Home work lecture 3 hand in Feb 9 2011

1a) Consider a H2 molecule described by the Hubbard Hamiltonian. Assume only 1s hydrogen like wave functions and inter atomic hoping t on site interaction U. Derive the energy and wave function for the ground state and the excited states of the N (i.e.2) electron system. Derive the Heisenberg exchange Hamiltonian for U>>t .

b) What is the energy splitting betweeGn the spin singlet and triplet states for U>>t?

c) Derive the eigenfunctions and eigenvalues for the N-1 and N+1 electron states. i.e. 1 electron and 3 electrons respectively

d) What would the photoemission and inverse photoemission spectrum look like for U=0, U=t/2, U=t and U>>t. Note the difference when U=0 ( molecular orbital limit ) and U >> t Heitler London Limit)

e) In the large U limit but for finite t why do we see two peaks in the photoemission spectrum?

2. Derive the expression for the reduction of U due to the polarizability of the nearest n neighbor molecules as used for C6o solid.

3. Suggest a form for the Hamiltonian that would include the occupation dependent hoping terms which is so important for a H lattice. Would you expect it to be as important for the difference in hoping of a 3d hole and 3d electron starting from 9 d electrons as in the cuprates?

4. Derive the Dyson equation in the form where

and G=1/(E-H)