Kondo Effect in a Metal with Correlated Conduction Electrons

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The large-degeneracy expansion for dilute magnetic alloys is extended to account for conduction electrons interactions. Particular attention is paid to the renormalization of the hybridization vertex which affects the low-energy excitations. As a first example, we calculate the enhanced characteristic energy \(k_B T_0\) in the limit of weakly correlated conduction electrons. The metallic regime with strongly correlated electrons is discussed.

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Correlations among the conduction electrons may strongly affect the ground state and the low-energy excitations of metals with magnetic ions. A typical example are doped cuprates with rare earth ions \(\text{Nd}_{2-x}\text{Ce}_{x}\text{CuO}_4\) where a novel type of heavy fermion-like behavior was recently discovered \([1]\). Although the thermodynamic properties in the normal state closely parallel the behavior of standard heavy fermion compounds \([2,3]\), the observed characteristic energy of the low-energy excitations cannot be related to a Kondo temperature estimated from the known coupling between the spins of the rare earth ions and the conduction electrons \([2,4]\).

In this paper, we study the influence of conduction electron correlations on the low-energy excitations of dilute magnetic alloys. The latter are characterized by an energy scale \(k_B T_0\) much smaller than the characteristic energies of the conduction electrons such as the bandwidth \(D\) or the local Coulomb repulsion \(U\). We thereby tacitly assume that the conduction electron correlations do not introduce low-energy anomalies i.e. that the conduction electron properties are smooth on the scale set by \(k_B T_0\). This separation of energy scales forms the basis of our theory. It allows us to reduce the general problem of a magnetic impurity in a metal with strongly correlated electrons to a form which can be solved in close analogy to the well-studied case of uncorrelated conduction electrons. Of particular interest is the characteristic energy \(k_B T_0\) which in the case of uncorrelated conduction electrons depends exponentially upon the inverse of the coupling between localized and conduction electrons \([2,4]\). This exponential many-body scale is a direct consequence of the existence of Fermi liquid low frequency excitations in a normal metal. Theoretical studies of an impurity spin embedded in a one-dimensional Luttinger liquid \([4,13]\), on the other hand, predict a power law for the variation of the characteristic temperature with the coupling in the limit of large on-site Coulomb interaction \(U\).

The modifications introduced by the conduction electron interactions into the low-energy excitations arise from the subtle interplay of three different types of influences. First, the density of conduction states at the Fermi level is changed. Second, the virtual transitions between f- and conduction states are reduced. Third, the effective spin coupling between the conduction and f-electrons is enhanced by the increased number of uncompensated spins in the correlated conduction electron system. Considering these facts, it is not surprising that model studies accounting only for selected aspects arrive at rather controversial conclusions concerning the Kondo effect in metals with correlated electrons \([14,17]\).

For a microscopic description, we consider an Anderson impurity coupled to interacting electrons. The latter are described by a one-band Hubbard model. The resulting Hamiltonian reads

\[
H = \sum_{\kappa \sigma} \epsilon_{\kappa} c_{\kappa \sigma}^\dagger c_{\kappa \sigma} + \frac{U}{2} \sum_{\kappa \kappa' \sigma \sigma'} c_{\kappa \sigma}^\dagger c_{\kappa' \sigma'}^\dagger c_{\kappa' \sigma'} c_{\kappa \sigma} + \sum_{m} \epsilon_f n_{f m} + \frac{U_f}{2} \sum_{m \neq m'} n_{f m} n_{f m'} + \sum_{\kappa \sigma} \left( V_{\kappa m} f_m^\dagger c_{\kappa \sigma} + h.c. \right)
\]

The operators \(c_{\kappa \sigma}^\dagger (c_{\kappa \sigma})\) create (annihilate) conduction electrons with momentum \(\kappa\) and band energy \(\epsilon_{\kappa}\) and spin \(\sigma\). The local Coulomb repulsion between two conduction electrons at the same site is \(U\). The \(f_m^\dagger (f_m)\) are the creation (annihilation) operators for f-electrons on the impurity site. They are characterized by the total angular momentum \(J\) and a quantum number \(m\) which denotes the different states \(m = 1, \ldots, N_f\) within the \(N_f\)-fold degenerate ground state multiplet with orbital energy \(\epsilon_f\). All energies are measured relative to the Fermi level. The Coulomb repulsion \(U_f\) is assumed to be much larger than the energy scales and therefore we may let \(U_f \rightarrow \infty\). We consider here an orbitally non-degenerate Anderson im-
purity putting in Eq. (1) \( m = \sigma \) and the hybridization coupling \( V_{km\sigma} = V \).

