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Ground-state properties of the generalized ferromagnetic Kondo lattice model

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Abstract. A special kind of bosonization technique and renormalization group theory are employed to study an extended ferromagnetic Kondo lattice model. An effective Hamiltonian is deduced. On the basis of this effective Hamiltonian the phase diagram is discussed, and the effects of the introduced Hund anisotropy and antiferromagnetic interaction between the local spins are clarified. The on-site interaction between the conduction electrons contributes to the effective ferromagnetic interaction between the local spins through the Hund interaction.

1. Introduction

Recently, colossal magnetoresistance (MR) was discovered in the Mn oxide perovskites $R_{1-x}A_xMnO_3$ (R = La, Nd, Pr; A = Ca, Sr, Ba, Pb) [1] and layered $(La, Sr)_{n+1}Mn_nO_{3n+1}$ ($n = 2$) [2] materials. In these materials, the Mn^{3+} has three electrons in the t_{2g} state forming a localized $S = 3/2$ spin, and one electron in the e_g state hopping between nearest-neighbour Mn ions. The t_{2g} electrons are coupled ferromagnetically to the itinerant e_g electrons through a very large Hund coupling, and this coupling leads the local $S = 3/2$ spins of the three Mn t_{2g} electrons to effectively ferromagnetically couple. Experiments [1] showed that these materials have a very rich phase diagram. When $x < 0.2$, there is an insulator state, and when the doping concentration exceeds 0.5 an antiferromagnetic insulator state will appear. In the doping range $0.2 < x < 0.5$, these materials undergo a phase transition from paramagnetic (PM) to ferromagnetic (FM) metal on cooling, and have a sharp resistivity peak near the Curie temperature T_c. In this doping range the relative magnetoresistance can be as large as 99% or more. This novel phenomenon may have potential for technical applications, so study of these materials is becoming intensive. In theoretical work, how to explain the existing experimental results has become a central problem. Usually, the following double-exchange Hamiltonian is the most appropriate model for Mn oxide studies:

$$H = -t\sum_{j,\sigma}(C^{\dagger}_{j,\sigma}C_{j+1,\sigma} + \text{h.c.}) - J_H\sum_{j,\sigma,\sigma'}\boldsymbol{S}_j\cdot\boldsymbol{\tau}_j \tag{1}$$

where the spin of the conduction electron $\boldsymbol{\tau}_j = \sum_{\sigma,\sigma'}C^{\dagger}_{j,\sigma}(\vec{\boldsymbol{\tau}}_{\sigma,\sigma'}/2)C_{j,\sigma'}$ and $\boldsymbol{S}_j$ is the local spin. The first term represents the e_g-electron hopping between the nearest-neighbour Mn ions; the second term is the Hund coupling ($J_H > 0$) between the $S = 3/2$ t_{2g} localized spin and the spin of the itinerant e_g electron. Solving this Hamiltonian is a rather difficult task. This is why even as regards this simple form of the Hamiltonian little is known and one has

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to treat the model under some approximation, e.g. $J_H \to \infty$ [3], localized spin $S \to \infty$, or treating the localized spin as a classical spin. In a popular approach [3], the localized spins are regarded as classical spins, and the e_g electrons move between the neighbouring sites in this background of classical spins with an effective hopping strength. But very recently Dagotto *et al* [4] studied this model numerically, and found an extraordinarily rich phase diagram, in which there is a coexistence state—namely, a phase separation state; this novel regime may be connected with some experiments. These results indicate that studying Hamiltonian (1) analytically is still necessary. This effort will be helpful in understanding the full features of Mn oxides. In addition, the numerical findings suggest that results for the three-dimensional case are similar to those for the one-dimensional case, and in the low-dimensional layered materials a very large MR is also detected. So, as regards both theory and experiments, study of Hamiltonian (1) in the low-dimensional case is required.

