Formation of the magnetic state of a Kondo lattice

V. Yu. Irkhin and M. I. Katsnel'son
Institute of Metal Physics, Ural Branch of the Russian Academy of Sciences, 620219, Ekaterinburg

(Submitted 7 April 1992)
Pis'ma Zh. Eksp. Teor. Fiz. **55**, No. 10, 567–569 (25 May 1992)

The mutual influence of the Kondo effect and the intersite exchange interaction is analyzed by a simple version of the renormalization-group method for a periodic *s*–*f* exchange model. Any of several situations can arise—an ordinary magnetic state, a Kondo magnetic state, and a nonmagnetic Kondo lattice—depending on the relation between the one-impurity Kondo temperature and the seed frequency of the spin fluctuations. Explicit expressions are derived for the saturation moment and for the renormalization of the spin dynamics for the case of a "ferromagnetic" *s*–*f* exchange.

Many experimental studies in recent years have shown convincingly that magnetic ordering is quite common among systems with heavy fermions and other anomalous *f* compounds, which are called "Kondo lattices" (see the review[1]). A characteristic feature of magnetic Kondo lattices is a pronounced sensitivity of the saturation moment M_s to external agents (doping or pressure). The values of M_s range from on the order of $10^{-2}\,\mu_B$ (in, for example, UPt_3, $CeAl_3$, and $CeInCu_2$) to on the order of μ_B [UCd_{11}, U_2Zn_{17}, TmS, $U(Pt_{0.95}Pd_{0.05})_3$, $U_{0.95}Th_{0.05}Pt_3$, and $CeAl_2$]. It was suggested in Refs. 1 and 2 that this behavior results from a mutual influence of the Kondo effect and an intersite exchange interaction. This suggestion contradicts the earlier belief that a competition between these factors would lead to the complete suppression of one of them.[3] In the present letter we generalize that hypothesis, and we explain the pronounced sensitivity of M_s.

We start from the Hamiltonian of a periodic *s*–*f* model:

$$H=\sum_{\vec{k}\sigma}\epsilon_{\vec{k}}c^{+}_{\vec{k}\sigma}c_{\vec{k}\sigma}-I\sum_{\vec{k}\vec{q}\alpha\beta}\vec{S}_{\vec{q}}\vec{\sigma}_{\alpha\beta}c^{+}_{\vec{k}+\vec{q}\alpha}c_{\vec{k}\beta}-\sum_{\vec{q}}J_{\vec{q}}S_{\vec{q}}S_{-\vec{q}}, \tag{1}$$

where the operators $c^{+}_{\vec{k}\sigma}$ create conduction electrons, $\vec{S}_{\vec{q}}$ are Fourier components of the spin operators, and $\vec{\sigma}$ are Pauli matrices. To analyze the renormalization of the *s*–*f* exchange parameter *I* in a paramagnet (PM), a ferromagnet (FM), and an antiferromagnet (AFM), we use a simple version of the renormalization-group method ("poor man scaling"[4]). We use a perturbation theory in *I* to calculate the eigenenergy parts of the electron Green's function $\Sigma_\sigma(\vec{k},E)$. For a ferromagnet, for example, we find

$$\Sigma_\sigma(\vec{k},E)=-\sigma IS+2I^2S\sum_{\vec{q}}\frac{\delta_{\sigma,-}+\sigma f_{\vec{q},-\sigma}}{E-\epsilon_{\vec{q},-\sigma}+\sigma\omega_{\vec{q}-\vec{k}}},\quad \sigma=\pm(\uparrow,\downarrow), \tag{2}$$

where $\epsilon_{\vec{k}\sigma}=\epsilon_{\vec{k}}-\sigma IS$, $\omega_{\vec{q}}$ is the magnon frequency, and $f_{\vec{k}\sigma}=f(\epsilon_{\vec{k}\sigma})$ is a Fermi function. We find the effective s–f parameter through a renormalization of the spin splitting on the Fermi surface.

$$I_{cf} = \frac{[\Sigma_\downarrow(\vec{k}, E) - \Sigma_\uparrow(\vec{k}, E)]}{2S}, \quad \epsilon_{\vec{k}\sigma} = E = 0.$$

