VARIATIONAL PRINCIPLE AND HARMONIC OSCILLATOR: A MORE GENERAL TRIAL FUNCTION

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 7.12.

In an earlier problem we used the variational principle to estimate the ground state of the harmonic oscillator. The trial function there was

$$\psi=\frac{A}{x^{2}+b^{2}} \tag{1}$$

We can generalize this by introducing another parameter n:

$$\psi=\frac{A}{\left(x^{2}+b^{2}\right)^{n}} \tag{2}$$

As usual, we first normalize ψ:

$$A^{2}\int_{-\infty}^{\infty}\frac{dx}{\left(x^{2}+b^{2}\right)^{2n}}=1 \tag{3}$$

As far as I know, there is no simple version of this integral, so we can use tables or Maple to work it out:

$$\int_{-\infty}^{\infty}\frac{dx}{\left(x^{2}+b^{2}\right)^{2n}}=\frac{1}{b^{4n}}\frac{\sqrt{\pi}b\Gamma\left(2n-\frac{1}{2}\right)}{\Gamma\left(2n\right)} \tag{4}$$

where $\Gamma\left(x\right)$ is the gamma function. Therefore

$$A=b^{2n}\left[\frac{\Gamma\left(2n\right)}{\sqrt{\pi}b\Gamma\left(2n-\frac{1}{2}\right)}\right]^{1/2} \tag{5}$$

We can now calculate $\langle H\rangle$:

$$\langle H\rangle = \langle\psi|H|\psi\rangle = \langle\psi|T+V|\psi\rangle \tag{6}$$

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

$$= \frac{\hbar^2\left(16n^3-16n^2+3n\right)+b^4m^2\omega^2\left(4n+2\right)}{4mb^2\left(2n+1\right)\left(4n-3\right)} \tag{8}$$

where Maple was used to do the integrals and simplify the result.

We now take the derivative w.r.t. b and set to zero to find $\langle H\rangle_{min}$:

$$b_{min} = \left[\frac{n\left(16n^2-16n+3\right)}{2\left(2n+1\right)}\right]^{1/4}\sqrt{\frac{\hbar}{m\omega}} \tag{9}$$

$$= \left[\frac{n\left(4n-1\right)\left(4n-3\right)}{2\left(2n+1\right)}\right]^{1/4}\sqrt{\frac{\hbar}{m\omega}} \tag{10}$$

This gives an upper bound of

$$\langle H\rangle_{min} = \sqrt{\frac{n\left(4n-1\right)}{2\left(2n+1\right)\left(4n-3\right)}}\hbar\omega \tag{11}$$

For $n=1$ this reduces to the solution we had earlier:

$$\langle H\rangle_{n=1} = \frac{1}{\sqrt{2}}\hbar\omega \tag{12}$$

Also, as $n\to\infty$, this tends to the exact answer:

$$\lim_{n\to\infty}\langle H\rangle = \frac{1}{2}\hbar\omega \tag{13}$$

We can use the corollary to estimate the first excited state's energy. Since we know the exact ground state wave function ψ_0 of the harmonic oscillator is even (it's a Gaussian), we can take as a trial function the odd function:

$$\psi = \frac{Bx}{\left(x^2+b^2\right)^n} \tag{14}$$

Following the same procedure as above, we get for B:

$$B^2 \int_{-\infty}^{\infty} \frac{x^2 dx}{\left(x^2+b^2\right)^{2n}} = 1 \tag{15}$$

$$B = b^{2n} \left[\frac{2\Gamma(2n)}{\sqrt{\pi} b^3 \Gamma\left(2n-\frac{3}{2}\right)} \right]^{1/2} \tag{16}$$

For the energy, we get

(17)

$$\langle H \rangle = \langle \psi | H | \psi \rangle = \langle \psi | T + V | \psi \rangle$$

$$= B^2 \int_{-\infty}^{\infty} \left[-\frac{\hbar^2}{2m} \frac{x}{\left(x^2+b^2\right)^n} \frac{d^2}{dx^2} \left(\frac{x}{\left(x^2+b^2\right)^n} \right) + \frac{m\omega^2 x^4}{2\left(x^2+b^2\right)^{2n}} \right] dx \tag{18}$$

$$= 3 \frac{\hbar^2\left(16n^3-32n^2+15n\right) + b^4 m^2 \omega^2 (4n+2)}{4mb^2 (2n+1)(4n-5)} \tag{19}$$

Finding the b that minimizes $\langle H \rangle$ gives

$$b_{min} = \left[\frac{n\left(16n^2-32n+15\right)}{2(2n+1)} \right]^{1/4} \sqrt{\frac{\hbar}{m\omega}} \tag{20}$$

$$= \left[\frac{n(4n-5)(4n-3)}{2(2n+1)} \right]^{1/4} \sqrt{\frac{\hbar}{m\omega}} \tag{21}$$

$$\langle H \rangle_{min} = \sqrt{\frac{n(4n-3)}{2(2n+1)(4n-5)}} \hbar\omega \tag{22}$$

Again, for large n we tend to the exact answer:

$$\lim_{n\to\infty} \langle H \rangle_{min} = \frac{3}{2}\hbar\omega \tag{23}$$

To see why the limit of large n gives the exact answer, we can use Maple's limit function to find the limit of the trial functions for large n. We find (remembering to substitute for A and B by their expressions from above):

$$\lim_{n\to\infty} \frac{A}{\left(x^2+b^2\right)^n} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar} = \psi_0 \tag{24}$$

$$\lim_{n\to\infty} \frac{Bx}{\left(x^2+b^2\right)^n} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \sqrt{\frac{2m\omega}{\hbar}} x e^{-m\omega x^2/2\hbar} = \psi_1 \tag{25}$$

That is, in the limit of large n, both trial functions tend to the exact wave functions.