Competition between the Kondo effect and magnetic ordering in a model which is exactly solvable asymptotically

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A model which includes a Kondo effect and a transition to a magnetically ordered state is proposed. In the limit of a high multiplicity of the degeneracy, this model is exactly solvable. The competition between the Kondo effect and the ferromagnetic ordering of localized moments is analyzed.

One of the most interesting aspects of the Ce- and U-based heavy-fermion compounds is the competition between the Kondo effect and magnetic ordering.[1,2] Despite extensive theoretical work (see, for example, some recent papers[2–4] and the papers cited therein), this problem remains unresolved.

In this letter we wish to propose a model which describes the interaction of conduction electrons with localized moments and which has the following important features: (1) In the limit of a high multiplicity of the degeneracy, $N\to\infty$, the mean-field theory yields an exact solution. (2) A transition to either a Kondo state or a magnetically ordered state is possible within this exact solution. (3) The nature of the magnetically ordered state is determined by that magnitude of the wave vector at which the seed magnetic susceptibility of the gas of conduction electrons has its maximum. The determining factors here are the specified band structure, topology of the Fermi surface, and distribution of localized moments over the lattice of the skeleton.

We are reporting a study of a competition between the Kondo effect, which leads to the formation of a heavy-fermion state, and the ferromagnetic ordering of localized moments. For a certain specific value of the parameters of the model (as discussed below), we find that if the Kondo temperature T_K is higher than the ferromagnetic-ordering temperature T_m, then the appearance of Kondo screening of localized moments suppresses the ferromagnetic transition. In the opposite case ($T_K < T_m$), the appearance of a spontaneous magnetic moment suppresses the Kondo effect.

We should point out that the model proposed here provides us with a regular method for constructing a perturbation theory in the reciprocal of the multiplicity of the degeneracy (a $1/N$ expansion). In the limit $N=2$, the model is equivalent to a Kondo model with an anisotropic interaction.

Let us examine the system described by the Hamiltonian

$$H=\sum_{m,\vec{k}}\epsilon_{\vec{k}}c^{+}_{m\vec{k}}c_{m\vec{k}}-\frac{J}{2N}\sum_{\alpha,m,m'}\{c_{m'\alpha}f^{+}_{m'\alpha}f_{m\alpha}c^{+}_{m\alpha}+f_{m\alpha}c^{+}_{m\alpha}c_{m'\alpha}f^{+}_{m'\alpha}\}$$
$$+J_1N^{-1}\sum_{\alpha}S^{z}_{\alpha}s^{z}_{\alpha}. \qquad (1)$$

Here the operators $c^+_{m\vec{k}}$, $c_{m\vec{k}}$ create and annihilate conduction electrons with a wave vector $\vec{k}$ and an orbital quantum number m. This quantum number takes on values $-j \leqslant m \leqslant j$. The degeneracy multiplicity is $N = 2j + 1$. The operators $f^+_{m\alpha}$, $f_{m\alpha}$ create and annihilate localized electrons at the points with the coordinates $\vec{R}_\alpha$. We define the spin operators S^z and s^z by

$$S^z_\alpha = \frac{1}{N}\sum_m m f^+_{m\alpha} f_{m\alpha}, \quad s^z_\alpha = \frac{1}{N}\sum_m m c^+_{m\alpha} c_{m\alpha}. \tag{2}$$

The number of f electrons at the points $\vec{R}_\alpha$ is fixed by the condition

$$\sum_m f^+_{m\alpha} f_{m\alpha} = q_0 N. \tag{3}$$

With $J_1 = 0$ and $J > 0$, Hamiltonian (1) is the Coqblin–Schrieffer Hamiltonian,[6] which is widely used in describing the thermodynamic and kinetic properties of heavy-fermion compounds.[7–9] Making use of the commutation properties of Fermi operators, we can show that at $N = 2$, i.e., for spins $j = 1/2$, Hamiltonian (1) is the same as the anisotropic Kondo Hamiltonian

