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**LETTER TO THE EDITOR**

# On the mean-field theory of magnetically ordered Kondo lattices

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**Abstract.** Magnetic solutions for the problem of the Kondo lattice ground state are analysed within the mean-field approximation. For the constant bare density of states, the saturated ferromagnetic Kondo state is stable at not too large intersite interactions $J$, and with increasing $J$ a first-order transition to the usual ferromagnetic state takes place. The criterion of antiferromagnetism is determined by the non-uniform magnetic susceptibility and reads $|J| \sim T_K$ with $T_K$ the Kondo temperature.

Recent experimental data [1–3] demonstrate that a large number of anomalous rare-earth and actinide compounds, including 'classical' heavy-fermion systems $CeAl_3$, $UPt_3$ and $CeCu_2Si_2$, possess magnetic ordering at low $T$, the magnetic state being highly sensitive to external pressure and additions of impurities. In this connection, the problem of the coexistence of the Kondo state and magnetic ordering acquires great importance. In the present letter, we treat this problem within the periodic s–f model with spin $S = \frac{1}{2}$ using the mean-field approach of Coleman and Andrei [4].

Unlike [4] where anomalous averages corresponding to a spin-liquid state were picked out from the Heisenberg Hamiltonian $H_f$ of localized spins, we consider the (more simple) case of magnetic long-range order. Performing the saddle-point approximation in the path integral (cf [4]), the Hamiltonian of the s–f exchange interaction is replaced in the mean-field approximation as

$$-I\sum_{\alpha\beta} c_{i\alpha}^{+}c_{i\beta}(\sigma_{\alpha\beta}\cdot S_i - \tfrac{1}{2}\delta_{\alpha\beta}) \to c_i^{+}\hat{V}_i f_i + \text{HC} - \frac{1}{2I}\text{Tr}(V_i^{+}V_i)$$

where $c_i^{+} = (c_{i\uparrow}^{+}, c_{i\uparrow}^{+})$, etc, $f_{i\sigma}^{+}$ are pseudofermion operators and $\hat{V}_i$ is an effective-hybridization matrix determined from the minimization of the free energy. For a ferromagnet we have

$$V_i^{\sigma\sigma'} = V_\sigma\delta_{\sigma\sigma'} \qquad H_f = -J\bar{S}\sum_{i\sigma}\sigma f_{i\sigma}^{+}f_{i\sigma} \qquad \bar{S} = \langle S^z\rangle$$

$$H - \mu\hat{N} = \sum_{k\sigma}[(\varepsilon_k - \mu)c_{k\sigma}^{+}c_{k\sigma} + W_\sigma f_{k\sigma}^{+}f_{k\sigma} + V_\sigma(c_{k\sigma}^{+}f_{k\sigma} + \text{HC}) + \text{constant} \qquad (1)$$

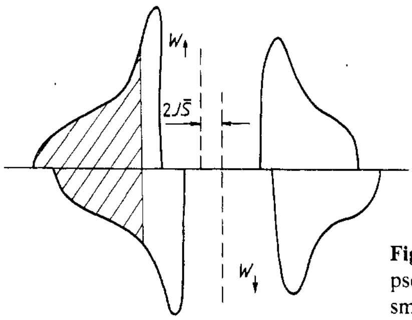


**Figure 1.** Total density of states (including that of pseudofermions) of a Kondo ferromagnet with a small spin splitting, $c < 1$ (schematic).

with $W_\sigma = W - \sigma J\bar{S}$ and $W$ of the order of the Kondo temperature $T_K$. Diagonalizing (1), we obtain

$$c_{k\sigma} = \cos(\theta_{k\sigma}/2)\,\alpha_{k\sigma} - \sin(\theta_{k\sigma}/2)\,\beta_{k\sigma} \qquad f_{k\sigma} = \sin(\theta_{k\sigma}/2)\,\alpha_{k\sigma} + \cos(\theta_{k\sigma}/2)\,\beta_{k\sigma}$$
$$\sin\theta_{k\sigma} = 2V_\sigma/E_{k\sigma} \qquad \cos\theta_{k\sigma} = (\varepsilon_k - \mu - W_\sigma)/E_{k\sigma} \tag{2}$$
$$\varepsilon_{k\sigma}^{1,2} = \tfrac{1}{2}(\varepsilon_k - \mu + W_\sigma \pm E_{k\sigma}) \qquad E_{k\sigma} = [(\varepsilon_k - \mu - W_\sigma)^2 + 4V_\sigma^2]^{1/2}$$

