VARIATIONAL PRINCIPLE AND HARMONIC OSCILLATOR: A 
MORE GENERAL TRIAL FUNCTION

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

\[ \psi = A x^2 + b^2 \]  
(1)

We can generalize this by introducing another parameter \( n \):

\[ \psi = A (x^2 + b^2)^n \]  
(2)

As usual, we first normalize \( \psi \):

\[ A^2 \int_{-\infty}^{\infty} \frac{dx}{(x^2 + b^2)^{2n}} = 1 \]  
(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:

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

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

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

We can now calculate \( \langle H \rangle \):
\[ \langle H \rangle = \langle \psi | H | \psi \rangle = \langle \psi | T + V | \psi \rangle \]
\[ = A^2 \int_{-\infty}^{\infty} \left[ -\frac{\hbar^2}{2m} \frac{1}{(x^2 + b^2)^n} dx^2 \left( \frac{1}{(x^2 + b^2)^n} \right) + \frac{m\omega^2 x^2}{2(x^2 + b^2)^{2n}} \right] dx \]
\[ = \frac{\hbar^2 (16n^3 - 16n^2 + 3n) + b^4 m^2 \omega^2 (4n + 2)}{4mb^2 (2n + 1) (4n - 3)} \]

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 \( \langle H \rangle_{\text{min}} \):

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

This gives an upper bound of

\[ \langle H \rangle_{\text{min}} = \sqrt{\frac{n (4n - 1)}{2(2n + 1) (4n - 3)}} \hbar \omega \]

For \( n = 1 \) this reduces to the solution we had earlier:

\[ \langle H \rangle_{n=1} = \frac{1}{\sqrt{2}} \hbar \omega \]

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

\[ \lim_{n \to \infty} \langle H \rangle = \frac{1}{2} \hbar \omega \]

We can use the corollary to estimate the first excited state’s energy. Since we know the exact ground state wave function \( \psi_0 \) of the harmonic oscillator is even (it’s a Gaussian), we can take as a trial function the odd function:

\[ \psi = \frac{Bx}{(x^2 + b^2)^n} \]

Following the same procedure as above, we get for \( B \):
For the energy, we get

\[ \langle H \rangle = \langle \psi | H | \psi \rangle = \langle \psi | T + V | \psi \rangle \]  
\[ = B^2 \int_{-\infty}^{\infty} -\frac{\hbar^2}{2m} \frac{x}{(x^2 + b^2)^n} \frac{d^2}{dx^2} \left( \frac{x}{(x^2 + b^2)^n} \right) + \frac{m \omega^2 x^4}{2(x^2 + b^2)^{2n}} \]  
\[ = 3 \frac{\hbar^2 (16n^3 - 32n^2 + 15n) + b^4 m^2 \omega^2 (4n + 2)}{4mb^2 (2n + 1)(4n - 5)} \]  

Finding the \( b \) that minimizes \( \langle H \rangle \) gives

\[ b_{\text{min}} = \left[ \frac{n (16n^2 - 32n + 15)}{2 (2n + 1)} \right]^{1/4} \sqrt{\frac{\hbar}{m \omega}} \]  
\[ = \left[ \frac{n (4n - 5) (4n - 3)}{2 (2n + 1)} \right]^{1/4} \sqrt{\frac{\hbar}{m \omega}} \]  
\[ \langle H \rangle_{\text{min}} = \sqrt{\frac{n (4n - 3)}{2 (2n + 1)(4n - 5)}} \hbar \omega \]  

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

\[ \lim_{n \to \infty} \langle H \rangle_{\text{min}} = \frac{3}{2} \hbar \omega \]  

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):

\[ \lim_{n \to \infty} \frac{A}{(x^2 + b^2)^n} = \left( \frac{m \omega}{\pi \hbar} \right)^{1/4} e^{-m \omega x^2/2 \hbar} = \psi_0 \]  
\[ \lim_{n \to \infty} \frac{B x}{(x^2 + b^2)^n} = \left( \frac{m \omega}{\pi \hbar} \right)^{1/4} \sqrt{\frac{2m \omega}{\hbar}} x e^{-m \omega x^2/2 \hbar} = \psi_1 \]
That is, in the limit of large \( n \), both trial functions tend to the exact wave functions.