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INSTABILITY OF THE FERMI-LIQUID FIXED POINT IN AN EXTENDED KONDO MODEL

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Abstract. We study an extended $SU(N)$ single-impurity Kondo model in which the impurity spin is described by a combination of Abrikosov fermions and Schwinger bosons. Our aim is to describe both the quasiparticle-like excitations and the locally critical modes observed in various physical situations, including non-Fermi liquid (NFL) behavior in heavy fermions in the vicinity of a quantum critical point and anomalous transport properties in quantum wires. In contrast with models with either pure bosonic or pure fermionic impurities, the strong coupling fixed point is unstable against the conduction electron kinetic term under certain conditions. The stability region of the strong coupling fixed point coincides with the region where the partially screened, effective impurity repels the electrons on adjacent sites. In the instability region, the impurity tends to attract $(N - 1)$ electrons to the neighboring sites, giving rise to a double-stage Kondo effect with additional screening of the impurity.

Key words: Non-Fermi Liquid, Strong versus Intermediate Coupling Fixed Point, Extended $SU(N)$ Kondo Model

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1. Introduction

One of the most striking properties discovered in Heavy-Fermion systems in recent years is the existence of a non-Fermi-liquid behavior (11, 21, 12) in the disordered phase close to the magnetic quantum critical point with a temperature dependence of the physical quantities which differs from that of a standard Fermi-liquid. Recent results obtained in $CeCu_{5.9}Au_{0.1}$ by inelastic neutron scattering experiments (19, 20) have shown the existence of anomalous ω/T scaling law for the dynamical spin susceptibility at the antiferromagnetic wavevector which persists over the entire Brillouin zone. This indicates that the spin dynamics are critical not only at large length scales as in the itinerant magnetism picture (7, 13) but also at atomic length scales. It strongly suggests the presence of locally critical modes beyond the standard spin-fluctuation theory. Alternative theories have been proposed to describe such a local quantum critical point. In this direction, we will mention recent calculations (18) based on dynamical mean field theory (DMFT) which seem to lead to encouraging results such as the prediction of a scaling law for the dynamical susceptibility. The other approach which has been put forward to describe the local QCP is based on supersymmetric theory (6, 17, 3, 4) in which the spin is described in a mixed fermionic-bosonic representation. The interest of the supersymmetric approach is to describe the quasiparticles and the local moments on an equal footing through the fermionic and the bosonic part of the spin respectively. It appears to be specially well-indicated in the case of the locally critical scenario in which the magnetic temperature scale T_N , and the Fermi scale T_K (the Kondo temperature) below which the quasiparticles die, vanish at the same point δ_C .

Let us now emphasize another aspect in the discussion of the breakdown of the Fermi-liquid theory. It has to do with the question of the instability of the strong coupling (SC) fixed point. A stable SC fixed point is usually associated with a local Fermi-liquid behavior. On the contrary, an instability of the SC fixed point is an indication for the existence of an intermediate coupling fixed point with non-Fermi-liquid behavior. The traditional source of instability of the SC fixed point in the Kondo model is the presence of several channels for the conduction electrons with the existence of two regimes, the underscreened and the overscreened ones with very different associated behavior. In the one-channel antiferromagnetic single-impurity Kondo model, it is well known from renormalization group arguments, that the system flows to a stable SC fixed point (2) with a behavior of the system identified with that of a local Fermi liquid (14). The situation is rather different in the case of the multichannel Kondo model with a number K of channels for the conduction electrons ($K > 1$) (15). In

the underscreened regime when $K < 2S$ (where S is the value of the spin in $SU(2)$), the SC fixed point is stable. It becomes unstable in the other regime $K > 2S$, known as the overscreened regime. The underscreened regime corresponds to the one-stage Kondo effect with the formation of an effective spin $(S - 1/2)$ resulting from the screening of the impurity spin by the conduction electrons located on the same site. The system described by the SC fixed point behaves as a local Fermi liquid. The instability of the SC fixed point in the overscreened regime is associated with a multi-stage Kondo effect in which successively the impurity spin is screened by conduction electrons on the same site, and then the dressed impurity is screened by conduction electrons on the neighboring site and so forth. The overscreened regime leads to the existence of an intermediate coupling fixed point with non-Fermi-liquid excitation spectrum and an anomalous residual entropy at zero temperature. It has been recently put forward (3, 4) that other sources of instability of the SC fixed point may exist other than the multiplicity of the conduction electron channels. Recent works have shown that the presence of a more general Kondo impurity where the spin symmetry is extended from $SU(2)$ to $SU(N)$, and the impurity has mixed symmetry, may also lead to an instability of the SC fixed point already in the one-channel case. In the large N limit, Coleman et al. (3) have found that the SC fixed point becomes unstable as soon as the impurity parameter q (defined below) is larger than $N/2$ whatever the value of $2S$ (defined below) is, giving rise to a two-stage Kondo effect. This result opens the route for the existence of an intermediate coupling fixed point with eventually non-Fermi-liquid behavior.

