Phase Diagram of the Anisotropic Kondo Chain

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We establish the phase diagram of the one-dimensional anisotropic Kondo lattice model at $T = 0$ using a generalized two-dimensional classical Coulomb gas description. We analyze the problem by means of a renormalization group treatment. We find that the phase diagram contains regions of paramagnetism, partial and full ferromagnetic order.

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The question of the behavior of localized magnetic moments in metals bears on a variety of important materials, from heavy fermion systems to manganites. Central to most theoretical studies is the Kondo lattice model (KLM) with both antiferromagnetic (AFM) and ferromagnetic (FM) couplings. The former case results from superexchange and is associated with heavy fermion behavior in rare-earth and transition metal intermetallic systems [1]. On the other hand, direct exchange leads to intratomic FM interactions of the Hund's rule type, also leading to a KLM description of systems such as the manganites [2]. In both cases, there is strong interest in the determination of the phase diagram and, more importantly, in the nature of the quantum phase transitions that separate the various phases at $T = 0$ [3].

Because of the occurrence of nonperturbative Kondo correlations, in addition to critical order parameter fluctuations, quantum phase transitions in the AFM KLM are still a hotly debated issue [4] as compared to their counterparts in other metallic magnetic systems [5] (see [6] for a recent attempt). In this Letter, we present a renormalization group (RG) treatment of the KLM that, although confined to one spatial dimension, has the advantage of being able to incorporate *both types of low-energy processes on an equal footing.* The RG analysis has been very fruitful in the single-impurity case and is the adequate tool to address the issue of competing ground states. Our treatment generalizes to the lattice case the mapping of the single-impurity problem into a classical Coulomb gas [7]. This enables us to decimate both the conduction electrons and the spins simultaneously. We establish the phase diagram (Fig. 1) for both signs of the coupling constant in a unified fashion. Our results may prove directly useful for quasi-one-dimensional organic compounds with localized moments, such as $(DMET)_2FeBr_4$ [8].

The anisotropic KLM chain is described by

$$H = -t \sum_{j,\sigma} (c_{j+1\sigma}^{\dagger} c_{j\sigma} + \text{H.c.}) + J_z S_j^z s_j^z + J_{\perp} \sum_{\alpha=x,y} S_j^{\alpha} s_j^{\alpha},$$

where $c_{j\sigma}$ annihilates a conduction electron in site j with spin projection σ, $\mathbf{S}_j$ is a localized spin-$\frac{1}{2}$ operator, and $\mathbf{s}_j = \frac{1}{2}\sum_{\alpha\beta} c_{j\alpha}^{\dagger} \boldsymbol{\sigma}_{\alpha\beta} c_{j\beta}$, the conduction electron spin density. At long wavelengths and low energies one can linearize the dispersion around the Fermi points $\pm k_F$ ($k_F a = \frac{\pi}{2} n_c$, where n_c is the conduction electron number density) and take the continuum limit of the fermionic operators. Following Ref. [9] we use bosonization identities and neglect the backscattering terms, which are irrelevant away from commensurability. In this limit the bosonic charge fields decouple giving rise to gapless collective modes. On the other hand, the bosonic spin field is coupled to the local spins, leading to the Hamiltonian

$$H = \frac{v_F}{2} \int dx\, [\partial_x \phi_s(x)]^2 + [\partial_x \theta_s(x)]^2 + \sum_i \left\{ J_z a \sqrt{\frac{2}{\pi}}\, \partial_x \phi_s(i) S^z(i) + \left[\frac{J_{\perp} a}{2\pi\alpha}\, e^{-i\sqrt{2\pi}\,\theta_s(i)} \cos[\sqrt{2\pi}\,\phi_s(i)] S^-(i) + \text{H.c.} \right] \right\}, \tag{1}$$

where $v_F = 2t \sin k_F a$ is the Fermi velocity and the bosonic fields are defined as in Ref. [9].

