

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

$$(0.1) \quad \psi = \frac{A}{x^2 + b^2}$$

We can generalize this by introducing another parameter n :

$$(0.2) \quad \psi = \frac{A}{(x^2 + b^2)^n}$$

As usual, we first normalize ψ :

$$(0.3) \quad A^2 \int_{-\infty}^{\infty} \frac{dx}{(x^2 + b^2)^{2n}} = 1$$

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

$$(0.4) \quad \int_{-\infty}^{\infty} \frac{dx}{(x^2 + b^2)^{2n}} = \frac{1}{b^{4n}} \frac{\sqrt{\pi} b \Gamma(2n - \frac{1}{2})}{\Gamma(2n)}$$

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

$$(0.5) \quad A = b^{2n} \left[\frac{\Gamma(2n)}{\sqrt{\pi} b \Gamma(2n - \frac{1}{2})} \right]^{1/2}$$

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

(0.6)

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

$$(0.7) \quad = A^2 \int_{-\infty}^{\infty} \left[-\frac{\hbar^2}{2m} \frac{1}{(x^2 + b^2)^n} \frac{d^2}{dx^2} \left(\frac{1}{(x^2 + b^2)^n} \right) + \frac{m\omega^2 x^2}{2(x^2 + b^2)^{2n}} \right] dx$$

$$(0.8) \quad = \frac{\hbar^2 (16n^3 - 16n^2 + 3n) + b^4 m^2 \omega^2 (4n + 2)}{4mb^2 (2n + 1) (4n - 3)}$$

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 $\langle H \rangle_{min}$:

$$(0.9) \quad b_{min} = \left[\frac{n(16n^2 - 16n + 3)}{2(2n + 1)} \right]^{1/4} \sqrt{\frac{\hbar}{m\omega}}$$

$$(0.10) \quad = \left[\frac{n(4n - 1)(4n - 3)}{2(2n + 1)} \right]^{1/4} \sqrt{\frac{\hbar}{m\omega}}$$

This gives an upper bound of

$$(0.11) \quad \langle H \rangle_{min} = \sqrt{\frac{n(4n - 1)}{2(2n + 1)(4n - 3)}} \hbar\omega$$

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

$$(0.12) \quad \langle H \rangle_{n=1} = \frac{1}{\sqrt{2}} \hbar\omega$$

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

$$(0.13) \quad \lim_{n \rightarrow \infty} \langle H \rangle = \frac{1}{2} \hbar\omega$$

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:

$$(0.14) \quad \psi = \frac{Bx}{(x^2 + b^2)^n}$$

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

$$(0.15) \quad B^2 \int_{-\infty}^{\infty} \frac{x^2 dx}{(x^2 + b^2)^{2n}} = 1$$

$$(0.16) \quad B = b^{2n} \left[\frac{2\Gamma(2n)}{\sqrt{\pi} b^3 \Gamma(2n - \frac{3}{2})} \right]^{1/2}$$

For the energy, we get

$$(0.17)$$

$$(0.18) \quad \langle H \rangle = \langle \psi | H | \psi \rangle = \langle \psi | T + V | \psi \rangle$$

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

$$(0.19) \quad = 3 \frac{\hbar^2 (16n^3 - 32n^2 + 15n) + b^4 m^2 \omega^2 (4n + 2)}{4mb^2 (2n + 1) (4n - 5)}$$

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

$$(0.20) \quad b_{min} = \left[\frac{n(16n^2 - 32n + 15)}{2(2n + 1)} \right]^{1/4} \sqrt{\frac{\hbar}{m\omega}}$$

$$(0.21) \quad = \left[\frac{n(4n - 5)(4n - 3)}{2(2n + 1)} \right]^{1/4} \sqrt{\frac{\hbar}{m\omega}}$$

$$(0.22) \quad \langle H \rangle_{min} = \sqrt{\frac{n(4n - 3)}{2(2n + 1)(4n - 5)}} \hbar\omega$$

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

$$(0.23) \quad \lim_{n \rightarrow \infty} \langle H \rangle_{min} = \frac{3}{2} \hbar\omega$$

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):

$$(0.24) \quad \lim_{n \rightarrow \infty} \frac{A}{(x^2 + b^2)^n} = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-m\omega x^2/2\hbar} = \psi_0$$

$$(0.25) \quad \lim_{n \rightarrow \infty} \frac{Bx}{(x^2 + b^2)^n} = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \sqrt{\frac{2m\omega}{\hbar}} x e^{-m\omega x^2/2\hbar} = \psi_1$$

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