1) If \( \hat{A} f(x) = a f(x) \) then \( f(x) \) is an eigenfunction of the operator \( \hat{A} \) with eigenvalue \( a \) (a number).

Is \( f(x) = e^{-ax^2} \) an eigenfunction of the operator \( x \frac{d}{dx} \)? If so, what is the eigenvalue?

2) As we discussed in class, a real polyene differs from a particle in an infinite box in that the "walls" are not infinite. On the left are the energies and two lowest wavefunctions for a particle in an infinite box. The potential on the right is for a particle in a finite box. Draw the energies and wavefunctions for the two lowest states of the new potential. Please indicate how the energies and wavefunctions of the new potential are different from those of the original potential.

3) The wavefunctions of the particle in a box for a box of length \( L \) are

\[
\psi_n(x) = \sqrt{\frac{2}{L}} \sin \left( \frac{n\pi x}{L} \right) \quad \text{with} \quad n = 1, 2, 3, ...
\]

Useful integrals for this problem:

\[
\int \sin^2(ax) \, dx = \frac{1}{2} x - \frac{1}{4a} \sin(2ax)
\]

\[
\int x \sin^2(ax) \, dx = \frac{1}{4} x^2 - \frac{x}{4a} \sin(2ax) - \frac{1}{8a^2} \cos(2ax)
\]

a) For the ground state wavefunction, what is the probability that the particle is in the rightmost third of the box \( (x > 2L/3) \)?

b) Compute the expectation values \( \langle x \rangle \) and \( \langle x^2 \rangle \) for the state \( \psi_n \). Use these to determine the root-mean-square deviation of the particle’s position from its average:

\[
\Delta x = \left( \langle x^2 \rangle - \langle x \rangle^2 \right)^{\frac{1}{2}}
\]
c) Calculate the expectation values $\langle p \rangle$ and $\langle p^2 \rangle$ for $\psi_n$.

d) Use these to determine the root mean square deviation of the particle's momentum from its average:

$$\Delta p = \left( \langle p^2 \rangle - \langle p \rangle^2 \right)^{\frac{1}{2}}$$

e) The Heisenberg Uncertainty Principle states that, for any wavefunction,

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

Calculate $\Delta x \Delta p$ for the particle in a box and compare it to the Heisenberg value.

4) Shown below are cyclopropenyl cation and anion structures:

\[ \begin{array}{c}
\text{Cation} \\
\text{Anion}
\end{array} \]

\[ \begin{array}{c}
\Theta \\
\Theta
\end{array} \]

a) Using the mnemonic taught in class, construct the $\pi$- molecular orbitals for these molecules.

b) Using the energy levels as a guide, briefly explain which of these two molecules is more stable & why.

c) If you did not have these energy levels handy, you would have still predicted which of these molecules is more stable. How would you have done that? Briefly explain.

5) The following reaction is called the Nazarov cyclization, which involves a pericyclic reaction. Write a mechanism and explain the reason for the stereospecificity of the product.
In the above stereospecific reaction, \( X = H \) and \( Y = D \) in one product and \( X = D \) and \( Y = H \) in the other. Identify the products and give reasons for your prediction.

7) Consider a [4+ 4] cycloaddition reaction between two molecules of 1,3-butadiene.
   a) What is the product?
   b) Using the frontier orbital theory, predict whether the reaction is thermally or photochemically allowed.