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1993 J. Phys.: Condens. Matter 5 6483

(http://iopscience.iop.org/0953-8984/5/35/013)

J. Phys.: Condens. Matter 5 (1993) 6483–6490. Printed in the UK

Antiferromagnetic correlation of the heavy-fermion system by the Gutzwiller approach

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Received 4 January 1993, in final form 27 April 1993

Abstract. In this paper, an antiferromagnetic correlation term beyond the RKKY interaction is derived from the Anderson model by the Gutzwiller projection technique. The competition between the Kondo coupling and antiferromagnetic correlation in heavy-fermion systems is discussed. The propagators, spectrum and dynamic spin susceptibility show that magnetic instability may occur at low frequencies.

The highly unusual behaviours of heavy-fermion systems (HFSs), from the Fermi liquid (FL) state through antiferromagnetic (AFM) ordering to superconductive ordering, have stimulated various attempts to derive these properties on the basis of microscopic theory [1]. In the development of our understanding of the physics of HFSs, two kinds of model Hamiltonian play instrumental roles: one is the Kondo lattice (or impurity) model; the other is the periodic (or impurity) Anderson model. For the impurity case, Schrieffer and co-workers [2, 3] proved that the Anderson model is equivalent to the Kondo model by a unity transformation. Various exact and approximate solutions to impurity models have been developed [4–6]; the theoretical results agree very well with the experimental data on dilute alloys.

However, many efforts need to be made for the lattice case (HFS) . Because of the lattice characteristic, HFSs cannot be regarded as arrays of a single Kondo resonance state [7]. The delocalization and coherence of f electrons in HFSs will heavily affect the properties of systems. Our previous work [8] shows that, after the unity transformation [3] to the periodic Anderson model, the effective Hamiltonian includes both the Kondo lattice interaction and a delocalized f-electron term, which not only renormalizes the f level but also forms a narrow f band; this delocalized term could explain the unusual magnetic properties in the low-temperature range of HFSs [8].

The transition of an HFS from an FL state to an AFM ground state has always been of interest [9–11]. To explore the coexistence of FL and AFM states, the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction between f electrons is added to the Kondo lattice Hamiltonian [12]. This method is not self-consistent because the RKKY interaction can be regarded as the second-order approximation of the Kondo or Anderson model [13]. All the Coulomb and exchange s–s, s–f, and f–f electron interactions are also considered in order to discuss the breakdown of the Kondo effect [14]; it shows that a sufficiently strong ferromagnetic exchange interaction between f electrons may change the sign of the exponent of the Kondo temperature and destroy the Kondo single state; nevertheless, it cannot explain why most magnetically ordered HFSs have an AFM nature.

When one assumes the Coulomb repulsion to be infinite in the Anderson model, it seems that some physics related to the Coulomb interaction is lost. For such a strongly

0953-8984/93/356483+08$07.50

correlated system, the Gutzwiller [15] projection approach can be used to project the double occupancy of f electrons. The approach may be more suitable for real HFSs than is the slave-boson method in which the on-site Coulomb repulsion U between f electrons is assumed to approach infinity. The Gutzwiller variational technique has been used for the one-electron hybridization wavefunction of the periodic Anderson model to remove the double occupancy in the same state by Rice and Ueda [16]; they found that it results in the renormalization of the hybridization matrix element V by a factor. The Gutzwiller approach has also been applied to the Kondo lattice Hamiltonian by Shiba and Fazekas [17]; it shows that the local f electrons participate in forming the large Fermi surface.

In this paper, we prove that an AFM correlation and Kondo coupling may coexist by the Gutzwiller projection approach in the periodic Anderson Hamiltonian, we evaluate the ground-state energy variationally and we examine the propagator, self-energy and dynamic spin susceptibility from the derived effective Hamiltonian.