and

$$\langle H - \mu\hat{N}\rangle = \sum_{k\sigma}\sum_{j=1,2} \varepsilon_{k\sigma}^j n_{k\sigma}^j + J\bar{S}^2 - \frac{1}{2I}\sum_\sigma V_\sigma^2 \tag{3}$$

where $n_{k\sigma}^j = \exp[(\varepsilon_{k\sigma}^j/T) + 1]^{-1}$. The quantities $V_\sigma$, $W$, the chemical potential $\mu$ and the magnetization $\bar{S}$ are determined from the equations

$$V_\sigma \equiv 2I\sum_k \langle c_{k\sigma}^+ f_{k\sigma}\rangle = -2IV_\sigma \sum_k \frac{n_{k\sigma}^{(2)} - n_{k\sigma}^{(1)}}{E_{k\sigma}} \tag{4}$$

$$c \equiv \sum_{k\sigma} \langle c_{k\sigma}^+ c_{k\sigma}\rangle = \tfrac{1}{2}\sum_{k\sigma j}[1 - (-1)^j \cos\theta_{k\sigma}]n_{k\sigma}^j \tag{5}$$

$$n_\sigma \equiv \sum_k \langle f_{k\sigma}^+ f_{k\sigma}\rangle = \tfrac{1}{2} + \sigma\bar{S} = \tfrac{1}{2}\sum_{kj}[1 + (-1)^j \cos\theta_{k\sigma}]n_{k\sigma}^j. \tag{6}$$

For $T = 0$ and small $|V_\sigma|$ we have $\cos\theta_{k\sigma} \simeq \mathrm{sgn}(\varepsilon_k - \mu - W_\sigma)$, and equations (4)–(6) are simplified. We restrict ourselves to the case where the conduction electron concentration $c < 1$ (the results for $c > 1$ are obtained after the particle–hole transformation $c \to 2 - c$, $\sigma \to -\sigma$). Define the function $\mu(n)$ by

$$n = 2\int_0^{\mu(n)} \mathrm{d}\varepsilon\,\rho(\varepsilon)$$

with $\rho(\varepsilon)$ $(0 < \varepsilon < D)$ the bare density of states. Then equation (5) at $|W_\sigma| \ll \mu$ reduces to $\mu(c) = \mu$.

Consider different types of ferromagnetic solution. If $\bar{S}$ is not too large, the condition $W_\sigma > V_\sigma^2/(D - \mu)$ holds, as well as at $\bar{S} = 0$, for both $\sigma$ (figure 1). Then we get from (4)–(6)

$$1 = -2I\int_0^{\mu+\lambda_\sigma} \frac{\mathrm{d}\varepsilon\,\rho(\varepsilon)}{[(\varepsilon - \mu)^2 + 4V_\sigma^2]^{1/2}} \tag{7}$$

$$\lambda_\sigma \equiv V_\sigma^2/W_\sigma = \mu(c + 2n_\sigma) - \mu. \tag{8}$$

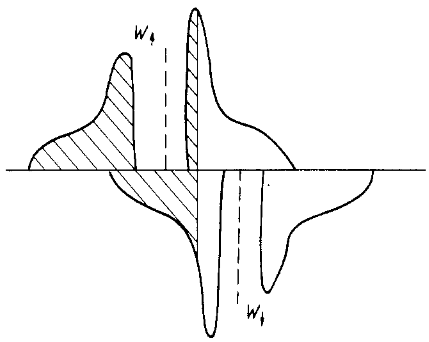

**Figure 2.** Density of states in the case where the splitting exceeds the energy gap.

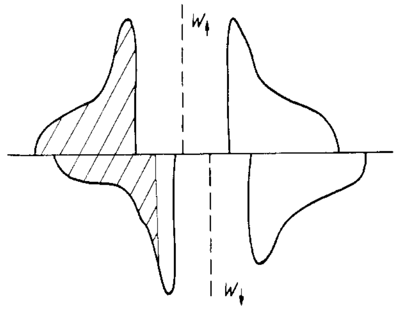

**Figure 3.** Density of states of a 'half-metallic' Kondo ferromagnet.

Introducing the cut-off parameter $L$ which does not enter the final results and using the relation

