Assigned Tuesday, November 3, 2005. Due Tuesday, November 15, 2005

1. Exact solution for the two site Hubbard dimer.

   The two-site Hubbard dimer is a model for a molecule with two sites 1 and 2. Each site has one basis state, e.g. an H atom in which we consider only the 1s state. The molecule may have 0,1,2,3, or 4 electrons. There is a hopping term t between sites and interaction term on each site giving the Hamiltonian:

   $$H = t \sum_{\sigma} (c^{+}_{1\sigma} c_{2\sigma} + c^{+}_{2\sigma} c_{1\sigma}) + U(n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow}) \tag{1}$$

   Give the exact solution for all possible cases. The solutions for 0 and 1 electrons are very straightforward. Show that the solution for 4 and 3 electrons are equivalent to 0 and 1 electrons (an example of particle-hole duality).

   For two electrons, the solution can be found exactly with nothing harder than solving a 2x2 matrix equation. (This can be done by classifying the states according to spin and to states that even or odd under reflection about the midpoint between the two sites.) Find the energies of all states with two electrons and show that the lowest energy state is always a singlet.

   Consider the case of two electrons.
   a. For $U = 0$ show that the solution is bonding and antibonding states, with the ground state is a spin singlet with up and down electrons in the bonding state. In this state show that the probability of finding two electrons on one site is $P_2 = 1/4$. For $0 < U << t$ show that the solution is similar but $P_2 < 1/4$. (This is picture of a chemical bond, e.g, in H_2 at the equilibrium distance.)
   b. For $t = 0$ show that the low energy solution is degenerate and the states correspond to one electron on each site with all possible spin orientations. For $0 < t << U$, show that the lowest energy state is a singlet and that the first excited state is a triplet. Derive the expression for the singlet-triplet energy difference in terms of t and U.
   c. Discuss the low energy solutions for for $0 < t << U$ and show that they correspond to a Heisenberg spin model with antiferromagnetic interactions between the spins.

2. Typical orders of magnitude.
   Consider the case with two electrons and $U >> t$. The singlet-triplet energy difference can be used to find a quantitative estimate of the coupling J in the Heisenberg model. Taking reasonable estimates of $t = 0.5eV$, $U = 4eV$, estimate J.