

Since $\langle \psi | \psi_0 \rangle = 0$, $c_0 = 0$ so

$$\psi = \sum_{n=1}^{\infty} c_n \psi_n$$

(2)

$$\langle \psi | H | \psi \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n$$

(3)

$$\geq E_1 \sum_{n=1}^{\infty} |c_n|^2$$

(4)

$$= E_1$$

(5)

In practice, this corollary’s usefulness is limited, since we won’t, in general, know $\psi_0$ so we can’t be sure our trial function $\psi$ is orthogonal to it. However, if we know that $\psi_0$ is even or odd, then we can take $\psi$ to be odd or even, respectively.

Example. We can apply this to the harmonic oscillator. Since the potential is even, we know that a solution can be taken as even or odd. As it happens, the ground state of the harmonic oscillator is even, as we’ve seen earlier:

$$\psi_0 = \left( \frac{m \omega}{\pi \hbar} \right)^{1/4} e^{-m \omega x^2 / 2\hbar}$$

(6)
We can therefore illustrate the corollary in this case. We take as the odd trial function:

\[ \psi = Axe^{-bx^2} \]  

(7)

First work out \( A \) from normalization:

\[ A^2 \int_{-\infty}^{\infty} x^2 e^{-2bx^2} dx = 1 \]  

(8)

\[ A^2 \frac{\sqrt{2\pi}}{8b^{3/2}} = 1 \]  

(9)

\[ A = \frac{2^{5/4}b^{3/4}}{\pi^{1/4}} \]  

(10)

We can now work out \( \langle H \rangle \) in the usual way:

\[ \langle H \rangle = \sqrt{\frac{2^5 b^3}{\pi}} \int_{-\infty}^{\infty} \left[ -\frac{\hbar^2}{2m} x e^{-bx^2} \frac{d^2}{dx^2} \left( x e^{-bx^2} \right) + x^2 e^{-2bx^2} \frac{m\omega^2}{2} x^2 \right] dx \]

(11)

\[ \langle H \rangle = \frac{3}{2} \frac{\hbar b^2}{m} + \frac{3}{8} \frac{m\omega^2}{b} \]  

(12)

where we did the calculus with Maple.

We find the value of \( b \) that minimizes \( \langle H \rangle \):

\[ \frac{d \langle H \rangle}{db} = \frac{3}{2} \frac{\hbar^2}{m} - \frac{3}{8} \frac{m\omega^2}{b^2} = 0 \]  

(13)

\[ b_{min} = \frac{m\omega}{2\hbar} \]  

(14)

\[ \langle H \rangle_{min} = \frac{3}{2} \frac{\hbar \omega}{2} \]  

(15)

This is the exact answer, which is to be expected since \( \psi \) happens to be the exact form of the wave function for the first excited state.

Pingbacks

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