$$\int_0^B \frac{\mathrm{d}\varepsilon\,\rho(\varepsilon+\mu)}{(\varepsilon^2+4V^2)^{1/2}} \simeq \rho(\mu)\ln\left|\frac{L}{V}\right| + \int_L^B \mathrm{d}\varepsilon\,\frac{\rho(\varepsilon+\mu)}{\varepsilon}$$

($|V| \ll L \ll B$) we derive the equation for $\bar{S}$:

$$\tanh\left(\frac{1}{4\rho(\mu)}\int_{\mu(c+2n_\downarrow)}^{\mu(c+2n_\uparrow)} \mathrm{d}\varepsilon\,\frac{\rho(\varepsilon)-\rho(\mu)}{\varepsilon-\mu}\right) = \frac{J\bar{S}}{W}. \tag{9}$$

If $W_\downarrow > V_\downarrow^2/(D-\mu)$, $W_\uparrow < -V_\uparrow^2/\mu$ (figure 2), equations (7) and (8) hold for $\sigma \equiv \downarrow$; for $\sigma \equiv \uparrow$, one has

$$1 = -2I\int_{\mu+\lambda_\uparrow}^{D} \frac{\mathrm{d}\varepsilon\,\rho(\varepsilon)}{[(\varepsilon-\mu)^2+4V_\uparrow^2]^{1/2}} \tag{10}$$

$$\lambda_\uparrow = \mu(c-2+2n_\uparrow) - \mu. \tag{11}$$

Then we obtain in analogy with (9)

$$\mathrm{cotanh}\left[\frac{1}{4\rho(\mu)}\left(\int_{\mu_1-\mu}^{\mu-\mu_2} \mathrm{d}\varepsilon\,\frac{\rho(\varepsilon+\mu)-\rho(\mu)}{\varepsilon} + \int_{\mu}^{D-\mu} \mathrm{d}\varepsilon\,\frac{\rho(\varepsilon+\mu)}{\varepsilon}\right)\right] = \frac{J\bar{S}}{W}$$

$$\mu_1 \equiv \mu(c+2n_\downarrow) \qquad \mu_2 \equiv \mu(c-2+2n_\uparrow). \tag{12}$$

If $W_\downarrow > V_\downarrow^2/(D-\mu)$, $-V^2/\mu < W_\uparrow < V^2/(D-\mu)$, i.e. $W_\uparrow$ lies in the energy gap (the 'half-metallic' case (figure 3)), the magnetization is determined by the number of conduction electrons only: $n_\uparrow = 1 - c/2$, $n_\downarrow = c/2$, $\bar{S} = (1-c)/2$. This solution exists at

$$-\varphi/\mu < [\mu(2c)-\mu]^{-1} - J(1-c)/V_\downarrow^2 < \varphi/(D-\mu) \tag{13}$$

$$\varphi = \left(\frac{V_\uparrow}{V_\downarrow}\right)^2 = \exp\left(\frac{1}{\rho(\mu)}\int_{\mu(2c)}^{D} \frac{\mathrm{d}\varepsilon\,\rho(\varepsilon)}{\varepsilon-\mu}\right). \tag{14}$$

Let us discuss the case $\rho(\varepsilon) = \rho = 1/D$ = constant. Then equation (9) has no non-trivial solutions (although solutions with $\bar{S} \neq 0$ may arise for some $\rho(\varepsilon)$ at $J \sim W \sim T_K$). Equation (12) turns out to have the solution

$$2J\bar{S} = D\exp(1/2I\rho) \equiv T_K \qquad \tfrac{1}{2}(1-c) < \bar{S} < \tfrac{1}{2} \tag{15}$$

at $T_K < J < T_K/(1-c)$. The condition (13) takes the form $J < T_K/(1-c)$ for $\rho$ = constant.