As in the Kondo problem, it is convenient to rescale the Hamiltonian by the Fermi velocity, introducing the dimensionless coupling constants $\tilde{J}_{z,\perp} = \frac{a J_{z,\perp}}{v_F}$. We follow an approach analogous to the Anderson-Yuval-Haman mapping of the Kondo impurity problem onto a classical Coulomb gas (CG) [7,10]. This is achieved by going to a path integral formulation in the coherent state basis of the bosonic fields and the S^z basis of the local moments. The z part is unmodified whereas the transverse terms generate spin flips along the Euclidean time direction leading to the partition function:

$$Z = \int D\phi_s\, D\theta_s \sum_{\{S_z\}} \sum_{v=\pm 1} y^N e^{-S}. \tag{2}$$

Here, $y = \frac{|\tilde{J}_{\perp}|}{2}$, N is the number of flips for a certain spin configuration $\{S_z\}$, and the Euclidean action is

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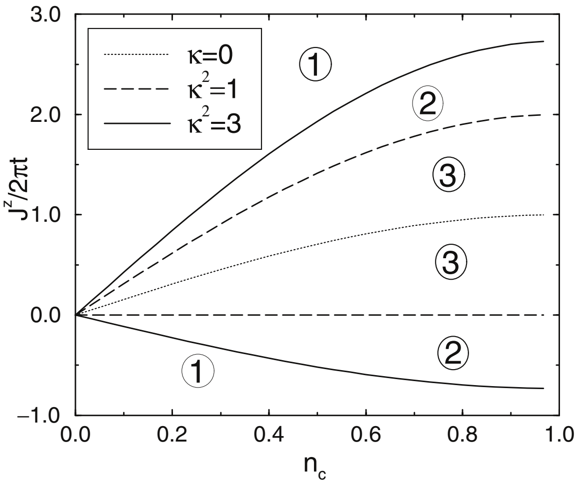

FIG. 1. Ground state phase diagram of the KLM as a function of the Kondo coupling J_z and the band filling n_c. (1) corresponds to the ordered phase of the spin array with $\langle S^z \rangle = 1/2$, (2) is an ordered phase with $\langle S^z \rangle < 1/2$, and (3) is a paramagnetic phase, $\langle S^z \rangle = 0$.

$$S = S_0 + \tilde{J}_z \sqrt{\frac{2}{\pi}} \sum_x \int d\tau\, \partial_x \phi_s(x,\tau) S^z(x,\tau) + -i\sqrt{2\pi} \sum_j [v(j)q(j)\phi_s(j) - \theta_s(j)q(j)], \quad (3)$$

where S_0 is the free Gaussian bosonic action in both variables ϕ_s and θ_s [11], $\sum_j$ is a sum over kink (spin flip) coordinates, and $q = S^z(\tau + \delta\tau) - S^z(\tau) = \pm 1$ is called the "magnetic charge" [11]. Because of the cosine in the $\tilde{J}_\perp$ term of (1), for each spin flip the ϕ_s field comes in with two different signs [11]. We denote them by $v(j) = \pm 1$ [$v(j)q(j)$ is called the "electric charge"]. Thus, each particle corresponds to a spin flip and has both a magnetic and an electric charge, which are related to the original term that produced the flip. The fugacity of the particles is y. For instance, a spin flip produced by the right moving fermions corresponds to a particle with electric and magnetic charges with the same sign, whereas one produced by the left moving fermions gives rise to a particle with opposite signs on its charges. There are two restrictions on the charge configurations *for each space coordinate:* (i) the magnetic charge q must alternate along the time direction (because its origin is a spin-$\frac{1}{2}$ flip) and (ii) the total charges must be zero, $\sum q = \sum qv = 0$ (because of periodic boundary conditions in the time direction). We note that these conditions are more stringent than in the usual 1D bosonic field theories [11]. We therefore call them strong neutrality conditions.

The final step consists of tracing out the bosonic fields in (3) in order to obtain an effective action for the spins and kinks. When this is done, both short- and long-range interactions are generated. The latter are universal but the short-range ones depend on the cutoff procedure [12]. These short-range terms are essentially the same found in Refs. [13,14] by means of a modified bosonization approach. We will focus on the universal long-range part of the action. Upon integrating by parts in imaginary time, spin time derivatives become kink variables. We rewrite all long-range terms in the form of a generalized CG action in two-dimensional Euclidean space for the kinks [15]:

$$S_{\mathrm{eff}} = N \ln y + \frac{1}{2} \sum_{ij} \left[\frac{\kappa^2}{g} \ln |r_{ij}| m(i)m(j) + g \ln |r_{ij}| e(i)e(j) - i\kappa\varphi_{ij} e(i)m(j) \right], \quad (4)$$

