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Phase diagram of the one-dimensional Kondo-lattice model

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The phase diagram of the one-dimensional Kondo lattice is determined by numerical diagonalization of both the original and an effective Hamiltonian describing the strong-coupling limit. The ground state in the strong-coupling region is ferromagnetic for all electron concentrations away from half filling. The weak-coupling region is characterized by a paramagnetic Luttinger liquid. For the finite-size systems studied here, the dominant spin and charge correlations are at $2k_F$ of the conduction band.

The Kondo-lattice model (KLM) is one of the most intensively studied models of strongly correlated electron systems. The KLM is expected to describe the basic physics of the heavy-electron materials which show a rich variety of different phases, e.g., a paramagnetic (PM) metal with extraordinarily heavy mass, antiferromagnetism or spiral phases, and unconventional superconductivity, etc. Nevertheless, strong correlation effects leave many fundamental questions open and the validity and limits of the model are still unclear. It is therefore important to understand first the simplest one-dimensional (1D) case.[1]

Recently, the ground state at two limits of electron concentration was carefully studied. In the low-concentration limit, it was proven that the one-electron case is ferromagnetic (FM) for all nonzero Kondo couplings J in any spatial dimensions.[2] For the opposite limit, the half-filled KLM in 1D was found to be a spin-liquid insulator for all $J > 0$.[3]

The less-than-half filling case in 1D was studied by Troyer and Würtz using a quantum Monte Carlo (MC) simulation at electron concentration $\rho_c = \frac{1}{3}$ and $\frac{2}{3}$. They found a FM behavior in the strong- and intermediate-coupling regions.[4] This result contradicts the phase diagrams obtained earlier, mainly based on the mean-field approximation,[5] which has a FM phase in the small J region and the Kondo singlet phase in the large J region. The magnetic properties of the KLM are usually discussed in terms of the competition between the Ruderman-Kittel-Kasuya-Yosida (RKKY) mechanism and Kondo screening: the former is believed to favor magnetically ordered states while the latter favor a PM state. The paradoxical MC results indicate that this naive picture must be reexamined. In order to study the strong-coupling limit, the authors have derived an effective Hamiltonian by using the $1/J$ expansion, and proved that the ground state of a *finite* system has the maximum total spin if J is large enough.[6] However, the question whether a FM phase exists in *infinite-size* systems is still open.

In this paper, we will determine the ground-state phase diagram of the 1D KLM in the J-ρ_c plane, by using numerical diagonalization. Generally, the only possible long-range order in 1D would be ferromagnetism,[7] because the total magnetization is a constant of motion. Other magnetic and charge-density-wave order parameters cannot become finite because of the divergence of long wavelength fluctuations. Phase separation also seems unlikely, since there is no trivial limit in which it is favored. Therefore, we concentrate on the FM-PM phase boundary. We find that the FM phase exists in the strong- and intermediate-coupling regions for *all* ρ_c. It is consistent with all known limiting cases and also with the MC simulation, but qualitatively different from the earlier mean-field-type results. In this sense, the phase diagram determined here by exact diagonalization is the first reliable one. We will discuss the character of the PM phase in the last part.

The Hamiltonian of the 1D KLM is written as

$$H_K = -t\sum_{j\sigma}\left(c_{j\sigma}^\dagger c_{j+1\sigma} + \text{H.c.}\right) + J\sum_j \mathbf{S}_{cj}\cdot\mathbf{S}_{fj}\ , \qquad (1)$$

where $\mathbf{S}_{cj} \equiv \sum_{\tau\tau'} c_{j\tau}^\dagger(\frac{1}{2}\boldsymbol{\sigma})_{\tau\tau'}c_{j\tau'}$ and $\mathbf{S}_{fj}$ is a localized spin with $S=\frac{1}{2}$. Hereafter we will set $t=1$ as units of energy. Since the Hamiltonian (1) has an electron-hole symmetry, we will restrict ourselves to the case of less-than-half filling, $0 \leq \rho_c \equiv N_c/L \leq 1$ (N_c, the number of conduction electrons; L, the number of sites).

