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Physikalisches Institut
Prof. Dr. H. Kroha, Z. Y. Lai, J. Martens
http://www.thp.uni-bonn.de/kroha

Advanced Theoretical Condensed Matter Physics — SS11

Exercise 9

(Please return your solutions before Tue. 05.07.2011)

In this exercise sheet we will calculate the *electronic* self-energy to 2nd and 3rd order in the coupling constant J, assumed to be constant. We will utilize Abrikosov's *pseudofermion formalism* for the diagrammatic expansion of the electron-impurity scattering term in the Hamiltonian. The interaction Hamiltonian takes the form

$$\mathcal{H}_{int} = -\frac{1}{N}\sum_{\mathbf{p},\mathbf{p}'}\left\{J_1(\mathbf{p}',\mathbf{p})\delta_{\alpha'\alpha}\delta_{\beta'\beta} + J_2(\mathbf{p}'\mathbf{p})\sigma^i_{\alpha'\alpha}S^i_{\beta'\beta}\right\}\times \\ \times \hat{a}^\dagger_{n\beta'}\hat{a}_{n\beta}\hat{c}^\dagger_{\mathbf{p}'\alpha'}\hat{c}_{\mathbf{p}\alpha}\exp\left[\mathrm{i}(\mathbf{p}-\mathbf{p}')\cdot\mathbf{R}_n\right] \quad (1)$$

With the expression of the interaction Hamiltonian in terms of the pseudofermions, one can simplify the calculation of diagrams since one can now resort to Wick's theorem. In fact, the self-energy diagrams can be evaluated without the help of the pseudofermions, but the evaluation is much more complicated since in that case one needs to explicitly take care of the time-ordering of the spin operators. If you want to know how this works, see the book by Mahan[1].

There is however a caveat for the use of the pseudofermion formalism: one needs to project out some spurious degrees of freedom which are included due to the fact that in introducing the pseudofermions, we have in fact introduced new states in our Hilbert space which does not correspond to single occupancy of the impurity site (in other words, there should only be single spin at the impurity site). In a practical sense, the procedure of projecting out the extra states is equivalent to including an additional *normalization factor* $\frac{e^{\lambda/T}}{2S+1}$, where λ is the free energy of the pseudofermions and S is the spin of the impurity, and taking the limit $\lambda/T \to \infty$ at a certain point in the calculation.

To simplify the calculations we define the free propagators for the electrons and pseudofermions. The free-electron propagator is given by

$$G^{(0)}_{\alpha\alpha'}(\mathbf{p}, i\epsilon) = \frac{\delta_{\alpha\alpha'}}{i\epsilon_n - \xi_{\mathbf{p}}}, \qquad \epsilon_n = (2n+1)\pi T \quad (2)$$

while the pseudofermion operator is given by

$$\mathcal{G}^{(0)}_{\beta\beta'}(i\omega) = \frac{\delta_{\beta\beta'}}{i\omega_l - \lambda}, \qquad \omega_l = (2l+1)\pi T \quad (3)$$

In this exercise we will for simplicity discard the δ-functions on both the propagators (they get summed in the calculation of the self-energy).

[1] See website for the reference; pages 376 - 382

9.1. Electronic self-energy for the Kondo model to 2nd order.

The diagrams corresponding to the electronic self-energy is shown in Fig. **??** with all the energy and momentum variables labeled.

a) Write down the expression corresponding to Fig. 1 in accordance to Feynman's rules.

