The Variational Method: Solved Problems

1. Compute the variational upper bounds for the ground state energy of a particle in the linear potential

\[ V(x) = \alpha |x| \]

and in the quartic potential

\[ V(x) = \alpha x^4 \]

using the Gaussian trial wavefunction

\[ \psi(x) = A e^{-bx^2}. \]

(a) Calculate the normalization constant \( A \). You should find \( A = (2b/\pi)^{1/4} \).

(b) Calculate the expectation value of the kinetic energy \( < T > \) for the Gaussian trial wavefunction. Explain why this calculation is the same for the linear and quartic potentials. You should find \( < T > = (\hbar^2b/2m) \).

(c) Calculate the expectation value of the potential energy \( < V > \) for the Gaussian trial wavefunction in the linear potential. You should find \( < V > = (\alpha/\sqrt{2\pi b}) \).

(d) Calculate the expectation value of the total energy \( < H > \) for the Gaussian trial wavefunction in the linear potential by adding the expectation values of the kinetic and potential energy \( < H > = < T > + < V > \). Then find the value of \( b \) that minimizes the expectation value of the total energy. You should find \( b = (m\alpha/\sqrt{2\pi}\hbar^2)^{1/4} \).

(e) Calculate the minimum of the expectation value of the total energy \( < H > \) for the Gaussian trial wavefunction in the linear potential. You should find \( < H >_{\text{min}} = \frac{3}{2}(\alpha^2\hbar^2/2\pi m)^{3/8} \).

(f) Calculate the expectation value of the potential energy \( < V > \) for the Gaussian trial wavefunction in the quartic potential. You should find \( < V > = (3\alpha/16b^2) \).

(g) Calculate the expectation value of the total energy \( < H > \) for the Gaussian trial wavefunction in the quartic potential by adding the expectation values of the kinetic and potential energy \( < H > = < T > + < V > \). Then find the value of \( b \) that minimizes the expectation value of the total energy. You should find \( b = (3\alpha m/4\hbar^2)^{1/4} \).

(h) Calculate the minimum of the expectation value of the total energy \( < H > \) for the Gaussian trial wavefunction in the quartic potential. You should find \( < H >_{\text{min}} = \frac{3}{4}(3\alpha^2\hbar^4/4m^2)^{3/4} \).
This problem involves the linear and quartic potentials and the Gaussian trial wavefunction:

\[ V(x) = \alpha |x| , \quad V(x) = \alpha x^4 \quad \text{and} \quad \psi(x) = Ae^{-bx^2}. \]

1.(a) First, calculate the normalization constant:

\[
< \psi | \psi > = 1 = \int_{-\infty}^{\infty} (Ae^{-bx^2})^* Ae^{-bx^2} \, dx = |A|^2 \int_{-\infty}^{\infty} e^{-2bx^2} \, dx = |A|^2 \sqrt{\frac{\pi}{2b}}
\]

\[
\Rightarrow A = \left( \frac{2b}{\pi} \right)^{1/4}.
\]

1.(b) Next, calculate the expectation value of the kinetic energy. Note that this will be exactly the same for both potentials, so we only need to do it once:

\[
\langle T \rangle = \langle \psi | T | \psi \rangle = \int_{-\infty}^{\infty} (Ae^{-bx^2})^* \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right) Ae^{-bx^2} \, dx = -|A|^2 \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} e^{-bx^2} \frac{d^2}{dx^2} e^{-bx^2} \, dx.
\]

We need the second derivative, so calculating we find

\[
\frac{d}{dx} e^{-bx^2} = -2bx e^{-bx^2}
\]

\[
\Rightarrow \frac{d^2}{dx^2} e^{-bx^2} = \frac{d}{dx}(-2bx e^{-bx^2}) = -2b \left( e^{-bx^2} + x(-2bx)e^{-bx^2} \right) = -2be^{-bx^2} + 4b^2 x^2 e^{-bx^2}.
\]

So, the expectation value of the kinetic energy becomes

\[
\langle T \rangle = -|A|^2 \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} e^{-bx^2} \left( -2be^{-bx^2} + 4b^2 x^2 e^{-bx^2} \right) \, dx
\]

\[
= -|A|^2 \frac{\hbar^2}{2m} \left[ -2b \int_{-\infty}^{\infty} e^{-2bx^2} \, dx + 4b^2 \int_{-\infty}^{\infty} x^2 e^{-bx^2} \, dx \right]
\]

\[
= - \left( \frac{2b}{\pi} \right)^{1/2} \frac{\hbar^2}{2m} \left[ -2b \sqrt{\frac{\pi}{2b}} + 4b^2 \frac{1}{2\sqrt{2b}} \sqrt{\frac{\pi}{2b}} \right]
\]

\[
= \frac{\hbar^2}{2m} \left[ -2b \sqrt{\frac{2b}{\pi}} \sqrt{\frac{\pi}{2b}} - b \sqrt{\frac{2b}{\pi}} \sqrt{\frac{\pi}{2b}} \right] = \frac{\hbar^2}{2m} \left[ 2b - b \right]
\]

