Practice Questions for CHEM 4010

In addition to the questions below, it is a good practice for you to try to answer the Multiple Choice Questions at the end of each chapter in Lowe and Peterson's "Quantum Chemistry".

1) Write an expression for the zero point energy of the particle in a one-dimensional box in terms of the particle's mass m, the length of the box L, and Planck's constant h.

2) Sketch the wavefunctions of the particle in a one-dimensional box for $n = 1, 2$, and 3.

3) The free-particle is like a particle in a infinitely large one-dimensional box. Give two *qualitative* differences between the allowed energies of the free-particle and the allowed energies of the particle in a box.

4) Describe in a few words what is the "photoelectric effect".

5) What is the DeBroglie wavelength of an electron with a kinetic energy of 5.0 eV? $h = 6.626176 \times 10^{-34}\,\mathrm{J\,s}$, $m_e = 9.109534 \times 10^{-31}\,\mathrm{kg}$, and $1\,eV = 1.6021892 \times 10^{-19}\,\mathrm{J}$.

6) Describe briefly the two-slit experiment (diffraction experiment) and explain how it reveals the wave-particle dual nature of electrons.

7) For the particle-in-a-ring, all energy levels are doubly degenerate except the lowest one. Why?

8) Calculate, or estimate as best as you can, this integral:
$\int_0^L sin(\pi x/L) sin(2\pi x/L)\, dx$

9) The allowed energies of a particle of mass m in a 3-dimensional box of dimensions L_x, L_y, L_z, are $E = (h^2/8m)(n_x^2/L_x^2 + n_y^2/L_y^2 + n_z^2/L_z^2)$, with n_x, n_y, n_z =1, 2, 3, ... What is the degeneracy of the second energy level for a particle in a 3-dimensional cubic box?

10) For the H atom, there are three wavefunctions solutions to the Schrödinger equation with quantum numbers $n = 2$ and $l = 1$: one with $m_l = 1$, one with $m_l = 0$, and one with $m_l = -1$. The $m_l = 0$ wavefunction is also called a "$2p_z$" orbital. But the $m_l = 1$ and $m_l = -1$ wavefunctions are neither "$2p_x$" or "$2p_y$" orbitals. Yes or No: is the "$2p_x$" orbital a solution to the Schrödinger equation for the H atom? Explain.

11) Perform dimensional analysis and show what are the SI units attached to the wavefunctions of the particle in a 3-dimensional box.

12) Sketch the 1s and 2s orbitals of the H atom, ψ_{100} and ψ_{200}, as a function of r (distance to the nucleus). Then, on another diagram, sketch $r^2\psi_{100}^2$ and $r^2\psi_{200}^2$ as a function of r.

13) Orbitals with very high n quantum numbers are called "Rydberg states". How many nodes does the H atom orbital with $n = 20$, $l = 14$ and $m = -8$ have? How many of these are radial nodes, and how many are planar nodes?

14) On one diagram, sketch the harmonic potential ($\frac{1}{2}kx^2$), the $n = 2$ wavefunction of the harmonic oscillator ($\psi_2(x)$), and the three lowest energy levels E_1, E_2 and E_3. Indicate the classical turning points for the $n = 2$ state and show how the wavefunction $\psi_2(x)$ extends into the classically forbidden region.

15) The ground state energy of the quantum harmonic oscillator is
$E_0 = \frac{1}{2}h\nu = \frac{h}{4\pi}\sqrt{\frac{k}{m}}$.
(a) What is the lowest possible energy for the *classical* harmonic oscillator?
(b) What is the *average* kinetic energy of the quantum harmonic oscillator in its ground state?
(c) By dimensional analysis, find what are the SI units attached to k.

16) Write down the time-independent Schrödinger equation for a particle of mass μ that is attached to a rigid wall by a ideal harmonic weightless spring of force constant k and which moves along x under the influence of that potential.