

## Objectives for Exam 1

Exam 1 will be available after class on Friday, March 1. It will be a take-home exam in which you will be allowed a total of **8 hours** of “*active attention*” to the exam between the time you pick up the exam to the time you turn it in, or 1:10 pm on Friday, March 8, whichever happens first. This is on the **Honor System**. *Active attention* is defined here as time in which you are actually thinking about solving a part of the exam, calculating, and writing out the answers. Other things such as sleeping exercising, conversing on other topics, etc., i.e., anything else that takes over your complete attention is not part of the 8 hours.

This is the Honor System. Unlike homework, you are to work on the exam strictly on your own. Questions of clarifications can only be discussed with the Professor, either verbally, by phone, or email. You may use the books, class notes, handouts, homework solutions, but **not** solutions of similar problems taken from the internet, or other convenient sources.

### Know or be able to do:

1. Quantum concepts, including tunneling.
2. Apply the Virial theorem to electronic energy and harmonic oscillator.
3. General nature of the 1-dimensional wavefunctions of a bound particle; relationship of wavefunction curvature, kinetic energy, and tunneling to a correct solution.
4. Calculate expectation values of a linear combination of basis functions, given the matrix elements and overlap integrals for the basis set.
5. Find a mathematical expression for the probability of measuring a certain dynamical variable eigenvalue for a system in a specified state function (as in Homework #3).
6. Importance of the variation principle to quantum chemistry. Non-linear and linear variation methods, including the perturbation limit. Know the general behavior of the eigenvalues and eigenvectors of the 2x2 dimensional variation method.
7. Get eigenvalues and vectors for up to 6x6 matrices using the Colby Diagonalizer or an equivalent program.
8. Draw pictures of atomic orbitals showing nodal planes, cones, and spheres, given  $n$ ,  $l$ , and  $|m|$  quantum numbers.

9. The Hamiltonian of a simple molecular system. Hartree-Fock SCF ideas and shortcomings and the criterion for reaching the minimum energy by the linear variation method. Know the meaning of “orbital energy”, one- and two-electron operators, J and K electron repulsion operators, Koopman’s Theorem. Given sufficient numerical information regarding these, find the total energy of a small molecule or an atom.
  
10. Extract the optimized energy, the MO “energies”, the ionization potential and electron affinity, and the general appearance of the MOs from the Gaussian 09 output for a small molecule.
  
11. Concept of electron correlation, the need for it, and methods by which it is obtained.
  
12. Understand how to quickly obtain matrix elements of an operator, given the density matrix and the operator matrix.
  
13. Show that optimizing the ratio of “ionic” and “covalent” terms of the energy of the H<sub>2</sub> molecule ground state in the molecular orbital wavefunction is exactly equivalent to doing a CI calculation by adding in some of the doubly excited configuration in which the two electrons are each in the antibonding MO.