\[
\Rightarrow \langle T \rangle = \frac{\hbar^2 b}{2m}.
\]
Note that the second integral can be evaluated using form 15.3.1.26 on page 249 of *Handbook of Mathematical Formulas and Integrals* by Jeffrey,
\[
\int_0^\infty x^{2n} e^{-px^2} \, dx = \frac{(2n-1) \cdots 5 \cdot 3 \cdot 1}{2(2p)^n} \sqrt{\frac{\pi}{p}} \quad \text{for} \quad p > 0, \quad \text{and} \quad n = 0, 1, 2, 3, \ldots
\]
For our integral, we have \( n = 1 \) and \( p = 2b \).

1.(c) Now consider the expectation value of the potential energy for \( V(x) = \alpha |x| \). We must calculate
\[
\langle V \rangle = \langle \psi | V | \psi \rangle = \int_{-\infty}^{\infty} \left( Ae^{-bx^2} \right)^* (\alpha |x|) Ae^{-bx^2} \, dx = \alpha A^2 \int_{-\infty}^{\infty} |x| e^{-2bx^2} \, dx = 2\alpha A^2 \int_0^\infty x e^{-2bx^2} \, dx.
\]
Form 15.3.1.27 on page 249 of *Handbook of Mathematical Formulas and Integrals* by Jeffrey, is
\[
\int_0^\infty x^{2n+1} e^{-px^2} \, dx = \frac{n!}{2p^{n+1}} \quad \text{for} \quad p > 0, \quad \text{and} \quad n = 0, 1, 2, 3, \ldots,
\]
which has the form of our \( \langle V \rangle \) integral with \( n = 0 \) and \( p = 2b \). So, we obtain
\[
2\alpha A^2 \int_0^\infty x e^{-2bx^2} \, dx = \frac{2\alpha A^2 (0!)}{2(2b)} = \frac{2\alpha}{4b} \sqrt{\frac{2b}{\pi}}
\]
\[
\Rightarrow \quad \langle V \rangle = \frac{\alpha}{\sqrt{2\pi b}}.
\]

1.(d) The expectation value of the total energy is the sum of the expectation values of the kinetic energy and the potential energy, so we have
\[
\langle H \rangle = \langle T \rangle + \langle V \rangle = \frac{\hbar^2 b}{2m} + \frac{\alpha}{\sqrt{2\pi b}}.
\]
The variational parameter in the trial wavefunction is \( b \). We will find the value of \( b \) which minimizes the total energy by taking the partial derivative with respect to \( b \), and then solving for the value of \( b \) which makes the derivative equal to zero:
\[
\frac{\partial}{\partial b} \left( \frac{\hbar^2 b}{2m} + \frac{\alpha}{\sqrt{2\pi}} b^{-1/2} \right) = \frac{\hbar^2}{2m} - \frac{1}{2} \frac{\alpha}{\sqrt{2\pi}} \frac{1}{b^{3/2}} = 0
\]
\[
\Rightarrow \quad b_0^{3/2} = \frac{\alpha}{2\sqrt{2\pi}} \frac{2m}{\hbar^2} = \frac{\alpha m}{2\pi \hbar^2}
\]
\[
\Rightarrow \quad b_0 = \left( \frac{\alpha m}{\sqrt{2\pi \hbar^2}} \right)^{2/3}.
\]
Here \( b_0 \) denotes the value of \( b \) which minimizes the total energy.

1.(e) Now that we have \( b_0 \), we can substitute it into the total energy expression to obtain the minimum energy \( \langle H \rangle \):

\[
\langle H \rangle = \langle T \rangle + \langle V \rangle = \frac{\hbar^2 b_0}{2m} + \frac{\alpha}{\sqrt{2\pi} b_0}
\]

\[
= \frac{\hbar^2}{2m} \left( \frac{\alpha m}{\sqrt{2\pi} \hbar^2} \right)^{2/3} + \frac{\alpha}{\sqrt{2\pi} b_0} \left[ \frac{2\pi}{\alpha m \sqrt{2\pi} \hbar^2} \right]^{1/2}
\]

\[
= \frac{\hbar^2}{m^{2/3}} \alpha^{2/3} m^{2/3} + \frac{\alpha^{1/6} \pi^{1/6} \hbar^{2/3}}{21/2 \pi^{1/2} \alpha^{1/3} m^{1/3}}
\]

\[
= \frac{1}{2} \frac{\hbar^2}{21/3 \pi^{1/3} m^{1/3}} + \frac{\hbar^{2/3} \alpha^{2/3}}{21/3 \pi^{1/3} m^{1/3}}
\]

\[
\Rightarrow \langle H \rangle_{\text{min}} = \frac{3}{2} \left( \frac{\hbar^2 \alpha^2}{2\pi m} \right)^{1/3}
\]

