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 ψas a test function for the hamiltonian H and get an upper bound on the ground state energy E_0:

$$\boxed{E_0 \le \langle\psi|H|\psi\rangle \equiv \langle H\rangle} \tag{1}$$

In this case, the potential is given by

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

and we'll take as the test function

$$\psi = \frac{A}{x^2+b^2} \tag{3}$$

where A and b are parameters.

We can find A from normalization:

$$\begin{aligned}
|A|^2\int_{-\infty}^{\infty}\frac{dx}{\left(x^2+b^2\right)^2} &= 1 &(4)\\
\frac{|A|^2\pi}{2b^3} &= 1 &(5)\\
A &= \sqrt{\frac{2}{\pi}}b^{3/2} &(6)
\end{aligned}$$

where we used Maple for the integral.

Following the usual procedure, we calculate:

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

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

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

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

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

$$E_0 \le \frac{1}{\sqrt{2}}\hbar\omega \tag{11}$$

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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