It is worth noting that the supersymmetry theory, or more specifically the taking into account of general Kondo impurities appears to offer valuable insights into the two issues raised by the breakdown of the Fermi liquid theory that we have summarized above, i.e. both the existence of locally critical modes and the question of the instability of the SC fixed point. Somehow it seems that the consideration of general Kondo impurities captures the physics present in real systems with the coexistence of the screening of the spin by conduction electrons responsible for the formation of quasiparticles, and the formation of localized magnetic moment that persists and eventually leads to a phase transition as the coupling to other impurities becomes dominant.

The aim of this work is to study the $SU(N)$, extended single-impurity Kondo model in the one-channel case (10). We would like to investigate how the system behaves when not only the values of the parameters $(2S, q)$ of the representation vary, but also the number n_d of conduction electrons on the neighboring site does. We want to discuss the effect of n_d on the stability of the SC fixed point and to further understand the nature of the

screening with the possibility of achieving either a one-stage, two-stage or multi-stage Kondo effect depending on the regime considered. Implications for the behavior of physical quantities will be given.

2. Extended $SU(N)$ single-impurity Kondo model

We consider a generalized, single-impurity, Kondo model with one channel of conduction electrons and a spin symmetry group extended from $SU(2)$ to $SU(N)$. An impurity spin, $\mathbf{S}$, is placed at the origin (site 0). We deal with impurities that can be realized by a combination of $2S$ bosonic ($b_\alpha^\dagger$) and $q - 1$ fermionic ($f_\alpha^\dagger$) operators. The hamiltonian describing the model is written as

$$H = \sum_{\mathbf{k}, \alpha} \varepsilon_{\mathbf{k}} c_{\mathbf{k}, \alpha}^\dagger c_{\mathbf{k}, \alpha} + J \sum_A \mathbf{S}^A \sum_{\alpha, \beta} c_\alpha^\dagger(0) \tau_{\alpha\beta}^A c_\beta(0), \quad (1)$$

where $c_{\mathbf{k}, \alpha}^\dagger$ is the creation operator of a conduction electron with momentum $\mathbf{k}$, and $SU(N)$ spin index $\alpha = a, b, \dots, r_N$, $c_\alpha^\dagger(0) = \frac{1}{\sqrt{N_S}} \sum_{\mathbf{k}} c_{\mathbf{k}, \alpha}^\dagger$, where N_S is the number of sites, and $\tau_{\alpha\beta}^A$ ($A = 1, \dots, N^2 - 1$) are the generators of the $SU(N)$ group in the fundamental representation, with $Tr[\tau^A \tau^B] = \delta_{AB}/2$. The conduction electrons interact with the impurity spin $\mathbf{S}^A$ ($A = 1, \dots, N^2 - 1$), placed at the origin, via Kondo coupling, $J > 0$. When the impurity is in the fundamental representation, we recover the Coqblin-Schrieffer model (5, 8) describing conduction electrons in interaction with an impurity spin of angular momentum j , ($N = 2j + 1$, $a = j$, $b = j - 1, \dots, r_N = -j$), resulting from the combined spin and orbit exchange scattering.

2.1. STRONG-COUPLING FIXED POINT

We consider the case where $J \rightarrow \infty$ and we can neglect the kinetic energy in Eq. 1. In this limit the model can be solved exactly in terms of the invariants associated to the spin of the electrons and of the impurities (9). The eigenvalues are of the form

$$E_{SC} = \frac{J}{2} [\mathcal{C}_2(R_{SC}) - \mathcal{C}_2(I) - \mathcal{C}_2(Y)] \quad (2)$$

where I denotes the impurity spin, Y the spin of the n_c conduction electrons coupled to the impurity at the origin, and R_{SC} the spin of the resulting SC state at the impurity site. The quantities $\mathcal{C}_2$ are the $SU(N)$ generalization of the $SU(2)$ eigenvalues, $S(S+1)$, and can be readily evaluated (for details, see Ref. (10)).

