RENORMALIZATION IN THE 1-D KONDO LATTICE

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ABSTRACT

We use the perturbative renormalization group and a functional integral method to study the one-dimensional Kondo lattice for a 1/6 filled conduction band, as a function of the Kondo coupling strength J_o and the Coulomb interaction between the carriers. We find that this system is always unstable towards the formation of RKKY spin density waves at the wavenumber $2k_F$ for all values of J_o falling within the weak coupling limit. Our results are in agreement with the Nozières criterion for partial Kondo screening.

INTRODUCTION

We have recently discussed the static magnetic susceptibility of the one-dimensional Kondo lattice for a 1/6 filled (with holes) conduction band [1]. We had postulated, based on an analogy with the half-filled band case but without real proof for partial filling, that the RKKY interaction, that is the spin-spin interaction mediated by the carriers, was the dominant one. We intend to show that this is the case for any value of the strength of the Kondo interaction J_o between the localised spins and the carrier spins or of the Coulomb interaction between the carriers falling within the weak coupling limit of our renormalization procedure.

RENORMALIZATION PROCEDURE

We propose to use a model similar to the one in [1] but using a functional integral expression for the partition function, which uses Grassmann variables for the localized spins and the carriers, as developed by Vieira [2] for the spins and Bourbonnais [3] for the carriers:

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$$Z = \mathrm{Tr}\,\exp(-\beta H) \propto \int \delta\zeta\ \delta\psi^*\ \delta\psi\ \exp(S[\zeta,\psi^*,\psi]), \tag{1}$$

where the action is

$$\begin{aligned}
S([\zeta,\psi^*,\psi]) = {} & \tfrac{1}{2} \sum_{i} \sum_{m,n} \sum_{\omega} \zeta_{im}(-\omega)\mathcal{G}^{-1}_{mn}(\omega)\zeta_{in}(\omega) + \sum_{p} \sum_{k} \sum_{s} \psi^*_{pks}(\omega)G^{-1}_{pks}(\omega)\psi_{pks}(\omega) \\
& - \tfrac{1}{2}J_o \sum_{\{\omega_i\}} N^{-1} \sum_{i} \sum_{k,k'} \sum_{s,s'} \sum_{p,p'} \psi^*_{p'k's'}(\omega_4)\psi_{pks}(\omega_3)\ \sigma_r^{ss'}\ \zeta_{im}(-\omega_2)\zeta_{in}(\omega_1) \\
& \qquad \times \exp[i(k'-k)R_i]\ (-\tfrac{1}{2}i\,\varepsilon_{rmn})\ \delta(\omega_1+\omega_3-\omega_2-\omega_4) \qquad\qquad (2) \\
& - \tfrac{1}{2}g_2 \sum_{\{\omega_i\}} N^{-1} \sum_{\substack{k,k'\\q}} \sum_{s,s'} \sum_{p,p'} \psi^*_{p(k+q)s}(\omega_4)\psi^*_{-p(k'-q)s'}(\omega_3)\psi_{-pk's'}(\omega_2)\psi_{pks}(\omega_1) \\
& \qquad \times \delta(\omega_1+\omega_3-\omega_2-\omega_4),
\end{aligned}$$

where $\mathcal{G}_{mn}(\omega)=-i\omega^{-1}\delta_{mn}$ and $G_{pks}(\omega)=[i\omega - v_F(pk-k_F)]^{-1}$ are the localized spin and carrier bare propagators respectively, ζ_{im} and ψ_{pks} are the Grassmann anticommuting variables associated with the spins (site i and component m) and the carriers ($p=\pm 1$ refers to right (+) or left (-) going carriers of momentum k and spin s) respectively, v_F is the carrier Fermi velocity, ω is the Matsubara Fermion frequency, σ_r is the Pauli spin matrix of component r, J_o is the bare Kondo interaction between spin and carrier while g_2 is the bare Coulomb forward scattering amplitude (we neglect g_1 which quickly renormalises to zero). Furthermore, we characterize the "bandwidth" of our linearized band by the parameter E_o such that the band occupation be $\mathcal{D}(E)E_o/2=1/6$, where the density of states per spin $\mathcal{D}(E)$ is $(\pi v_F)^{-1}$, that is $E_o=\pi v_F/3$. The renormalization group (RG) procedure we shall use on (2) is that of Solyom [4] or equivalently (in this case) of Bourbonnais [3]. It is a weak coupling perturbative RG.

RESULTS

In the absence of Coulomb interaction, the Kondo instability is characterized by the Kondo temperature T_K which corresponds to the pole of the first-order (Parquet) renormalization equation (the t-matrix equation between spin and carrier) $\partial\tilde{J}/\partial\ell = \tilde{J}^2$ where $\tilde{J}=J\mathcal{D}(E)$ is the invariant Kondo coupling. Here, $\ell=\ln(0.57/\tilde{T})$ as deduced by numerical fit of the bare carrier magnetic response function and $\tilde{T}=T/v_F$. Coulomb interactions introduce vertex corrections to this equation. This vertex correction is for the backward scattering *carrier* vertex only. This immediatlely implies a splitting of the invariant Kondo coupling into forward $\tilde{J}_2$ and backward $\tilde{J}_1$ part. The RG equations now are:

$$\partial\tilde{J}_2/\partial\ell = \tfrac{1}{2}\tilde{J}_2^{\,2} + \tfrac{1}{2}\tilde{J}_1^{\,2} \quad ; \quad \partial\tilde{J}_1/\partial\ell = \tilde{J}_1\tilde{J}_2 + \tfrac{1}{2}\tilde{g}_2\tilde{J}_1 \quad . \tag{3}$$

Here $\tilde{g}_2 = g_2/(\pi v_F)$ is the invariant Coulomb coupling. The boundary condition is that $\tilde{J}_\alpha = J_o$ at $\ell=0$. Note that g_2 is unchanged by renormalization [4].