We find a renormalization-group equation by breaking up the sum with $f_{\vec{q}, -\sigma}$ in (2) into layers $C < \epsilon_{\vec{q}, -\sigma} < C + \delta C$, calculating the contribution from each layer, and making the replacement $I \to I_{ef}$ in the expression for $\partial I_{ef}/\partial C$. Correspondingly, we can determine I_{ef} in an antiferromagnet through a renormalization of the antiferromagnetic gap in the electron spectrum. For this purpose we need to calculate Σ to third order in I (Ref. 5). Finally, I_{ef} in a paramagnet is determined from the imaginary part of Σ calculated in third order in I with allowance for the spin dynamics.[1,5] Introducing the dimensionless coupling constant $g_{ef} = -2\rho I_{ef}$ (ρ is the density of states at the Fermi level), we find

$$\frac{\partial g_{ef}(C)}{\partial C} = \frac{g_{ef}^2(C)}{C}\phi\left(\frac{\bar{\omega}_{ef}(C)}{C}\right).$$

The function $\phi(x)$, which satisfies the condition $\phi(0) = 1$, depends on the type of magnetic structure and the dimensionality of the space, d:

$$\phi(x) = \begin{cases} (1/x)\arctan x, & \text{PM}, d = 3 \\ (1/2x)\ln[(1+x)/(1-x)], & \text{FM}, d = 3 \\ -(1/x^2)\ln(1-x^2), & \text{AFM}, d = 3 \\ (1-x^2)^{-1/2}, & \text{AFM}, d = 2 \end{cases} \tag{4}$$

Here $\overline{\omega}$ is a characteristic frequency of the spin fluctuations ($\overline{\omega} = \omega_{2k_F}$ in a ferromagnet or antiferromagnet; $\overline{\omega} = 4Dk_F^2$ in a paramagnet, where D is the spin diffusion coefficient, and k_F the Fermi momentum). In turn, $\overline{\omega}$ is replaced by $\overline{\omega}_{ef}$, which depends on the cutoff parameter C through the Kondo contributions from filled electron states. The logarithmic corrections to $\overline{\omega}$ on the order of I^3 were found for a paramagnet in Ref. 2 from the second moment of the spin correlation function. Using the approximation of nearest neighbors (at a distance R) for f–f exchange, we find

$$\frac{\partial \ln \bar{\omega}_{ef}(C)}{\partial C} = -\frac{1-\alpha}{2C} g_{ef}^2(C)\phi\left(\frac{\bar{\omega}_{ef}(C)}{C}\right), \quad \alpha = \left(\frac{\sin k_F R}{k_F R}\right)^2, \tag{5}$$

where $\phi(x) = \arctan x/x$. Formally, the Kondo corrections to $\overline{\omega}$ for a ferromagnet or antiferromagnet arise from terms which describe the anharmonicity of magnons when the logarithmic corrections to their occupation numbers $N_{\vec{p}}$ at $T = 0$ are taken into account. (They arise from the s–f exchange damping). For a ferromagnet, for example, we have

$$\delta\omega_{\vec{q}} = 2\sum_{\vec{p}}(J_{\vec{p}} + J_{\vec{q}} - J_{\vec{p}-\vec{q}} - J_0)\delta N_{\vec{p}},$$

$$\delta N_{\vec{p}} = 2I^2 S \sum_{\vec{k}} \frac{f_{\vec{k}\downarrow}(1 - f_{\vec{k}+\vec{p}\uparrow})}{(\epsilon_{\vec{k}\downarrow} - \epsilon_{\vec{k}+\vec{p}\uparrow} - \omega_{\vec{p}})^2}.$$

For all magnetic states we find Eq. (5); the function $\phi(x)$ is defined in (4).

Equations (3) and (5) can be put in the form

$$\bar{\omega}_{ef}(\xi) = \bar{\omega} \exp\left\{\frac{1-\alpha}{2}[g - g_{ef}(\xi)]\right\}, \tag{6}$$

$$\frac{1}{g_{ef}(\xi)} = \frac{1}{g} - \int_0^{\xi} d\xi' \psi\left(\beta + \frac{1-\alpha}{2} g_{ef}(\xi') - \xi'\right), \tag{7}$$

$$g = -2\rho I \ll 1, \quad \beta = \ln\left(\frac{W}{\bar{\omega}}\right) \gg 1, \quad \xi = \ln\left|\frac{W}{C}\right|, \tag{8}$$

where W is the width of the conduction band, and $\psi(x) = \phi(e^{-x})$ is a monotonically increasing function. Here $\psi(x \gg 1) \simeq 1$. Analysis of Eq. (7) reveals three distinctive regions of parameter values in the model, which are determined by the relation between the seed values of $\overline{\omega}$ and the single-dopant Kondo temperature $T_K = W\exp(-1/g)$ $(g>0)$.