1.(f) Now we will go through the analogous procedure for the quartic potential. The expectation value of the potential energy \( V(x) = \alpha x^4 \), is given by

\[
\langle V \rangle = \langle \psi | V | \psi \rangle = \int_{-\infty}^{\infty} \left( A e^{-bx^2} \right)^* (\alpha x^4) A e^{-bx^2} dx = \alpha A^2 \int_{-\infty}^{\infty} x^4 e^{-2bx^2} dx
\]

\[
= 2\alpha A^2 \int_{0}^{\infty} x^4 e^{-2bx^2} dx.
\]

Form 15.3.1.26 on page 249 of Jeffrey is

\[
\int_{0}^{\infty} x^{2n} e^{-px^2} dx = \frac{(2n - 1) \cdots 5 \cdot 3 \cdot 1}{2(2p)^n} \sqrt{\frac{\pi}{p}} \quad \text{for} \quad p > 0, \quad \text{and} \quad n = 0, 1, 2, 3, \ldots
\]

This is the form of our \( \langle V \rangle \) integral, with \( n = 2 \) and \( p = 2b \). So our integral is given by

\[
2\alpha A^2 \int_{0}^{\infty} x^4 e^{-2bx^2} dx = \frac{2\alpha A^2}{2(2 \cdot 2b)^2} \sqrt{\frac{\pi}{2b}} = \frac{3\alpha}{16b^2} \sqrt{\frac{2b}{\pi}} \sqrt{\frac{\pi}{2b}}
\]

\[
\Rightarrow \langle V \rangle = \frac{3\alpha}{16b^2}.
\]

1.(g) Now the expectation value of the total energy is given by

\[
\langle H \rangle = \langle T \rangle + \langle V \rangle = \frac{\hbar^2 b}{2m} + \frac{3\alpha}{16b^2}.
\]
Minimizing the total energy by taking the partial derivative with respect to \( b \), and then finding the value of \( b \) that makes the derivative equal to zero, we find

\[
\frac{d}{db} \left( \frac{\hbar^2}{2m} b + \frac{3\alpha}{16} b^{-2} \right) = \frac{\hbar^2}{2m} - 2 \frac{3\alpha}{16} \frac{1}{b^3} = 0
\]

\[\Rightarrow \quad b^3_0 = \frac{3\alpha}{8} \frac{2m}{\hbar^2}\]

\[\Rightarrow \quad b_0 = \left( \frac{3\alpha m}{4\hbar^2} \right)^{1/3}.
\]

1.(h) Now, using \( b_0 \) to obtain the minimum value of \( \langle H \rangle \), we find

\[
\langle H \rangle_{\text{min}} = \langle T \rangle + \langle V \rangle = \frac{\hbar^2 b_0}{2m} + \frac{3\alpha}{16 b_0^2}
\]

\[= \frac{\hbar^2}{2m} \left( \frac{3\alpha m}{4\hbar^2} \right)^{1/3} + \frac{3\alpha}{16} \left( \frac{4\hbar^2}{3\alpha m} \right)^{2/3}
\]

\[= \frac{\hbar^2}{2m} \frac{3^{1/3} \alpha^{1/3} m^{1/3}}{4^{1/3} \hbar^{2/3}} + \frac{3\alpha}{16} \frac{4^{2/3} \alpha^{4/3} \hbar^{4/3}}{3^{2/3} \alpha^{2/3} m^{2/3}}
\]

\[= \frac{1}{2} \frac{\hbar^{4/3} 3^{1/3} \alpha^{1/3}}{m^{2/3} 4^{1/3}} + \frac{1}{4} \frac{\hbar^{4/3} 3^{2/3} \alpha^{2/3}}{m^{2/3} 4^{1/3}}
\]

\[\Rightarrow \quad \langle H \rangle_{\text{min}} = \frac{3}{4} \left( \frac{3\alpha \hbar^4}{4m^2} \right)^{1/3}.
\]
2. Compute the variational upper bound for the ground state energy of a particle in a harmonic oscillator using the trial wavefunction

$$\psi(x) = A \left(x^2 + b^2\right)^{-1}.$$ 

(a) Calculate the normalization constant $A$. You should find $A = \left(\frac{2b^3}{\pi}\right)^{\frac{1}{2}}$.

(b) Calculate the expectation value of the kinetic energy $< T >$ for this trial wavefunction. You should find $< T > = \left(\frac{\hbar^2}{4mb^2}\right)$.

(c) Calculate the expectation value of the potential energy $< V >$ for this trial wavefunction in the harmonic oscillator potential. You should find $< V > = \frac{1}{2}m\omega^2b^2$.

(d) Calculate the expectation value of the total energy $< H >$ for this trial wavefunction in the harmonic oscillator potential by adding the expectation values of the kinetic and potential energy $< H > = < T > + < V >$. Then find the value of $b$ that minimizes the expectation value of the total energy. You should find $b^2 = \left(\frac{\hbar}{\sqrt{2} m\omega}\right)$.

