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LETTER TO THE EDITOR

Fermi liquid model for Kondo lattice systems

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Abstract. We present a Fermi liquid theory for Kondo lattice systems in which spin–orbit effects are specifically included. We assume the ground state of the Kondo lattice to be single-ion Kondo singlets built coherently into the lattice. We explain the advantage of our model over that of Zou and Anderson.

It is well known that the ground state of a Kondo ion is a singlet, and its low-energy behviour is strongly constrained by the Friedel sum rule. Renormalisation group analysis and exact solution (Nozieres 1974, 1978, Nozieres and Blandin 1980, Wilson 1975, Andrei 1980, Andrei *et al* 1983, Tsvelick and Wiegmann (1983) suggest that a renormalised resonant level (RL) is a good description of the low-energy behaviour of such a system. The RL, which is characterised by an effective width Δ^* and an effective f level position E_f^*, describes a renormalised f state with $2J + 1 = N$ scattering channels, each with a specified azimuthal quantum number (Haldane 1978) m_j. In the Kondo regime, $\Delta^* \simeq D \exp(-\pi|E_f|/N\Delta)$ for $-E_f \gg N\Delta$ where Δ and E_f are the bare hybridisation width and f level position and $2D$ is the band width.

In a Kondo lattice, the energy scale for lattice coherence effects is smaller than the Kondo temperature, and the contribution to the free energy from inter-site coherence effects are of higher order in $1/N$ than intra-site effects (Ramakrishnan 1982, Kuramoto 1983, Grewe 1983, Coleman 1983). In view of the above, Razahfimandimby *et al* (1984) and d'Ambrumenil and Fulde (1985) have assumed that, for a Kondo lattice, the scattering at each Kondo site can be described by a phase shift

$$\delta_\nu(\varepsilon) = \delta(\mu) + (\varepsilon - \mu)/T_K + \sum_{\nu'\varepsilon'} \varphi_{\nu\nu'} \delta n_{\nu'}(\varepsilon') \tag{1}$$

where ν and ν' denote the spin–orbital states of the localised f level, T_K is the Kondo temperature and $\delta(\mu)$ is fixed by the valence of the Kondo ion and by using the Friedel sum rule. Requiring that the scattering for the lattice at $T = 0$ ($\delta n_{\nu'} = 0$) is coherent leads to the KKRZ equations (Ziman 1965) whose solutions near μ, E_K, correspond to the energies of single quasi-particle excitations. Two quasi-particles interact when one 'senses' the virtual polarisation of a Kondo ion induced by another. This interaction is characterised by the parameters $\varphi_{\nu\nu'}$. By using the well known results from the theory of transition metals due to Heine (1967), Pettifor (1972) and Razafimandimby *et al* (1984) cast their results into a hybridisation model. However, they made the drastic

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assumption that the additional phase shift caused by the Kondo ions is of s electrons instead of f electrons, thereby neglecting spin–orbit effects which are very important for heavy fermions.

In this Letter, we present a Fermi liquid theory for Kondo lattice systems in which spin–orbit effects are specifically included. We assume the ground state of the Kondo lattice to be single-ion Kondo singlets built coherently into the lattice. However, this assumption is not always justified. For example, in CeB_6, the RKKY interaction is thought to dominate the single-ion effects forcing CeB_6 into a magnetic ground state (Aarts 1984, Rossat-Mignod *et al* 1981). Thus we specifically refer to $CeCu_2Si_2$ or $CeAl_3$ when we discuss a Kondo lattice. In this Letter we outline the formulation of our theory. We shall report the results of our calculation of the effective magnetic moment and the Wilson ratio of Kondo lattice systems in a future paper. We have also explained the non-linear relation between Knight shift and magnetic susceptibility of a Kondo lattice by using our model, a preliminary version of which has recently been presented (Misra and Callaway 1986) (the details will be published elsewhere). Subsequently Zou and Anderson (1986) have also formulated a Fermi liquid model for the formation of heavy-fermion bands by using a similar technique. They have shown that only one specific linear combination of the six local f states can hybridise with a conduction state of given $\boldsymbol{k}$ and spin and hence the magnetic moments of heavy fermions are sharply quenched. Their results for effective magnetic moments are in fair agreement with experimental results. However, our theory is more general than that of Zou and Anderson (1986) and has several advantages which we shall discuss later when we compare the two models.