We first review some previous results briefly. Our starting point is the periodic Anderson Hamiltonian

$$H = \sum_{k\sigma} \epsilon_k c^+_{k\sigma} c_{k\sigma} + \sum_{k\sigma} (V_{ki} c^+_{k\sigma} f_{i\sigma} + \mathrm{HC}) + \sum_{i\sigma} E_0 f^+_{i\sigma} f_{i\sigma} + \sum_{k\sigma} \tfrac{1}{2} U n_{i\sigma} n_{k\bar{\sigma}} \tag{1}$$

where the conduction band dispersion ϵ_k and f energy level E_0 are measured from the chemical potential μ. The hybridization matrix element $V_{ki} = [V \exp(-\mathrm{i}kR_i)]/\sqrt{N}$; the on-site Coulomb interaction U between f electrons is large (but finite) compared with ϵ_k, E_0 and V. The orbital degeneracy of electrons is neglected for simplicity.

A unity transformation [3] applied to the Anderson model (1) leads to the effective Hamiltonian (to the order of V^2)

$$\begin{aligned} H_1 = \sum_{k\sigma} \epsilon_k c^+_{k\sigma} c_{k\sigma} + \sum_{kk'i} J_{kk'} \exp[-\mathrm{i}(k-k')R_i]\, \boldsymbol{S}_i \cdot \boldsymbol{s}_{\mu\mu'} c^+_{k\mu} c_{k'\mu'} + \sum_{i\sigma} E_0 f^+_{i\sigma} f_{i\sigma} \\ + \sum_{i\sigma} \tfrac{1}{2} U n_{i\sigma} n_{i\bar{\sigma}} + \sum_{ij\sigma} [t^{(1)}_{ij}(1-n_{i\bar{\sigma}}) + t^{(2)}_{ij} n_{i\bar{\sigma}}] f^+_{i\sigma} f_{j\sigma} + \mathrm{HC} \end{aligned} \tag{2}$$

with

$$\begin{aligned} J_{kk'} &= (V^2/N)\Big[1/(\epsilon_k - E_0) + 1/(\epsilon_k - E_0 - U) + 1/(\epsilon_{k'} - E_0) + 1/(\epsilon_{k'} - E_0 - U)\Big] \\ t^{(1)}_{ij} &= \frac{1}{N} \sum_k \frac{V^2}{\epsilon_k - E_0} \exp[-\mathrm{i}k(R_i - R_j)] \\ t^{(2)}_{ij} &= \frac{1}{N} \sum_k \frac{V^2}{\epsilon_k - E_0 - U} \exp[-\mathrm{i}k(R_i - R_j)]. \end{aligned} \tag{3}$$

Here the first two terms are just the Kondo lattice Hamiltonian, an extension of the result of Coqblin and Schrieffer [2] to the lattice case, which describes the FL and heavy-electron characteristics of an HFS. The last term corresponds to a transfer process of f electrons; the coefficient $t^{(1)}_{ij}$ or $t^{(2)}_{ij}$ is obviously the transfer matrix element of an f electron hopping from site j to site i when site i is empty or occupied by a spin-flipped electron; the charge-transfer process may be traced back to the lattice characteristics of an HFS. So Hamiltonian (2) is a two-band Kondo model and the HFS could be described as a two-weak-coupling fluid, as Coleman and co-workers [9] suggested.

One should keep in mind that the hopping process is indirect, or via the conduction band. The formation of a narrow f band implies another contribution to the effective mass of the heavy electron. It can be seen that, if the Coulomb interaction is far larger than the conduction band width D and the f energy level $|E_0|$, the value of the matrix element $t^{(2)}$ is less than $t^{(1)}$. If conditions $U \to \infty$ and $n_{i\bar{\sigma}} \to 1$ are satisfied, the transfer term in equation (2) tends to zero; the slave-boson method is then needed. The last three terms resemble a single-band Hubbard Hamiltonian; this similarity is very interesting. The effective Hamiltonian including the Kondo part and the Hubbard part may give a clue as to the coexistence or competition of FL state and antiferromagnetism in the same heavy-electron system.