On the other hand, Hamiltonian (1) is also called the Kondo lattice model; this model has been intensively studied in the antiferromagnetic (AFM) case [5], but the FM case is rarely considered, especially at partial band fillings. Recently, Hur [6] studied the effects of hole doping and disorder with Hamiltonian (1) by using standard bosonization techniques. As a restriction of the method, the results are limited to the range of very low doping and weak coupling. For Hamiltonian (1), the influence [4] of an on-site Coulombic repulsion has been recently discussed. In view of the large Hund interaction, this term has always been neglected, and it has been shown [4] that it does not produce qualitative changes in the ground state. But recent study [7] shows that strong Coulomb interaction is very important. In our paper, the Coulombic interaction will be included. In addition, to achieve a full understanding of the phase diagram of the Mn oxides, treatment of the competition between ferromagnetic and antiferromagnetic interaction is necessary. Thus, an AFM interaction is naturally introduced into the model Hamiltonian. This interaction may arise from direct interaction, indirect RKKY coupling [8] or superexchange interaction [9]. In the single-impurity Kondo problem, the exchange anisotropy is known to play an important role in the low-temperature behaviour, so the effect of this kind of anisotropy in the Kondo lattice model may also be interesting, especially at partial band fillings.

In this paper, we will extend the usual double-exchange model by adding the AF interaction between the local spins and introducing the anisotropy of the Hund interaction to Hamiltonian (1). As the first step towards treating the higher-dimensional problem, we will study the extended model in the one-dimensional case, employing a special kind of bosonization technique invented by Honner and Gulácsi [10, 11] and successfully used in the Kondo lattice model at partial band filling and Hamiltonian (1). In the following treatment, we will follow this scheme, and deduce an effective Hamiltonian. On the basis of this effective Hamiltonian, we will concentrate on studying the low-temperature phase diagram.

2. The model Hamiltonian and its effective form

The model Hamiltonian is

$$\begin{aligned} H = & -t\sum_{j,\sigma}(C^{\dagger}_{j,\sigma}C_{j+1,\sigma} + \text{h.c.}) + U\sum_{j} C^{\dagger}_{j,\uparrow}C_{j,\uparrow}C^{\dagger}_{j,\downarrow}C_{j,\downarrow} \\ & - \sum_{j}\left\{\frac{J^{\perp}_{H}}{2}\left[S^{+}_{j}\tau^{-}_{j} + \text{h.c.}\right] + J^{\parallel}_{H}S^{Z}_{j}\tau^{Z}_{j}\right\} \\ & + \sum_{j}\left\{\frac{J^{\perp}_{AF}}{2}\left[S^{+}_{j}S^{-}_{j+1} + \text{h.c.}\right] + J^{\parallel}_{AF}S_{j}S_{j+1}\right\} \end{aligned} \tag{2}$$

where $J_H^{\perp}$ and $J_H^{\parallel}$ are the anisotropic Hund interactions. U is the Hubbard interaction term, and $J_{AF}^{\perp}$ and $J_{AF}^{\parallel}$ are the nearest-neighbour anisotropic antiferromagnetic exchanges between the localized spins. Following reference [10], decomposing the site operator into the right- and left-moving parts, and defining Bose fields $\phi_\sigma(j)$ and $\Pi_\sigma(j)$, in the thermodynamic limit we find that the Fermi operator can be expressed as

$$c_{\pm,\sigma}(j) \approx \mathcal{N}(\alpha) \exp\left\{\pm \mathrm{i}\sqrt{4\pi}\left[\Phi_{\pm,\sigma}(j) + k_F j a\right]\right\}$$

where $\Phi_{\pm,\sigma}(j)$ is defined as

$$\Phi_{\pm,\sigma}(j) = \left[\phi_\sigma(j) \mp \int_{-\infty}^{ja} \Pi_\sigma(x)\,\mathrm{d}x\right] \Big/ 2$$

and from the commutator of ϕ_σ and its canonical conjugate Π_σ it follows that

$$\left[\phi_\sigma(j), \Pi_{\sigma'}(j')\right] = \mathrm{i}\delta_{\sigma,\sigma'} J_{j-j'}(\alpha)$$

where

$$J_{j-j'}(\alpha) = \int_{-\infty}^{+\infty} \cos\left[k(j-j')a\right] \Lambda^2(k)\,\mathrm{d}k$$

