Chem 249 Cumulative Exam. R. Corn. Spring 2006.

1) Simple Harmonic Oscillator (25 points)

Consider a quantum mechanical simple harmonic oscillator with a resonance frequency of $\omega_0 = (k/m)^{1/2}$.

We add a time independent perturbation W to the SHO of the form $W = ax^3$.

a) What is the first order perturbation theory energy correction to the ground state $|0\rangle$?

b) What states mix with the ground state in the first order correction to the eigenstates? (Hint: $x = (h/2m\omega_0)^{1/2}(a^\dagger + a)$)

2) Two Level System (25 points)

Consider the density matrix for a two level system with energies E1 and E2.

a) If the two states have no permanent dipole moments but a nonzero transition dipole moment $\mu 12$, write down the general expression for the dipole moment $\langle\mu(t)\rangle$ in terms of the density matrix elements ρ_{11}, ρ_{12}, ρ_{21} and ρ_{22}.

b) How is $\mu(t)$ related to the dielectric susceptibility $\chi(\omega)$?

3) Term Symbols and Atomic Spectroscopy (25 points)

a) What are the term symbols for the ground state configuration of Aluminum ($1s^2 2s^2 2p^6 3s^2 3p$)?

b) Consider the excited state of Al ($1s^2 2s^2 2p^6 3s^2 4s$). What are the term symbols for this state?

c) What transitions are allowed (if any) from the ground state to the excited state?

d) If we apply a weak magnetic field to perform Zeeman Atomic Spectroscopy, draw a diagram of how the ground and excited state manifolds split.

e) How many lines will be observed in this weak field Zeeman Atomic Spectrum?

4) Spin Systems and NMR (25 points)

Boron-10 (^{10}B) has a spin of 3. In a particular macrocyclic molecule, the Boron-10 nuclear spin states have energies given by the equation:

$$E = -h\omega_0 M_I + ha\, M_I^2$$

where $a << \omega_0$ and M_I is the quantum number for I_z.

Sketch an energy level diagram for Boron-10 in this molecule, and then draw in the allowed transitions. Be sure to label the states and any energy level splittings. Draw the NMR spectrum you would expect to see.