Home work for lectures 10 and 11 due April 6 2011

1. Discuss briefly why the Madelung potential enters into the gap of a charge transfer gap insulator and not in the gap of a Mott Hubbard gap system. If we have a charge transfer gap system how would you expect the gap to change at the surface of such a system. Take a 110 surface of NiO (NaCl) structure as an example.
2. Determine the impurity density of states for an impurity with an s atomic level at an energy D from the center of a host band. Assume that the hybridization matrix element V between the impurity and host is independent of energy and momentum k and that the host density of states (1 state per eV) is constant within a band width of W and zero outside of this. Using the Dyson equation to solve for the impurity greens function and determine the impurity density of states including possible bound states outside of the band. Describe the condition for finding these bound states.
3. Consider an Octahedron with O2- ions at the corners and a TM2+ ion at the center like Ni2+ which has two holes in an eg orbital. Consider only the O 2p orbitals with lobes pointing to the Ni2+ and a tpp hoping integral between the nearest neighbor O p orbitals with this orientation . determine the single hole molecular orbital eigenstates and then including a large repulsive U for two holes on the same O determine the nature of the two hole eigenstates of both singlet and triplet character. This is like the model discussed in the lecture but a bit simplified.
4. What is the expectation value for $\langle S_i \bullet S_j \rangle$ for spins of 1/2 , i and j nearest neighbors for a singlet state, a ferromagnetically ordered material, a Neel like antiferromagnetically ordered material