In cerium systems, only the $l = 3$ phase shift is important. The spin–orbit splitting between $J = \frac{5}{2}$ and $J = \frac{7}{2}$ is much larger than Δ^*, and therefore $\delta_3(\varepsilon)$ is large in the $J = \frac{5}{2}$ state. Ignoring the crystal-field effects, the phase shift around the Fermi energy is of the form $\delta_3(\varepsilon) \simeq \tan^{-1}(\Delta^*/(E_f^* - \varepsilon))$. The position of E_f^* is determined by the Friedel sum rule, $N\delta_3(\mu)/\pi = n_f$. The phase shifts are assumed to be caused by a scattering potential which is non-zero within a muffin tin of radius R. It is easy to show, by using a procedure similar to the KKRZ method (Ziman 1965) (including spin-orbit effects), that the band structure is obtained from

$$\det\|(k_n^2 - E)\delta_{\boldsymbol{k}_n s, \boldsymbol{k}_{n's'}} + \Gamma_{\boldsymbol{k}_n s, \boldsymbol{k}_{n's'}}\| = 0 \tag{2}$$

where

$$\Gamma_{\boldsymbol{k}_n s, \boldsymbol{k}_{n's'}} = -\frac{(4\pi)^2}{K\Omega}\sum_{\lambda\mu}\tan\eta_{l(\lambda)}\frac{j_{l(\lambda)}(k_n R)j_{l(\lambda)}(k_{n'}R)}{j^2_{l(\lambda)}(KR)} \times C(l\tfrac{1}{2}j, \mu - m_s, m_s)C(l\tfrac{1}{2}j, \mu - m_{s'}, m_{s'})Y^{\mu-m_s}_{l(\lambda)}(\hat{\boldsymbol{k}}_n)Y^{*\mu-m_{s'}}_{l(\lambda)}(\hat{\boldsymbol{k}}'_n). \tag{3}$$

Here, $\boldsymbol{k}_n = \boldsymbol{k} + \boldsymbol{G}_n$, $K = (2mE)^{1/2}$, Ω is the volume of the unit cell, s is the spin index, the C are Clebsch–Gordon coefficients, $\det\|\mathbf{U}\|$ means determinant of matrix $\mathbf{U}$. In addition

$$l = \lambda \qquad j = l - \tfrac{1}{2} \qquad (\lambda > 0)$$

$$l = -\lambda - 1 \qquad j = l + \tfrac{1}{2} \qquad (\lambda < 0)$$

$$\cot\eta_{l(\lambda)} = \cot\delta_{l(\lambda)} - n_{l(\lambda)}(KR)/j_{l(\lambda)}(KR)$$

and $j_l(x)$ and $n_l(x)$ are the spherical Bessel functions. We redefine

$$E_f = E_f^* - (n_3(KR)/j_3(KR))\Delta^*. \tag{4}$$

It may be noted that $\Gamma \propto \Delta^*/(E_f - E)$ and is strongly energy dependent. In addition, there is a singularity at resonance which can be tamed by a transformation in which RLS are added as basis states.

We construct Bloch states

$$\psi_{ks}(\boldsymbol{r}) = \frac{1}{\sqrt{N}} \sum_{i\mu} \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_i) A^{ks}_{\lambda\mu} \varphi_\lambda(|\boldsymbol{r} - \boldsymbol{R}_i|)\chi_{\lambda\mu}(i) \tag{5}$$

where

$$A^{ks}_{\lambda\mu} = (4\pi/3)^{1/2}\, \mathrm{i}^l C(l\tfrac{1}{2}j, \mu - m_s, m_s) Y_l^{*\mu - m_s}(\hat{\boldsymbol{k}}) \tag{6}$$

and

$$\chi_{\lambda\mu}(i) = \sum_{m_s} C(l\tfrac{1}{2}j, \mu - m_s, m_s) Y_l^{\mu - m_s}(\boldsymbol{r} - \boldsymbol{R}_i)\chi^{m_s}. \tag{7}$$