in which $\Lambda(k)$ is the cut-off function; α characterizes the delocalization [10]—it describes the characteristic spatial spread of the conduction electron. It should be noted that the factors $\mathcal{N}(\alpha)$ and $J_{j-j'}(\alpha)$ depend on the form of the cut-off $\Lambda(k)$, and in the following discussion we will specify it. From this procedure, we obtain the bosonized Hamiltonian. In order to derive an effective interaction between the localized spins from the Hamiltonian deduced, a unitary transformation:

$$R = \exp\left\{\mathrm{i}\frac{J_H a}{\sqrt{2\pi^3} v_F} \sum_j S_j^z \theta_s(j)\right\}$$

($v_F = at\sin(k_F a)$, $k_F = n\pi/2a$, $n = 1 - x$) is introduced. After this preparation, keeping the nearest-neighbour interaction, and replacing the Bose field of the conduction electron band by the expectation values in the non-interacting ground state, finally we get an effective Hamiltonian:

$$\tilde{H} = \sum_j \left\{\frac{J_{AF}^{\perp}}{2}\left[S_j^+ S_{j+1}^- + \text{h.c.}\right] - \Delta S_j^z S_{j+1}^z - h_j S_j^x\right\} \tag{3}$$

where

$$\Delta = \frac{(\Delta_H J_H^{\perp})^2 a^2 J_1(\alpha)}{2\pi^2 v_F}\left(1 + \frac{U}{v_F \pi}\right) - J_{AF}^{\parallel} \tag{4}$$

$$h_j = 2J_H^{\perp}\mathcal{N}^2(\alpha). \tag{5}$$

In the above equations, the Hund anisotropic parameter $\Delta_H = J_H^{\parallel}/J_H^{\perp}$ is introduced for convenience.

3. The phase diagram

If we are just considering the incommensurate filling case, $\cos(2kj_F a)$ can be regarded as a random variable; then $\tilde{H}$ is nothing but the one-dimensional quantum XXZ-model with a random transverse field. It is clear that Δ consists of two parts; the first part results from the double-exchange mechanics and always leads to a FM coupling between the local spins. The second part is the contribution of the AFM interaction between the local spins. The first term

of Hamiltonian (3) has its origin in the AFM interaction of local spins and drives the system to the XY-phase. The last term arises from the transverse Hund interaction, and contributes an effective transverse field which always tends to destroy any kind of order. Thus the competition of the three terms in Hamiltonian (3) will lead to a complex phase diagram. In the following, we will quantitatively discuss the properties of Hamiltonian (1) in several different cases using model (3).

3.1. $J_{AF}^{\perp} = 0$

When $J_{AF}^{\perp} = 0$, the Hamiltonian can be reduced to the Ising model with a random field:

$$H_{\text{Ising}} = -\sum_j \Delta S_j^z S_{j+1}^z - \sum_j h_j S_j^x. \tag{6}$$

For equation (6) we only consider the case of $\Delta > 0$, since for $\Delta < 0$ the model can be transformed to the positive case. The critical behaviour [12] is described by the function

$$\overline{\ln(\Delta)} = \overline{\ln(h_i)}$$

from which we get the critical line

$$(\Delta_H J_H^{\perp c})^2 \frac{a^2 J_1(\alpha)}{2\pi^2 v_F}\left(1 + \frac{U}{v_F \pi}\right) - J_H^{\perp c}\mathcal{N}^2(\alpha) - J_{AF}^{\parallel} = 0. \tag{7}$$

When $J_H^{\perp} > J_H^{\perp c} > 0$, the system is in the FM phase, while when $J_H^{\perp} < J_H^{\perp c}$, the system is in the paramagnetic (PM) state.

