

## Physics 503, Problem Set 1

### Due by beginning of class on Thursday, January 19

Please note that the solutions are due by the beginning of class, 11:00. Late problem sets will not be accepted for credit. Typed solutions will be posted on the course web site later that day.

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

$$H = \sum_{i=1}^2 \sum_{\sigma} \epsilon_i c_{i\sigma}^{\dagger} c_{i\sigma} - \sum_{\sigma} t (c_{1\sigma}^{\dagger} c_{2\sigma} + h.c.) \quad (1)$$

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

- Calculate the ground state energy, and the ground state wavefunction.
- What is the average number of electrons at each site in the ground state? What about at finite temperature, in the canonical ensemble, with the number of electrons held fixed at 2?
- What is the average value of the hopping operator ( $c_{1\sigma}^{\dagger} c_{2\sigma} + h.c.$ ) in the ground state?
- 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  $\Delta$ ? At fixed  $\Delta$ , what happens to the average number at large temperature?

2) Consider a simple spinless interacting tight binding model with only 2 sites:

$$H = -t(c_1^{\dagger} c_2 + c_2^{\dagger} c_1) + V \hat{n}_1 \hat{n}_2, \quad (2)$$

where  $\hat{n}_i$  is the electron number operator on site  $i$ . Find all eigenvalues of this Hamiltonian and specify the total number of electrons and parity for each eigenstate. (By parity I refer to the symmetry which interchanges the 2 sites.) (HINT: The total number of states is 4.)

It is not necessary to use any mathematical software if you take advantage of the fact that the Hilbert space decomposes into sectors with definite total electron number and parity which are not mixed by the Hamiltonian. You will learn much more from solving this problem by taking advantage of the symmetries than by brute force diagonalization of a large matrix.

3) Consider a simple 2-band non-interacting tight-binding model with 2 orbitals per site, with the corresponding annihilation operators denoted  $c_{\vec{R}}$  and  $d_{\vec{R}}$ . Suppose that the direct hopping of electrons in the  $d$ -orbitals is negligible but that there is some on-site mixing of the  $c$  and  $d$  orbitals (i.e. they are not orthogonal). The Hamiltonian is:

$$H = -t \sum_{\vec{R}} \left[ \sum_{\vec{\delta}} c_{\vec{R}}^{\dagger} c_{\vec{R}+\vec{\delta}} + V (c_{\vec{R}}^{\dagger} d_{\vec{R}} + h.c.) \right]. \quad (3)$$

Here  $h.c.$  denotes the hermitean conjugate of the previous term. Find the dispersion relations of the two bands in this problem, as a function of wave-vector  $\vec{k}$ , considering the case of a three dimensional simple cubic lattice with spacing  $a$ . The sum over  $\vec{\delta}$  is over the 6 nearest neighbour vectors.

4) Let  $G_{\text{ret}}(\vec{p}, \omega)$  be the retarded Green's function for the electron operators:

$$G_{\text{ret}}(\vec{p}, \omega) \equiv -i \int_0^{\infty} dt e^{i\omega t} \langle \{c_{\vec{p}}(t), c_{\vec{p}}^{\dagger}(0)\} \rangle. \quad (4)$$

Here  $\langle \dots \rangle$  denotes the Boltzmann average at temperature  $T$ , as usual. Assuming that the time-evolution is given by the Hamiltonian  $H$ , prove the following sum rule:

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} n_F(\omega) \omega^s \text{Im} G_{\text{ret}}(\vec{p}, \omega) = C \langle [H, c_{\vec{p}}^{\dagger}] [H, c_{\vec{p}}] \rangle \quad (5)$$

where  $n_F(\omega)$  is the Fermi distribution function:

$$n_F(\omega) \equiv \frac{1}{e^{\beta\omega} + 1} \quad (6)$$

and  $s$  and  $C$  are constants which you are to find. In general, when I write an expression like Eq. (5) without indicating the time at which the operators are evaluated, you may assume that all operators are at  $t = 0$  (or, equivalently any other time which is the same for all operators).  $\langle \dots \rangle$  denotes the thermal average.