The heavy-fermion compounds are strongly correlated systems, which are similar to the high-T_c superconductive materials. This motivates us to apply the Gutzwiller projector to the Hamiltonian (2). The projectors

$$P_1 = \prod_i (1 - n_{i\uparrow} n_{i\downarrow})$$
$$P_2 = 1 - P_1 = 1 - \prod_i (1 - n_{i\uparrow} n_{i\downarrow}) \tag{4}$$

are the Gutzwiller projectors onto the states with no double occupancy and with double occupancy of the f-electron configuration, respectively. Then a unity transformation leads to the resulting effective Hamiltonian

$$H' = \sum_{k\sigma} \epsilon_k c_{k\sigma}^+ c_{k\sigma} + \sum_{kk'i} J_{kk'} \exp\left[-\mathrm{i}(k-k')R_i\right] S_i \cdot s_{\mu\mu'} c_{k\mu}^+ c_{k'\mu'} + \sum_{i\sigma} E_0 f_{i\sigma}^+ f_{i\sigma}$$
$$+ \sum_{ij\sigma} (t_{ij}^{(1)} f_{i\sigma}^+ f_{j\sigma} + \mathrm{HC}) + \sum_{ij} A_{ij} S_i \cdot S_j \tag{5}$$

with

$$A_{ij} = 2(t_{ij}^{(1)} + t_{ij}^{(2)})^2 / U$$

where the high-energy band of f electrons (double occupancy) is neglected in the low-energy range. For simplicity, $J_{kk'}$ is assumed to be approximately a positive constant J near the Fermi surface, and A_{ij}, which is only the nearest-neighbour interaction A, is not zero. Therefore the last three terms of the Hamiltonian (5) display an AFM correlation between f electrons which has been extensively studied for high-T_c superconductors [18, 19].

As shown in equation (5), with the delocalization and coherence of f electrons arising from the charge-transfer term and the strong correlation from the Coulomb repulsion between f electrons, the nearest-neighbour spins of magnetic f electrons tend to antiparallel alignment to decrease the ground-state energy. So, at low energies, the effective interaction will develop into an AFM term rather than the oscillatory RKKY interaction at high energies. With equation (5), one could understand why most magnetically ordered HFSs behave as AFM rather than ferromagnetic.

Although the spin of f electrons has a tendency to antiparallel alignment, the spin-compensated Kondo coupling between s and f electrons will weaken it. Therefore the effective Hamiltonian (5) exhibits explicitly competition and coexistence of Kondo coupling and the AFM correlation. One would expect naturally that many properties of HFSs consist of contributions from both the FL component and the AFM component.

With the effective Hamiltonian (5), we consider a paramagnetic state. A many-body variational wavefunction for the HFS is constructed as follows:

$$|\psi\rangle = \sum_{\langle ij\rangle} \sum_{kk'} \sum_{\sigma\sigma'} \exp\left(-\mathrm{i}kR_i - \mathrm{i}k'R_j\right) \Gamma_{kk'} c_{k\sigma}^+ c_{k'\sigma'}^+ |FS\rangle |\bar{\sigma}_i \bar{\sigma}_j'\rangle \tag{6}$$

where $|FS\rangle$ represents the Fermi spherical ground state of the conduction electron, $|\bar{\sigma}_i\bar{\sigma}'_j\rangle$ the spin wavefunction of f electrons with spin $\bar{\sigma}$ on site i and spin $\bar{\sigma}'$ on site j (the restriction $i \neq j$ excludes the doubly occupied state on the same site). The invariance of $|\psi\rangle$ in commutating index k and k' requires that

$$\Gamma_{kk'} = -\Gamma_{k'k} \text{ and hence } \Gamma_{kk} = 0. \tag{7}$$

The variational to the ground-state energy of the HFS leads to the bound energy of a Kondo single state:

$$E_b = A - D \exp[-\tfrac{1}{6} JN(0)] \tag{8}$$

where D is the conduction band width and $N(0)$ the density of states on the Fermi surface. According to equation (8), the AFM correlation will lift the energy of the Kondo state and, if it is strong enough (i.e. if the parameter A is large), the bound energy E_b becomes zero or positive; the Kondo single state is thus destroyed.