where r_{ij} is the length of the vector in the Euclidean plane from particle j to particle i, whereas φ_{ij} is the angle it makes with a fixed axis. In (4), $\kappa = 1 - \tilde{J}_z/\pi$, $g = 1$, $m(j) = q(j)$ is the magnetic charge, and $e(j) = v(j)q(j)$ is the electric one. The coefficient of the term in φ_{ij} is usually an integer (the conformal spin, [11]) and the ambiguity of $2\pi n$ in the angle is then irrelevant. However, in this case, κ can assume noninteger values. The theory remains well defined nevertheless, due to the strong neutrality condition, which leads to a cancellation of the Riemann surface index.

In order to investigate the physics of the action (4), we employ a RG procedure [15]. The most interesting situation is the dense limit, where the distance between impurities is of the order of the smallest bosonic wavelength available in the system. Even though we begin with unitary charges, higher charges are generated by renormalization, which come from the fusion of elementary kinks [16]. They correspond to new action terms with spin flip *pairs* and four fermion operators:

$$O_{ph} \sim \tilde{G}[\psi^\dagger_{R\uparrow}(x)\psi_{R\downarrow}(x)\psi^\dagger_{L\uparrow}(x)\psi_{L\downarrow}(x) \times S^-(x+\delta)S^-(x) + \mathrm{H.c.}], \quad (5)$$

$$O_{pp} \sim G[\psi^\dagger_{R\uparrow}(x)\psi_{R\downarrow}(x)\psi^\dagger_{L\downarrow}(x)\psi_{L\uparrow}(x) \times S^+(x+\delta)S^-(x) + \mathrm{H.c.}], \quad (6)$$

where δ is a distance of order α. These operators do not appear in the original Hamiltonian but are generated by the RG procedure. Notice that they are associated with exchange processes generated by electron-electron interactions. It is natural, from this viewpoint, to think of the localized spins as generating interactions among the electrons. The O_{ph} term flips two nearby spins simultaneously and its action generates a particle with charges $(m, e) = (\pm 2, 0)$, whereas O_{pp} creates $(0, \pm 2)$ charges. Thus, G and $\tilde{G}$ are the fugacities of these charge 2 particles. Higher charges are irrelevant. The RG equations are

$$\frac{dy}{d\ell} = \left[2 - \frac{1}{2}\left(\frac{\kappa^2}{g} + g\right)\right] y + \pi\varepsilon y (G + \tilde{G}),$$
$$\frac{d\tilde{G}}{d\ell} = 2\left(1 - \frac{\kappa^2}{g}\right)\tilde{G} + \pi y^2, \qquad (7)$$
$$\frac{dG}{d\ell} = 2(1 - g)G + \pi y^2,$$

$$\frac{1}{(2\pi^2)} \frac{d\ln g}{d\ell} = \frac{\varepsilon}{2} \frac{\kappa^2 - g^2}{g} y^2 + \frac{\kappa^2}{g}\tilde{G}^2 - gG^2,$$

where $\varepsilon = \sin(2\pi\kappa)/(2\pi\kappa)$, with initial conditions: $g(0) = 1$, $y(0) = \tilde{J}_\perp/2$, and $G(0) = \tilde{G}(0) = 0$.

The Coulomb coupling g starts at 1 for noninteracting conduction electrons. However, the same RG equations apply to the case of conduction electrons with an SU(2) noninvariant forward scattering interaction. In this case, the initial value of g is the corresponding Luttinger liquid parameter [11]. We do not consider this case here, but its phase diagram is analogous to the one below.

By considering the solutions of Eqs. (7), we can trace three distinct regions characterized by different fugacity flows. In Fig. 1 these regions are plotted as a function of the original Kondo coupling J_z and the band filling n_c. Since the RG equations depend only on $|\kappa|$, those regions are mirror reflections on the $\kappa = 0$ line. The full and dashed lines trace out borders between different phases, whereas the dotted line, which is embedded in region 3, is the "Toulouse line" of Ref. [9].