(e) Calculate the minimum of the expectation value of the total energy $< H >$ for this wavefunction in the harmonic oscillator potential. You should find $< H >_{\text{min}} = \left(\sqrt{2} \frac{\hbar\omega}{2}\right)$. Note that this upper bound is about 40 percent larger than the true ground state energy $\frac{1}{2}\hbar\omega$.

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2.(a) First, calculate the normalization constant for the wave function

$$\psi(x) = |\psi(x)| = A \left(x^2 + b^2\right)^{-1}$$

using $< \psi | \psi > = 1$

$$\Rightarrow \int_{-\infty}^{\infty} \left(\frac{A}{(x^2 + b^2)}\right)^* \left(\frac{A}{(x^2 + b^2)}\right) dx = |A|^2 \int_{-\infty}^{\infty} \frac{dx}{(x^2 + b^2)^2} = 2|A|^2 \int_{0}^{\infty} \frac{dx}{(x^2 + b^2)^2} = 1.$$ 

Form 15.1.1.16 on page 244 of Jeffrey is

$$\int_{0}^{\infty} \frac{dx}{(x^2 + a^2)(x^2 + c^2)} = \frac{\pi}{2ac(a + c)}$$ 

which is our integral with $a = c = b$. Here $b$ is the variational parameter in the trial wave function, and our integral is given by

$$2|A|^2 \int_{0}^{\infty} \frac{dx}{(x^2 + b^2)^2} = 2|A|^2 \frac{\pi}{2b \cdot b (b + b)} = \frac{|A|^2 \pi}{2b^3} = 1 \Rightarrow |A|^2 = \frac{2b^3}{\pi}$$

$$\Rightarrow A = \left(\frac{2b^3}{\pi}\right)^{1/2}.$$
2. (b) Next, find the expectation value of the kinetic energy

\[
\langle T \rangle = \langle \psi | T | \psi \rangle = \int_{-\infty}^{\infty} \left( \frac{A}{x^2 + b^2} \right) \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right) \left( \frac{A}{x^2 + b^2} \right) \ dx.
\]

Calculate the second derivative

\[
\frac{d}{dx} (x^2 + b^2)^{-1} = -1 (x^2 + b^2)^{-2} \ 2x = -2x (x^2 + b^2)^{-2}
\]

\[
\frac{d^2}{dx^2} (x^2 + b^2)^{-1} = \frac{d}{dx} \left( -2x (x^2 + b^2)^{-2} \right) = -2 (x^2 + b^2)^{-2} - 2x (x^2 + b^2)^{-3} (-2)(2x)
\]

\[
\Rightarrow \ \frac{d^2}{dx^2} (x^2 + b^2)^{-1} = -\frac{2}{(x^2 + b^2)^2} + \frac{8x^2}{(x^2 + b^2)^3}.
\]

Then our integral becomes

\[
\langle T \rangle = -\frac{A^2 \hbar^2}{2m} \int_{-\infty}^{\infty} \left( \frac{1}{x^2 + b^2} \right) \left( -\frac{2}{(x^2 + b^2)^2} + \frac{8x^2}{(x^2 + b^2)^3} \right) \ dx
\]

\[
= \frac{A^2 \hbar^2}{2m} \left[ -8 \int_{-\infty}^{\infty} \frac{x^2 \ dx}{(x^2 + b^2)^4} + 2 \int_{-\infty}^{\infty} \frac{dx}{(x^2 + b^2)^3} \right]
\]

\[
= \frac{A^2 \hbar^2}{2m} \left[ -16 \int_{0}^{\infty} \frac{x^2 \ dx}{(x^2 + b^2)^4} + 4 \int_{0}^{\infty} \frac{dx}{(x^2 + b^2)^3} \right]. \quad (1)
\]

Form 3.241.4 on page 292 of Table of Integrals, Series, and Products by Gradshteyn and Ryzhik is

\[
\int_{0}^{\infty} \frac{x^{\mu-1} \ dx}{(p + qx^n)^{n+1}} = \frac{1}{\nu p^{n+1}} \left( \frac{p}{q} \right)^{\mu/\nu} \frac{\Gamma \left( \frac{\mu}{\nu} \right) \Gamma \left( 1 + n - \frac{\mu}{\nu} \right)}{\Gamma(1 + n)} \quad \text{for} \quad 0 < \frac{\mu}{\nu} < n + 1, \ p \neq 0, \ \text{and} \ q \neq 0.
\]