If $\omega < T_K$ (if g is greater than $\beta - 1$), there is clearly no value ξ^* at which g_{ef} diverges. The quantity $T_K^* = W\exp(-\xi^*)$ plays the role of a Kondo temperature for the lattice. As $\xi \to \xi^*$, the quantity $\overline{\omega}_{ef}(\xi)$ vanishes as $\exp[-(\xi - \xi^*)^{-1}]$. One might suggest that in this case all the current carriers are coupled with f spins in singlet states, that the spin–spin interaction is suppressed, and that we are dealing with the case of a nonmagnetic Kondo lattice. This case also corresponds to dilute Kondo systems $\overline{\omega} \to 0$, $\beta \to \infty$.

If $1 < (\beta g)^{-1} < 1 + \text{const}\cdot g$, or equivalently, if $T_K < \overline{\omega} < AT_K$ $[A = O(1)$ as $g \to 0]$, there exists a fixed point with a finite g^* as $\xi \to \infty$. The magnetic moment is not completely canceled. Calculating the corrections to the sublattice magnetization $\overline{S}$ in the ferromagnetic and antiferromagnetic phases, or the corrections to the Curie constant in the paramagnetic phase,[5] we find

$$\frac{\bar{S}_{ef}(\xi)}{S} = \left(\frac{\bar{\omega}_{ef}(\xi)}{\bar{\omega}}\right)^{\frac{1}{1-\alpha}} \simeq \exp\left[-\frac{g_{ef}(\xi) - g}{2}\right]. \tag{9}$$

Consequently, as the seed constant g varies over a small interval on the order of g^2 in size, the value of $g^* = g_{ef}(\xi = \infty)$ changes from on the order of unity to infinity, while $\overline{S}^* = \overline{S}_{ef}(\xi = \infty)$ falls off from values on the order of S to zero. These results can apparently explain the pronounced sensitivity of the M_s values in heavy-fermion systems.

Finally, for $\beta g \ll 1$, i.e., for $\overline{\omega} \gg T_K$, $g^* \simeq g$, the Kondo divergences are cut off at $|C| \sim \overline{\omega}$, and it is sufficient to consider only the logarithmic corrections of second order in g. In other words, we are dealing with the case of an ordinary magnetic material.

We need to stress that neither the very fact that there is a magnetic ordering nor the type of ordering is of particular importance in determining the regime: The only changes are in the form of the function $\phi(x)$ and thus in the constant A.

For s–f ferromagnetic exchange, with $I>0$ $(g<0)$, we have $|g_{ef}(\xi)|<|g|$. In this case, Eqs. (3), (5), and (9) are useful for more than a qualitative analysis; they lead to explicit expressions for $\overline{S}^*$ and $\overline{\omega}^*=\overline{\omega}_{ef}(\xi=\infty)$. Ignoring $g_{ef}(\xi)$ in comparison with β in the argument of the function ψ in (7), we find

$$\bar{\omega}^* = \bar{\omega}\exp\left[-\frac{(1-\alpha)g^2\beta}{2(1-g\beta)}\right], \tag{10}$$

$$\bar{S}^* = S\exp\left[-\frac{1}{2}\frac{g^2\beta}{1-g\beta}\right]. \tag{11}$$

In the case $g\beta \ll 1$, expression (10) becomes the corresponding result of Ref. 5. For pure rare-earth metals we would have $g \sim 10^{-2}$, and the renormalizations in (10) and (11) are unimportant. They may, on the other hand, be important for compounds with a high density of states at the Fermi level.

[1]V. Yu. Irkhin and M. I. Katsnel'son, Fiz. Met. Metalloved. **1**, 16 (1991).
[2]V. Yu. Irkhin and M. I. Katsnelson, Z. Phys. B **82**, 77 (1991).
[3]V. V. Moshchalkov and N. B. Brandt, Usp. Fiz. Nauk **149**, 585 (1986) [Sov. Phys. Usp. **29**, 725 (1986)].
[4]P. W. Anderson, J. Phys. C **3**, 2346 (1970).
[5]Y. Yu. Irkhin and M. I. Katsnelson, Z. Phys. B **75**, 67 (1989).

Translated by D. Parsons