In region 1 ($\kappa^2 > 3$), single spin flip processes are irrelevant ($y \to 0$) just as in the FM phase of the single impurity Kondo problem [7]. Besides, this phase has one of the higher charges G flowing to strong coupling [see (6)]. In contrast, both single and double spin flip processes are relevant in regions 2 and 3. What distinguishes them is the fact that in region 2 the flow of y is slower and $G > \tilde{G}$. The flow in the dashed line between 2 and 3 can be solved analytically: $y(\ell) = y(0)e^{\ell}$ and $G(\ell) = \tilde{G}(\ell) = \pi y^2(0)(e^{2\ell} - 1)/2$. This defines a characteristic length $a \sim 2a_0 \ln(2/|\tilde{J}_\perp|)$, where $y(a/a_0) \sim 1$. In this case, there is a precise balance between the electric and magnetic charges, which prevents them from being screened. As a consequence, $g = 1$ and does not renormalize, though the ground state is a plasma. All correlations fall in a power law fashion implying a gapless system. On the other hand, outside the line $|\kappa| = 1$, the interactions are screened ($g \to 0$ or ∞). A particularly simple case of this kind of flow occurs in the Toulouse line ($\kappa = 0$), where $g \to 0$ and all fugacities grow.

Although the RG flows are clear, their physical interpretation is less straightforward. Since we used Abelian bosonization, we treated in different ways the z and the transverse components of the spins. Therefore, while short-range transverse spin correlations are generated by fusion of elementary particles [Eqs. (5) and (6)], the corresponding z correlations appear only through their annihilation and no fugacity is associated with this process. Nevertheless, we can make progress by writing down the operators describing this annihilation. After point splitting the fermionic part, we get

$$O_z \sim 2(\tilde{G}^2 - G^2)S^z(x + \delta)S^z(x) + \frac{y^2}{2} S^-(x + \delta)S^+(x) + \text{H.c.}, \tag{8}$$

which are the counterparts of the transverse terms coming from the fusion of particles. This enables us to determine the magnetic phase diagram assigning an effective spin Hamiltonian to some special cases. Taking δ to be the lattice spacing at the final RG scale in the O_{pp}, O_{ph}, and O_z definitions, we find an effective Hamiltonian

$$H_{\text{eff}} \sim H_0(\bar{\phi}_s, \bar{\theta}_s) + \sum_j 2[\tilde{G}^2 - G^2]S^z(j + 1)S^z(j) + y\cos[\sqrt{2\pi g}\,\bar{\phi}_s(j)]e^{-i\sqrt{2\pi/g}\,\kappa\bar{\theta}_s(j)}S^-(j) + \left[G\cos[\sqrt{8\pi g}\,\bar{\phi}_s(j)] + \frac{y^2}{2}\right]S^-(j + 1)S^+(j) + \tilde{G}e^{i\sqrt{8\pi/g}\,\kappa\bar{\theta}_s(j)}S^-(j + 1)S^-(j) + \text{H.c.} \tag{9}$$

It reproduces the same CG that we studied above. In region 1, this reduces to the FM Heisenberg model in its ordered phase ($G \sim 1, \langle S^z\rangle = 1/2$). The effective Hamiltonian for the $\kappa = 0$ line is also independent of the bosonic field. It is an AFM *XYZ* model in an external field. In this case, the effective spin Hamiltonian is ordered in the *XY* plane, $G \sim \tilde{G} \sim y \sim 1$. Nevertheless, this does not imply any order of the *original* spins. A unitary transformation connects the spins of Eq. (9) to the ones of the original model (1) ensuring that the latter are disordered even if the former are ordered [see the discussion after Eq. (10) and Ref. [9]]. Another situation that can be insightful is the $|\kappa| = 1$ line. In this case, we cannot write an effective model for the spins independent of the bosonic field. However, due to the symmetric flow of G and $\tilde{G}$, the z term vanishes and the order parameter $\langle S^{x,y,z}\rangle$ is still zero. With these assignments in mind, we propose that the entire region 3 is a paramagnetic phase with short-range AFM fluctuations. There is no simple effective Hamiltonian within region 2, but the disordering term, proportional to y, starts to grow more slowly and the short-range z correlations turn from antiferro- to ferromagnetic. We thus find that this is an ordered phase with unsaturated magnetization of the spins.

