

VARIATIONAL PRINCIPLE AND THE FIRST EXCITED STATE

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Post date: 27 September 2021.

A corollary to the variational principle goes like this:

Corollary 1. *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.*

Proof. We can expand ψ in terms of the eigenfunctions of H in the usual way:

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

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

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

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

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

$$= E_1 \quad (5)$$

□

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 1. 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:

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

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

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

First work out A from normalization:

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

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

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

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

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

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

where we did the calculus with Maple.

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

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

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

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

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.

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