To investigate the energy stability of the solutions obtained, we calculate from (3) the corresponding values of the total energy:

$$E(N) = \langle H - \mu\hat{N}\rangle + \mu N + W \qquad N = \langle\hat{N}\rangle \equiv c \qquad \mu = \mu(N)$$

(the quantity $-W$ plays the role of the chemical potential for pseudofermions with $N_f = 1$). For the non-magnetic Kondo state, solution (15) and the saturated Kondo ferromagnetic state we obtain

$$E = c^2/4\rho - \tfrac{1}{2}cT_K \tag{16}$$

$$E = c^2/4\rho + J\bar{S}^2 + \tfrac{1}{2}(1-c)T_K \tag{17}$$

$$E = c^2/4\rho - J\bar{S}^2 - \tfrac{1}{2}cT_K \tag{18}$$

respectively. Thus, in the mean-field approximation with $\rho$ = constant, only the case of the saturated Kondo ferromagnet is realized. In this state, each conduction electron 'compensates' one localized spin, as in the s–f model with $I \to -\infty$ or the narrow-band Hubbard model [5]. Ferromagnetism is caused by exchange interaction between the moments which remain uncompensated. Equation (18) should be compared with the energy of the usual ferromagnetic state with $V_\sigma = 0$, $\bar{S} = \tfrac{1}{2}$, $E = N^2/4\rho - J/4$. One can see that the latter state becomes energetically favourable for $J(1 - c/2) > T_K$, and at the critical point a first-order transition takes place.

Quantum fluctuations may result in the formation of a non-saturated state (cf [5]). Note that the case $\rho$ = constant (where $T_K$ does not vanish at $c \ll 1$) imitates that of two dimensions.

We have demonstrated that the dependence $V$ of $\sigma$ plays a crucial role in the criterion of ferromagnetism. This is not the case for antiferromagnetic ordering where, in the mean-field approximation,

$$H_f = -J_Q\bar{S}_Q \sum_k (f^+_{k+Q\uparrow} f_{k\downarrow} + \text{HC})$$

($\bar{S}_Q$ is the staggered magnetization; $J_Q = J_{max}$) since corrections to $V$ and $W$ are of the order of $(J_Q\bar{S}_Q)^2/D$. Thus at $\bar{S}_Q \to 0$ the criterion of antiferromagnetism has the usual form $J_Q\chi_Q > 1$ with $\chi_Q$ being the non-enhanced staggered susceptibility of localized electrons (pseudofermions) in the effective hybridization model (1). The dominant contribution comes from intersubband transitions (cf [6, 7])

$$\delta\chi_Q = 2\sum_k \cos^2\left(\frac{\theta_k}{2}\right)\sin^2\left(\frac{\theta_{k+Q}}{2}\right)\frac{n_k^{(2)} - n_{k+Q}^{(1)}}{\varepsilon_{k+Q}^{(1)} - \varepsilon_k^{(2)}} \sim \frac{D}{V^2} \sim \frac{1}{T_K}$$

so that the criterion reads $J_Q >$ constant $\times\, T_K$.

Although we are dealing with an itinerant model of magnetism (with the hybridization spectrum of conduction electrons), one can see that the criterion of magnetic ordering is essentially different from the Stoner criterion. In particular, intra-site interaction, entering the latter, is replaced by intersite interaction. In this sense, the magnetism of Kondo lattices is of a 'localized' nature. At the same time, magnetic moments are non-integer, as in 'diluted' (by non-magnetic atoms) systems.

In real Kondo ferromagnets ($CeRh_3B_2$, $CeSi_x$, $Ce_4Bi_3$, etc) the effects of spin dynamics seem to play an important role (e.g. the paramagnon specific-heat enhancement has been observed in $CeSi_x$ [8]). Such effects are not taken into account in the mean-field approximation; for $T > T_K$ they were considered in [9]. For the case of low $T$ these questions will be treated elsewhere [10]. However, the main result of the present paper concerning possible instability of the Kondo lattice ground state with respect to magnetic ordering seems to be reliable.

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