

VARIATIONAL PRINCIPLE AND THE HARMONIC OSCILLATOR

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 7.2.

Here's another example of the variational principle, this time applied to the one-dimensional harmonic oscillator. We use a normalized function ψ as a test function for the hamiltonian H and get an upper bound on the ground state energy E_0 :

$$E_0 \leq \langle \psi | H | \psi \rangle \equiv \langle H \rangle \quad (1)$$

In this case, the potential is given by

$$V(x) = \frac{1}{2}m\omega^2x^2 \quad (2)$$

and we'll take as the test function

$$\psi = \frac{A}{x^2 + b^2} \quad (3)$$

where A and b are parameters.

We can find A from normalization:

$$|A|^2 \int_{-\infty}^{\infty} \frac{dx}{(x^2 + b^2)^2} = 1 \quad (4)$$

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

$$A = \sqrt{\frac{2}{\pi}} b^{3/2} \quad (6)$$

where we used Maple for the integral.

Following the usual procedure, we calculate:

$$\langle H \rangle = \frac{2}{\pi} b^3 \int_{-\infty}^{\infty} \left[-\frac{\hbar^2}{2m} \frac{1}{x^2 + b^2} \frac{d^2}{dx^2} \left(\frac{1}{x^2 + b^2} \right) + \frac{1}{(x^2 + b^2)^2} \frac{m\omega^2 x^2}{2} \right] dx \quad (7)$$

$$= \frac{\hbar^2 + 2m^2\omega^2 b^4}{4mb^2} \quad (8)$$

$$= \frac{\hbar^2}{4mb^2} + \frac{1}{2} m\omega^2 b^2 \quad (9)$$

Taking the derivative with respect to b and setting to zero, we get

$$b_{min} = \frac{1}{2^{1/4}} \sqrt{\frac{\hbar}{m\omega}} \quad (10)$$

$$E_0 \leq \frac{1}{\sqrt{2}} \hbar\omega \quad (11)$$

The exact ground state energy is $E_0 = \frac{1}{2} \hbar\omega$ so this upper limit is higher by a factor of $\sqrt{2}$.

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