The ground state corresponds to having $n_c = (N - q)$ electrons at the origin, partially screening the impurity. It can be written explicitly as the action of $(2S - 1)$ bosonic operators on a singlet state. For instance the *highest spin* state can be written as

$$|GS\rangle_{\{a\}aa}^{[2S-1]} = \frac{1}{\sqrt{(2S-1)!}} (b_a^\dagger)^{2S-1} \left[\frac{1}{\gamma} \mathcal{A}(b_{i_1}^\dagger (\prod_{\alpha=i_2}^{i_q} f_\alpha^\dagger) (\prod_{\beta=i_{q+1}}^{i_N} c_\beta^\dagger)) \right] |0\rangle \quad (3)$$

with $\gamma \equiv \sqrt{(2S + N - 1)C_{N-1}^{q-1}}$. Here, $c_\alpha^\dagger \equiv c_\alpha^\dagger(0)$. We denote the ground state energy by E_0 .

The effect of the kinetic term in Eq. 1 is, to lowest order in perturbation theory, to mix the ground state with excited states where the number of electrons changes by one. There are three such states, which we denote by $|GS + 1\rangle^S$, $|GS + 1\rangle^A$ and $|GS - 1\rangle$. The labels S(A) indicate that the additional electron is coupled symmetrically(antisymmetrically) to the ground state. The states are readily obtained by deriving the relevant SU(N) Clebsch-Gordan coefficients (10).

2.2. STABILITY OF THE STRONG COUPLING FIXED POINT

In order to understand better the low-energy physics of the system, we should consider the finite Kondo coupling, allowing virtual hopping from and to the impurity site. These processes generate interactions between the composite at site 0 and the conduction electrons on neighboring sites, that can be treated as perturbations of the SC fixed point. The energy shifts due to the perturbation can be reproduced by introducing an interaction between the spin at the impurity site and the spin of the electrons on the neighboring site, with effective coupling J_{eff} . Applying an analysis similar to that of Nozières and Blandin (15) to the nature of the excitations, we can argue whether or not the SC fixed point remains stable once virtual hopping is allowed.

Thus, if the coupling between the effective spin at the impurity site and that of the electrons on site 1 is ferromagnetic we know, from the scaling analysis at weak coupling, that the perturbation is irrelevant, and the low energy physics is described by a SC fixed point. That is, an underscreened, effective impurity weakly coupled to a gas of free electrons with a phase shift indicating that there are already $(N - q)$ electrons screening the original impurity.

If, on the contrary, the effective coupling is antiferromagnetic, the perturbation is relevant, the SC fixed point is unstable and the low-energy physics of the model corresponds to some intermediate coupling fixed point, to be identified.

We explicitly calculate the effects of hopping on the SC fixed point to the lowest order in perturbation theory, that is, second order in t . We consider the case with an arbitrary number n_d of conduction electrons on site 1 generalizing the case $n_d = 1$ considered in ref. (4).

Adding n_d electrons on site 1 leads to two different states, that we will call symmetric (S) and antisymmetric (A). These states, degenerate in the SC limit, acquire energy shifts, ΔE_0^A and ΔE_0^S due to the perturbation given, in the large- N limit, by

$$\Delta E_0^A = - \left(\frac{2t^2}{J} \right) \left[\left(\frac{N-q}{q} \right) - \frac{n_d}{N} \left(\frac{N(N-2q)}{q(N-q)} \right) \right] , \quad (4)$$

$$\begin{aligned} \Delta E_0^S - \Delta E_0^A &= - \left(\frac{2S + n_d - 1}{2S + N - q} \right) \left(\frac{2t^2}{JN} \right) \left(\frac{N(N-2q)}{q(N-q)} \right) , \quad (5) \\ &= \frac{J_{eff}}{2} (2S + n_d - 1) . \end{aligned}$$