$$H = \sum_{m,\vec{k}} \epsilon_{\vec{k}} c^+_{m\vec{k}} c_{m\vec{k}} + \frac{1}{4}\sum_\alpha (J_z \hat{\tau}^z_{c\alpha}\hat{\tau}^z_{f\alpha} + J\hat{\tau}^x_{c\alpha}\hat{\tau}^x_{f\alpha} + J\hat{\tau}^y_{c\alpha}\hat{\tau}^y_{f\alpha}), \tag{4}$$

where $\hat{\tau}^\mu_{c\alpha} = \Sigma c^+_{m\alpha}\tau^\mu_{mm'}c_{m'\alpha}$, $\hat{\tau}^\mu_{f\alpha} = \Sigma f^+_{m\alpha}\tau^\mu_{mm'},c_{m'\alpha}$, and τ^μ are the Pauli matrices. The exchange interaction constant is $J_z = J + J_1/8$. The value $J_1 = 0$ thus corresponds to the isotropic case. For definiteness we assume J, $J_1 > 0$ below.

In the Matsubara temperature technique, the partition function for model (1) under condition (3) can be written as a functional integral over Grassmann fields c^+, c, f^+, f and Bose fields b^*, b, ψ^*, ψ, λ:

$$Z = \int D(c^+ c f^+ f b^* b \psi^* \psi \lambda) \exp\left(-\int_0^\beta d\tau \mathcal{Z}(\tau)\right), \tag{5}$$

$$\begin{aligned}\mathcal{Z}(\tau) = &\sum_{m\vec{k}} c^+_{m\vec{k}}(\partial_\tau + \epsilon_{\vec{k}} - \mu)c_{m\vec{k}} \\ &+ \sum_{m\alpha} f^+_{m\alpha}\partial_\tau f_{m\alpha} + N\sum_\alpha (J^{-1} b^*_\alpha b_\alpha + J_1 \psi^*_\alpha \psi_\alpha) \\ &- \sum_{m\alpha}(b^*_\alpha f^+_{m\alpha} c_{m\alpha} + b_\alpha c^+_{m\alpha} f_{m\alpha}) + J_1 \sum_\alpha (\psi^*_\alpha s^z_\alpha - \psi_\alpha S^z_\alpha) \\ &+ i\sum_{\alpha m}\lambda_\alpha\left(f^+_{m\alpha} f_{m\alpha} - q_0 + \frac{1}{2}\right).\end{aligned} \tag{6}$$

For $N \gg 1$, the integration over the Bose fields can be carried out by the method of steepest descent. At the saddle point we set

$$b_\alpha(\tau) = b_\alpha^*(\tau) = b_\alpha, \quad J_1\psi_\alpha(\tau) = h_\alpha, \quad \psi_\alpha^*(\tau) = M_\alpha, \quad i\lambda_\alpha(\tau) = \epsilon_{f\alpha} - \mu. \tag{7}$$

Here is the physical meaning of these parameters: b_α determines the effective parameter of the hybridization of c and f electrons at point α; h_α determines the local spontaneous magnetic field which acts on the local moment at point α; M_α is the magnitude of the spontaneous moment ($M_\alpha = \langle S^z \rangle /N$); and $\epsilon_{f\alpha}$ determines the effective position of the degenerate f level. As a result, we find the following expression for the free energy:

$$\mathcal{F}_{MF} = N \sum_\alpha (J^{-1}b_\alpha^2 + h_\alpha M_\alpha - (q_0 - \frac{1}{2})(\epsilon_{f\alpha} - \mu)) + \Phi[\epsilon_\alpha, b_\alpha, h_\alpha, M_\alpha], \tag{8}$$

$$\Phi[\epsilon_\alpha, b_\alpha, h_\alpha, M_\alpha] = -T \ln \int D(c^+ c f^+ f) \exp\{ \sum_{\omega m \vec{k}} (i\omega - \epsilon_{\vec{k}}$$

