The Variational Method: Solved Problems

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

$$V(x) = \alpha \ \mid x \mid$$

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 $A = (2b/\pi)^{\frac{1}{4}}$.

(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 $< T > = \ (\hbar^2 b/2m)$.

(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 $b = (m\alpha/\sqrt{2\pi}\hbar^2)^{\frac{2}{3}}$.

(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 $< H >_{min} = \ \frac{3}{2}(\alpha^2\hbar^2/2\pi m)^{\frac{1}{3}}$.

(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 $b = (3\alpha m/4\hbar^2)^{\frac{1}{3}}$.

(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 $< H >_{min} = \ \frac{3}{4}(3\alpha\hbar^4/4m^2)^{\frac{1}{3}}$.

This problem involves the linear and quartic potentials and the Gaussian trial wavefunction:

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

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

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

$$\boxed{\Rightarrow \quad A = \left(\frac{2b}{\pi}\right)^{1/4}.}$$

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:

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

We need the second derivative, so calculating we find

$$\frac{d}{dx} e^{-bx^2} = -2bxe^{-bx^2}$$

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

So, the expectation value of the kinetic energy becomes

$$\begin{aligned}
\langle T\rangle &= -|A|^2 \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} e^{-bx^2} \left(-2be^{-bx^2} + 4b^2x^2e^{-bx^2}\right) dx \\
&= -|A|^2 \frac{\hbar^2}{2m} \left[-2b \int_{-\infty}^{\infty} e^{-2bx^2}\, dx + 4b^2 \int_{-\infty}^{\infty} x^2 e^{-bx^2}\, dx\right] \\
&= -\left(\frac{2b}{\pi}\right)^{1/2} \frac{\hbar^2}{2m} \left[-2b\sqrt{\frac{\pi}{2b}} + 4b^2 \frac{1}{2(2b)} \sqrt{\frac{\pi}{2b}}\right] \\
&= \frac{\hbar^2}{2m} \left[2b\sqrt{\frac{2b}{\pi}}\sqrt{\frac{\pi}{2b}} - b\sqrt{\frac{2b}{\pi}}\sqrt{\frac{\pi}{2b}}\right] = \frac{\hbar^2}{2m}[2b - b]
\end{aligned}$$

$$\boxed{\Rightarrow \quad \langle T\rangle = \frac{\hbar^2 b}{2m}.}$$

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

$$\langle V\rangle = \langle\psi|V|\psi\rangle = \int_{-\infty}^{\infty}\left(Ae^{-bx^2}\right)^*(\alpha|x|)\,Ae^{-bx^2}\,dx = \alpha A^2\int_{-\infty}^{\infty}|x|e^{-2bx^2}\,dx = 2\alpha A^2\int_0^\infty xe^{-2bx^2}\,dx.$$

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 $<V>$ integral with $n=0$ and $p=2b$. So, we obtain

$$2\alpha A^2\int_0^\infty xe^{-2bx^2}\,dx = \frac{2\alpha A^2(0!)}{2(2b)} = \frac{2\alpha}{4b}\sqrt{\frac{2b}{\pi}}$$

$$\boxed{\Rightarrow \quad \langle V\rangle = \frac{\alpha}{\sqrt{2\pi b}}\ .}$$

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:

$$\frac{\partial}{\partial b}\left(\frac{\hbar^2}{2m}b + \frac{\alpha}{\sqrt{2\pi}}b^{-1/2}\right) = \frac{\hbar^2}{2m} - \frac{1}{2}\frac{\alpha}{\sqrt{2\pi}}\frac{1}{b^{3/2}} = 0$$

$$\Rightarrow \quad b_0^{3/2} = \frac{\alpha}{2\sqrt{2\pi}}\frac{2m}{\hbar^2} = \frac{\alpha m}{\sqrt{2\pi}\hbar^2}$$

$$\boxed{\Rightarrow \quad b_0 = \left(\frac{\alpha m}{\sqrt{2\pi}\hbar^2}\right)^{2/3}.}$$

