Homework 1 (due on April 5th)

Problem 1

Prove a very useful identity:

$$\sum_{\sigma_1,\sigma_2} a^\dagger_{k\sigma_1} a_{k\sigma_2} a^\dagger_{l\sigma_2} a_{l\sigma_1} = \frac{1}{2}\left(\hat{n}_k \hat{n}_l + 4\hat{S}_k \cdot \hat{S}_l\right)$$

where $\hat{n}_k = \sum_\sigma a^\dagger_{k\sigma} a_{k\sigma}$ and $\hat{S}_k \cdot \hat{S}_l = S^x_k S^x_l + S^y_k S^y_l + S^z_k S^z_l$ with S^i_k being operators of spin component i for electron in orbital k.
Hints: Spin operators in 2nd quantization are given by $\hat{S}^i_k = \frac{1}{2}\sum_{ss'} a^\dagger_{ks}[\sigma^i]_{ss'} a_{ks'}$ where $[\sigma^i]_{ss'}$ is the ss' matrix element of Pauli matrix σ^i ($i = x, y, z$). Remember also that it is sometimes easier to use spin ladder operators, $\hat{S}^\pm = \hat{S}^x \pm i\hat{S}^y$ than $\hat{S}^{x,y}$ operators.

Problem 2

Take a Heisenberg Hamiltonian for two electrons (one in orbital L and the other in orbital R):

$$-J\hat{S}_L \cdot \hat{S}_R$$

and find its eigenstates and eigenvalues. You can work either in basis of $|\sigma_L \sigma_R\rangle$ states or the basis of total S of two electrons and its projection on z axis, $|S m_S\rangle$ (what is the relation between these bases?).
Hints: Remember about the ladder operators. Take $\hat{S} = \hat{S}_L + \hat{S}_R$ and square it, while recalling things that you learned a long time ago about eigenvalues of $\hat{S}^2$.
This is really a problem belonging to Quantum Mechanics 1 course (the part on spin operator algebra), but since we've talked so much about the problem of two interacting electrons mapping on the problem of two coupled spins, let's refresh the addition of two spins here.

Problem 3

Let us look at the problem of a dimer (two sites) / double quantum dot. Our single-particle Hilbert space is spanned by two orbitals, $|\Phi_L\rangle, |\Phi_R\rangle$, one localized in the left well of the potential, the other in the right well. The orbitals are orthogonal. We take into account the tunneling coupling between them, and the on-site Coulomb repulsion, so that the Hamiltonian is given by

$$\hat{H}_{LR} = -t\sum_\sigma (a^\dagger_{L\sigma} a_{R\sigma} + a^\dagger_{R\sigma} a_{L\sigma}) + U\hat{n}_{L\uparrow}\hat{n}_{L\downarrow} + U\hat{n}_{R\uparrow}\hat{n}_{R\downarrow} \ .$$

Consider now two electrons. The Hilbert space is then spanned by 6 states. We will call them $|\uparrow_L\downarrow_L, 0\rangle$, $|0, \uparrow_R, \downarrow_R\rangle$, $|\uparrow_L, \downarrow_R\rangle$, $|\downarrow_L, \uparrow_R\rangle$, $|\uparrow_L, \uparrow_R\rangle$, $|\downarrow_L, \downarrow_R\rangle$.

1. Write these states using creation operators acting on the vaccum state.
2. Write our the Hamiltonian matrix in this basis. It should look similar (sic!) to this one

$$\begin{pmatrix} U & 0 & t & -t & 0 & 0 \\ 0 & U & t & -t & 0 & 0 \\ t & t & 0 & 0 & 0 & 0 \\ -t & -t & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

3. Two connected questions. Did you get the same Hamiltonian? Where does the minus factor in front of some of ts come from?

4. Diagonalize the Hamiltonian. Try doing it by "brute force" and then by changing the basis in $|\downarrow_L, \uparrow_R\rangle$, $|\uparrow_L, \downarrow_R\rangle$ subspace (the new basis is formed by symmetric and antisymmetric combinations of these two states). See how one of new states decouples from all the other states. This is the so-called "dark state". Note that it works in this way because some of ts come with minus signs.

Problem 4

Take a one-dimensional chain of sites with electron hopping between the nearest neighbors:

$$\hat{H} = -t \sum_{j,\delta=\pm 1} a^\dagger_{j+\delta} a_j$$

The site spacing (the lattice parameter) is a. Use periodic boundary conditions for a finite chain consisting of N sites. Show that the Hamiltonian is diagonal after change of basis from localized states (electron created on site j) to "plane-wave" states (electron created in a superposition of being on various sites, with amplitudes modulated in a wave-like manner):

$$a_j = \frac{1}{\sqrt{N}} \sum_k e^{ikja} c_k \ .$$

What is the energy dispersion (within the first BZ - and by the way, what is the 1st BZ in this case?). What is the bandwidth?
Hints: What are the allowed values of k when using periodic boundary conditions, and when we have a lattice constant a? What is the value of $\sum_k e^{ikma}$ (where m is integer) when summed over the relevant set of k?