$$+\mu) c^+_{m\vec{k}}(\omega) c_{m\vec{k}}(\omega) + \sum_{\omega m \alpha} [(i\omega - \epsilon_{f\alpha} + \mu + \frac{m}{N} h_\alpha) f^+_{m\alpha} f_{m\alpha} \tag{9}$$

$$- \frac{m}{N} J_1 M_\alpha c^+_{m\alpha}(\omega) c_{m\alpha}(\omega) + b_\alpha (f^+_{m\alpha}(\omega) c_{m\alpha}(\omega) + c^+_{m\alpha}(\omega) f_{m\alpha}(\omega))]\}.$$

The Gaussian functional integral in (9) can be evaluated easily once the structure of the ground state has been determined. The values of $\epsilon_{f\alpha}$, b_α, h_α, and M_α are found from the solution of the system of equations

$$\frac{\partial \mathcal{F}_{MF}}{\partial \epsilon_{f\alpha}} = \frac{\partial \mathcal{F}_{MF}}{\partial b_\alpha} = \frac{\partial \mathcal{F}_{MF}}{\partial h_\alpha} = \frac{\partial \mathcal{F}_{MF}}{\partial M_\alpha}. \tag{10}$$

To determine the type of magnetic order, we consider the static magnetic susceptibilities of the sublattice of localized moments and of the gas of conduction electrons. For this purpose we need to find the following correlation functions:

$$\chi_{f\alpha\beta} = \frac{T}{N} \langle S_\alpha^z(\omega_n = 0) S_\alpha^z(\omega_n = 0) \rangle, \quad \chi_{c\alpha\beta} = \frac{T}{N} \langle s_\alpha^z(\omega_n = 0) s_\beta^z(\omega_n = 0) \rangle. \tag{11}$$

These functions are related to the magnetic susceptibility by the simple expression $\chi^{zz}_{\alpha\beta} = g^2 \mu_B^2 \chi_{\alpha\beta}$. An exact summation of the perturbation-theory series in the leading order in $1/N$ leads to the following results for temperatures $T > T_m$, T_K:

$$\chi_f(\vec{q}) = \frac{\chi_f^0}{1 - J_1^2 \chi_f^0 \chi_c^0(\vec{q})}, \quad \chi_c(\vec{q}) = \frac{\chi_c^0(\vec{q})}{1 - J_1^2 \chi_f^0 \chi_c^0(\vec{q})},$$

$$\chi_c^0(\vec{q}) = \sum_\alpha \exp(i\vec{q}\vec{R}_\alpha) \chi_c^0(R_\alpha), \tag{12}$$

where $g^2\mu_B^2\chi_f^0$ is the susceptibility of a free local moment ($\chi_f^0 = j(j+1)q_0(1-q_0)/3N^2T$ and $g^2\mu_B^2\chi_c^0(\vec{R})$ is a seed susceptibility of the gas of conduction electrons ("seed" in the sense that the interaction with f electrons is ignored). The summation in (12) is carried out over all sites $\vec{R}_\alpha$ of the sublattice of f electrons; $\vec{q}$ is a wave vector in this sublattice. It follows from (12) that the temperature of the magnetic transition, T_m, can be found under the condition $T_m > T_k$ from the equation

$$J_1^2\chi_f^0 \max \chi_c^0(\vec{q}) = 1. \tag{13}$$

The value of $\vec{q}_m$ at which $\chi_c^0(\vec{q})$ has a maximum determines the structure of the magnetically ordered phase. The value $q_m = 0$, for example, corresponds to a transition to a ferromagnetic state. The q dependence of χ_c^0 is determined by the band structure of the skeleton, by the topology of the Fermi surface, and by the parameters of the sublattice of localized moments (Refs. 10–12, for example). According to (12), the magnetic phase transition in model (1) results from an intensification of features in the magnetic susceptibility of the gas of conduction electrons as the result of an exchange interaction with localized moments.