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 $\langle H\rangle$:

$$\begin{aligned}\langle H\rangle = \langle T\rangle + \langle V\rangle &= \frac{\hbar^2 b_0}{2m} + \frac{\alpha}{\sqrt{2\pi b_0}} \\ &= \frac{\hbar^2}{2m}\left(\frac{\alpha m}{\sqrt{2\pi}\hbar^2}\right)^{2/3} + \frac{\alpha}{\left[2\pi\left(\frac{\alpha m}{\sqrt{2\pi}\hbar^2}\right)^{2/3}\right]^{1/2}} \\ &= \frac{\hbar^2\alpha^{2/3}m^{2/3}}{m 2^{4/3}\pi^{1/3}\hbar^{4/3}} + \frac{\alpha 2^{1/6}\pi^{1/6}\hbar^{2/3}}{2^{1/2}\pi^{1/2}\alpha^{1/3}m^{1/3}} \\ &= \frac{1}{2}\frac{\hbar^{2/3}\alpha^{2/3}}{2^{1/3}\pi^{1/3}m^{1/3}} + \frac{\hbar^{2/3}\alpha^{2/3}}{2^{1/3}\pi^{1/3}m^{1/3}}\end{aligned}$$

$$\boxed{\Rightarrow \quad \langle H\rangle_{\min} = \frac{3}{2}\left(\frac{\hbar^2\alpha^2}{2\pi m}\right)^{1/3}.}$$

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

$$\begin{aligned}\langle V\rangle = \langle\psi|V|\psi\rangle &= \int_{-\infty}^{\infty}\left(Ae^{-bx^2}\right)^*\left(\alpha x^4\right)Ae^{-bx^2}\,dx = \alpha A^2\int_{-\infty}^{\infty}x^4e^{-2bx^2}\,dx \\ &= 2\alpha A^2\int_0^{\infty}x^4e^{-2bx^2}\,dx\,.\end{aligned}$$

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 $<V>$ integral, with $n=2$ and $p=2b$. So our integral is given by

$$2\alpha A^2\int_0^{\infty}x^4e^{-2bx^2}\,dx = \frac{2\alpha A^2 3\cdot 1}{2(2\cdot 2b)^2}\sqrt{\frac{\pi}{2b}} = \frac{3\alpha}{16b^2}\sqrt{\frac{2b}{\pi}}\sqrt{\frac{\pi}{2b}}$$

$$\boxed{\Rightarrow \quad \langle V\rangle = \frac{3\alpha}{16b^2}\,.}$$

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

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

$$\Rightarrow \quad b_0^3 = \frac{3\alpha}{8}\frac{2m}{\hbar^2}$$

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

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

$$\begin{aligned}
\langle H \rangle_{\text{min}} = \langle T \rangle + \langle V \rangle &= \frac{\hbar^2 b_0}{2m} + \frac{3\alpha}{16 b_0^2} \\
&= \frac{\hbar^2}{2m}\left(\frac{3\alpha m}{4\hbar^2}\right)^{1/3} + \frac{3\alpha}{16}\left(\frac{4\hbar^2}{3\alpha m}\right)^{2/3} \\
&= \frac{\hbar^2}{2m}\frac{3^{1/3}\alpha^{1/3}m^{1/3}}{4^{1/3}\hbar^{2/3}} + \frac{3\alpha}{16}\frac{4^{2/3}\hbar^{4/3}}{3^{2/3}\alpha^{2/3}m^{2/3}} \\
&= \frac{1}{2}\frac{\hbar^{4/3}3^{1/3}\alpha^{1/3}}{m^{2/3}4^{1/3}} + \frac{1}{4}\frac{\hbar^{4/3}3^{1/3}\alpha^{1/3}}{m^{2/3}4^{1/3}}
\end{aligned}$$

$$\boxed{\Rightarrow \quad \langle H \rangle_{\text{min}} = \frac{3}{4}\left(\frac{3\alpha\hbar^4}{4m^2}\right)^{1/3}.}$$

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2. Compute the variational upper bound for the ground state energy of a particle in a harmonic oscillator using the trial wavefunction

$$\psi(x) = A\,[x^2 + b^2]^{-1}.$$

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

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

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

(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 $b^2 = (\hbar/\sqrt{2}\, m\omega)$.

