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COHERENCE EFFECTS IN THE TWO-IMPURITY KONDO PROBLEM

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The coherence between the spin-flip of two Kondo impurities is treated in a decoupling scheme within the functional integral method leading to two characteristic temperatures $T_K^\pm \sim D \exp[2D/J(1 \pm \sin k_F R/k_F R)]$. This enables us to establish three successive resistivity regimes when the temperature is lowered: the usual logarithmic behaviour succeeded by an intermediate regime of linear variation, followed finally by a T^2 -dependence typical of a Fermi liquid.

1. Introduction

Following the ideas developed by Doniach [1], most of the authors working on the N -impurity Kondo problem deal mainly with the competition between the Kondo interaction (leading to the formation of a singlet) and the RKKY's (favouring a magnetic order). Doniach [1], and the Jullien et al. [2] found a critical value of J/D (J being the Kondo interaction and $2D$ the width of the conduction band) above which the 1-dimensional lattice passes from a magnetic to a Kondo phase. This result was later generalised in the 3-dimensional case by Lacroix and Cyrot [3] using a functional integral method which transforms the Kondo exchange interaction into a fictitious s–f hybridisation. Lavagna et al. [4] then related the scattering of the conduction electrons to the spatial fluctuations of the s–f hybridisation. Those evaluated to $kT/2|J|$ lead to a linear T -dependence of the metallic resistivity at low temperature, as predicted in the general theory of Mott [5]. Nevertheless, this model does not permit one to obtain the usual Fermi liquid regime (T^2 -dependence as obtained easily in the case of the single impurity [6]), a behaviour not well understood.

The question of the coherence between the spin-flip of the N Kondo impurities has been much less studied. This effect seems however to play an essential role in the low temperature properties as shown by thermal dilatation and specific heat measurements [7,8]. The aim of the present paper is to treat this problem with the number of impurities $N = 2$. This simpler case already contains most of the features of the many-impurity problem. Let us mention the previous work of Jayaprakash, Krishna-Murthy and Wilkins [9] (scaling technique) pointing out, in the case of strong ferromagnetic RKKY interactions, three regimes of susceptibility as the temperature is lowered, corresponding to the ferromagnetic locking together of the two-impurity spins followed by a two-stage freezing out of the local moments. In this paper, we put forward an original decoupling scheme within the functional integral method leading to two distinct temperatures corresponding to the progressive establishment of the coherence. This solves at the same time the problem previously raised, as an additional Fermi-liquid regime appears as soon as the coherence is completely ensured.

2. Decoupling scheme in the functional integral method

Using the functional integral approach, the partition function of the two-impurity Kondo system can be written [3]:

$$Z = \int_{-\infty}^{+\infty} dx_1(\tau) dx_2(\tau) Z(x_1, x_2) \exp \left[\int_0^\beta \frac{J}{2} (x_1^2 + x_2^2) d\tau \right], \quad (1)$$

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with

$$Z(x_1, x_2) = \text{Tr} T_\tau \exp \left[- \int_0^\beta H(\tau) d\tau \right] \text{ and} \quad (2)$$

$$H(\tau) = \sum_k \tilde{\epsilon}_k c_{k\sigma}^+ c_{k\sigma} + \sum_{i=1,2} E_0 d_{i\sigma}^+ d_{i\sigma} + \sum_\sigma \frac{1}{2} J x_1(\tau) (d_{1\sigma}^+ c_{1\sigma} + c_{1\sigma}^+ d_{1\sigma}) + \sum_\sigma \frac{1}{2} J x_2(\tau) (d_{2\sigma}^+ c_{2\sigma} + c_{2\sigma}^+ d_{2\sigma}), \quad (3)$$

where $\tilde{\epsilon}_k$ and $\tilde{E}_0$ are the s and f effective levels. $x_1(\tau)$ and $x_2(\tau)$ are the matrix elements of a fictitious s-f hybridisation. T_τ is the time-ordering operator.

