

## 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  $\psi$  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:

$$(0.1) \quad \psi = \sum_{n=0}^{\infty} c_n \psi_n$$

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

$$(0.2) \quad \psi = \sum_{n=1}^{\infty} c_n \psi_n$$

$$(0.3) \quad \langle \psi | H | \psi \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n$$

$$(0.4) \quad \geq E_1 \sum_{n=1}^{\infty} |c_n|^2$$

$$(0.5) \quad = E_1$$

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:

$$(0.6) \quad \psi_0 = \left( \frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-m\omega x^2/2\hbar}$$

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

$$(0.7) \quad \psi = Axe^{-bx^2}$$

First work out  $A$  from normalization:

$$(0.8) \quad A^2 \int_{-\infty}^{\infty} x^2 e^{-2bx^2} dx = 1$$

$$(0.9) \quad A^2 \frac{\sqrt{2\pi}}{8b^{3/2}} = 1$$

$$(0.10) \quad A = \frac{2^{5/4} b^{3/4}}{\pi^{1/4}}$$

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

$$(0.11) \quad \langle H \rangle = \sqrt{\frac{2^5 b^3}{\pi}} \int_{-\infty}^{\infty} \left[ -\frac{\hbar^2}{2m} x e^{-bx^2} \frac{d^2}{dx^2} (x e^{-bx^2}) + x^2 e^{-2bx^2} \frac{m\omega^2}{2} x^2 \right] dx$$

$$(0.12) \quad = \frac{3 b \hbar^2}{2 m} + \frac{3 m \omega^2}{8 b}$$

where we did the calculus with Maple.

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

$$(0.13) \quad \frac{d\langle H \rangle}{db} = \frac{3 \hbar^2}{2 m} - \frac{3 m \omega^2}{8 b^2} = 0$$

$$(0.14) \quad b_{min} = \frac{m\omega}{2\hbar}$$

$$(0.15) \quad \langle H \rangle_{min} = \frac{3}{2} \hbar \omega$$

This is the exact answer, which is to be expected since 0.7 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