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

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

$$2|A|^2 \int_0^{\infty} \frac{dx}{(x^2+b^2)^2} = \frac{2|A|^2\pi}{2b\cdot b\,(b+b)} = \frac{|A|^2\pi}{2b^3} = 1 \quad \Rightarrow \quad |A|^2 = \frac{2b^3}{\pi}$$

$$\boxed{\Rightarrow \quad A = \left(\frac{2b^3}{\pi}\right)^{1/2}.}$$

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

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

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

$$\Rightarrow \quad \frac{d^2}{dx^2}\left(x^2+b^2\right)^{-1} = \frac{-2}{\left(x^2+b^2\right)^2} + \frac{8x^2}{\left(x^2+b^2\right)^3}\ .$$

Then our integral becomes

$$\begin{aligned}\langle T\rangle &= -\frac{A^2\hbar^2}{2m}\int_{-\infty}^{\infty}\left(\frac{1}{(x^2+b^2)}\right)\left(\frac{-2}{\left(x^2+b^2\right)^2}+\frac{8x^2}{\left(x^2+b^2\right)^3}\right)dx \\ &= \frac{A^2\hbar^2}{2m}\left[-8\int_{-\infty}^{\infty}\frac{x^2\,dx}{\left(x^2+b^2\right)^4} + 2\int_{-\infty}^{\infty}\frac{dx}{\left(x^2+b^2\right)^3}\right] \\ &= \frac{A^2\hbar^2}{2m}\left[-16\int_0^{\infty}\frac{x^2\,dx}{\left(x^2+b^2\right)^4} + 4\int_0^{\infty}\frac{dx}{\left(x^2+b^2\right)^3}\right]. \qquad (1)\end{aligned}$$

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

$$\int_0^{\infty}\frac{x^{\mu-1}\,dx}{\left(p+qx^{\nu}\right)^{n+1}} = \frac{1}{\nu p^{n+1}}\left(\frac{p}{q}\right)^{\mu/\nu}\frac{\Gamma\left(\frac{\mu}{\nu}\right)\Gamma\left(1+n-\frac{\mu}{\nu}\right)}{\Gamma(1+n)} \quad \text{for} \quad 0<\frac{\mu}{\nu}<n+1,\ p\neq 0, \quad \text{and} \quad q\neq 0.$$

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

$$\begin{aligned}-16\frac{A^2\hbar^2}{2m}\int_0^{\infty}\frac{x^2\,dx}{\left(x^2+b^2\right)^4} &= -16\frac{A^2\hbar^2}{2m}\left[\frac{1}{2\cdot b^{2(3+1)}}\left(\frac{b^2}{1}\right)^{3/2}\frac{\Gamma\left(\frac{3}{2}\right)\Gamma\left(1+3-\frac{3}{2}\right)}{\Gamma(1+3)}\right] \\ &= -4\frac{A^2\hbar^2}{m}\cdot\frac{b^3}{b^8}\cdot\frac{\Gamma\left(\frac{3}{2}\right)\Gamma\left(\frac{5}{2}\right)}{\Gamma(4)} = -\frac{4A^2\hbar^2}{mb^5}\cdot\frac{\Gamma\left(\frac{3}{2}\right)\Gamma\left(\frac{5}{2}\right)}{\Gamma(4)}.\end{aligned}$$

