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Strongly Correlated Electrons
4. Übung

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1. Poor man's scaling and the Kondo problem **3 points**

In this exercise, we will follow the original formulation of P. W. Anderson, and discuss the Kondo problem from the simplest renormalization-group (RG) perspective. Our starting point is the generalized anisotropic Kondo model

$$\hat{H} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}} \hat{c}_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{k},\mathbf{k}'} \Big(J^+ \hat{S}^+ \hat{c}^\dagger_{\mathbf{k}',\downarrow} \hat{c}_{\mathbf{k},\uparrow} + J^- \hat{S}^- \hat{c}^\dagger_{\mathbf{k}',\uparrow} \hat{c}_{\mathbf{k},\downarrow} + J^z \hat{S}^z (\hat{c}^\dagger_{\mathbf{k}',\uparrow} \hat{c}_{\mathbf{k},\uparrow} - \hat{c}^\dagger_{\mathbf{k}',\downarrow} \hat{c}_{\mathbf{k},\downarrow}) \Big) . \tag{1}$$

The idea is to incorporate the effect of the high-energy degrees of freedom in new effective couplings for the low-energy theory. We therefore want to integrate out electronic degrees of freedom close to the band edges at energies $\pm D$ (and iterate this procedure consistently).

a) **1 point**

Argue that the component of the Hamiltonian scattering a conduction electron into an unoccupied state close to the upper band edge is given by

$$\hat{H}_{\mathrm{D-particle}} = \frac{1}{2} \sum_{\mathbf{q},\mathbf{k}} \Big(J^+ \hat{S}^+ \hat{c}^\dagger_{\mathbf{q},\downarrow} \hat{c}_{\mathbf{k},\uparrow} + J^- \hat{S}^- \hat{c}^\dagger_{\mathbf{q},\uparrow} \hat{c}_{\mathbf{k},\downarrow} + J^z \hat{S}^z (\hat{c}^\dagger_{\mathbf{q},\uparrow} \hat{c}_{\mathbf{k},\uparrow} - \hat{c}^\dagger_{\mathbf{q},\downarrow} \hat{c}_{\mathbf{k},\downarrow}) \Big) \tag{2}$$

where $D - \delta D < q < D$. In an analogous way, write down $\hat{H}_{\mathrm{D-hole}}$ that scatters a conduction electron in an high-energy hole close to the lower band edge.

b) **1 point**

Argue (somewhat similarly to exercise 2 on the last sheet) that the second order diagrams of Fig. 1 renormalize the diagonal coupling constant $J^z \to J^z + \delta J^z$ according to

$$\delta J^z \approx J^+ J^- \rho_0 \frac{|\delta D|}{D} \tag{3}$$

where ρ_0 is the density of states per spin (that we assume to be a constant in the interval $-D < \epsilon < D$). From the diagrams of Fig. 2, derive also the renormalization of the couplings $J^\pm$.

$$\delta J_\pm \approx J^\pm J^z \rho_0 \frac{|\delta D|}{D} \tag{4}$$

The following suggestions may be useful:

- Account for both the processes with a virtual high energy particle and with a virtual high energy hole.
- Use the identities $S^+ S^- = 1/2 + S^z$ and $S^- S^+ = 1/2 - S^z$.
- Assume, to simplify your expressions, that $D \gg \epsilon_{\mathbf{k}}$ is always the largest and the only relevant energy scale.

c) **1 point**

From the above result, and using $J^+ = J^-$, read off the RG equations for the coupling constants

$$\frac{dJ^\pm}{d\ln D} = -\rho_0 J^z J^\pm \tag{5}$$

$$\frac{dJ^z}{d\ln D} = -\rho_0 J^+ J^- . \tag{6}$$

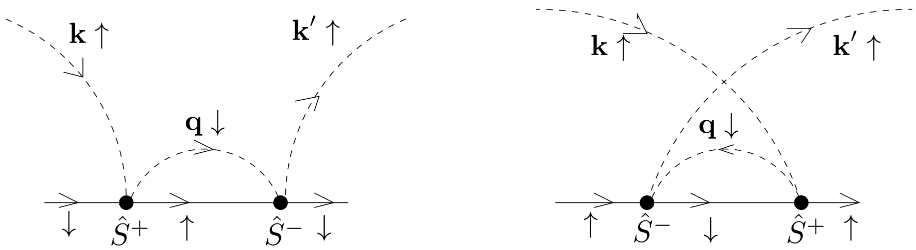

Figure 1: Second-order diagrams which involve either a particle, Fig. 1a, or a hole, Fig. 1b, in an intermediate state $\mathbf{q}$ at a band edge.