The excitation spectra are calculated from the Green’s functions of the empty state \( |0> \) (i.e. the \( f^0 \) or \( f^{14} \) configuration) and the occupied \( f \) states \( |\sigma> \), respectively, denoted by \( G_0(z) \) and \( G_\sigma(z) \)

\[
G_\alpha(z) = \frac{1}{z - \epsilon_\alpha - \Sigma_\alpha(z)}
\]

where \( \epsilon_\alpha = 0, \epsilon_f \) for \( \alpha = 0, \sigma \) respectively. The interactions among the conduction electrons affect the self-energies \( \Sigma_0 \) and \( \Sigma_\sigma \) which are coupled. They are determined by the self-consistent large degeneracy expansion in close analogy to the Non Crossing Approximation [18] for non-interacting conduction electrons.

The derivation of the generalized NCA equations proceeds in two steps starting from a conventional perturbation expansion for the self-energies \( \Sigma_0 \) and \( \Sigma_\sigma \) in terms of the bare conduction electron propagators, the bare Green’s functions for the relevant \( f \)-configurations, the Coulomb interaction \( U \) and the hybridization \( V \). By reordering and partial summation the series is converted into an expansion in terms of bare Green’s functions for the \( f \)-configurations, Coulomb-renormalized propagators for the conduction electrons and effective hybridization vertices which account for the correlations among the conduction electrons. The resulting diagrams are classified with respect to their order in the inverse degeneracy in close analogy to the case \( U = 0 \). Self-consistent summation of the leading terms yields the self-energies displayed in Figures 1a,b for the empty \( f \)-state and occupied \( f \)-states, respectively, while Figure 1c illustrates the general structure of the effective hybridization vertex for the case of two-particle correlations. The correlation-induced vertex corrections generally contain an \( n \)-electron Green’s function where \( 2n-1 \) external lines are connected by \( n \) Green’s functions for empty and occupied \( f \)-configurations, respectively, via \( 2n-1 \) bare hybridization vertices. On the relevant low-energy scale the variation with energy of the effective vertices and of the selfenergies is determined by the structure of the diagrams and the Green’s functions \( G_0 \) and \( G_m \). This fact follows directly from the separation of energy scales.

For the Hubbard model, the dominant contribution originates from two-particle correlations. We shall therefore restrict ourselves to the self-consistency equations displayed in Figure 1.

Neglecting the vertex corrections from the Coulomb interaction yields self-energies

\[
\Sigma^{(0)}_0(\omega) = \frac{V^2}{N} \sum_{k\xi} d\xi n_F(\xi) A_\sigma(k, \xi) G_\sigma(\omega + \xi)
\]

\[
\Sigma^{(0)}_\sigma(\omega) = \frac{V^2}{N} \sum_{k\xi} d\xi n_F(-\xi) A_\sigma(k, \xi) G_0(\omega - \xi)
\]

in close analogy to the case of non-interacting electrons [20]. In Eq. (3), \( n_F(\xi) \) is the Fermi function while \( A_\sigma(k, \xi) \) denotes the spectral function of interacting electrons which for \( U = 0 \), reduces to \( \delta(\xi - \epsilon_k) \). For non-interacting conduction electrons, the self-consistent solution has three characteristic features: The occupied \( f \)-spectrum shifts to peak at a value \( E_f \) the dominant contribution to the level shift coming from the continuum of charge fluctuations. The resonance in the occupied \( f \)-spectrum acquires a small width. Finally, the empty state spectral function exhibits a pronounced structure at \( \omega_0 = E_f - k_B T_0 \) which develops with decreasing temperature and which sets the scale for the low-temperature behavior. This feature is the direct manifestation of the Kondo effect reflecting the admixture of \( f^0 \)-contributions to the ground state and the low-energy excitations.

It is obvious [19] that also for interacting conduction electrons the dominant effect of hybridization on the \( 4f^1 \) configurational spectrum is a shift \( E_f(U) - \epsilon_f = Re \Sigma_\sigma \) of the resonance energy which, however, is renormalized by the Coulomb repulsion \( U \) and its influence on the charge fluctuations. The interaction-induced shift, however, is rather small [19] and will be neglected in the subsequent discussion. The central quantity to be studied here is the empty state self energy and, in particular, its variation with energy close to \( E_f \) which can be deduced form rather general considerations. The smooth variation with energy of \( \Sigma^{(0)}_\sigma(\omega) \) implies that the basic analytic structure of \( \Sigma^{(0)}_\sigma(\omega) \) is not altered as compared to the case of non-interacting conduction electrons, the characteristic feature being a logarithmic variation in the vicinity of the \( f \)-energy \( E_f \). The prefactor, however, is proportional to the interaction-renormalized density of states at the Fermi level \( \rho(0) \). The low-energy scale, \( k_B T_0 \), i.e. the distance between the pole in the empty \( f \)-state Green’s function and the \( 4f^1 \) peak depends on the renormalized parameters in the usual exponential way. The vertex correction displayed in Figure 1c accounts for the two-particle correlations in the interacting conduction electron system. The corresponding contribution to the empty state self energy is denoted by \( \Sigma^{(1)}_\sigma(\omega) \). We should like to emphasize that the latter is proportional to \( V^4 N_f (N_f - 1) \) and hence of the same order in the inverse local degeneracy \( (1/N_f)^0 \) as the leading term \( \Sigma^{(0)}_\sigma(\omega) \). The same classification applies to the \( 4f^1 \) configurational self energies \( \Sigma^{(0)}_\sigma \) and \( \Sigma^{(1)}_\sigma \) which are both of the order \( (1/N_f)^1 \).