To evaluate the Γ functions, remember that

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

so we obtain

$$-\frac{4A^2\hbar^2}{mb^5}\cdot\frac{\Gamma\left(\frac{3}{2}\right)\Gamma\left(\frac{5}{2}\right)}{\Gamma(4)} = -\frac{4A^2\hbar^2}{mb^5}\cdot\frac{\left(\frac{1\cdot\sqrt{\pi}}{2}\right)\left(\frac{3\cdot 1\cdot\sqrt{\pi}}{4}\right)}{3\cdot 2\cdot 1} = -\frac{\pi A^2\hbar^2}{4mb^5}. \qquad (2)$$

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

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

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

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

$$\boxed{\Rightarrow \quad \langle T\rangle = \frac{\hbar^2}{4mb^2} \; .}$$

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

$$\begin{aligned}\langle V\rangle = \langle\psi|V|\psi\rangle &= \int_{-\infty}^\infty \left(\frac{A}{(x^2+b^2)}\right)\left(\frac{1}{2}m\omega^2x^2\right)\left(\frac{A}{(x^2+b^2)}\right)dx\\ &= \frac{A^2m\omega^2}{2}\int_{-\infty}^\infty \frac{x^2\,dx}{(x^2+b^2)^2}\\ &= A^2m\omega^2\int_0^\infty \frac{x^2\,dx}{(x^2+b^2)^2}.\end{aligned}$$

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

$$\begin{aligned}A^2m\omega^2\int_0^\infty \frac{x^2\,dx}{(x^2+b^2)^2} &= \frac{A^2m\omega^2}{2\cdot b^{2(1+1)}}\left(\frac{b^2}{1}\right)^{3/2}\frac{\Gamma\left(\frac{3}{2}\right)\Gamma\left(1+1-\frac{3}{2}\right)}{\Gamma(1+1)}\\ &= m\omega^2\left(A^2\right)\frac{b^3}{2\cdot b^4}\frac{\Gamma\left(\frac{3}{2}\right)\Gamma\left(\frac{1}{2}\right)}{\Gamma(2)}\\ &= m\omega^2\left(\frac{2b^3}{\pi}\right)\frac{b^3}{2\cdot b^4}\frac{\Gamma\left(\frac{3}{2}\right)\Gamma\left(\frac{1}{2}\right)}{\Gamma(2)}\\ &= \frac{m\omega^2b^2}{\pi}\frac{\frac{\sqrt{\pi}}{2}\sqrt{\pi}}{1}\end{aligned}$$

$$\boxed{\Rightarrow \quad \langle V\rangle = \frac{1}{2}m\omega^2b^2.}$$

2.(d) Now find the value of b that minimizes the expectation value of the total energy:

$$\frac{\partial}{\partial b}\left(\frac{\hbar^2}{4mb^2} + \frac{1}{2}m\omega^2 b^2\right) = -\frac{\hbar^2}{2mb^3} + m\omega^2 b = 0$$

$$\Rightarrow \quad b_0^4 = \frac{\hbar^2}{2m^2\omega^2}$$

$$\boxed{\Rightarrow \quad b_0^2 = \frac{\hbar}{\sqrt{2}\, m\omega}\,.}$$

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

$$\begin{aligned}
\langle H\rangle_{\min} &= \frac{\hbar^2}{4mb_0^2} + \frac{1}{2}m\omega^2 b_0^2 \\
&= \frac{\hbar^2}{4m(\hbar/\sqrt{2}m\omega)} + \frac{1}{2}m\omega^2(\hbar/\sqrt{2}m\omega) \\
&= \frac{\sqrt{2}\hbar\omega}{4} + \frac{\hbar\omega}{2\sqrt{2}} \\
&= \left(\frac{\sqrt{2}}{4} + \frac{\sqrt{2}}{4}\right)\hbar\omega = \frac{2\sqrt{2}}{4}\hbar\omega
\end{aligned}$$

$$\boxed{\Rightarrow \quad \langle H\rangle_{\min} = \frac{\sqrt{2}}{2}\hbar\omega\,.}$$

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 $\langle H\rangle_{\min} = 0.71\,\hbar\omega$. Note, however, that if we used a Gaussian trial wave function, we would have obtained $\langle H\rangle_{\min} = 0.5\,\hbar\omega$.