We turn now to the simple case in which the state density ρ_F in the conduction band is nearly constant, in which the f and c sublattices coincide, and in which the susceptibility χ_c^0 of the gas of c-electrons has its standard form, with a maximum at $q_m = 0$. In this case a ferromagnetic transition can occur in the system. The temperature of this transition can be found easily from (13):

$$T_m = \left[\frac{j(j+1)}{3N^2}\right]^2 J_1^2\rho_F q_0(1-q_0). \tag{14}$$

The behavior of the spontaneous moment $M(T)$ and of $h(T)$ is found from system of equations (10), which takes the following form in the case $M_\alpha = M$, $h_\alpha = h$, $\epsilon_{f\alpha} = \epsilon_f$, and $b_\alpha = 0$:

$$q_0 = \frac{1}{N}\sum_m n(\epsilon_f - mh/N), \quad M = \frac{1}{N}\sum_m \frac{m}{N} n(\epsilon_f - mh/N), \tag{15}$$

$$h = (J_1/N\mathcal{N})\sum_{m\vec{k}} \frac{m}{N} n(\epsilon_{\vec{k}} - mJ_1M/N),$$

where $n(\epsilon) = [\exp((\epsilon-\mu)/T)+1]^{-1}$, and $\mathcal{N}$ is the number of unit cells.

To determine the temperature of the transition to a coherent Kondo state, we seek a solution of Eqs. (10) with $M_\alpha h_\alpha = 0$, $b_\alpha = b \neq 0$, and $\epsilon_{f\alpha} = \epsilon_f$. The equations for b and ϵ_f are in the standard form for the Coqblin–Schrieffer model.[7,9] For a half-filled conduction band and the value $q_0 = 1/2$, i.e., if the f level is nearly half-filled, we also have

$$T_K = \mu \exp(-1/J\rho_F - 0.126). \tag{16}$$

We turn now to the problem of the competition between the Kondo effect and ferromagnetism. According to (14) and (16), by varying J and J_1 we can arrange arbitrary relations between T_m and T_K. We first consider the case $T_M > T_K$. At $T < T_m$ a spontaneous field $h(T)$ then arises. We know quite well that a coherent Kondo state is destroyed if the field acting on a localized moment exceeds a critical field $h_K(T)$. It is thus clear that at $h(T) > h_K(T)$ a transition to a coherent Kondo state in the region $T < T_m$ becomes impossible. In the case of a half filling we find $h_K(T) = 7.5 T_K \ln^{1/2}(T_K/T)$ and $h(T) \simeq 8.9 T_m (1 - T/T_m)^{1/2}$. It follows that if $T_m > T_K$, but T_m and T_K are not far apart, then the field $h(T)$ increases more rapidly than $h_k(T)$, indicating a suppression of the Kondo effect by the ferromagnetism

If $T_K > T_m$, there is first a transition to a coherent Kondo state with an effective hybridization $b(T) \simeq [(T\mu/2q_0(1-q_0)\ln(T_K/T)]^{1/2}$ for T near T_K. Analysis of the stability of the Kondo state with respect to magnetic fluctuations shows that, in the particular case which we are discussing here (in terms of the choice of the band ϵ_K and a half filling), the appearance of a value $b \neq 0$ suppresses the transition to the ferromagnetic state. Consequently, the total magnetic susceptibility behaves in the following way at $T_K > T_m$. As the temperature decreases to $T = T_K$, the susceptibility increases in accordance with $\chi^{zz} = C/(T - T_m)$. At $T = T_K$, the susceptibility changes slope and begins to decrease with decreasing temperature. It reaches a finite but large value C/T_0, where $T_0 \sim T_K$.

In conclusion we repeat that the results found for model (1) are sensitive to the choice of the band structure of the skeleton and the choice of the sublattice of localized moments. The corresponding band structures must thus be used to analyze experimental data with the help of model (1). In particular, it is very important to study the behavior of the magnetic susceptibility of the gas of conduction electrons, $\chi_c^0(\vec{q})$. This behavior is important for determining the structure of the magnetically ordered phase.

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