

598SCM Fall 2004 Homework 4

Handed out Tuesday, November 16, 2004

Due Tuesday, December 7, 2004

There will be an "Office hour" session before the due date. Anyone is welcome to come to discuss the solutions to the problems. Time to be announced.

1. Properties of the self energy

In this problem you are asked to describe the form of the Greens function $G_\lambda(E)$ near a resonance $E = \epsilon_\lambda$ where there is some broadening due to many-body effects. (Here λ is a label that denotes a conserved quantum number, e.g., \mathbf{k} in a crystal. It is just a label and does not affect the solution.) Note that solution of this problem requires only simple algebraic manipulation of the terms. It does NOT require and knowledge of the details of the self-energy.

Use the general expression for the Green's function in terms of the proper self-energy

$$G_\lambda(E) = \frac{1}{E - \epsilon_\lambda^0 - \Sigma_\lambda^*(E)} \quad (1)$$

and expand the self-energy $\Sigma_\lambda^*(E)$ in powers of the energy difference $E - \epsilon_\lambda$. From this show that near $E = \epsilon_\lambda$ the Greens function is approximated by

$$G_\lambda(E) = \frac{Z_\lambda}{E - \epsilon_\lambda - i\gamma_\lambda}, \quad (2)$$

where

$$\epsilon_\lambda = \epsilon_\lambda^0 + \text{Re}\Sigma_\lambda^*(E = \epsilon_\lambda), \quad (3)$$

$$Z_\lambda = \left[1 - \frac{d \text{Re}\Sigma_\lambda^*(E)}{dE} \right]_{E=\epsilon_\lambda}^{-1}, \quad (4)$$

and

$$\gamma_\lambda = Z_\lambda \text{Im}\Sigma_\lambda^*(E = \epsilon_\lambda) \quad (5)$$

The consequence of this result is that the "quasiparticle" with quantum number λ has a broadened peak (width given by Eq. 5) centered at a shifted energy (Eq. 3), with a reduced total weight in the peak (the factor Z_λ in Eq. 4).

2. 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:

$$H = t \sum_{\sigma} (c_{1\sigma}^+ c_{2\sigma} + c_{2\sigma}^+ c_{1\sigma}) + U(n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow}) \quad (6)$$

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. Show that for two electrons the lowest state is always a singlet.

Show that for two electrons and small U ($U \ll t$) one has the usual bonding and antibonding states, like is appropriate for hydrogen at the equilibrium distance. For two electrons large U ($U \gg t$) the system is more like a spin system with total spin equal zero and antiferromagnetic correlation of the spins.

3. Anderson Impurity Model in the Hartree Fock Approximation

The object of this problem is to carry out the unrestricted Hartree-Fock approximate solution of the Anderson Model for impurities in a metal. The primary result will be to find the ranges of parameters where the solution is a) a singlet state with no magnetic moment and b) a degenerate pair of states each with a moment. The latter case is called the "local moment regime". The best reference is the original paper (P. W. Anderson, Phys. Rev. 124, 41 (1961).) In this local moment regime in fact the true ground state is a singlet; this is the famous Kondo problem that was finally solved by Wilson using the renormalization group methods which he invented.

The Hamiltonian is given by

$$H = \sum_{\sigma} \epsilon_L c_{L,\sigma}^{\dagger} c_{L,\sigma} + U n_{L,\uparrow} n_{L,\downarrow} + \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^{\dagger} c_{k,\sigma} + V \sum_{k,\sigma} (c_{k,\sigma}^{\dagger} c_{L,\sigma} + h.c.) \quad (7)$$

For the non-interacting ($U = 0$) case you may use the form of the Green's function (retarded form) derived in the class notes for a "flat" density of states (the real part of the self energy is zero in this case because the spectrum is symmetric from - infinity to plus infinity).

$$G_{\sigma}((L, L), \omega) = \frac{1}{\omega - \epsilon_L + i\Delta} \quad (8)$$

where $\Delta = \text{constant}$ and ϵ_L is assumed to include any shift from the real part of the self-energy.

In the H-F approximation, the Greens function for each spin is given by the above equation with

$$\epsilon_L \rightarrow \epsilon_{L,\sigma} = \epsilon_L + U \langle n_{L,-\sigma} \rangle. \quad (9)$$

a) Show that in the H-F approximation the number of localized electrons of each spin type is given by

$$n_{L,\sigma} = \int_{-\infty}^{E_F} dE \rho_{L,\sigma}(E) = \frac{1}{\pi} \cot^{-1} \left(\frac{\epsilon_L + U \langle n_{L,-\sigma} \rangle - E_F}{\Delta} \right) \quad (10)$$

b) In terms of the variables $x = \frac{E_F - \epsilon_L}{U}$, $y = \frac{U}{\Delta}$, $n_1 = n_{L\uparrow}$ and $n_2 = n_{L\downarrow}$, show that the equations can be written:

$$\cot n_1 - y(n_2 - x) = 0$$

$$\cot \pi n_2 - y(n_1 - x) = 0.$$

c) Show graphically that for some values of x and y there is only one non-magnetic solution with $n_1 = n_2$, whereas for other values of x and y , there are three solutions.

Show this by graphing n_2 as a function of n_1 from the first equation and n_1 as a function of n_2 from the second equation. Plot the solutions for n_2 vs. n_1 and show examples of the two types of solutions.

d) Show that the boundary between the non-magnetic and magnetic regimes is given by the condition that the two curves have the same slope at the point $n_1 = n_2$, and that this leads to the relation of critical values of n_c and y_c given by

$$\frac{\pi}{\sin^2 \pi n_c} = y_c.$$

e) Show qualitatively that the boundary of the magnetic regime has the form found by Anderson:

Optional Problems

4. Divergence of individual terms in expansion of correlation energy in powers of e^2 for the homogeneous electron gas.

Consider the direct term in the expansion of the correlation energy to the lowest order beyond Hartree-Fock in Jellium. The Hartree-Fock wavefunction is the filled Fermi sea and the energy is first order in the interaction. In the next order one has sums over all excited states generated by the interaction

$$H_{int} = \frac{1}{2} \sum_{k,\sigma,k',\sigma',q} V_q \left(c_{k+q,\sigma}^+ c_{k'-q,\sigma'}^+ c_{k',\sigma'} c_{k,\sigma} \right) \quad (11)$$

where V_q is the Coulomb interaction in Fourier space. Give the standard second order perturbation expression for the energy to second order in $V_q \approx e^2$, and identify the direct and the exchange terms. Consider the direct term and show that it diverges. (This is sufficient to show that the perturbation series formally does not converge, which is the reason that the series must be resummed in a different way to get a finite expression.)