In this paper we shall evaluate and discuss the contribution to lowest order in the effective interaction. The conclusions we shall arrive at can easily be extended to intermediate values of \( U \) by inserting a more sophisticated approximation to the appropriate two-particle \( t \)-matrix. However, the latter cannot be simply expressed in terms of Landau parameters since the microscopic expression involves conduction electron energies far from the Fermi surface. To study the analytic behavior in the energy range of interest, we insert the unperturbed conduction electron propagator and obtain
\[ \Sigma_0^{(1)}(\omega) = -\frac{2UV^4}{N^3} \sum_{\kappa, \kappa', q} \frac{g_{\kappa, \kappa', q} - g_{\kappa, q'}}{\epsilon_{\kappa} - \epsilon_{\kappa'} + \epsilon_{\kappa' + q} - \epsilon_{\kappa + q}} \]  

(4)

\[ g_{\kappa, \kappa', q} = G_0(\omega + \epsilon_{\kappa} - \epsilon_{\kappa'} - \epsilon_{q})G_0(\omega + \epsilon_{\kappa})n_{F}(\epsilon_{\kappa})n_{F}(\epsilon_{\kappa'} + \epsilon_{q}) \]

\[ n_{F}(\epsilon_{\kappa})G_\sigma(\omega + \epsilon_{\kappa}) - n_{F}(\epsilon_{\kappa'}).G_\sigma(\omega + \epsilon_{\kappa'} + \epsilon_{q}) \]

The occupied state self-energy \( \Sigma_0^{(1)}(\omega) \) is expressed analogically [21]. To make things simpler we calculate \( \Sigma_0^{(1)}(\omega) \) for \( T = 0 \) in the local approximation, hence neglecting the momentum conservation in Eq. (8), and obtain

\[ \Sigma_0^{(1)}(\omega) = -\frac{1}{\pi^2}U\rho(0) \frac{\Gamma}{D} I_0^{(1)}(\omega) \Sigma_0^{(0)}(\omega) \]

(5)

\[ I_0^{(1)}(\omega) = \int_{-D}^{0} d\xi \int_{0}^{D} dn \int_{-D}^{0} d\zeta \frac{2}{(\omega - \epsilon_f + \xi)(\omega - \epsilon_f - \xi - \eta + \zeta)} \]

(6)

A similar expression is obtained for the second integral, \( I_0^{(2)} \) [22]. Indeed on this first iteration stage of the NCA equations we already face an integral equation for the second integral, \( I_0^{(2)}(\omega) \) are dimensionless functions of \( \omega/D \). For the square DOS and half-filling \( I_0^{(1)}(\omega) \) is given by the following equation

\[ \Gamma \to \Gamma \left( 1 - \frac{U}{2\pi^2 \rho(0)} \frac{\Gamma}{D} I_0^{(1)}(\omega_0) \right) \]

(8)

\[ \epsilon_f \to \epsilon_f + \frac{U}{2\pi^2}(\frac{\Gamma}{D})^2 I_0^{(2)}(\omega_0) \]

Both integrals \( I_{1,2}(\omega_0) \) are negative, so the former renormalization leads to an increase of \( T_0(U) \) whereas the latter leads to a decrease ( see also [13] ). Calculations of integrals in Eq. (8) show that the \( \Gamma \)-renormalization wins and \( T_0(U) \) increases with \( U \) in agreement with [14]. The "on-shell" results for \( T_0(U) \) which are included in Figure 2 for comparison tend to overestimate the renormalization.