Here $\varphi_\lambda(r)$ is the radial part of the exact solution of the Schrödinger equation within one Wigner–Seitz cell for a given scattering potential with eigenvalue E but for $r > R$, the φ decay into plane wave states. It can be easily shown that

$$\sum_\mu A^{ks}_{\lambda\mu} A^{ks'}_{\lambda\mu} = \delta_{ss'}. \tag{8}$$

One can transform the determinant in equation (2) by using the states in equation (5) and the integral formula for phase shift by adapting a technique used originally by Heine (1967) for transition metals. After some algebra, one obtains

$$\|\mathbf{U}\| \cdot \left\| \frac{(k_n^2 - E)\delta_{k_n s'', k_n' s'''} + W_{k_n s'', k_n' s'''}}{\gamma^*_{k_n s'', ks'}} \middle| \frac{\gamma_{ks, k_n' s'''}}{(E_f - E)\delta_{ks, ks'}} \right\| = 0. \tag{9}$$

Here $W_{k_n s'', k_n' s'''}$ is the pseudopotential, s is spin index, $\mathbf{U}$ is a matrix with a non-vanishing determinant, and the hybridisation form factors $\gamma^{3,5/2}_{ks,k_n s''}$ and $\gamma^{3,7/2}_{ks,k_n s''}$ are given by

$$\begin{aligned}\gamma^{3,5/2}_{ks,k_n s''} &= (3B_{3,5/2}/8\pi)[5(\boldsymbol{k}\cdot\boldsymbol{k}_n)^3 - 3(\boldsymbol{k}\cdot\boldsymbol{k}_n)k^2k_n^2]\mathbf{I}_{ss''} \\ &\quad + (3\mathrm{i}B_{3,5/2}/8\pi)[5(\boldsymbol{k}\cdot\boldsymbol{k}_n)^2 - k^2k_n^2|\boldsymbol{k}\times\boldsymbol{k}_n\cdot\boldsymbol{\sigma}_{ss''}\end{aligned} \tag{10}$$

and

$$\begin{aligned}\gamma^{3,7/2}_{ks,k_n s''} &= (B_{3,7/2}/2\pi)[5(\boldsymbol{k}\cdot\boldsymbol{k}_n)^3 - 3(\boldsymbol{k}\cdot\boldsymbol{k}_n)k^2k_n^2]\mathbf{I}_{ss''} \\ &\quad + (3\mathrm{i}B_{3,7/2}/8\pi)[5(\boldsymbol{k}\cdot\boldsymbol{k}_n)^2 - k^2k_n^2|\boldsymbol{k}\times\boldsymbol{k}_n\cdot\boldsymbol{\sigma}_{ss''}\end{aligned} \tag{11}$$

where

$$\begin{aligned}B_{3,5/2} &= -[(4\pi)^3/3]^{1/2}(\Delta_{5/2}/K\Omega)^{1/2}(1/k^3K^3) \\ B_{3,7/2} &= -[(4\pi)^3/3]^{1/2}(\Delta_{7/2}/K\Omega)^{1/2}(1/k^3K^3)\end{aligned} \tag{12}$$

$\mathbf{I}$ is an identity matrix and $\boldsymbol{\sigma}$ is the Pauli spin matrix.

The hybridisation potential is obtained by multiplying the form factor by the structure factor. It may be noted that the hybridisation potential includes spin–orbit coupling and

mixes the dispersionless resonance states with extended states of all Brillouin zones. In fact, equation (9) can be considered as the secular equations of a hybridisation Hamiltonian of the form

$$H = \sum_{k,n,s} \varepsilon_n(\boldsymbol{k}) C^+_{kns} C_{kns} + \sum_{k,s,J} E_{fJ} f^+_{ksJ} f_{ksJ} + \sum_{k,n,s,s',J} \gamma^J_{ks,k_n s'} (f^+_{ksJ} C_{kns'} + C^+_{kns'} f_{ksJ}). \tag{13}$$

Here $\varepsilon_n(\boldsymbol{k})$ is the energy of the nth Brillouin zone obtained by diagonalising the Hamiltonian containing the kinetic energy term and the corresponding spin–orbit pseudopotential terms (including $l = 3$), $\gamma^J_{ks,k_n s'}$ are the hybridisation potentials derived by us and $C_{kns}(C^+_{kns})$; $f_{ksJ}(f^+_{ksJ})$ are the usual fermion operators destroying (creating) an extended state and a localised state respectively. We note that the energy E_{fJ} is dispersionless but the hybridisation term mixes the localised states with extended states of all Brillouin zones. The Hamiltonian (13) can be transformed into one with one extended band only by a projection method suggested by Heine (1967). If this procedure is adopted, one obtains the hybridisation of one conduction band with localised states which have dispersion in their energy. This characteristic dispersion of the resonance levels is a consequence of the reduction of the hybridisation Hamiltonian to the lowest Brillouin zone. This procedure would lead us to the derivation of a periodic Anderson Hamiltonian in which spin–orbit effects are explicitly included.