A phase diagram is calculated in terms of the parameter A/D and $JN(0)$, as shown in figure 1. It shows that a small AFM correlation could suppress the formation of a Kondo single state; the FL character in the HFS emerges only when the Kondo coupling between the conduction and f electrons is sufficiently large.

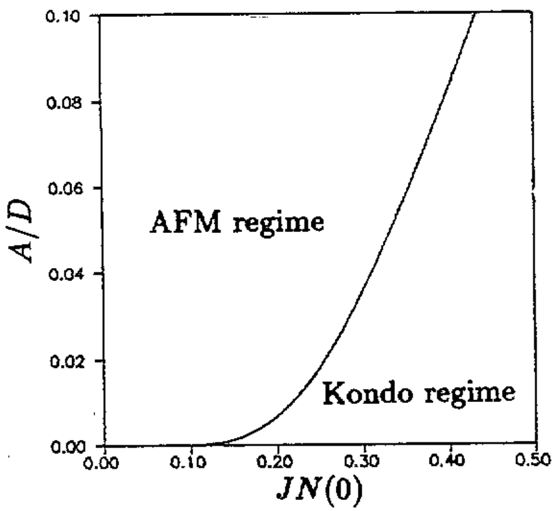

Figure 1. A phase diagram when the Kondo coupling and the AFM correlation coexist.

Next we consider the dynamic spin susceptibility of the HFS. The susceptibility is the dynamic response function of spin:

$$\chi(\omega, q) = \langle\langle S^-(q); S^+(-q)\rangle\rangle_{\omega+i\eta} \tag{9}$$

where $G(\omega, q) = \langle\langle S^-(q); S^+(-q)\rangle\rangle$ is the propagator of spin components. For an HFS with an AFM correlation, the susceptibility matrix has nine components χ_{cc}, χ_{ac}, χ_{bc} etc; here the subscripts c, a and b represent the conduction band electrons, the spin-up f electrons and the spin-down f electrons in the sublattice, respectively.

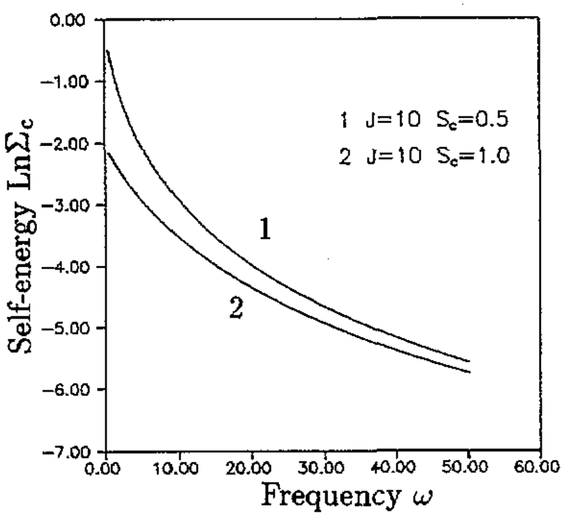

Figure 2. The dependence of the self-energy $\Sigma_c(\omega, q)$ of conduction electrons on frequency ω for the precise screening $|s_c| = S$ and underscreening $S > |s_c|$ cases. The energy scale is the parameter $A = 1$.