Note: You should insert a prefactor of $\delta_{\alpha\alpha'}S(S+1)(2S+1)$ *by hand which results from tracing over the spin variables. Also do not forget the normalization factor* $\frac{e^{\lambda/T}}{2S+1}$.

b) First perform the relevant Matsubara summations in part (a). In order to deal with the arising distribution functions remember the periodicity characteristic of the Matsubara frequencies. We note that the quantity $n_F(\lambda) \to e^{-\lambda/T}$ as $\lambda/T \to \infty$, wher $n_F(\varepsilon)$ is the Fermi distribution. Note that it is true that $n_F(i(\epsilon_n - \omega_l) + \xi_p) = n_F(\xi_p)$ in general. In addition, the following is also true

$$\lim_{\lambda/T\to\infty} n_F(i\epsilon - \xi_p + \lambda) \to -e^{-\lambda/T}e^{\xi_p/T}$$

to lowest order. You should obtain an expression of the form

$$\Sigma^{(2)}(\mathbf{p}, i\epsilon) = \lim_{\lambda/T\to\infty} \delta_{\alpha\alpha'}S(S+1)\left(\frac{J}{N}\right)^2 \int \frac{d^3p'}{(2\pi)^3}\frac{1}{i\epsilon - \varepsilon_{\mathbf{p}'}} \tag{4}$$

c) Now perform the final momentum integration in (4). You can use the usual replacement of

$$\int \frac{d^3p'}{(2\pi)^3}\, f(\xi_{\mathbf{p}'}) \to \int d\varepsilon\, \rho(\varepsilon)\, f(\varepsilon) \to \rho(0)\int d\varepsilon\, f(\varepsilon)$$

where $\rho(\varepsilon)$ is the density of states. Show that you obtain a term which is proportional to $S(S+1)(J/N)^2\rho(0)$. This term is not that interesting, since it has the same form as ordinary impurity scattering in the second Born approximation. The spin only enters as an effective interaction of the form $S(S+1)J^2$.

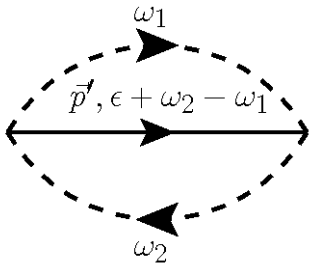

Figure 1: The second order self-energy diagram. Note that the full line denotes the electron propagator, while the dotted lines are the pseudofermion propagators.

9.2. Electronic self-energy for the Kondo model to 3rd order.

In the previous exercise, you have seen that the self-energy calculation to 3rd order does not yield any interesting results. Here we will see that in order to finally obtain the temperature dependence that is characteristic of the Kondo effect. The diagrams to be calculated are to be seen in Fig. 2 and 3

a) As above, write down the expression for Fig. 2 and 3. The spin prefactor and normalization coefficient given in (a) in 9.1 should still be inserted.

b) Perform the Matsubara summation, much as you did in part (b) of 9.1 for both diagrams. You should obtain an expression of the form

$$\Sigma^{(3b)}(\mathbf{p}, i\epsilon) = \delta_{\alpha\alpha'} 2S(S+1) \left(\frac{J}{N}\right)^3 \int\int \frac{d^3p_1}{(2\pi)^3} \frac{d^3p_2}{(2\pi)^3} \frac{n_F(\varepsilon_{p_2})}{(i\epsilon - \varepsilon_{\mathbf{p}_1})(\epsilon_{\mathbf{p}_1} - \epsilon_{\vec{p}_2})} \tag{5}$$

for the diagram in Fig. 3. The expression for the diagram in Fig. 2 is almost exactly the same, apart from a prefactor in the argument of the Fermi function.

c) The momentum integration in (5) can also be rewritten in this case as energy integrals. However, further evaluation of these expressions will require some approximations, and these will be discussed in the exercise class.

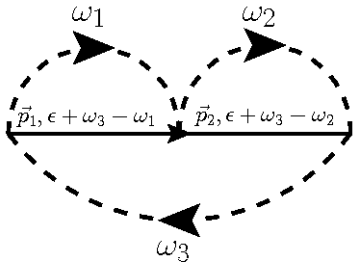

Figure 2: The 3rd order self-energy diagram

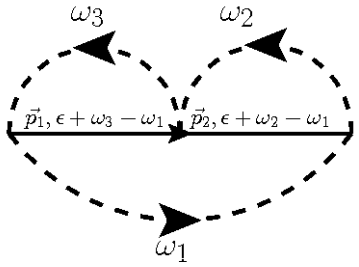

Figure 3: Another configuration for the self-energy diagram