Notice that the behavior of both Eq. 4 and Eq. 5 are controlled by the same factor. This result has the immediate following physical consequence. The change of sign of J_{eff} (Fig. 1, Right) -and hence of the stability of the SC fixed point- is directly connected to the change in the behavior of $\Delta E_0^A \sim \Delta E_0^S$ with n_d . In particular, when $\Delta E_0^S = \Delta E_0^A$, $\Delta E_0^A = -(2t^2/J)$ independently¹ of n_d , q or $2S$. In the regime where the SC fixed point is stable, $q/N < 1/2$, $J_{eff} < 0$, the lowest energy corresponds to $n_d = 1$, whereas for $q/N > 1/2$, $J_{eff} > 0$, the energy expressed in Eq. (4) is minimized for $n_d = (N - 1)$ (Fig. 1, Left). This is precisely the mechanism behind the two-stage quenching. The accumulation of electrons on site 1 is not related to J_{eff} which is independent of n_d , but results from the dependence of $\Delta E_0^A \sim \Delta E_0^S$ with n_d .

We finish by making some remarks on the physical properties of the model in the different regimes. As is common to all models with an antiferromagnetic Kondo coupling, there will be a crossover from weak coupling above a given Kondo scale, T_K , to a low-energy regime. When the SC fixed point is stable, we should expect for $T \ll T_K$ a weak coupling of the effective impurity at site-0 with the rest of the electrons. The physical properties at low temperature are controlled by the degeneracy of the effective impurity, $d([2S-1]) = C_{N+2S-2}^{N-1}$. Thus, we should expect a residual entropy $\mathcal{S}^i \sim \ln C_{N+2S-2}^{N-1}$ and a Curie susceptibility, $\chi^i \sim C_{N+2S-2}^{N-1}/T$, with logarithmic corrections (9, 16). This is the result that we would expect for a purely symmetric impurity. Contrary to the purely bosonic case, only

¹ This is true for arbitrary values of N , and $2S$.

Figure 1. (Left) Leading term in the energy shift, $\Delta E_0^A \sim \Delta E_0^S$, as a function of q/N , for $1 < n_d < N - 1$ (shaded region), and in the limiting cases $n_d/N \ll 1$ (dashed line), and $n_d/N \approx 1$ (solid line). Notice that the value at $q/N = 1/2$ is equal to $-2t^2/J$, for any n_d . (Right) Energy difference, $(\Delta E_0^S - \Delta E_0^A)$, as a function of q/N , for different values of $2S$ in the large- N limit.

$(N - q)$ electrons are allowed at the origin in the SC limit, instead of $(N - 1)$. Thus, we would expect to find different results for quantities that involve the scattering phase shift of electrons off the effective impurity.

In the $q > N/2$, we do not have access to the intermediate coupling fixed point that determines the low-energy behavior. Nevertheless, it is reasonable to think that there would be a magnetic contribution to the entropy, and a Curie-like contribution to the susceptibility, since the impurity remains unscreened. This behavior is different from that of the multichannel Kondo model, which is also characterized by an intermediate coupling fixed point, but where the impurity magnetic degrees of freedom are completely quenched. The degeneracy of the true ground state is an open question, but we can assume that the entropy will be smaller than that of the SC fixed point (1). It is in the scattering properties that we might be able to see the anomalous features of this new fixed point more clearly.

3. Conclusions

We have studied a Kondo model where the spin of the impurity has mixed symmetry, as a way of incorporating the phenomena of local moment screening and magnetic correlation that is observed in some heavy fermion compounds. Such model is naturally realized by extending the spin symmetry to $SU(N)$, and it displays a rich phase diagram. We find that as long as the bosonic component of spin is of order N , there is a transition around

the point where the fermionic component of the impurity is $q = N/2$. At this particular point, the energy shift is, to lowest order in perturbation theory around the SC fixed point, equal to $-2t^2/J$, independent of the impurity parameters, q , S and N . When $q < N/2$, the low-energy physics corresponds to the SC fixed point. For $q > N/2$ the SC fixed point is unstable and anomalous behavior is expected, in particular, the two-stage quenching effect. This phase diagram is not accidental, but is due to the relation of the effective impurity site in the SC regime to the conduction electrons in neighboring sites, as our study of the dependence of the energy shifts on n_d reveals. If $q < N/2$, the energy is minimized when the dressed impurity repels the electrons on the next site. That is, when $n_d = 1$. At $q = N/2$, the energy shift is also independent of n_d . Finally, the lowest energy shift for $q > N/2$ corresponds to a maximal n_d , indicating the accumulation of electrons leading to the two-stage Kondo quenching.

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