8.513 Problem Set 1

(Dated: September 15, 2004)

Due Sept 21

Practice with creation / annihilation operators

1. Consider a situation where an electron can hop between two different localized regions of space (eg: the vicinity of each nucleus in a diatomic molecule, or two different impurity sites in a solid, etc). A model for such a situation is to consider a lattice with just two sites, and a Hamiltonian

$$H = \sum_{i=1,2} \epsilon_i a^\dagger_{i\alpha} a_{i\alpha} - t \left(a^\dagger_{1\alpha} a_{2\alpha} + h.c \right) \tag{1}$$

Here $\alpha = \uparrow, \downarrow$ is the spin index and $t > 0$. Assume that there are two electrons in the system. To begin with assume $\epsilon_1 = \epsilon_2 = \epsilon$.

   (a) Calculate the ground state energy, and the ground state wavefunction.

   (b) What is the average number of electrons at each site in the ground state? What about at finite temperature?

   (c) What is the average value of the hopping operator $a^\dagger_{1\alpha} a_{2\alpha} + h.c$ in the ground state?

   (d) Now consider the case where $\epsilon_1 = \epsilon + \Delta$ and $\epsilon_2 = \epsilon - \Delta$ with $\Delta > 0$. What is the average number of electrons at each site in the ground state? What happens in the limit of large Δ? At fixed Δ, what happens to the average number at large temperature?

2. Consider the Hamiltonian

$$H = \epsilon a^\dagger a + \frac{\Delta}{2} \left(a^2 + (a^\dagger)^2 \right) \tag{2}$$

where $a, a^\dagger$ are bosonic operators. Assume $\Delta < \epsilon$. Diagonalize the Hamiltonian (i.e find the excitation energies). (Hint: Find linear combinations of a and $a^\dagger$ which preserve the commutation algebra but in terms of which the Hamiltonian is diagonal).