VARIATIONAL PRINCIPLE AND THE FIRST EXCITED STATE

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 7.4.

A corollary to the variational principle goes like this:

Corollary. *If $\langle\psi|\psi_0\rangle = 0$ where ψ is the trial function and ψ_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 ψ in terms of the eigenfunctions of H in the usual way:

$$\psi = \sum_{n=0}^{\infty} c_n \psi_n \tag{1}$$

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

$$\begin{aligned} \psi &= \sum_{n=1}^{\infty} c_n \psi_n && (2) \\ \langle\psi|H|\psi\rangle &= \sum_{n=1}^{\infty} |c_n|^2 E_n && (3) \\ &\geq E_1 \sum_{n=1}^{\infty} |c_n|^2 && (4) \\ &= E_1 && (5) \end{aligned}$$

In practice, this corollary's usefulness is limited, since we won't, in general, know ψ_0 so we can't be sure our trial function ψ is orthogonal to it. However, if we know that ψ_0 is even or odd, then we can take ψ 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:

$$\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar} \tag{6}$$

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

$$\psi = Axe^{-bx^2} \tag{7}$$

First work out A from normalization:

$$A^2\int_{-\infty}^{\infty}x^2e^{-2bx^2}dx = 1 \tag{8}$$

$$A^2\frac{\sqrt{2\pi}}{8b^{3/2}} = 1 \tag{9}$$

$$A = \frac{2^{5/4}b^{3/4}}{\pi^{1/4}} \tag{10}$$

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

$$\langle H\rangle = \sqrt{\frac{2^5b^3}{\pi}}\int_{-\infty}^{\infty}\left[-\frac{\hbar^2}{2m}xe^{-bx^2}\frac{d^2}{dx^2}\left(xe^{-bx^2}\right)+x^2e^{-2bx^2}\frac{m\omega^2}{2}x^2\right]dx \tag{11}$$

$$= \frac{3}{2}\frac{b\hbar^2}{m}+\frac{3}{8}\frac{m\omega^2}{b} \tag{12}$$

where we did the calculus with Maple.

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

$$\frac{d\langle H\rangle}{db} = \frac{3}{2}\frac{\hbar^2}{m}-\frac{3}{8}\frac{m\omega^2}{b^2} = 0 \tag{13}$$

$$b_{min} = \frac{m\omega}{2\hbar} \tag{14}$$

$$\langle H\rangle_{min} = \frac{3}{2}\hbar\omega \tag{15}$$

This is the exact answer, which is to be expected since 7 happens to be the exact form of the wave function for the first excited state.

PINGBACKS

Pingback: Variational principle and the harmonic oscillator - 2

Pingback: Variational principle and harmonic oscillator: a more general trial function