The propagator of conduction band electrons is especially interesting and is easily calculated to the leading-order approximation:

$$G_{cc}(\omega, q) = G^0_{cc}\{1 + AJ^2S^2[1 - \gamma(q)]/\det(\omega, q)G^0_{cc}\} \tag{10}$$

where G^0_{cc} is the propagator of a non-interacting electron gas (FL) and $\det(\omega, q)$ an abbreviation of the expression

$$\det(\omega, q) = (\omega + Js_c)^2 - (\omega_q)^2 - AJ^2S^2[1 - \gamma(q)]G^0_{cc}$$

with $\gamma(q) = (1/z)\sum_\delta \exp(-i\delta k)$; δ denotes the nearest-neighbour position vector, z the number of the nearest neighbours and $\omega_q = AS\sqrt{1 - \gamma^2(q)}$, the AFM spin-wave spectrum. s_c and S represent the spin statistical average values of s and f electrons, respectively.

Accordingly, to the leading-order approximation,the self-energy of conduction electrons in systems with an AFM internal field is

$$\Sigma_c(\omega, q) = AJ^2S^2[1 - \gamma(q)]/\det(\omega, q). \tag{11}$$

The relation of the self-energy to the frequency ω is shown in figure 2. The evaluation is performed for the exact screening case $S = |s_c|$ (the case of a precise balance between the f spin and the s spin), and for the underscreening case $S > |s_c|$. It seems that there is no discontinuity in the self-energy in the low-energy range.

Since the self-energy is related to the energy shift of conduction electrons, the smooth variation in self-energy with frequency shows that, when the AFM correlation is switched on in an HFS, the transition of the HFS from the FL to the AFM ordering state may be smooth.

The dynamic susceptibility of conduction electrons gives

$$\chi_{cc}(\omega, q) = \chi^0_{cc}(\omega, q)\left[1 + \{AJ^2S^2[1 - \gamma(q)]/\det(\omega + i\eta, q)\}\chi^0_{cc}(\omega, q)\right] \tag{12}$$

where the spin susceptibility in the FL state without the AFM correlation is denoted χ^0_{cc}, which is given by the Lindhard-type functions when $\omega = 0$. A similar result was obtained by Doniach [10], in which the magnetic instability is discussed in the periodic Anderson model by the slave-boson method, provided that $\chi^0_{ff} = AS^2[1-\gamma(q)]/\det(\omega + i\eta, q)$. Similarly, the cross susceptibilities χ_{ac} and χ_{bc} could be calculated readily.

From equation (12), the response of conduction electrons consists of two parts: one is the contribution $\chi^{(0)}_{cc}$ from the FL, which gives the RKKY coupling in the low-temperature range; the other is the contribution from the coupling between the FL and AFM correlation.

The dynamic spin susceptibility $\chi_{cc}(\omega, q)$ of conduction electrons is shown in figure 3. It exhibits an oscillation at low frequencies and approaches the FL susceptibility at high frequencies. This indicates that the interaction between the FL component and the AFM correlation is strong in the low-energy range, while it becomes asymptotically free in the high-energy range.

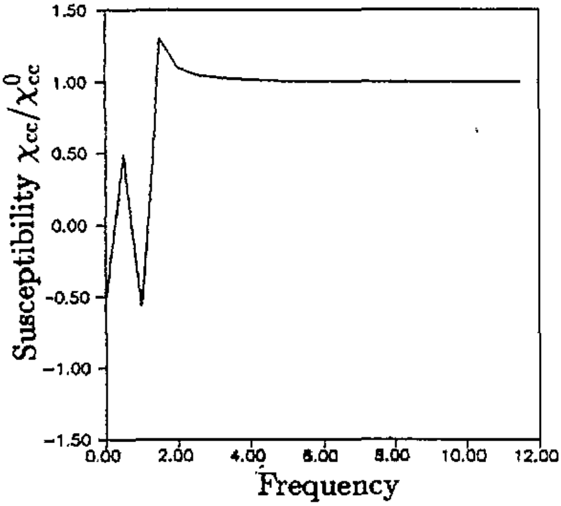

Figure 3. The dependence of the reduced dynamic spin susceptibility χ_{cc}/χ^0_{cc} on frequency ω for $J = 5$ and $|s_c| = S$. The energy scale is $A = 1$.