In order to discuss the phase diagram, we must know the form of $\mathcal{N}(\alpha)$. We choose a sharper cut-off function, the Gaussian. After examining the non-interacting expectation values, we find that, when $\Lambda(k) = \exp(-\alpha^2 k^2/2)$, we have

$$\mathcal{N}(\alpha) \approx 1/\sqrt{4\sqrt{\pi}\alpha} \qquad J_1(\alpha) = (\sqrt{\pi}/2\alpha)\exp[-(a/2\alpha)^2].$$

We insert $\mathcal{N}(\alpha)$ and $J_1(\alpha)$ into the critical function (7); then the critical line can be obtained. But here we must know the behaviour of α. This parameter characterizes the spatial spread of the conduction electrons. In the half-filling case the conduction electrons spread within a very narrow space because double occupation at the same site is forbidden. When the band filling is lowered from half-filling, the conduction electron average spatial spread will be magnified. We describe this effect simply by using $\alpha = c/n$, in which c is a constant, treated as a fitting parameter for numerical results [4]. Similar behaviour is also obtained in reference [11] by comparison with numerical results. To get the value of c, we set $\Delta_H = 1$, $U = 0$, and $J_{AF}^{\parallel} = 0$. Then we find $c \approx 0.28$ by fitting the numerical results in reference [4]. The full phase diagram is plotted in figure 1, from which it can be seen that our results agree well with the numerical results over a wide range. In our following treatment, we assume that the behaviour of α is independent of other parameters and that this holds in all cases.

On the basis of equation (7), we can discuss the effect of Hund anisotropy. The critical line can be obtained from equation (7):

$$\Delta_H^2 J_H^{\perp c} = f(n, U)/2 + \sqrt{f^2(n, U)/4 + \Delta_H g(n, U, J_{AF}^{\parallel})}. \tag{8}$$

When $\Delta_H = 1$, we recover the isotropic case. As $\Delta_H \neq 1$, the anisotropy will move the phase boundary between the FM and PM regions. For $\Delta_H > 1$, the FM region will be extended; this anisotropy effectively increases the FM interaction between local spins. For $\Delta_H < 1$, the phase boundary moves towards the FM phase. This effect of Δ_H is also shown in figure 1. The Hund anisotropy directly changes the effective FM interaction between the local spins, so it will play an important role in the phase transition.

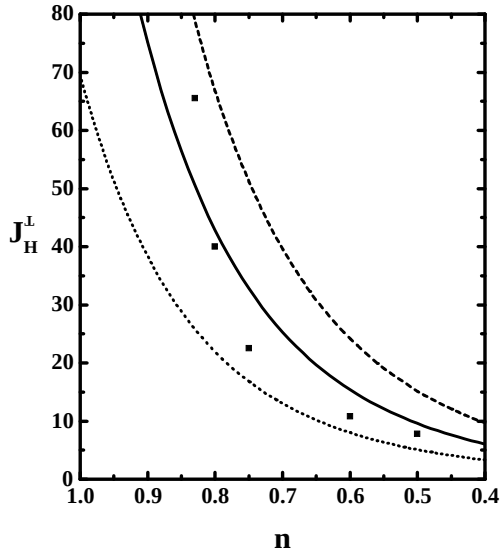

Figure 1. The phase diagram of the FM Kondo lattice model with $S = 1/2$ localized spins. The solid boxes are the results from reference [4] and the solid curve is the result from our theory. For the dotted curve, $U = 0$, $J_{AF} = 0.05$, $\Delta_H = 1.4$, and for the dashed curve, $U = 0$, $J_{AF} = 0.05$, $\Delta_H = 0.8$.

The effect of the Hubbard U can also be easily deduced from equation (7). These effects are plotted in figure 2(a) for different kinds of parameter. It is obvious that the on-site Coulomb U can stabilize the FM ground state, because the forbidding of double occupation can decrease the probability of neighbouring conduction electrons having different spin directions. This effect

