Each problem is worth 20 points. You may use a calculator, your text and notes but not a laptop. If you need extra room, you may use scratch paper, but put all final answers on the exam itself. Read all problems carefully. Set up problems methodically, show your work, and be neat. Partial credit will be given when it is possible for me to follow your work. If you are having trouble with a problem, go on to the next and come back. GOOD LUCK!

1. Electrons have been used to determine molecular structure by diffraction. Calculate the speed of an electron for which the wavelength is equal to a typical bond length, namely 0.150 nm.

\[
\rho = m v = \frac{\hbar}{2} \frac{kg \cdot m^2 \cdot s^{-2}}{6.626 \times 10^{-34} \cdot \surd 3} \\
\rho = \frac{h}{m \lambda} = \frac{0.150 \text{ nm}}{1.50 \times 10^{-10} \text{ m}} \\
\lambda = 9.109 \times 10^{-31} \text{ kg} \\
v = 4.849 \times 10^6 \text{ m/s}
\]
2. Consider the set of functions \( f_n(\omega) = Ne^{i\omega n} \), defined over the range \( 0 \leq \omega \leq 2\pi \) (\( \omega \) is an angle), and where \( n \) is an integer.

(a) Normalize the functions. That is, determine the value of the normalization constant \( N \). You must show your work for credit.

\[
\frac{1}{2\pi} \int_{0}^{2\pi} f_n^* f_n \, d\omega = N^2 \int_{0}^{2\pi} e^{-i\omega n} e^{i\omega n} \, d\omega = N^2 \int_{0}^{2\pi} 1 \, d\omega = 2\pi N^2 \Rightarrow N = \frac{1}{\sqrt{2\pi}}
\]

(b) Show that the set of functions \( \{f_n(\omega)\} \) is an orthonormal set. That is, show that \( f_n \) and \( f_m \) are orthogonal if \( m \neq n \) (you ensured normality in part (a)).

\[
\frac{1}{2\pi} \int_{0}^{2\pi} f_m^* f_n \, d\omega = \int_{0}^{2\pi} \left( \frac{1}{\sqrt{2\pi}} e^{-i\omega m} \right) \left( \frac{1}{\sqrt{2\pi}} e^{i\omega n} \right) \, d\omega = \frac{1}{2\pi} \int_{0}^{2\pi} e^{i(\omega n - \omega m)} \, d\omega
\]

If \( m = n \)

\[
\frac{1}{2\pi} \int_{0}^{2\pi} e^{i\omega} \, d\omega = \frac{1}{2\pi} \int_{0}^{2\pi} e^{i\omega} \, d\omega = 1 \quad \checkmark \text{normalized}
\]

If \( m \neq n \)

\[
\int_{0}^{2\pi} e^{i(n-m)\omega} \, d\omega = \frac{1}{2\pi i(n-m)} e^{i(n-m)\omega} \bigg|_{0}^{2\pi} = \frac{1}{2\pi i(n-m)} \left( e^{i2\pi(n-m)} - 1 \right) = \frac{1}{2\pi i(n-m)} \left( \cos 2\pi(n-m) + i \sin 2\pi(n-m) \right) = 0 \quad \checkmark \text{orthogonal}
\]

(Or use \( e^{2\pi i(n-m)} = 1 \) for \((n-m)\) an integer)
3. Below is depicted a one-dimensional potential energy barrier (thick lines). Three different energy levels are indicated by a, b, c.

(i) Sketch Re(\(\psi\)), that is, the real part of the wave function, for each of the energy levels, along the dotted line. Your sketches will be qualitative but should include as many features as possible from the given information.

(ii) Describe and explain any differences between the wave functions for the energy levels.

(iii) Identify energy levels and regions where tunneling occurs.

(iv) Discuss the phenomenon of tunneling and how it differs from classical behavior.
4. Consider a particle in a 2-dimensional, square box with sides of length L. The wave function will be \( \psi(x, y) = N \sin \left( \frac{n_x \pi x}{L} \right) \sin \left( \frac{n_y \pi y}{L} \right) \).

