

Objectives for the Final Exam

Chmy 564-17

27 April 2017

The final exam will be a take-home exam, on which you are to work completely independently (you may direct questions of clarification to the Professor only). You may use only your notes, handouts, readings from this course, and personal textbooks.

The final exam will be available **starting at 2:00 pm on Friday**, April 28 and must be **turned in no later than Wed, May 3 at 12 noon**. The cumulative time limit is **8 hours** of *active* work. You may break the time into sections such that periods of time (sleeping, etc) for which you are not consciously solving an exam problem do not count as part of the 8 hours.

The final is worth 200 points. The midterm and the homework will each be worth 100 points.

Objectives:

1. General: You may expect problems similar to those on the homework and on the midterm exam.

Specifically: Know or be able to do:

1. Quantum concepts.
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.
4. Calculate expectation values of a linear combination of basis functions, given the matrix elements and overlap integrals for the basis set.
5. 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.
6. Get eigenvalues and vectors for up to 6x6 matrices using the Colby Diagonalizer or an equivalent program.

7. Draw pictures of atomic orbitals showing nodal planes, cones, and spheres, given n , l , and $|m|$, quantum numbers.
8. LCAO-Hartree-Fock SCF to the extent examined in HW#4. Understand the shortcomings of HF-SCF.
9. Meaning of transition density. Understand how to quickly obtain matrix elements of an operator, given a density matrix or transition density matrix and the operator matrix.
10. Concept of electron correlation, the need for it, and methods by which it is obtained.
11. Be able to perform ab initio electronic energy calculations Using Gaussian 09 for small molecules, including use of DFT. Be able to find the lowest excited state energy and description of it in terms of singly excited configurations (CIS).
12. The difference between molecular orbital (MO) and valence bond (VB) methods.
13. Symmetry: character, character tables, representations, irreducible representation, how to use a character table for the purpose of determining when certain matrix elements must be zero “due to symmetry”
14. Born-Oppenheimer approximation and wavefunction and how this provides the vibronic transitions and intensities by Franck-Condon (FC) factors. Calculate FC factors given the information necessary to use the simple formula for $0 \rightarrow v$ vibrational transitions in Lec. 27
15. (a) What generally happens to a state function when the Hamiltonian operates on it.
(b) What the time dependent Schrödinger equation says about the phase and magnitude of the time derivative of an energy eigenfunction.
16. Behavior of a wavefunction and density for a two-level system (TLS) for different cases of real and imaginary Hamiltonian:
 - (a) using the notation $|\Psi\rangle = c_1|1\rangle + c_2|2\rangle$, where c_1 and c_2 are complex, and $H_{11} = H_{22}$ for different cases of H_{12} .
 - (b) using the Feynman-Vernon-Hellwarth equation notation.
17. Pure and mixed states of ensembles; the concept of coherence and dephasing for an ensemble density. The meaning of T_1 , T_2 , and T_2^* relaxation times for a non-equilibrium ensemble density.