The susceptibility describes the dynamical response of the HFS under a varying magnetic field, and its imaginary part relates to the correlation function of spin through the fluctuation–dissipation theorem. In the static state (i.e. $\omega \to 0, q \to 0$), the divergence of the susceptibility implies the long-range correlation of spin and the formation of magnetic order. The AFM interaction in equation (5) will excite local or intersite spin fluctuations, as shown in neutron scattering experiments.

The low-frequency oscillation of the dynamical susceptibility χ implies magnetic instability; it predicts that, under a small AFM interaction, the HFS deviates from the normal FL state [20] and drives the system to an AFM ordered state at a certain temperature T. Further investigation is carrying on.

Magnetic instability occurs when the denominator $\det(\omega + i\eta, q)$ vanishes:

$$(\omega + Js_c)^2 - \omega_q^2 - AJ^2S^2[1-\gamma(q)]\chi^0_{cc} = 0. \tag{13}$$

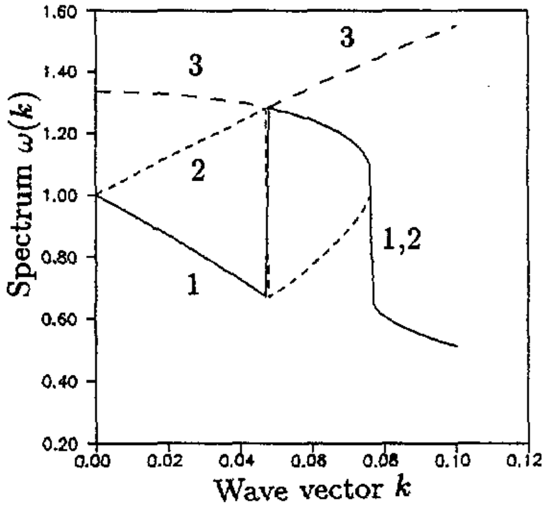

Figure 4. The energy spectrum of the magnetic instability $\omega(q)$ as a function of wavevector q for $J = 1$ and $|s_c| = S$. The energy scale is the parameter $A = 1$; the crystal constant $a = 1$.

The solution to equation (13) for the long-wavelength approximation is shown in figure 4. There exist three branches of the spectra. The branches $\omega_1(k)$ and $\omega_2(k)$ correspond to AFM spin fluctuation. $\omega_3(k)$ is the response of interaction between conduction electrons and AFM spin fluctuation.

We noticed that, physically, the projection of the Gutzwiller operator onto the ground-state wavefunction as Rice and Ueda did in [16] should be equivalent to projection onto equation (1). However, for the latter, one can explore the details of interaction occurring in the HFS. Our results would be consistent with the work of Shiba and Fazekas [17] if the charge-transfer term t_{ij} or the AFM correlation A_{ij} term disappear and the ground-state wavefunction is constructed as their singlet wavefunction.

As pointed out in [17, 21], since some virtual processes, such as the charge-transfer process here, are taken into account through the canonical transformation in the strong-coupling limit, the variation in the effective Hamiltonian (5) is superior to a similar variation in the original Hamiltonian (1).

Here an experimental fact has been noticed for some heavy-electron systems [12]; the critical temperature T_c of the superconductive transition is about a tenth of the AFM Néel temperature T_N, or $T_N \approx 10T_c$. This implies that the relation between the AFM correlation and superconductive ordering is direct. Is it a scaling behaviour in some HFSs? This universal character is very interesting.

Finally we summarize our results. On the basis of the modified periodic Anderson model, we derived an effective Hamiltonian describing the coexistence of Kondo coupling and AFM correlation. The variational calculation shows that the AFM correlation will lift the bound energy of a single state. The dynamic spin susceptibility may exhibit magnetic instability resulting from the competition between the Kondo coupling and the AFM correlation.

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