The picture that emerges from these results is that there are two continuous phase transitions in the KLM. The first transition from region 1 to region 2 in Fig. 1, reminiscent of the Berezinskii-Kosterlitz-Thouless transition of the single impurity Kondo model [7], separates regions of relevance and irrelevance of the single flip process. The effective model [Eq. (9)] in region 1 has FM order, with full saturation of the *localized* spins. A regime with FM order is beyond the present bosonization treatment, since the spin polarization of the conduction electrons must be incorporated. However, the RG flow is still able to indicate its existence through the irrelevance of single spin flips. In a highly anisotropic model, this leads to the ordering of the localized spin array so that the electrons can gain kinetic energy (resembling the double exchange mechanism). In Refs. [17,18], the authors showed that in the isotropic case this is indeed what happens. Within this scenario, the total spin per site (electrons + spins) would be $S^z_{\rm tot} = \langle S^z \rangle - n_c/2 = (1 - n_c)/2$ in the AFM case and $S^z_{\rm tot} = (1 + n_c)/2$ in the FM one. Within the region where the couplings are relevant, there is another continuous phase transition from region 2 to region 3 in Fig. 1, similar to the transition of the Ising model in a transverse field [19], that separates a paramagnetic phase (region 3 of Fig. 1) from a region with unsaturated magnetization of localized spins, which grows continuously until the border of the first transition (region 2 of Fig. 1). This interpretation is consistent with the numerical studies of both the isotropic FM KLM of Dagotto *et al.* [2] and the isotropic AFM KLM of Tsunetsugu *et al.* [18]. The methods used here cannot describe the region of phase separation found in the numerical simulations for the FM KLM, because in that case the magnetic energies are of the order of the electron bandwidth. In this limit the bosonization scheme is not applicable.

We now make contact with previous treatments of the KLM with Abelian bosonization. In Refs. [9,13,14], a family of unitary transformations,

$$U = e^{-if(J_z)\sum_i \theta_s(i) S^z(i)}, \tag{10}$$

is used to define new fields that mix spin and boson degrees of freedom. The charges of the CG we obtained arise from vortices of these mixed fields. As can be readily checked, the integration by parts that we performed in the effective action for spins and kinks is equivalent to this unitary transformation. Therefore, our effective Hamiltonians in the different regions of RG flow [Eq. (9)] should be understood *in this rotated basis*. This is of special importance in the analysis of the $\kappa = 0$ line, where $\langle \theta_s \rangle = 0$. Thus, even if the spins acquire order in the XY plane, they still remain disordered in the original basis. Zachar *et al.* [9] argued that along the $\kappa = 0$ line the system has a spin gap. Since the effective Hamiltonian (9) in this line is in a gapped phase, our results are consistent with this conclusion. However, this is at variance with the available numerical evidence [18,20] for the *isotropic* KLM. This discrepancy raises the question about whether the anisotropic model can capture the physics of the isotropic one. In addition, the subsequent work of Zachar [21] proposes additional phases away from $\kappa = 0$, which may be related to our regions 1 and 2. Honner and Gulácsi [13,14] have also proposed a phase diagram for the *isotropic* 1D KLM. They predict a paramagnetic phase for ferromagnetic coupling. This is in disagreement with our results and the work of Dagotto *et al.* [2]. A full discussion of their methods and results in contrast to ours will be published elsewhere.

In conclusion, we have established the zero temperature phase diagram of the anisotropic 1D KLM with ferromagnetic and antiferromagnetic coupling. We have found three different phases: a paramagnetic phase where the Kondo effect dominates, a fully polarized magnetic phase where the "double exchange" correlations drive the system towards order, and a partially polarized phase where Kondo effect and magnetic correlations compete directly to generate partial polarization. The two quantum phase transitions have continuous nature, closely related to the Berezinskii-Kosterlitz-Thouless transition of the single impurity Kondo problem and to the Ising model in a transverse field. Although we have worked in 1D, many of the effects discussed here are generic and also occur in higher dimensions. In spite of the fact that we have used Abelian bosonization and worked on the anisotropic model, our findings are in agreement with the numerical simulations in the SU(2) KLM [2,18]. It would be interesting to have the numerical work extended to the anisotropic model as a further test of our results. Finally, we hope our results will be a stimulus for the study of the phase diagram of quasi-one-dimensional systems with localized moments such as $(DMET)_2FeBr_4$ [8].

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