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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 $\mid \psi >$ in energy eigenstates

$$\mid \psi > = \sum_{n=0}^{\infty} c_n \mid \psi_n > .$$

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

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

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 $< T > = \; (3\hbar^2 b/2m)$.

(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 $< H >_{min} = \frac{3}{2}\hbar\omega$. 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

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

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

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

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

$$<\!\psi|\psi_0\!> = 0 \quad \Rightarrow \quad \sum_{n=0}^{\infty} c_n \langle\psi_n|c_0\psi_0\rangle = 0.$$

Then, using the orthonormality, we find

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

$$\Rightarrow \quad c_0 = 0.$$

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

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

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

$$\begin{aligned}
\langle H\rangle = \,<\!\psi|H|\psi\!> \,&= \left(\sum_{m=1}^{\infty} c_m\langle\psi_m|\right) H \left(\sum_{n=1}^{\infty} c_n|\psi_n\rangle\right) \\
&= \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} c_m^* c_n E_n <\!\psi_m|\psi_n\!> \,= \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} c_m^* c_n E_n \delta_{mn} \\
&= \sum_{n=1}^{\infty} |c_n|^2 E_n \geq E_1 \sum_{n=1}^{\infty} |c_n|^2 = E_1 \, .
\end{aligned}$$

$$\boxed{\Rightarrow \quad \langle H\rangle \geq E_1 \, .}$$

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

$$<\psi|\psi> = 1 \;\Rightarrow\; \int_{-\infty}^{\infty} \left(Axe^{-bx^2}\right)^* \left(Axe^{-bx^2}\right) dx = |A|^2 \int_{-\infty}^{\infty} x^2 e^{-2bx^2}\, dx = 2|A|^2 \int_0^{\infty} x^2 e^{-2bx^2}\, dx.$$

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

$$2|A|^2 \int_0^{\infty} x^2 e^{-2bx^2}\, dx = 2|A|^2 \frac{(2(1)-1)!!}{2(2\cdot 2b)^1}\sqrt{\frac{\pi}{2b}} = \frac{|A|^2}{4b}\sqrt{\frac{\pi}{2b}} = 1$$

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

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

$$\begin{aligned}\langle T\rangle = <\psi|T|\psi(x)> &= \int_{-\infty}^{\infty} \left(Axe^{-bx^2}\right)^* \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right) \left(Axe^{-bx^2}\right) dx \\ &= -\frac{|A|^2\hbar^2}{2m} \int_{-\infty}^{\infty} \left(xe^{-bx^2}\right)^* \left(\frac{d^2}{dx^2}(xe^{-bx^2})\right) dx.\end{aligned}$$

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

$$\begin{aligned}\frac{d^2}{dx^2}(xe^{-bx^2}) &= \frac{d}{dx}\left(\frac{d}{dx}(xe^{-bx^2})\right) = \frac{d}{dx}\left(e^{-bx^2} - 2bx^2 e^{-bx^2}\right) \\ &= -2bxe^{-bx^2} - 4bxe^{-bx^2} + 4b^2x^3e^{-bx^2} \\ &= -6bxe^{-bx^2} + 4b^2x^3e^{-bx^2}.\end{aligned}$$