The on-shell approximation in Eq. (8) may be represented as \( \Gamma_{eff} = \Gamma[1 + C U \rho(0)] \) where \( C \) is itself a function of \( \Gamma \) and \( \epsilon_f \). For \( \epsilon_f/D = -0.67 \) and \( 0.16 \leq \Gamma/D \leq 0.3 \) we obtain \( 0.72 \geq C \geq 0.54 \) These values has to be compared with the \( C \approx 1 \) in the Kondo spin model of [14]. Analogically we obtain \( \epsilon_f = \epsilon_f (1 + C_1 U/[\epsilon_f]) \) with \( 0.02 \geq C_1 \geq 0.16 \).

For weak electron-electron interaction the increase of \( T_0 \) may be understood as resulting from the reduced probability of finding doubly occupied and empty lattice sites in the correlated conduction electron systems. The increased number of uncompensated conduction electron spins finally leads to the enhancement of the effective hybridization coupling. We may expect that for sufficiently large \( U \) and a half-filled conduction band the virtual transition from the f-state to the conduction state will cost too much energy inhibiting the \( T_0 \)-increase and leading eventually to the change in the trend. The analogy between the Kondo spin model and the Anderson impurity model in its local moment regime is not complete in the case of correlated conduction electrons ( see also [14] ). In the former case \( T_0 \) will increase monotonously with the \( U \) because of the enhancement of the exchange interaction. In the latter case the process is two-staged, it involves the formation of a local moment and its interaction with the conduction electrons.

The present results are based on the separation of energy scales. We therefore anticipate no qualitative changes when using more sophisticated approximations for the vertices \( \Gamma^{(i,\sigma)}(1, 2; 3, 4) \) (Figure 2 c) appropriate for the strong correlation regime. For a quantitative treatment of this problem there are two visible approaches. One is to introduce summation of the infinite subseries of the RPA and the ladder type. In this case we introduce in self-energies \( \Sigma_0^{(1)}(\omega) \) and \( \Sigma_0^{(1)}(\omega) \) dynamical Lindhard functions. The other way is to approximate the vertex correction by response functions ( dynamic susceptibilities ). This may be done with the use of the local approximation [23, 24]. The work in these directions is in progress [18]. In addition, the influence of conduction electron interactions on the spectral properties of magnetic impurities and their dependence upon the doping are also interesting topics for future investigations.
that due to the renormalisation of the hybridization interaction the characteristic energy is increased by the weak interactions.

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\[ \Sigma^{(1)}_{\sigma} \text{ may be obtained from the } \Sigma^{(1)}_{\sigma,0} \text{ by omitting the factor of 2, by changing in the function } g \text{ superscripts, } b \leftrightarrow f, \text{ and by inverting signs of all } \epsilon \text{ in this function.} \]

\[ \text{Our integral functions } I_{0}^{(1)} \text{ and } I_{0}^{(1)} \text{ are very close to ana-} \]

\[ \text{logical integrals in ref. [17], } -I_{A}^{(1)} \text{ and the sum } -(I_{B}^{(1)} + I_{D}^{(1)}) \text{ correspondingly.} \]

\[ \text{FIG. 1. Self-consistent f configuration self-energies and contributions to the vertex. The solid, dashed and wavy lines represent the dressed propagators for conduction electrons, occupied and empty f states. The open circle denotes the bare hybridization V while open and filled squares are the bare on-site Coulomb repulsion and the two-particle vertex } \Gamma_{\sigma,\bar{\sigma}}^{(1)}(1,2;3,4), \text{ respectively. (a) Empty state self-energy } \Sigma^{(1)}_{\sigma}(i\nu_{m}) \text{. (b) Occupied state self-energy } \Sigma^{(1)}_{\sigma}(i\omega_{n}). \text{ (c) Contribution to the effective hybridization vertex. (d) Lowest order correction.} \]

\[ \text{FIG. 2. } T_{K}(U) \text{ as function of } U/D = 0.5 \text{ and } \epsilon_{f}/D = -0.67. \text{ The solid refers to the solutions of Eq. (6) while the dashed line is for the on-shell approximation, Eq. (6); We also include the U=0 result for comparison (dot-dashed line).} \]
a) \[ \sigma, i(\omega_n + v_m) \]

b) \[ i(\omega_n - \omega_{n'}) \]

c) \[ \begin{array}{c}
\begin{array}{c}
\text{Diagram 1}
\end{array}
\end{array} \rightleftharpoons \begin{array}{c}
\begin{array}{c}
\text{Diagram 2}
\end{array}
\end{array} \]

d) \[ \begin{array}{c}
\text{Diagram 3}
\end{array} \rightarrow \begin{array}{c}
\text{Diagram 4}
\end{array} \]
\[ \ln \left( \frac{T_0}{D} \right) \]

- U = 0
- U/D = 0.5

Graph showing the relationship between \( \ln \left( \frac{T_0}{D} \right) \) and D/\( \Gamma \).