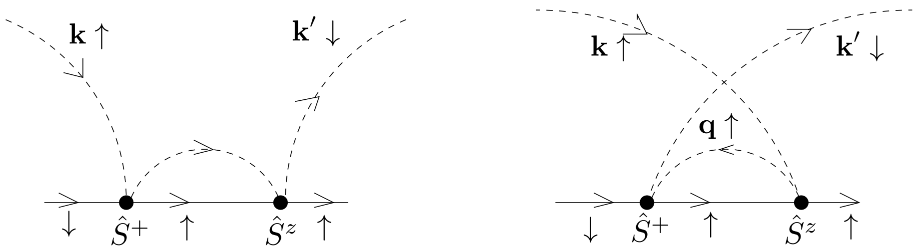

Figure 2: Second-order diagrams with spin flip scattering and a particle, Fig. 2a, or a hole, Fig. 2b, in an intermediate state $\mathbf{q}$ at a band edge.

Comment this result in the ferromagnetic and antiferromagnetic case, showing that $(J^z)^2 - (J^+J^-)^2$ is a RG invariant. Finally, integrate out the scaling equations for the isotropic case.

2. Slave-boson approximation for the Kondo model **8 points**

In this exercise, we will study the Kondo model within the so-called slave-boson approximation.
Let us consider the Kondo model $\hat{H} = \hat{H}_0 + \hat{H}_1$ with

$$H_0 = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}\,\sigma} \hat{c}_{\mathbf{k}\,\sigma} \tag{7}$$

$$\hat{H}_1 = J\hat{\mathbf{S}} \cdot \hat{\mathbf{s}}_0, \tag{8}$$

where $\hat{c}^\dagger_{\mathbf{k}\,\sigma}$ $(\hat{c}_{\mathbf{k}\,\sigma})$ creates (annihilates) a conduction electron with momentum $\mathbf{k}$ and spin $\sigma =\uparrow,\downarrow$, $\varepsilon_{\mathbf{k}}$ is the fermion dispersion, J is the Kondo coupling, $\hat{\mathbf{S}}$ is the impurity spin (spin-1/2), and $\hat{\mathbf{s}}_0$ is the conduction electron spin operator at the impurity site, i.e.,

$$\hat{\mathbf{s}}_0 = \frac{1}{2} \sum_{\mathbf{k},\mathbf{k}'} \hat{c}^\dagger_{\mathbf{k}\sigma} \hat{\tau}_{\sigma\sigma'} \hat{c}_{\mathbf{k}'\sigma}$$

where $\hat{\tau}$ is the vector of Pauli matrices, and the summation over repeated spin indices is assumed.

a) 1 point

It is convenient to write the impurity spin $\hat{\mathbf{S}}$ in terms of auxiliary fermion operators $\hat{f}_\sigma$ (the so-called Abrikosov fermions), i.e., $\hat{\mathbf{S}} = \frac{1}{2}\hat{f}^\dagger_\sigma \hat{\tau}_{\sigma\sigma'} \hat{f}_{\sigma'}$. In order to preserve the size of the Hilbert space, we need a constraint, $\sum_\sigma \hat{f}^\dagger_\sigma \hat{f}_\sigma = 1$, which is enforced by the introduction of a Lagrange multiplier λ. Show that, apart from global shifts of the energy and the chemical potential, $\hat{H}_1$ assumes the form

$$\hat{H}_1 = -\frac{J}{2} \hat{f}^\dagger_\sigma \hat{c}_\sigma(0) \hat{c}^\dagger_{\sigma'}(0) \hat{f}_{\sigma'}, \tag{9}$$

where $\hat{c}_\sigma(0) = \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}$ is the conduction electron operator at the impurity site.

b) 1 point

Decouple the four-fermion term $(J/2)\hat{f}^\dagger \hat{c}\hat{c}^\dagger \hat{f}$ in Eq. (9) by replacing the *bosonic* operator $\hat{c}^\dagger \hat{f}$ by its average value b (this mean-field approximation is equivalent to the one discussed in the lecture). Show that, again up to constants, the Hamiltonian assumes the form

$$H = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} - (b\, \hat{f}^{\dagger}_{\sigma} \hat{c}_{\sigma}(0) + h.c.) + \lambda(\hat{f}^{\dagger}_{\sigma} \hat{f}_{\sigma} - 1), \tag{10}$$

with

$$b = \frac{J}{2} \sum_{\sigma} \langle \hat{c}^{\dagger}_{\sigma}(0) \hat{f}_{\sigma} \rangle. \tag{11}$$

Notice that b is in general a complex number.