We can use this form to evaluate both of the integrals in equation (1). For the first integral, the parameters are \( \mu = 3, \ \nu = 2, \ n = 3, \ q = 1, \ \text{and} \ p = b^2, \) so we obtain

\[
-16 \frac{A^2 \hbar^2}{2m} \int_{0}^{\infty} \frac{x^2 \ dx}{(x^2 + b^2)^4} = -16 \frac{A^2 \hbar^2}{2m} \left[ \frac{1}{2 \cdot b^{2(3+1)}} \left( \frac{b^2}{1} \right)^{3/2} \frac{\Gamma \left( \frac{3}{2} \right) \Gamma \left( 1 + 3 - \frac{3}{2} \right)}{\Gamma(1 + 3)} \right]
\]

\[
= -4 \frac{A^2 \hbar^2}{mb^5} \cdot \frac{b^3}{\Gamma(4)} \cdot \frac{\Gamma \left( \frac{3}{2} \right) \Gamma \left( \frac{5}{2} \right)}{\Gamma(4)} = -4 \frac{A^2 \hbar^2}{mb^5} \cdot \frac{\Gamma \left( \frac{3}{2} \right) \Gamma \left( \frac{5}{2} \right)}{\Gamma(4)}.
\]

To evaluate the \( \Gamma \) functions, remember that

\[
\Gamma \left( \frac{1}{2} \right) = \sqrt{\pi}, \ \Gamma(1) = \Gamma(2) = 1, \ \Gamma(n + 1) = n!, \ \text{and} \ \Gamma \left( n + \frac{1}{2} \right) = \frac{(2n - 1) \cdots 5 \cdot 3 \cdot 1}{2^n} \Gamma \left( \frac{1}{2} \right),
\]

so we obtain

\[
-4 \frac{A^2 \hbar^2}{mb^5} \cdot \frac{\Gamma \left( \frac{3}{2} \right) \Gamma \left( \frac{5}{2} \right)}{\Gamma(4)} = -4 \frac{A^2 \hbar^2}{mb^5} \cdot \frac{(1 \cdot \sqrt{\pi})}{3 \cdot 2 \cdot 1} = -\pi A^2 \hbar^2 \frac{4}{4mb^5}. \quad (2)
\]
We could also evaluate the second integral in equation (1) using the same form, but it is actually a simpler integral, and there is a simpler form in Gradshteyn and Ryzhik, namely form 3.249.1 on page 294, which is

\[ \int_0^\infty \frac{dx}{(x^2 + a^2)^n} = \frac{(2n - 3)!!}{2(2n - 2)!!} \frac{\pi}{a^{2n-1}}. \]

Here the double factorial means the product of only the odd factors, so for example \((2n + 1)!! = 1 \cdot 3 \cdot 5 \cdots (2n + 1)\). Our second integral becomes

\[ \frac{4A^2 h^2}{2m} \int_0^\infty \frac{dx}{(x^2 + b^2)^3} = \frac{2A^2 h^2}{m} \frac{3 \cdot 1}{2(4 \cdot 2)} \cdot \frac{\pi}{b^5} = \frac{3\pi A^2 h^2}{8mb^5}. \]

Adding these two integrals, we obtain the expectation value of the kinetic energy

\[ \langle T \rangle = -\frac{\pi A^2 h^2}{4mb^5} + \frac{3\pi A^2 h^2}{8mb^5} = 2b^3 \left( -\frac{2}{8mb^5} + \frac{3}{8mb^5} \right) \]

\[ \Rightarrow \quad \langle T \rangle = \frac{h^2}{4mb^2}. \]

2.(c) Now we must calculate the expectation value of the potential energy for \(V(x) = \frac{1}{2} m\omega^2 x^2\), which is given by

\[ \langle V \rangle = \langle \psi | V | \psi \rangle = \int_{-\infty}^\infty \left( \frac{A}{x^2 + b^2} \right) \left( \frac{1}{2} m\omega^2 x^2 \right) \left( \frac{A}{x^2 + b^2} \right) \ dx \]

\[ = \frac{A^2 m\omega^2}{2} \int_{-\infty}^\infty \frac{x^2 \ dx}{(x^2 + b^2)^3} \]

\[ = A^2 m\omega^2 \int_0^\infty \frac{x^2 \ dx}{(x^2 + b^2)^2}. \]

We can evaluate this integral using form 3.241.4 from Gradshteyn and Ryzhik, with the parameters \(\mu = 3\), \(\nu = 2\), \(n = 1\), \(q = 1\), and \(p = b^2\). Then we obtain

\[ A^2 m\omega^2 \int_0^\infty \frac{x^2 \ dx}{(x^2 + b^2)^2} = A^2 m\omega^2 \left( \frac{b^2}{1} \right)^{3/2} \frac{\Gamma \left( \frac{3}{2} \right) \Gamma \left( 1 + \frac{3}{2} \right)}{\Gamma(1 + 1)} \]

\[ = m\omega^2 \left( A^2 \right) \frac{b^3}{2 \cdot b^4} \frac{\Gamma \left( \frac{3}{2} \right) \Gamma \left( \frac{1}{2} \right)}{\Gamma(2)} \]