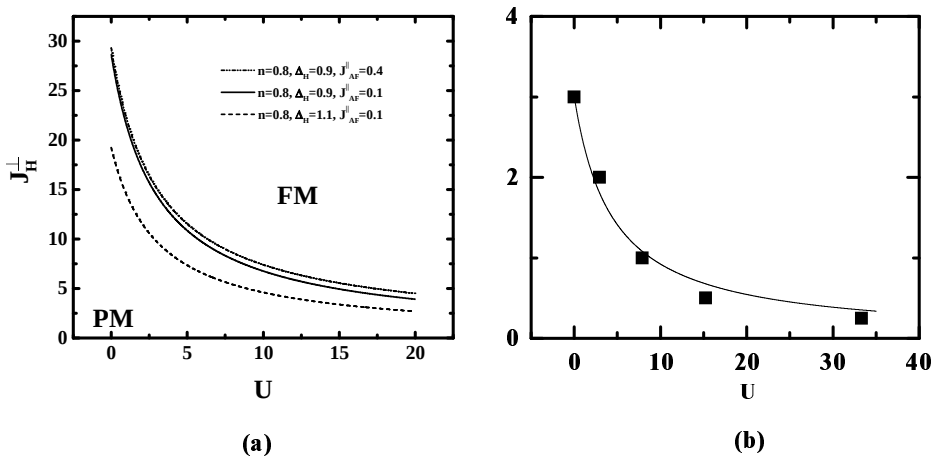

Figure 2. (a) The phase diagram of our $S = 1/2$ model in different cases. (b) The phase diagram of the FM Kondo lattice model with $S = 1/2$ localized spins at $x \approx 0.5$. The solid boxes are the results from reference [13]. The curve is our fitting result.

favours the FM ordering. In our treatment, the Hubbard U directly increases the strength of the effective FM coupling between the local spins. In reference [4], it was shown that for localized spins $S = 1/2$ and $S = 3/2$, the phase diagrams show similar results. So we believe that our above results are still valid for $S = 3/2$. Fortunately, there are existing results [13] which can be used to test our arguments. When $J_{AF}^{\perp} = 0$ and $\Delta_H = 1$, the effects of the Hubbard U can be simply expressed as

$$J_H^c \propto 1/(1 + U/2\pi \sin(n\pi/2)).$$

We use this to fit the numerical results. The fitting line and the numerical results are plotted in figure 2(b). It is found that throughout the parameter range, our fitting accords well with the numerical results.

When the anisotropy of the Hund interaction is strong enough, we consider the limit of $J_H^{\perp} = 0$. Equation (3) is reduced to the well-known XXZ-model. When $|\Delta| \leqslant J_{AF}^{\perp}$, the model is in the gapless quasi-long-range-ordered XY-phase [12]. For $\Delta < -J_{AF}^{\perp}$, the ground state is AF ordered along the Z-axis and a gap opens in the spin excitation. For $\Delta > J_{AF}^{\perp}$, the ground state is FM. When all of the spin parameters are fixed, we change the conduction electron band filling $n \propto 1/\alpha$. For appropriate parameters, if one lowers the band filling, the system may sequentially reach two phase transition points: AFM $\rightarrow$ XY and XY $\rightarrow$ FM. These transitions may also account for the complicated phase transition discovered in experiments.

3.2. $J_{AF}^{\perp} \neq 0$

As $J_H^{\perp}$ has finite value and is small, the model is very intricate; we have to employ renormalization group theory to study its phase diagram. First, using the Jordan–Wigner transformation, we get a spinless fermion model. To treat this model, it is convenient to use the bosonization method. Here only the final results are given. It should be noted that the transverse field in the S^x-direction is decomposed into slowly varying ($q \sim 0$) and oscillating ($q \sim \pi/a$) parts. The latter can be called backward scattering, which can lead to localization. However, in our model the oscillating part is exactly equal to zero. So localization will not be introduced into our system. The bosonized Hamiltonian is given by

$$\bar{H} = \frac{av}{2} \int \mathrm{d}x \left\{ \bar{\Pi}^2 + (\nabla\bar{\phi})^2 + \alpha_1 \cos(\sqrt{16\pi K}\bar{\phi}) + \alpha_2 \cos\left(\sqrt{4\pi K}\bar{\phi} + \sqrt{\frac{\pi}{K}}\bar{X} \right) \right\} \tag{9}$$

in which

$$K = \sqrt{\left(1 + \frac{2\Delta}{\pi J_{AF}^{\perp}}\right) \Big/ \left(1 - \frac{2\Delta}{\pi J_{AF}^{\perp}}\right)} \tag{10}$$