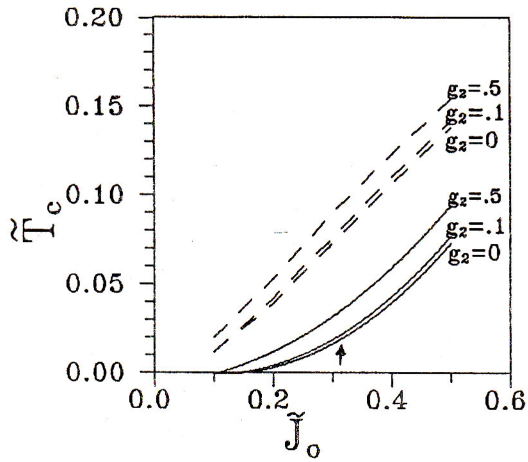

Fig. 1 Characteristic temperature for the Kondo (full lines) and the RKKY (dashed lines) instabilities as a function of the strength of the Kondo interaction. The arrow indicates the limit of weak coupling (see text).

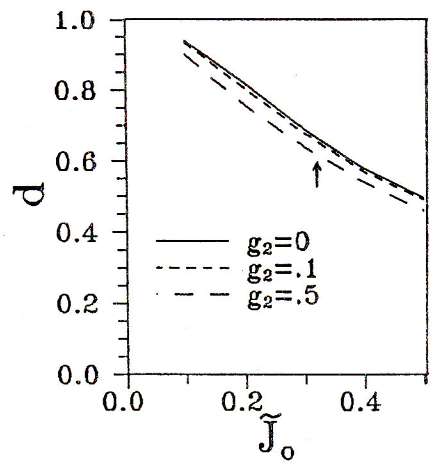

Fig. 2 Spin fraction untouched by the Kondo singlet pairing as a function of the strength of the Kondo interaction. The arrow indicates the limit of weak coupling (see text).

Fig. 1 shows the results of the solution of (3) for T_K. Repulsive Coulomb interactions enhance the magnetic response function and the vertex correction thereby increasing the Kondo temperature. The figure also indicates the limit of validity of the weak coupling approach we have used which corresponds to $J<E_o$ (the splitting between Kondo singlet and triplet levels must be less than the characteristic carrier energy of our model).

But this information by itself is of little interest. What we are interested in is the competition between the Kondo and RKKY instabilities. The RKKY spin response function at $2k_F$ can be determined in the RPA [1]. It has a pole at $\pi\tilde{J}_{RKKY}/(4.\tilde{T})=1$ where $\tilde{J}_{RKKY}=\tilde{J}_o^2\ell\ /4.$ is the carrier mediated spin-spin interaction. Calculations of this instability temperature T_{RKKY} show that $T_{RKKY}>T_K$ for all values of J_o in Fig. 1. This is in agreement with Nozières' argument [5] which states that there are not enough carriers present to screen all the spins (one for three). The Kondo effect must then be incomplete. This leaves enough of the spins free to become unstable through the RKKY interaction. A careful analysis of the fraction of unpaired spins shown that the RPA does a poor job with regard to this criterion. The reason is simple. There is no feedback from the Kondo to the RKKY in the RPA. One way to do this is by applying the RG procedure to the RKKY effective interaction for which one can write the following equation:

$$\partial\tilde{J}_{RKKY}/\partial\ell = \tfrac{1}{2}(\tilde{J}_1^{\,2} + \tilde{J}_2^{\,2})/4, \tag{4}$$

with the boundary condition $\tilde{J}_{RKKY}=0$ at $\ell=0$. The modified RPA pole is now at $\pi\tilde{J}_{RKKY}/(4.\tilde{T})=1$. It is quite obvious that one cannot use the first-order RG equations (3) with (4) since the Parquet structure of (3) will always produce a divergence in $\tilde{J}_{RKKY}$ for $T>T_K$, a situation that cannot be correct at all band fillings. Indeed, the results for a half-filled band [6] clearly indicate that the Kondo instability can dominate over the RKKY for a sufficiently large J_o. We must then go to second order RG in which case a correction term $-\tfrac{1}{2}(\tilde{J}_1^{\,2}+\tilde{J}_2^{\,2})$ must be added to each spin vertex in equations (3). As a result, the fixed point is shifted to $\tilde{J}_\alpha\approx 2$.

The results for T_{RKKY} are shown in Fig. 1. The RKKY still dominates the Kondo instability, as has been discussed above. More important, however, is the fact that the remaining unpaired spin fraction, which follows the renormalization equation $\partial\ln(d)/\partial\ell=-\tfrac{1}{2}(\tilde{J}_1^{\,2}+\tilde{J}_2^{\,2})$ (spin self-energy corrections), behaves quite properly. As a matter of fact $d\gtrsim 2/3$ in the region of validity of the RG. At the boundary to strong coupling ($\tilde{J}_o\approx 1/\pi$), $d\approx 2/3$ which is what one would expect since the Kondo pairing is then maximum; the carriers can only screen 1/3 of the spins at 1/6 band filling.

CONCLUSION

We have shown that the 1/6 filled Kondo 1D lattice with Coulomb interaction can only undergo incomplete Kondo effect and that it thus remains inherently unstable towards a RKKY spin modulation. The Nozières criterion is verified throughout the weak coupling region.

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