\[ = m\omega^2 \left( \frac{2b^3}{\pi} \right) \frac{b^3}{2 \cdot b^4} \frac{\Gamma \left( \frac{3}{2} \right) \Gamma \left( \frac{1}{2} \right)}{\Gamma(2)} \]

\[ = m\omega^2 b^2 \frac{\sqrt{\pi}}{\pi} \frac{\sqrt{\pi}}{1} \]

\[ \Rightarrow \quad \langle V \rangle = \frac{1}{2} m\omega^2 b^2. \]
2.(d) Now find the value of $b$ that minimizes the expectation value of the total energy:

\[
\frac{\partial}{\partial b} \left( \frac{\hbar^2}{4mb^2} + \frac{1}{2}m\omega^2b^2 \right) = -\frac{\hbar^2}{2mb^2} + m\omega^2b = 0
\]

\[\Rightarrow b_0^4 = \frac{\hbar^2}{2m^2\omega^2}\]

\[\Rightarrow b_0^2 = \frac{\hbar}{\sqrt{2}m\omega}.
\]

2.(e) The minimum expectation value of the total energy is given by

\[
\langle H \rangle_{\text{min}} = \frac{\hbar^2}{4mb_0^2} + \frac{1}{2}m\omega^2b_0^2
\]

\[= \frac{\hbar^2}{4m(h/\sqrt{2}m\omega)} + \frac{1}{2}m\omega^2(h/\sqrt{2}m\omega)\]

\[= \frac{\sqrt{2}\hbar\omega}{4} + \frac{h\omega}{2\sqrt{2}}\]

\[= \left( \frac{\sqrt{2}}{4} + \frac{\sqrt{2}}{4} \right) \hbar\omega = \frac{2\sqrt{2}}{4} \hbar\omega\]

\[\Rightarrow \langle H \rangle_{\text{min}} = \frac{\sqrt{2}}{2} \hbar\omega.
\]

We know that the ground state energy of the SHO is $\hbar\omega/2 = 0.5\hbar\omega$. From this problem, we see that the variational method only gives us an upper bound on the ground state energy, specifically in this case $\langle H \rangle_{\text{min}} = 0.71\hbar\omega$. Note, however, that if we used a Gaussian trial wave function, we would have obtained $\langle H \rangle_{\text{min}} = 0.5\hbar\omega$. 

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9
3. Generalize the ground state variational method to allow computation of variational upper bounds for the first excited state energy by using a trial wavefunction that is orthogonal to the ground state wavefunction.

(a) Modify the proof for the ground state case. First, expand the trial wavefunction $|\psi\rangle$ in energy eigenstates

$$|\psi\rangle = \sum_{n=0}^{\infty} c_n |\psi_n\rangle.$$  

Then use the fact that the trial wavefunction $|\psi\rangle$ is orthogonal to the exact ground state wavefunction $|\psi_0\rangle$, i.e., that

$$<\psi|\psi_0> = 0,$$

to rewrite the energy sum omitting the $n = 0$ ground state term—i.e., since $c_0 = 0$,

$$<H> = \sum_{n=1}^{\infty} E_n c_n^2.$$  

Finally, modify the derivation of the ground state variational principle.

(b) Calculate the normalization constant $A$ for the first excited state trial wavefunction

$$\psi(x) = A \, x \, e^{-bx^2}.$$  

You should find $A = \left[4b \, \sqrt{(2b/\pi)}\right]^{1/2} = \left[32b^3/\pi\right]^{1/4}$.

(c) Calculate the expectation value of the kinetic energy $<T>$ for this trial wavefunction. You should find $<T> = (3\hbar^2b/2m)$.

(d) Calculate the expectation value of the potential energy $<V>$ for this trial wavefunction in the harmonic oscillator potential. You should find $<V> = (3m\omega^2/8b)$.

(e) Calculate the expectation value of the total energy $<H>$ for this trial wavefunction in the harmonic oscillator potential by adding the expectation values of the kinetic and potential energy $<H> = <T> + <V>$. Then find the value of $b$ that minimizes the expectation value of the total energy. You should find $b = (m\omega/2\hbar)$.

(f) Calculate the minimum of the expectation value of the total energy $<H>$ for this wavefunction in the harmonic oscillator potential. You should find $<H>_{\text{min}} = 3/2 \hbar \omega$. Note that you obtain the exact energy of the first excited state because you “guessed” the exact excited state wavefunction!
3.(a) Any wave function can be expressed as a linear combination of the energy eigenstates, i.e.,

$$|\psi> = \sum_{n=0}^{\infty} c_n |\psi_n> = c_0 |\psi_0> + c_1 |\psi_1> + c_2 |\psi_2> + \cdots.$$ 

If we pick our trial wave function orthogonal to the ground state wave function, we have

$$<\psi |\psi_0> = 0, \text{ and } c_0 = 0.$$ 

Because they are orthogonal, the projection is zero. To show this, assume that the trial wave function is normalized, then we have

$$1 = <\psi |\psi> = \left(\sum_{m=0}^{\infty} c_m <\psi_m|\psi_m>\right) \left(\sum_{n=0}^{\infty} c_n |\psi_n>\right) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} c_m^* c_n <\psi_m |\psi_n>.$$ 