The time-dependence of the problem is neglected in the static approximation and:

$$\log \frac{Z(x_1, x_2)}{Z(x_1=0, x_2)} = \sum_\sigma \sum_{\omega_\nu} \text{Tr} \ln [1 - V_1 G_{11}(x_1=0, x_2)], \quad (4)$$

with

$$G_{11}(x_1=0, x_2) = G_{11}^o + G_{12}^o V_2 G_{21}^o, \quad (5)$$

where G_{ij}^o are the Green's functions in the absence of hybridisation and V_i are the hybridisation matrices.

(i) Making a first-order approximation reduces eq. (5) to

$$G_{11}(x_1=0, x_2) = G_{11}^o.$$

Substitution of this into (4) leads to

$$Z = \int dx_1 dx_2 \exp \left[-\beta \sum_{i=1,2} F_1(x_i) \right], \quad (6)$$

with

$$F_1(x_i) = -\frac{J x_i^2}{2} - \frac{1}{\beta} \sum_\sigma \sum_{\omega_\nu} \text{Tr} \ln (1 - V_i G_{ii}^o). \quad (7)$$

The last term, equivalent to $(J^2 x_i^2 / 2\pi) \int f(\omega) \text{Im} G_c^o G_d^o d\omega$, can be evaluated in the high temperature approximation, and we have in this limit:

$$F_1(x_i) = -A x_i^2 \quad \text{with} \quad A = \frac{1}{2} J [1 + (J/2D) \ln 1.14\beta D]. \quad (8)$$

The curvature A changes sign at a temperature $T_K = 1.14D \exp(2D/J)$. In the first-order approximation, the averaged hybridisation term vanishes above a characteristic temperature T_K , typical of an isolated Kondo impurity. All the effects of the coherence are neglected. Let us remind ourselves however, that there remain strong thermal fluctuations above T_K , playing an essential role in the high temperature limit [4].

(ii) Taking account of the full expression of G_{11} leads to the following exact results:

$$Z = \int dx_1 dx_2 \exp [-\beta F_1(x_1) - \beta F_1(x_2) - \beta F_2(x_1, x_2)], \quad (9)$$

with

$$F_2(x_1, x_2) = B x_1 x_2 \quad \text{and} \quad B = \frac{J^2}{2\beta} \sum_{\omega_\nu} \left(\sum_k \frac{e^{i\mathbf{k} \cdot \mathbf{R}} + e^{-i\mathbf{k} \cdot \mathbf{R}}}{\omega - \epsilon_k} \right) G d^o. \quad (10)$$

This way of introducing the coupling interaction is very similar to Cyrot's approach [10] in the Hubbard model. Using the usual [11] relation $\sum_k e^{i\mathbf{k} \cdot \mathbf{R}} / \omega - \epsilon_k = -\pi \rho_0 e^{i\mathbf{K} \cdot \mathbf{R}} / KR$ (with $\omega = \hbar^2 K^2 / 2m^*$), we have in the high temperature limit:

$$B = \frac{J^2}{2D} \frac{\sin k_F R}{k_F R} \ln 1.14\beta D. \quad (11)$$

At this stage, a decoupling scheme can be applied and the free energy can be written as the sum of two uncorrelated terms related to even and odd channels $x_1 \pm x_2$:

$$F = -\frac{1}{2}(A - B/2)(x_1 + x_2)^2 - \frac{1}{2}(A + B/2)(x_1 - x_2)^2. \quad (12)$$

The curvature relative to the decoupled variable $x_1 \pm x_2$ changes sign at the temperature:

$$T_K^\pm = 1.14 D \exp[2D/J(1 \pm \sin k_F R/k_F R)]. \quad (13)$$

This procedure is the direct adaptation of Jayapakash et al. 's [9] scaling method to the functional integral approach, and leads to similar results on the characteristic temperatures. Finally, it is not difficult to realize (the details will appear in a forthcoming publication) that the energy scales $T_K^\pm$ are directly related to the values of $\pi J^2(x_1 \pm x_2)^2/8D$ which minimize the free energy at zero temperature [3].

