Work in groups on these problems. You should try to answer the questions without referring to your textbook. If you get stuck, try asking another group for help.

Constructing the Variational Energy

The **variational method** is one way of finding approximations to the lowest energy eigenstate or ground state. The method consists of constructing a "trial wavefunction" depending on one or more parameters (e.g., $\langle \phi(\alpha, \beta, \gamma, \ldots) \rangle$) and then evaluating the "trial energy" (variational energy)

$$E_\phi(\alpha, \beta, \gamma, \ldots) = \frac{\langle \phi(\alpha, \beta, \gamma, \ldots) | \hat{H} | \phi(\alpha, \beta, \gamma, \ldots) \rangle}{\langle \phi(\alpha, \beta, \gamma, \ldots) | \phi(\alpha, \beta, \gamma, \ldots) \rangle} \label{W1}$$

where the Hamiltonian for the system. The wavefunction obtained by fixing the parameters to such values is then an approximation to the true wavefunction.

**Q1**

What are the limits on the number of parameters that a trial wavefunction $\langle \phi \rangle$ can have?

**Q2**

Identify which is hardest and why:

- Constructing the Hamiltonian for the system,
- Constructing the trial wavefunction for the system, or
- Evaluating the variational energy.

**Q3**

What is the origin of the denominator in Equation \ref{W1}? Does it always have to be in the equation? If not, when can you ignore it?
**Variational Theorem**

The variational theorem argues that this trial energy, \( E_\phi \) associated with the trial wavefunction for the known Hamiltonian is **always greater** than or equal to the true energy \( E_\psi \). Proof is not given.

\[ E_\phi (\alpha, \beta, \gamma, \ldots) \ge E_\psi \]

The variation method approximates the lowest energy eigenvalue, \( E_\psi \), and eigenfunction, \( \psi \), for a quantum mechanical system by guessing a function that is well-behaved over the limits of the system and minimizing the energy.

**Q4**

Under what condition(s) will this equation be true?

\[ E_\phi (\alpha, \beta, \gamma, \ldots) = E_\psi \]

**Q5**

Explain the power (utility) of Equation \ref{VM}. If this equation were not true, would we be able to approximate the true solutions to the Hamiltonian of the unsolveable system using the variational method?

**Minimizing the Variational Energy**

The variational theory argues that when the energy is minimized, then

\[ E_\phi (\alpha, \beta, \gamma, \ldots) \approx E_{\text{actual}} \]

and

\[ | \phi (\alpha, \beta, \gamma, \ldots) \rangle \approx | \psi \rangle \]

The better the trial wavefunction resembles the true wavefunction, the more accurate these approximations are.

**Q6**

Since one does not know the true eigenstate \(| \psi \rangle\), how would one conclude that the optimized trial wavefunction is a good approximation to the true wavefunction?
From the previous groupwork, we explore the trial wavefunction

\[
| \phi(x) (\beta) \rangle = \frac{1}{1+\beta x^2} \label{trial}
\]

where \( |\phi \rangle \) is the wavefunction that we guess and \( \hat{H} \) is the Hamiltonian for the system. The variational energy (from solving Equation \ref{W1}) was shown to be

\[
E_\phi (\beta) = \frac{\langle \phi | \hat{H} | \phi \rangle}{\langle \phi | \phi \rangle} = \frac{\hbar^2 \beta}{4 \mu} + \frac{k}{2 \beta}
\]

Some equations you may find useful for the following discussion:

\[
\hat{H}_{HO} = -\frac{\hbar^2}{2 \mu} \frac{d^2}{dx^2} + \frac{kx^2}{2}
\]

\[
E_{n,HO} = h\nu \left(n+\frac{1}{2}\right) = \hbar \omega \left(n+\frac{1}{2}\right)
\]

\[
| \psi(x) \rangle = \left(\frac{a}{\pi}\right)^{1/4} e^{-ax^2/2}
\]

Q7

Is the trial wavefunction (Equation \ref{trial}) normalized? And does it matter? Why or why not?

Q8

What is \( \frac{dE_\phi(\beta)}{d\beta} = 0 \) and why do you need to evaluate this derivative?

Q9

What value for \( \beta \) fulfills the minimized \( E_\phi (\beta) \)?

Q10

What is \( E_\phi(\beta) \) for the value for \( \beta \) that fulfills the minimization?
Q11
The variation method approximates the ground state energy for the system. What is the expression for the exact energy of the harmonic oscillator?

Q12
What is the value for the quantum number for the ground state of the harmonic oscillator?

Q13
What is the exact energy for the ground state of the harmonic oscillator?

Q14
Considering only energies, how well does the optimizing trial wavefunction (Equation \ref{trial}) approximate the lowest energy harmonic oscillator eigenstate?

Q15
How could you improve this approximation?

Q16
Given the knowledge you have of the true harmonic oscillator wavefunction, how well would a different trial wavefunction, |\phi(x) (\beta) \rangle = e^{\beta x^2} \rangle \rangle approximate the solution for the lowest energy state of the harmonic oscillator?