BCHM485 Graded HW#2 (25 points) Due date/time: March 10, 2026 by 12noon

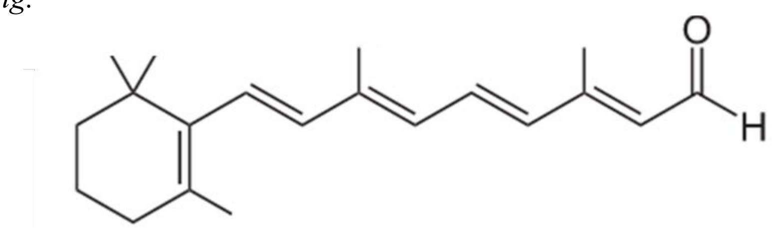
Problem 1 (9 points). Are the following wave functions orthogonal to each other? Support your answer by carrying out the appropriate integration.

(A) Wave functions of the harmonic oscillator corresponding to the states with $n = 1$ and $n = 2$.

(B) Wave functions of the harmonic oscillator corresponding to the states with $n = 1$ and $n = 3$.

(C) Wave functions of a particle on a ring corresponding to the states with $m_l = 3$ and $m_l = -3$.

Problem 2 (4 points). Consider electrons in the π-network in the retinal as particles in a 1-D box. For simplicity you can ignore carbons in the ring. Recall that each double-bonded carbon atom donates one electron to the π-network. The C=C bond length is 1.34 Å, the C–C bond length is 1.54 Å (1 Å = 10^{-10} m). What is the longest wavelength of light required to induce a transition from the ground state to one of the excited states of these electrons? *Briefly explain your reasoning.*



Problem 3 (12 points). Consider a hydrogen fluoride molecule absorbed on a flat surface. Assume that there is no coupling between the translational, vibrational, and rotational states, i.e. these motions are independent of each other. Here are some relevant characteristics of the molecule: the equilibrium bond length is 0.9168 Å (1Å=10^{-10} m), the force constant is 966 $\mathrm{N \cdot m^{-1}}$ (1 N=1 $\mathrm{kg \cdot m \cdot s^{-2}}$).

(A) Assume that vibrational states of the HF molecule can be described by the harmonic oscillator model. Calculate the quantum of energy that is absorbed when the molecule undergoes a transition from the ground state to the first excited vibrational state.

(B) What is the smallest quantum of energy that can be emitted by the HF molecule when it undergoes a transition from one rotational state to another? Assume that molecular rotations can be described by the particle on a ring model.

(C) How will your answers to questions A and B change if the hydrogen is substituted by deuteron? Support your answers by calculations. Assume that the equilibrium bond length and the force constant remain the same.

(D) When approximating the actual potential energy of inter-atomic interaction using the harmonic potential, we assumed that the amplitudes of bond vibrations are small compared to the equilibrium bond length. *Does this assumption hold for HF molecule?* To answer this question, estimate the vibrational amplitude of the HF molecule in the ground state by calculating $\Delta x = \sqrt{\langle x^2 \rangle}$, and compare your result with the equilibrium bond length.

The following table integrals might or might not turn useful:

$$\int_0^\infty e^{-ax^2} x^{2m}\, dx = \sqrt{\frac{\pi}{a}}\,\frac{1\cdot 3\cdot 5\cdot \ldots \cdot (2m-1)}{2^{m+1} a^m}\text{; (for } m \geq 1\text{)}$$

$$\int_0^\infty e^{-ax^2}\, dx = \frac{1}{2}\sqrt{\frac{\pi}{a}}$$

$$\int_0^\infty x^m e^{-ax}\, dx = \frac{m!}{a^{m+1}}$$