Next consider the inner product of the ground state and the first excited state trial wavefunction

$$<\psi |\psi_0> = 0 \Rightarrow \sum_{n=0}^{\infty} c_n <\psi_n |\psi_0> = 0.$$ 

Then, using the orthonormality, we find

$$\sum_{n=0}^{\infty} c_n^* c_0 <\psi_n |\psi_0> = \sum_{n=0}^{\infty} c_n^* c_0 \delta_{n0} = |c_0|^2 = 0$$

$$\Rightarrow c_0 = 0.$$ 

This means that the general expansion of our trial wavefunction can be written as usual, except that the sum starts at $n = 1$ instead of $n = 0$. For example, the normalization equation becomes

$$\sum_{m=0}^{\infty} \sum_{n=0}^{\infty} c_m^* c_n <\psi_m |\psi_n> = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} c_m^* c_n <\psi_m |\psi_n> = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} c_m^* c_n \delta_{mn} = \sum_{n=1}^{\infty} |c_n|^2 = 1.$$ 

Now we are ready to derive the inequality for the first excited state energy. Write down the expectation value of the energy:

$$\langle H \rangle = <\psi |H|\psi> = \left(\sum_{m=1}^{\infty} c_m <\psi_m|\psi_m>\right) H \left(\sum_{n=1}^{\infty} c_n |\psi_n>\right)$$

$$= \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} c_m^* c_n E_n <\psi_m |\psi_n> = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} c_m^* c_n E_n \delta_{mn}$$

$$= \sum_{n=1}^{\infty} |c_n|^2 E_n \geq E_1 \sum_{n=1}^{\infty} |c_n|^2 = E_1.$$ 

$$\Rightarrow \langle H \rangle \geq E_1.$$ 

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3.(b) Calculate the normalization constant for the first excited state trial wave function

\[ <\psi|\psi> = 1 \Rightarrow \int_{-\infty}^{\infty} (Axe^{-bx^2})^* (Axe^{-bx^2}) \, dx = |A|^2 \int_{-\infty}^{\infty} x^2 e^{-2bx^2} \, dx = 2|A|^2 \int_{0}^{\infty} x^2 e^{-2bx^2} \, dx. \]

One easy way to evaluate this integral is using form 15.3.1.26 from page 249 of Jeffrey, which we have encountered previously in Problem 1. Then we have

\[ \int_{0}^{\infty} x^{2n} e^{-px^2} \, dx = \frac{(2n-1) \cdots 5 \cdot 3 \cdot 1}{2(2p)^n} \sqrt{\frac{\pi}{p}} \quad \text{for} \quad p > 0, \quad \text{and} \quad n = 0, 1, 2, 3, \ldots . \]

For our integral, the parameters are \( n = 1 \) and \( p = 2b \), so we obtain

\[ 2|A|^2 \int_{0}^{\infty} x^2 e^{-2bx^2} \, dx = 2|A|^2 \left( \frac{2(1)}{2(2\cdot2b)^1} \right) \sqrt{\frac{\pi}{2b}} = \frac{|A|^2}{4b} \sqrt{\frac{\pi}{2b}} = 1 \]

\[ \Rightarrow |A|^2 = 4b \sqrt{\frac{2b}{\pi}} = 4 \sqrt{\frac{2b^3}{\pi}} \quad \text{or} \quad A = 2 \left( \frac{2b^3}{\pi} \right)^{1/4}. \]

3.(c) Calculate the expectation value for the kinetic energy

\[ \langle T \rangle = <\psi|T|\psi(x)> = \int_{-\infty}^{\infty} (Axe^{-bx^2})^* \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right) (Axe^{-bx^2}) \, dx \]

\[ = -\frac{|A|^2 \hbar^2}{2m} \int_{-\infty}^{\infty} (xe^{-bx^2})^* \left( \frac{d^2}{dx^2} (xe^{-bx^2}) \right) \, dx. \]

Again, we need the second derivative of the trial wave function. This is given by

\[ \frac{d^2}{dx^2} (xe^{-bx^2}) = \frac{d}{dx} \left( \frac{d}{dx} (xe^{-bx^2}) \right) = \frac{d}{dx} \left( e^{-bx^2} - 2bx^2 e^{-bx^2} \right) \]

\[ = -2bxe^{-bx^2} - 4bx^2 e^{-bx^2} + 4b^2 x^3 e^{-bx^2} \]

\[ = -6bxe^{-bx^2} + 4b^2 x^3 e^{-bx^2}. \]