where v is the spin velocity and K is the spin stiffness, $\bar{X}(x)$ is the dual field of $\bar{\Pi}(x)$, defined as $\bar{\Pi}(x) = \partial\bar{X}(x)/\partial x$, $\alpha_1 \sim \Delta$, and $\alpha_2 \sim J_H^{\perp}\mathcal{N}^2(\alpha)$. In the lowest order, the scaling equations can be derived using the standard Kadanoff [14] transformation. The scaling equations for α_1 and α_2 are given as follows:

$$\frac{\mathrm{d}\alpha_1(l)}{\mathrm{d}l} = [2 - 4K(l)]\,\alpha_1(l) \tag{11}$$

$$\frac{\mathrm{d}\alpha_2(l)}{\mathrm{d}l} = \left[2 - K(l) - \frac{1}{4K(l)}\right]\alpha_2(l). \tag{12}$$

Equation (12) implies that the transverse field is relevant only for $1 - \sqrt{3}/2 < K < 1 + \sqrt{3}/2$, and for a pure XXZ-model there are three phases, namely the AF phase, XY-phase, and FM phase. Thus we have five different cases:

(I) $K \to \infty$. A fully polarized FM phase will be formed. α_1 and α_2 are irrelevant under renormalization. In our theory this phase has $\Delta/J_{AF}^{\perp} > \pi/2$, which is somewhat larger than the exact result $\Delta/J_{AF}^{\perp} = 1$. This difference arises from the bosonization method. Notwithstanding the above, it can be concluded that there is a certain $(\Delta/J_{AF}^{\perp})^*$ such that when $\Delta/J_{AF}^{\perp} > (\Delta/J_{AF}^{\perp})^*$, the system will be in the FM phase.

(II) $1+\sqrt{3}/2 < K$ (and K is finite). Here both α_1 and α_2 are irrelevant under renormalization. So the only stable phase is the gapless XY-phase. For this case, Δ dominates over $J_{AF}^{\parallel}$.

(III) $1/2 < K < 1+\sqrt{3}/2$. In this range, α_1 is renormalized to zero. The pure system is the XY-phase; even an infinitesimal disordered h_i will destroy the gapless XY-phase and the result will be a PM phase. It should be noted that when h_i is strong, the problem will be beyond our renormalization group theory treatment.

(IV) $1-\sqrt{3}/2 < K < 1/2$. This case is very complex. α_1 and α_2 are both renormalized to infinity. If we consider a strongly anisotropic case, $J_H^{\perp}$ is very small. In this case, the singlet-to-triplet gap may not be destroyed by the small random $h_i \propto J_H^{\perp}$. The AF phase is still retained in this case. Moreover, in the system there is chance to avoid making the above assumption. From the above discussion, $h_i \propto \mathcal{N}^2(\alpha) \propto n$; thus when $n \to 0$, h_i will approach zero. So in this situation, our above argument still holds. When h_i is not very weak, there will be competition between Δ and h_i. Δ will lead to AF order and h_i will tend to destroy this order. So, in this range, the AF phase may be replaced by a PM phase.

(V) $K < 1-\sqrt{3}/2$. In this range, α_2 will be renormalized to zero and can be neglected. Then what is left is just a pure $S = 1/2$ XXZ-model. For this model when $K < 1-\sqrt{3}/2$, the ground state is AF with a singlet-to-triplet excitation gap. In this phase, $J_{AF}^{\parallel}$ must be strong enough to exceed the FM interaction of the local spin induced by the Hund interaction.

4. Discussion and conclusions

Combining the discussion of the $J_{AF}^{\perp} = 0$ and $J_{AF}^{\perp} \neq 0$ cases, we draw the following conclusions. The Coulomb interaction can stabilize the FM ground state. It directly increases the effective FM interaction between local spins. In contrast, the longitudinal AFM interaction of local spins will decrease the effective FM interaction and can drive the system to an AFM phase. And the transverse part of the AFM interaction can induce a long-range-ordered XY-phase. The Hund anisotropy will move the phase boundary. The contributions of the above interactions will lead to a very complex phase diagram.

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