In all cases indicate clearly how you get your answer. You only get partial credit for the correct result without explanation. This includes indicating conversions between different units. Carefully read the questions and verify you answer all parts of the question.

You have one hour and fifty minutes to answer the questions.

Table of Physical Constants:

\[ N_A = 6.02 \times 10^{23} \]
\[ e = 1.602 \times 10^{-19} \text{ C} \]
\[ R = 13.6 \text{ eV} = 2.18 \times 10^{-18} \text{ J} \]
\[ 1 \text{ eV} = 1.602 \times 10^{-19} \text{ J} = 8.066 \times 10^3 \text{ cm}^{-1} \]
\[ 4\pi\varepsilon_0 = 1.113 \times 10^{-10} \text{ C}^2 \text{ J}^{-1} \text{ m}^{-1} \]
\[ k_B = 1.381 \times 10^{-23} \text{ J K}^{-1} \]
\[ \pi = 3.14159 \]
\[ h = 6.63 \times 10^{-34} \text{ J sec} \]
\[ c = 2.998 \times 10^8 \text{ m/sec} \]
\[ a_0 = 0.529 \text{ Å} = 0.529 \times 10^{-10} \text{ m} \]
\[ m_e = 9.11 \times 10^{-31} \text{ kg} \]
\[ m_p = m_n = 1.67 \times 10^{-27} \text{ kg} \]
\[ 1 \text{ Å} = 1.0 \times 10^{-10} \text{ m} \]

1. **Rovibrational spectrum for \(^1H^{79}Br\) and \(^2D^{79}Br\) (30 %)**

a. The equilibrium bond distance (minimum of potential energy) for both \(^1H^{79}Br\) and \(^2D^{79}Br\) is 141.4 pm. Calculate the rotational constant in cm\(^{-1}\) for both species.

b. The vibrational wave number for \(^1H^{79}Br\) is 2649 cm\(^{-1}\). Calculate the corresponding value for \(^2D^{79}Br\).

c. Use the rigid rotor and harmonic oscillator approximation for \(^1H^{79}Br\). Calculate the 4 lowest lying rotational energy levels (in cm\(^{-1}\)) in both the \(v=0\) and \(v=1\) vibrational state. What is the degeneracy of each \((v,j)\) level?

d. Sketch a picture of the two sets of levels and clearly indicate the allowed transitions between the \(v=0\) and \(v=1\) levels.

e. Draw the spectrum to scale for the transitions between \(v=0\) and \(v=1\) levels.
   You can use the spacings between the spectral lines to characterize the energy differences (no need to report the full excitation energies).

f. For the real molecule the transitions are not equidistant. Provide a sketch how the energy levels are expected to change, indicating your reasoning. You can use formulas you need from your formula sheet. No need to derive.
2. Measurement of angular momentum for a particle on the ring (40 %).

The angular momentum operator associated with a particle on the ring is

\[ \hat{L}_z = -i\hbar \frac{\partial}{\partial \phi} \].

The boundary condition is the usual one for the particle on the ring.

We will perform a measurement of angular momentum on an ensemble described by the normalized function

\[ \Psi(\phi) = \frac{1}{5\sqrt{\pi}} \cos(\phi) + \frac{2}{5\sqrt{\pi}} \sin(2\phi) \]

a. Show that the functions \( \Phi_k(\phi) = \frac{1}{\sqrt{2\pi}} e^{ik\phi} \) are eigenfunctions of \( \hat{L}_z \). What are the corresponding eigenvalues?

b. What are the allowed values of \( k \), such that the wave functions satisfy the boundary conditions?

c. Show that the above eigenfunctions are normalized. Use integration over the interval \( \phi \in [0, 2\pi] \)

d. Show that the wave function \( \Psi(\phi) = \frac{1}{5\sqrt{\pi}} \cos(\phi) + \frac{2}{5\sqrt{\pi}} \sin(2\phi) \)

can be written as a sum \( \sum_k c_k \Phi_k(\phi) \). Explicitly: show

\[
\frac{1}{\sqrt{10}} \left( \frac{1}{\sqrt{2\pi}} e^{i\phi} - \frac{1}{\sqrt{2\pi}} e^{-i\phi} \right) + \frac{1}{\sqrt{10}} \left( \frac{2}{\sqrt{2\pi}} e^{2i\phi} + \frac{2}{\sqrt{2\pi}} e^{-2i\phi} \right) = \Psi(\phi)
\]

e. Given the above formula for the wave function that describes the sample being measured, what are the values one can measure for the angular momentum? What are the (non-zero) probabilities to find the values for the angular momentum?

f. What is the average value of the angular momentum (using your answer under e)?

g. Make a sketch of such a measurement, indicating the outcomes one would observe in this specific measurement (using your answer under e).
3. Two-dimensional harmonic oscillator (30 %).

Consider the Hamiltonian that describes harmonic motion in two dimensions (for example bending + symmetric stretch for water molecule).

\[ \hat{H} = \hbar \omega_x \left( \frac{p_x^2}{2} + \frac{x^2}{2} \right) + \hbar \omega_y \left( \frac{p_y^2}{2} + \frac{y^2}{2} \right) \]

The energy levels for this 2D harmonic oscillator are given by

\[ E_{n,m} = \hbar \omega_x (n + \frac{1}{2}) + \hbar \omega_y (m + \frac{1}{2}) \]

a. Consider the special case that \( \omega_y = 2 \omega_x \equiv 2 \omega \). Derive the simplified energy expression \( E_{n,m} = \frac{3}{2} \hbar \omega + \hbar \omega (n + 2m) \)

b. Using the simplified energy expression calculate the lowest 6 energy levels. Provide all of the corresponding quantum numbers \( n, m \) that yield each of your energies and indicate the degeneracy of each energy level.

c. The ladder operators for this Hamiltonian are defined as

\[ \hat{b}_x = \frac{1}{\sqrt{2}} (x + \frac{\partial}{\partial x}), \quad \hat{b}_x^\dagger = \frac{1}{\sqrt{2}} (x - \frac{\partial}{\partial x}) \]
\[ \hat{b}_y = \frac{1}{\sqrt{2}} (y + \frac{\partial}{\partial y}), \quad \hat{b}_y^\dagger = \frac{1}{\sqrt{2}} (y - \frac{\partial}{\partial y}) \]

Show by acting on the general function \( f(x,y) \) that \( [\hat{b}_x^\dagger, \hat{b}_y] = 0 \)

d. Using the ladder operators the Hamiltonian can be written as

\[ \hat{H} = \hbar \omega_x (\hat{b}_x^\dagger \hat{b}_x + \frac{1}{2}) + \hbar \omega_y (\hat{b}_y^\dagger \hat{b}_y + \frac{1}{2}) \]

The only non-zero commutators are

\[ [\hat{b}_x, \hat{b}_x^\dagger] = [\hat{b}_y, \hat{b}_y^\dagger] = 1 \]

Show that if \( \Psi(x,y) \) is an eigenfunction of \( \hat{H} \) with energy \( E \), then \( \hat{b}_x^\dagger \Psi \) is an eigenfunction of \( \hat{H} \) with eigenvalue \( E + \hbar \omega_x \). Likewise \( \hat{b}_y^\dagger \Psi \) is an eigenfunction of \( \hat{H} \) with eigenvalue \( E + \hbar \omega_y \) (no need to show).

Success!