So, the expectation value of kinetic energy is given by

\[ \langle T \rangle = -\frac{|A|^2 \hbar^2}{2m} \int_{-\infty}^{\infty} (xe^{-bx^2})^* \left( -6bxe^{-bx^2} + 4b^2 x^3 e^{-bx^2} \right) \, dx \]

\[ = \frac{|A|^2 \hbar^2}{2m} \left[ 6b \int_{-\infty}^{\infty} x^2 e^{-2bx^2} \, dx - 4b^2 \int_{-\infty}^{\infty} x^4 e^{-2bx^2} \, dx \right] \]

\[ = \frac{|A|^2 \hbar^2}{m} \left[ 6b \int_{0}^{\infty} x^2 e^{-2bx^2} \, dx - 4b^2 \int_{0}^{\infty} x^4 e^{-2bx^2} \, dx \right]. \]
We can evaluate both integrals using the same general integral from Jeffrey used in part b. For the first integral, \( n = 1 \) and \( p = 2b \), and for the second integral, \( n = 2 \) and \( p = 2b \). Then the expectation value of the kinetic energy becomes

\[
\langle T \rangle = \frac{|A|^2 \hbar^2}{m} \left[ 6b \left( \frac{(2(1) - 1)!!}{2(2 \cdot 2b)^1} \sqrt{\frac{\pi}{2b}} \right) - 4b^2 \left( \frac{(2(2) - 1)!!}{2 \cdot (2 \cdot 2b)^2} \sqrt{\frac{\pi}{2b}} \right) \right]
\]

\[
= \frac{\hbar^2}{m} \left( |A|^2 \right) \left[ 6b \left( \frac{1}{8b} \sqrt{\frac{\pi}{2b}} \right) - 4b^2 \left( \frac{3 \cdot 1}{32b^2} \sqrt{\frac{\pi}{2b}} \right) \right]
\]

\[
= \frac{\hbar^2}{m} \left( 4b \sqrt{\frac{2b}{\pi}} \right) \sqrt{\frac{\pi}{2b}} \left[ \frac{3}{4} - \frac{3}{8} \right]
\]

\[
\Rightarrow \langle T \rangle = \frac{3\hbar^2 b}{2m}.
\]

3.(d) Next, calculate the expectation value of the potential energy

\[
\langle V \rangle = \langle \psi | V | \psi(x) \rangle = \int_{-\infty}^{\infty} (Axe^{-bx^2})^* \left( \frac{1}{2} m \omega^2 x^2 \right) (Axe^{-bx^2}) \, dx
\]

\[
= \frac{|A|^2 m \omega^2}{2} \int_{-\infty}^{\infty} x^4 e^{-2bx^2} \, dx
\]

\[
= |A|^2 m \omega^2 \int_{0}^{\infty} x^4 e^{-2bx^2} \, dx
\]

\[
= |A|^2 m \omega^2 \left( \frac{(2(2) - 1)!!}{2 \cdot (2 \cdot 2b)^2} \sqrt{\frac{\pi}{2b}} \right)
\]

\[
= m \omega^2 \cdot 4b \sqrt{\frac{2b}{\pi}} \left( \frac{3 \cdot 1}{32b^2} \sqrt{\frac{\pi}{2b}} \right) = m \omega^2 \cdot \frac{12}{32b}
\]

\[
\Rightarrow \langle V \rangle = \frac{3m \omega^2}{8b}.
\]

3.(e) The expectation value of the total energy is the sum of the kinetic and potential energies, so

\[
\langle H \rangle = \langle T \rangle + \langle V \rangle = \frac{3\hbar^2 b}{2m} + \frac{3m \omega^2}{8b}.
\]

To find the value of \( b \) that minimizes the expectation value of total energy, we differentiate with respect to the variational parameter, set the resulting expression equal to zero, and solve for \( b_0 \) as before, \( i.e., \)

\[
\frac{\partial}{\partial b} \left( \frac{3\hbar^2 b}{2m} + \frac{3m \omega^2}{8b} \right) = \frac{3\hbar^2}{2m} - \frac{3m \omega^2}{8} b^{-2} = 0
\]

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\[ b_0^2 = \frac{3m\omega^2}{8} \frac{2m}{3\hbar^2} = \frac{m^2\omega^2}{4\hbar^2} \]

\[ \Rightarrow b_0 = \frac{m\omega}{2\hbar} \]

3.(f) The minimum value of the total energy is obtained by substituting \( b_0 \) into the equation for \( \langle H \rangle \). We find

\[ \langle H \rangle_{\text{min}} = \frac{3\hbar^2}{2m} b_0 + \frac{3m\omega^2}{8b_0} \]

\[ = \frac{3\hbar^2}{2m} \frac{2m\omega}{2\hbar} + \frac{3m\omega^2}{8(m\omega/2\hbar)} = \frac{3}{4} \hbar \omega + \frac{3}{4} \hbar \omega \]

\[ \Rightarrow \langle H \rangle_{\text{min}} = \frac{3}{2} \hbar \omega \]

Note that this is the exact energy of the first excited state of the quantum mechanical SHO because we have successfully “guessed” the exact first excited state wavefunction.