Exam 2, Chem 311, 60 minutes, Dr. H. Guo, Oct. 15, 2008

You are allowed to bring a one page sheet containing equations and a calculator

I. Answer the following multiple choice questions (5 pts each), choose one answer only!.

1. Which of the following is a Boson?
A. Electron.
B. Proton.
C. Photon.
D. The planet earth.
E. None of the above.

2. What is the unit of the wave function for a particle in a three-dimensional box?
A. meter^{-1}.
B. meter^{-2}.
C. meter^{-3}.
D. meter$^{-1/2}$.
E. meter$^{-3/2}$.

3. The probability to find a particle in the region [x, $x+dx$] is given by
A. $\Psi(x)$.
B. $\Psi(x)dx$.
C. $\Psi^*(x)dx$.
D. $\Psi^*(x)\Psi(x)$.
E. $\Psi^*(x)\Psi(x)dx$.

4. Which of the following equation represents the orthogonality of two one-dimensional wavefunctions?
A. $\phi^*\varphi = 0$.
B. $\phi^* = \varphi$.
C. $\int \phi^*\varphi dx = 0$.
D. $\int \phi^*\varphi dx = 1$.
E. $\phi^*\varphi dx = 0$.

5. Zero-point energy of a harmonic oscillator is
A. the energy of the lowest quantum state.
B. the potential energy at zero displacement.
C. the photon energy for the excitation of the ground state to the first excited state.
D. the vibrational frequency.
E. the energy gap between adjacent quantum levels.

II. Solve the following simple problems

6. (10 pts) Write down the Hamiltonian for a two-dimensional rigid rotor in polar coordinates. Prove that the wavefunction $\Psi = \frac{1}{\sqrt{2\pi}}\cos m\phi$ is an eigenfunction of the Hamiltonian and determine the eigenvalue.

7. (10 pts) For harmonic oscillator, we have $\hat{H}\Psi_0 = 0.5\hbar\omega\Psi_0$ Calculate the expectation value of the operator $\hat{\Omega} = (1 - 2\hat{H})/3$ for its ground state wavefunction (Ψ_0)?

III. Solve the following more complicated problems

8. (15 pts) For an electron in a 1.5 nm box, calculate the energy of its ground state and the photon frequency needed for exciting the electron from the ground state to its first excited state. Depict the wavefunctions of the two quantum states.

9. (20 pts) The infrared vibrational spectrum of gas phase $H^{81}Br$ has a dominant peak at 2650 cm^{-1}. Calculate the vibrational frequency, force constant, and the zero-point energy of the molecule assuming it is a harmonic oscillator.

10. (20 pts) A three-dimensional rigid rotor has a moment of inertia of 2.4×10^{-47} kg m^2. Calculate the energy difference between the l=1 and l=2 states and the corresponding photon wavelength for the transition. Depict all the possible degenerate states for l=2 in a vector model and label them with m.