Physics 556 Spring 2007 -- HW # 4 -- due Friday March 2

The Mn^{3+} ion occurs as a substitutional impurity for Al^{3+} in corundum and other insulators. It also forms the active ion in $LaMnO_3$, the "parent compound" of the "colossal magnetoresistance" materials. There are 4 d-electrons to distribute among 10 d orbitals. This can be done in 10x9x8x7/4x3x2x1=210 ways. This means that the space of possible states contains 210 orthonormal many-electron wavefunctions, each most simply written as a Slater determinant. The Coulomb electron-electron interaction v couples these 210 states. To solve by degenerate perturbation theory, you diagonalize the 210 x 210 matrix of v. Using irreducible representations of the space and spin rotations, you can reduce this matrix almost to diagonal form. Here is the numbers game you play to figure out the "L-S terms" like ^5D which constitute the irreducible representations. You make a table whose cells enumerate all ways of making states with given values of M_L and M_S. If the complete table were shown there would be 210 entries. Only the upper left part needs to be explicitly constructed. The notation (u,d,2,-,-) means that the various single electron orbitals with m_l values (2,1,0,-1,-2) are populated "up, down, twice, empty, empty." This entry appears in the box M_S=0, M_L=3. This Slater determinant is not an eigenstate of (L,M_L,S,M_S), but contributes partially to all existing L-S terms with L greater than or equal to 3, and S greater than or equal to 0. Your job is to figure out which terms exist. Here are two hints. In the last column, the "singlet I" term is indicated, because the state (2,2,-,-,-) can only belong to the term with L=6 (S,P,D,F,G,H,I,… are the labels for the L=0,1,2,… orbital angular momenta.) It can't belong to L greater than 6 because there is no way to make M_L greater than 6. It also must have S=0 because there are no entries in the M_S=1 or 2 columns. Cells lower in the table start to have lots of entries, especially the M_S=0 column, and less so the other columns. The first entry in the M_S=2 column is shown. This has to belong to the Hund's rule ground state ^5D. This "term" has 25-fold degeneracy before spin-orbit effects are included. Please (1) figure out all the allowed "terms," (2) verify that these terms contain 210 states, and (3) describe the structure of the reduced v matrix.

Mn^{3+} (d^4)	M_S=2	M_S=1	M_S=0	Rep.
M_L=6			(2,2,-,-,-)	^1I
M_L=5				
M_L=4				
M_L=3				
M_L=2	(u,u,u,u,-)			^5D
M_L=1				
M_L=0				