3. Predictions on the resistivity regimes

Let us first recall the method previously developed for the case of the Kondo lattice [4]. After having related the electron scattering to the spatial fluctuations of the s-f hybridisation ($\delta_i = x_i - \langle x_i \rangle$), the relaxation time can be written, using the T -matrix approximation, as:

$$\tau_i(\omega)^{-1} = -\text{Im}T_{ss} = \left(\frac{1}{2}J\delta_i\right)^2 \rho_d(\omega), \quad (14)$$

and the conductivity can be calculated by the use of the Boltzmann equation. It is:

$$\sigma = \frac{2}{3}e^2 \int \left(-\frac{df}{d\omega}\right) \rho_c(\omega) v^2(\omega) \tau(\omega) d\omega. \quad (15)$$

At low temperature, the spatial fluctuations $\langle \delta^2 \rangle$ are evaluated as $kT/2|J|$, and the conductivity is found to take the following form:

$$\sigma = \sigma(0) \left[1 + (T/T_1)^2\right] \quad \text{with} \quad \sigma(0) \approx \langle \delta^2 \rangle^{-1}. \quad (16)$$

The resistivity exhibits a linear thermal variation with a maximum at $T_1 \approx T_K(1-n)^{1/3}$.

In the high temperature limit, $\delta_i = x_i$ and (14) leads to the usual relation with the phase shift introduced by the isolated impurity. The resistivity follows a logarithmic decrease typical of incoherent impurities.

As this case appears to have some interest in what follows, we also recall the low temperature limit of the single impurity. In the saddlepoint approximation, the fluctuations $\langle \delta_i^2 \rangle = \langle x_i^2 \rangle$ (related to T_K) are independant of temperature. According to (15), this method leads to the usual T^2 -regime typical of a Fermi liquid.

Let us now return to our present problem of the two Kondo impurities. As above the relaxation time can be written:

$$\tau(\omega)^{-1} = \left[\frac{1}{2}J(x_1 - x_2)\right]^2 \rho_d(\omega), \quad (17)$$

where $\rho_d(\omega)$ is the conduction density of states in the presence of an average hybridisation $x_1 + x_2$.

The correlations $x_1 x_2$ are negligible at high temperatures and the classical logarithmic behaviour is obtained. Two regimes appear at low temperature:

(i) for $T_K^- < T < T_K^+$, the free energy is quadratic in $(x_1 - x_2)$ and the average value of $(x_1 - x_2)^2$ has a linear thermal variation. The corresponding resistivity varies linearly with T , as obtained in the case of the lattice.

(ii) for $T < T_K^-$, the free energy has a clear minimum for a value of $(x_1 - x_2)^2$ related to T_K^- (section 2). There is a direct equivalence with the single impurity in the low-temperature limit (with T_K^- instead of T_K). In the saddle-point approximation, one obtains a T^2 -regime typical of strong interacting fermions.

A schematic representation of the resistivity regimes is given in fig. 1. The crude model used for the Kondo-lattice reduces to taking $T_K^- = 0$, i.e. a linear thermal dependence of the fluctuations δ^2 . Hence, it is not surprising that only the T -regime was found. As a matter of fact, a correct description of the correlations provides at once an additional Fermi-regime at lower temperature. When the impurities get further apart (infinite distance), both T_K^+ and T_K^- tend to

Fig. 1. Schematic representation of the resistivity regimes in the two-impurity Kondo problem.

a single temperature T_K typical of an isolated impurity. One directly passes from a logarithmic to a Fermi-liquid regime, as expected for the single Kondo impurity.

To summarise, three resistivity regimes appear corresponding to the different steps in the establishment of the Kondo coherence. After total incoherence, seen via the logarithmic behaviour, the coherence progressively sets up, passing through a T -regime before giving the usual Fermi-liquid behaviour when the various spin flips become completely correlated. These predictions seem to be confirmed by the last results obtained, notably in CeAl_3 [12]. The coherence is certainly present in many other effects e.g. thermoelectric power, specific heat, thermal dilatation, susceptibility ... and it would be worthwhile to pursue further theoretical developments on the subject.

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