As noted earlier, Zou and Anderson (1986) have also formulated a Fermi liquid model for the formation of heavy-fermion bands by using a similar technique. However, our model is more general and has the following advantages.

(i) We have calculated the hybridisation potentials for both $J = \frac{2}{5}$ and $J = \frac{1}{2}$ while their model has only the $J = \frac{2}{5}$ hybridisation potential. Therefore our model can be easily extended to include crystal-field effects.

(ii) Our resonance states are Bloch functions, the formulation of which is essential for calculation of magnetic susceptibility (Misra *et al* 1982), Knight shift (Tripathy *et al* 1982) and other transport properties of heavy fermions.

(iii) It is easier to handle our model Hamiltonian since the creation and annihilation operators for both resonance and extended states refer to Bloch states.

(iv) The band-structure effects in our calculations are included in a pseudopotential formalism while their formulation essentially accounts for hybridisation between one plane wave and a localised state, which is far from realistic.

We have used degenerate perturbation theory to construct Bloch functions which are eigenfunctions of the Hamiltonian described in equation (13). We have used these functions to evaluate the momentum and spin matrix elements which occur in the general expressions for magnetic susceptibility (χ_s) of Misra *et al* (1982) and for Knight shift (K_s) of Tripathy *et al* (1982). Finally we obtain

$$\chi_s = -\mu_0^2 \sum_k \{\tfrac{1}{3} g_j^2 j(j+1)(2j+1) a_1^2(\boldsymbol{k}) + 2[(a_2(\boldsymbol{k}) + b_2(\boldsymbol{k}))^2 + (a_3(\boldsymbol{k}) + b_3(\boldsymbol{k}))^2 + (a_4(\boldsymbol{k}) + b_4(\boldsymbol{k}))^2]\} \frac{f'(\varepsilon_k)}{1 - \alpha(\boldsymbol{k})} \tag{14}$$

and

$$K_s = -\sum_k \Big[\tfrac{2}{3}\mu_0 g_j^2 (2j+1)\Big(\Big\langle \frac{1}{r_0^3} \Big\rangle_{nl} l(l+1) + \tfrac{4}{3}\pi \langle \delta(r_0) \rangle_{nl} [j(j+1) - l(l+1) + s(s+1)] \Big) a_1^2(\boldsymbol{k}) + \tfrac{16}{3}\pi \bar{\Omega} \langle |\psi_{kf}(0)|^2 \rangle_{av} [a_2(\boldsymbol{k})(a_2(\boldsymbol{k}) + b_2(\boldsymbol{k})) + a_3(\boldsymbol{k})(a_3(\boldsymbol{k}) + b_3(\boldsymbol{k})) + a_4(\boldsymbol{k})(a_4(\boldsymbol{k}) + b_4(\boldsymbol{k}))] \Big] \frac{f'(\varepsilon_k)}{1 - \alpha(\boldsymbol{k})}. \tag{15}$$

Here $a_n(\boldsymbol{k})$, $b_n(\boldsymbol{k})$ and $\alpha(\boldsymbol{k})$ are complicated functions of $\boldsymbol{k}$ and the other symbols have their usual meanings. It is evident from equation (14) and (15) that K_s is not directly proportional to χ_s. The details of our calculations will be published elsewhere.

To summarise, we have formulated a Fermi liquid model for Kondo lattice systems which includes spin–orbit effects. We have explained the advantages of our model over that of Zou and Anderson (1986). We have calculated the Knight shift (K_s) and magnetic susceptibility (χ_s) by using our model and shown that K_s is not proportional to χ_s, a result which is well known for Kondo-lattice systems.

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