

VARIATIONAL PRINCIPLE AND THE FIRST EXCITED STATE

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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:

$$(1) \quad \psi = \sum_{n=0}^{\infty} c_n \psi_n$$

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

$$(2) \quad \psi = \sum_{n=1}^{\infty} c_n \psi_n$$

$$(3) \quad \langle \psi | H | \psi \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n$$

$$(4) \quad \geq E_1 \sum_{n=1}^{\infty} |c_n|^2$$

$$(5) \quad = E_1$$

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:

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

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

$$(7) \quad \psi = Axe^{-bx^2}$$

First work out A from normalization:

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

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

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

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

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

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

where we did the calculus with Maple.

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

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

$$(14) \quad b_{min} = \frac{m\omega}{2\hbar}$$

$$(15) \quad \langle H \rangle_{min} = \frac{3}{2} \hbar\omega$$

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.

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