c) **1 point**

The Hamiltonian (10) is bilinear in fermion operators and is thus solvable. It is useful to introduce propagators for the f fermions, $G_{ff}(\tau) = -\langle T_{\tau} \hat{f}(\tau) \hat{f}^{\dagger}(0) \rangle$, and a mixed propagator $G_{fc}(\tau) = -\langle T_{\tau} \hat{f}(\tau) \hat{c}^{\dagger}(r = 0, 0) \rangle$ as well. Show that

$$G_{ff}(i\omega_n) = \left(i\omega_n - \lambda - |b|^2 G^0(r = 0, i\omega_n)\right)^{-1} \tag{12}$$

and

$$G_{fc}(i\omega_n) = -b\, G_{ff}(i\omega_n) G^0(r = 0, i\omega_n)\,, \tag{13}$$

where $G^0(r = 0, i\omega_n) = \sum_k (i\omega_n - \varepsilon_{\mathbf{k}})^{-1}$ is the local Green's function for the conduction electrons.
Hint: recall the discussion about the non-interacting Anderson model.

d) **1 point**

From now on, let us assume that b is real. The assumption made in item (b), namely that λ is constant, implies that the constraint $\sum_{\sigma} \hat{f}^{\dagger}_{\sigma} \hat{f}_{\sigma} = 1$ is fulfilled only on the average, i.e.,

$$\sum_{\sigma} \langle \hat{f}^{\dagger}_{\sigma} \hat{f}_{\sigma} \rangle = 1. \tag{14}$$

Rewrite Eqs.(11) and (14) in terms of the Green's functions (12) and (13). Notice that the two derived equations, combined with Eq.(12), form a set of self-consistent equations. Once the density of states of the conduction electrons $\rho_0(\omega)$ and J are known, the equations can be solved for a fixed temperature.

e) **1 point**

Use the results of the item d), convert the Matsubara sums into integrals over real frequencies, and show that Eq. (11) can be written as

$$\frac{1}{J} = -\int_{-\infty}^{\infty} d\omega\, n_f(\omega) \frac{\frac{\rho_0(\omega)}{\omega - \lambda}}{\left|1 - \frac{b^2 G^0(\omega + i\eta)}{\omega - \lambda}\right|^2} + \mathcal{O}(b^2), \tag{15}$$

if $b \neq 0$ and

$$\frac{1}{J} = -\int_{-\infty}^{\infty} d\omega\, n_f(\omega) \left(\frac{\rho_0(\omega)}{\omega - \lambda} + \mathrm{Re}\, G^0(\omega + i\eta) \delta(\omega - \lambda) \right), \tag{16}$$

if $b = 0$. Here, the spectral density (density of states) $\rho_0(\omega) = -\mathrm{Im} G^0(\omega + i\eta)/\pi$ and $n_f(x) = 1/[\exp(\beta x) + 1]$ is the Fermi function.
Hint: the identity $-(1/\beta) \sum_{i\omega_n} G(i\omega_n) = \int d\omega \rho(\omega) n_f(\omega)$, where $\rho(\omega)$ is the spectral density related to $G(\omega + i\eta)$, might be useful [see the discussion below Eq.(3.5.10) of Mahan's book for details].

f) **1 point**

Assume that $\rho_0(\omega)$ is constant for $-D < \omega < D$, where $2D$ is the bandwidth of the conduction electrons, and discuss the solutions of the mean-field equations. Show that it is possible to derive the correct (one-loop) expression for the Kondo temperature T_K from these equations.
Observation: recall the discussion during the lecture about the fact that the slave-boson approximation introduces an artificial phase transition at T_K.

g) **1 point**

Assume now that $\rho_0(\omega) \sim (\omega/D)^r$ with $r > 0$. Discuss the solutions of the mean-field equations for $T = 0$.
Observation: the case $r = 1$ corresponds to graphene.

h) **1 point**

The magnetic response of the impurity to a locally applied field is given by the so-called local susceptibility χ_{loc}. In our mean-field approximation, it is exactly given by the simple bubble diagram,

$$\chi_{\text{loc}}(T) = -\frac{1}{2}\int_0^\beta d\tau\, G_f(\tau)G_f(-\tau) = -\frac{1}{2\beta}\sum_{i\omega_n} G_f^2(i\omega_n) \tag{17}$$

Convert the Matsubara summation into real-axis integrals. Discuss $\chi_{\text{loc}}(T)$ for low and high T. Show that $\chi_{\text{loc}}(T) = 1/(8k_BT)$ at high T (where $b = 0$). Why is this result different from the usual one for spin $\frac{1}{2}$, i.e., $\chi(T) = 1/(4k_BT)$?