(a) Determine the normalization constant, N. You must show your reasoning for credit.

\[
1 = \int_{0}^{L} \int_{0}^{L} |\psi(x, y)|^2 \, dx \, dy = \int_{0}^{L} \int_{0}^{L} N^2 \sin^2 \left( \frac{n_x \pi x}{L} \right) \sin^2 \left( \frac{n_y \pi y}{L} \right) \, dx \, dy
\]

\[
\frac{1}{N^2} = \left( \int_{0}^{L} \sin^2 \left( \frac{n_x \pi x}{L} \right) \, dx \right) \left( \int_{0}^{L} \sin^2 \left( \frac{n_y \pi y}{L} \right) \, dy \right) = \frac{L^2}{4}
\]

\[N = \frac{2}{L}\]

(b) Determine the probability that, in the ground state, the particle will be found in the region \( L/4 < x < 3L/4 \text{ and } L/4 < y < 3L/4 \) (i.e., in shaded region in picture below).

\[
P = \frac{1}{L^2} \left( \int_{L/4}^{3L/4} \int_{L/4}^{3L/4} \sin^2 \left( \frac{n_x \pi x}{L} \right) \, dx \, dy \right)^2
\]

\[
= \frac{L^2}{8} \left( \frac{3L}{4} - \frac{L}{4} \sin \left( \frac{3\pi x}{L} \right) \right) \left( \frac{3L}{4} - \frac{L}{4} \sin \left( \frac{3\pi y}{L} \right) \right)
\]

\[
= \frac{L^2}{8} \left( \frac{3L}{4} \sin \left( \frac{3\pi y}{L} \right) - \sin \left( \frac{3\pi x}{L} \right) \sin \left( \frac{3\pi y}{L} \right) \right)
\]

\[
P = \frac{4}{L^2} \left( \frac{L}{4} + \frac{L}{2\ell} \sin \left( \frac{3\pi y}{L} \right) \right)^2 = \left( \frac{1}{2} + \frac{L}{2\ell} \sin \left( \frac{3\pi y}{L} \right) \right)^2 = 0.67
\]

(c) Specify the quantum numbers of all states with the given energy, and state the degeneracy (number of states with the same energy).

\[
(i) \quad E = \frac{5h^2}{8mL^2} \quad n_x, n_y = 1, 2 \text{ or } 2, 1 \quad \eta = 2
\]

\[
(ii) \quad E = \frac{3h^2}{8mL^2} \quad n_x, n_y = 2, 2 \quad \eta = 1
\]

"degeneracy"
5. The force constant for $^1\text{H}^{19}\text{F}$ is 966 N/m, and the average bond length is 0.092 nm.

(a) Calculate the zero point energy for $^1\text{H}^{19}\text{F}$, using the harmonic oscillator model.

$$2\hbar \omega = \frac{1}{2} \hbar \omega (\nu = 0)$$

$$\hbar \omega = \frac{\hbar}{2m} m = \frac{m_m m_F}{m_m + m_F} \cdot \frac{1.66 \times 10^{-27} \text{kg}}{1.66 \times 10^{-27} \text{kg}} = \frac{1.19}{20} \cdot 1.66 \times 10^{-27} \text{J}$$

$$2\hbar \omega = \frac{1}{2} \cdot 6.626 \times 10^{-34} \text{J} s \left( \frac{966 \text{N/m}}{1.66 \times 10^{-27} \text{kg}} \right) = 4.12 \times 10^{-20} \text{J}$$

(b) Determine the frequency of light needed to excite this molecule from the ground to the first excited vibrational state (via absorption of a photon of light).

$$h\nu = \Delta E = \frac{3}{2} \hbar \omega - \frac{1}{2} \hbar \omega = \frac{1}{2} \hbar \omega$$

$$\nu = \frac{1}{2\pi} \omega = \frac{1}{2\pi} (7.82 \times 10^{14} \text{ s}^{-1}) = 1.24 \times 10^{14} \text{ s}^{-1}$$ (cycles/s understood)

(c) Determine the most "most probable" bond distance(s) between the $^1\text{H}$ and $^{19}\text{F}$ atoms in a molecule of $^1\text{H}^{19}\text{F}$ in the second excited vibrational state ($\nu = 2$).

Most probable distance is when $U_2$ is maximum

$\nu = 2$

$U_2 = N^2 H_2(x) e^{-y^2}$

$u_2 = N^2 (4x^2 - 2)e^{-y^2}$

$$\frac{dU_2}{dx} = N^2 (2(4x^2 - 2)x) - 2y (4x^2 - 2)e^{-y^2}$$

$$0 = (4y^2 - 2)(y)(8 - 4y^2 + 2) = y(5 - 2y^2)(4y^2 - 2)$$

$$y = 0, \pm \sqrt{\frac{5}{2}}, \pm \sqrt{\frac{1}{2}}$$

Small maximum

$$x = 2y = \pm 2 \sqrt{\frac{5}{2}}$$

$$d = \left( \frac{1}{4\pi} \right)^{1/4} = 9.24 \times 10^{-8} \text{ m}$$

Most prob. dist. $= 0.092 \pm 0.015 = 0.107 \text{ nm}$

$x = \pm 0.015 \text{ nm}$