So, the expectation value of kinetic energy is given by

$$\begin{aligned}\langle T\rangle &= -\frac{|A|^2\hbar^2}{2m} \int_{-\infty}^{\infty} \left(xe^{-bx^2}\right)^* \left(-6bxe^{-bx^2} + 4b^2x^3e^{-bx^2}\right) dx \\ &= \frac{|A|^2\hbar^2}{2m}\left[6b\int_{-\infty}^{\infty} x^2 e^{-2bx^2}\, dx - 4b^2 \int_{-\infty}^{\infty} x^4 e^{-2bx^2}\, dx\right] \\ &= \frac{|A|^2\hbar^2}{m}\left[6b\int_0^{\infty} x^2 e^{-2bx^2}\, dx - 4b^2 \int_0^{\infty} x^4 e^{-2bx^2}\, dx\right].\end{aligned}$$

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

$$\begin{aligned}
\langle T\rangle &= \frac{|A|^2\hbar^2}{m}\left[6b\left(\frac{(2(1)-1)!!}{2(2\cdot 2b)^1}\sqrt{\frac{\pi}{2b}}\right) - 4b^2\left(\frac{(2(2)-1)!!}{2\cdot(2\cdot 2b)^2}\sqrt{\frac{\pi}{2b}}\right)\right] \\
&= \frac{\hbar^2}{m}\left(|A|^2\right)\left[6b\left(\frac{1}{8b}\sqrt{\frac{\pi}{2b}}\right) - 4b^2\left(\frac{3\cdot 1}{32b^2}\sqrt{\frac{\pi}{2b}}\right)\right] \\
&= \frac{\hbar^2}{m}\left(4b\sqrt{\frac{2b}{\pi}}\right)\sqrt{\frac{\pi}{2b}}\left[\frac{3}{4}-\frac{3}{8}\right]
\end{aligned}$$

$$\Rightarrow \quad \langle T\rangle = \frac{3\hbar^2 b}{2m}\,.$$

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

$$\begin{aligned}
\langle V\rangle = <\psi|V|\psi(x)> &= \int_{-\infty}^{\infty}\left(Axe^{-bx^2}\right)^*\left(\frac{1}{2}m\omega^2x^2\right)\left(Axe^{-bx^2}\right)dx \\
&= \frac{|A|^2 m\omega^2}{2}\int_{-\infty}^{\infty} x^4 e^{-2bx^2}\,dx \\
&= |A|^2 m\omega^2\int_{0}^{\infty} x^4 e^{-2bx^2}\,dx \\
&= |A|^2 m\omega^2\left(\frac{(2(2)-1)!!}{2\cdot(2\cdot 2b)^2}\sqrt{\frac{\pi}{2b}}\right) \\
&= m\omega^2\cdot 4b\sqrt{\frac{2b}{\pi}}\left(\frac{3\cdot 1}{32b^2}\sqrt{\frac{\pi}{2b}}\right) = m\omega^2\cdot\frac{12}{32b}
\end{aligned}$$

$$\Rightarrow \quad \langle V\rangle = \frac{3m\omega^2}{8b}\,.$$

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.*,

$$\frac{\partial}{\partial b}\left(\frac{3\hbar^2}{2m}b + \frac{3m\omega^2}{8}b^{-1}\right) = \frac{3\hbar^2}{2m} - \frac{3m\omega^2}{8}b^{-2} = 0$$

$$\Rightarrow \quad b_0^2 = \frac{3m\omega^2}{8}\frac{2m}{3\hbar^2} = \frac{m^2\omega^2}{4\hbar^2}$$

$$\boxed{\Rightarrow \quad b_0 = \frac{m\omega}{2\hbar}\ .}$$

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

$$\begin{aligned}\langle H\rangle_{\rm min} &= \frac{3\hbar^2}{2m}b_0 + \frac{3m\omega^2}{8b_0} \\ &= \frac{3\hbar^2}{2m}\frac{m\omega}{2\hbar} + \frac{3m\omega^2}{8\,(m\omega/2\hbar)} = \frac{3}{4}\hbar\omega + \frac{3}{4}\hbar\omega\end{aligned}$$

$$\boxed{\Rightarrow \quad \langle H\rangle_{\rm min} = \frac{3}{2}\hbar\omega\ .}$$

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.
