Physics 726: Assignment 5

(to be submitted by Thursday, March 10, 2016)

1. The trihydrogen cation H_3^+ consists of three protons in a triangular arrangement, populated with two electrons. Suppose that the electronic behaviour can be approximately described by the noninteracting, tight-binding Hamiltonian

$$\hat{H}_0 = \sum_{\alpha=\uparrow,\downarrow} \sum_{j=1,2,3} \left(-t \left[c_{j,\alpha}^\dagger c_{(j \bmod 3)+1,\alpha} + \text{h.c.} \right] + \epsilon c_{j,\alpha}^\dagger c_{j,\alpha} \right).$$

Here, t is real and positive.

   (a) What do each of t and ϵ signify? Could any other term appear in $\hat{H}_0$ without also breaking a symmetry of the system?

   (b) Argue that $\hat{H}_0$ can be written in the form

$$\hat{H}_0 = \sum_\alpha \begin{pmatrix} c_{1,\alpha}^\dagger & c_{2,\alpha}^\dagger & c_{3,\alpha}^\dagger \end{pmatrix} \begin{pmatrix} ? & ? & ? \\ ? & ? & ? \\ ? & ? & ? \end{pmatrix} \begin{pmatrix} c_{1,\alpha} \\ c_{2,\alpha} \\ c_{3,\alpha} \end{pmatrix},$$

   and determine the missing matrix elements.

   (c) Construct a transformation

$$c_{j,\alpha} = \sum_{k=1,2,3} U_{j,k} d_{k,\alpha}$$

   that produces the diagonal form

$$\hat{H}_0 = \sum_\alpha \sum_k E_k d_{k,\alpha}^\dagger d_{k,\alpha}.$$

   You should find that $\{E_1, E_2, E_3\} = \{\epsilon - 2t, \epsilon + t, \epsilon + t\}$.

   (d) The $j = 1,2,3$ appearing as a subscript on the operator $c_{j,\alpha}$ is an atomic site label. What does the $k = 1,2,3$ on $d_{k,\alpha}$ refer to?

   (e) What is the ground state of the two-electron system? What is the ground-state energy?

   (f) Write down an expression for the average electronic occupation on any one atomic site. Show that the result is the same, regardless of which site you choose.

2. Now imagine that the electrons exert a short-range repulsion on one another such that they pay an energy cost U when two electrons are on the same site. In other words, the Hamiltonian is augmented by a term

$$\hat{H}_1 = U \sum_j \hat{n}_{j\uparrow} \hat{n}_{j\downarrow},$$

where $\hat{n}_{j,\alpha} = c_{j,\alpha}^\dagger c_{j,\alpha}$ is the number operator.

   (a) What's different about how $\hat{H}_1$ acts on the states $|\psi_0^{S=0}\rangle = d_{1,\uparrow}^\dagger d_{1,\downarrow}^\dagger |\text{vac}\rangle$ and $|\psi_0^{S=1}\rangle = d_{1,\uparrow}^\dagger d_{2,\uparrow}^\dagger |\text{vac}\rangle$?

   (b) Compute the first-order energy shift for small U. Estimate the value of U above which the spin-polarized state is lower in energy.

   (c) Compute the ground-state degeneracy in the limit $U \to \infty$.

   (d) Consider the case of a *three*-electron system in the parameter regime $U \gg t, \epsilon$. Think about how you would carry out a perturbative calculation in $\hat{H}_0$ around the $\hat{H}_1$ ground state. What order of perturbation theory would you have to go to break the ground state degeneracy? Explain why t^2/U is the energy scale of the level splitting.