In the limit of $J = \infty$, the degrees of freedom per site are reduced from eight to three: a local singlet composed of one conduction electron and an f spin, and an unpaired f spin (up or down). By assigning these local singlets as vacant sites, the $J = \infty$ KLM is mapped to the $U = \infty$ Hubbard model with $N \equiv L - N_c$ particles (say f electrons). It is well known that the ground state of the 1D $U = \infty$ Hubbard model has a complete 2^N-fold spin degeneracy, because the nearest-neighbor hopping does not change the spin configuration. The wave functions in the ground-state multiplet are[8]

$$|\Gamma\{\sigma_j\}\rangle = \sum_{j_1<j_2<\cdots<j_N} \det|\phi_\alpha(j)|\; f^\dagger_{j_1\sigma_1}\cdots f^\dagger_{j_N\sigma_N}|0\rangle, \quad (2)$$

where the one-particle eigenfunctions $\{\phi_\alpha\}$ are chosen to be the lowest N levels of the kinetic term.

For finite but small t/J, second-order perturbation gives an effective model for small t/J:[9]

$$H_{\text{eff}} = \sum_{j\sigma}\left[-\frac{t}{2}f^\dagger_{j+1\sigma}f_{j\sigma} + \frac{t^2}{6J}f^\dagger_{j+2\sigma}f_{j\sigma}(1-n_{j+1}) + \frac{3t^2}{8J}f^\dagger_{j+2\sigma}f_{j\sigma}n_{j+1} + \text{H.c.}\right] - \frac{t^2}{4J}\sum_{j\tau\tau'}\left[f^\dagger_{j+2\tau}f_{j\tau'}(\boldsymbol{\sigma})_{\tau\tau'}\cdot\mathbf{S}_{fj+1} + \text{H.c.}\right] + \frac{5t^2}{6J}\sum_j n_j n_{j+1} + \text{const.}, \quad (3)$$

where $n_j \equiv \sum_\sigma f^\dagger_{j\sigma}f_{j\sigma}$. The f electrons should satisfy the local constraint of no double occupancy. The most important terms are the second-neighbor hopping over a particle, $f^\dagger_{j+2\sigma}f_{j\sigma}n_{j+1}$ and $f^\dagger_{j+2\tau}f_{j\tau'}\sigma^z_{\tau\tau'}S^z_{j+1f}$, because these two processes change the spin configuration and lift the spin degeneracy. If the t^2/J terms are small, the effective spin interactions in the ground state multiplet may be calculated, keeping the charge configuration fixed:

$$\langle\Gamma(\sigma'_1\cdots\sigma'_N)|H_{\text{eff}}|\Gamma(\sigma_1\cdots\sigma_N)\rangle = \langle\sigma'_1\cdots\sigma'_N|J_{\text{eff}}\textstyle\sum_j\mathbf{S}_j\cdot\mathbf{S}_{j+1}|\sigma_1\cdots\sigma_N\rangle + \text{const.},$$

$$J_{\text{eff}} = -\frac{t^2}{2\pi J}\left(\frac{2}{\pi\rho}\sin^2\pi\rho - \sin 2\pi\rho\right), \quad \rho \equiv N/L. \quad (4)$$

Thus this effective interaction is described by the Heisenberg model with FM coupling for all $0 < \rho < 1$, and the spin degeneracy is lifted yielding a ground state with the maximum spin $S_{\text{tot}} = \frac{1}{2}N$.

The above treatment with charge configuration fixed is justified when we fix the system size and then take the limit of small t/J. However, it is not guaranteed that a FM phase exists in infinite-size systems for large but finite J, because it is no longer justified to approximate the charge configuration by the single Slater determinant. In the following, first we will confirm the FM phase of H_{eff} by using numerical diagonalization.

We have calculated the total spin S_{tot} of the ground state of H_{eff} by the Lanczos method using open boundary conditions (BC). The open BC have the advantage of having a complete spin degeneracy in the $J = \infty$ limit, while periodic and antiperiodic BC partially lift this degeneracy by cyclic spin permutations. The result is shown in Fig. 1 for L =8, 10, 12, and 14. The maximum spin $S_{\text{tot}} = \frac{1}{2}N$ occurs in the large and intermediate J regions for all ρ_c (above the solid lines in the figures). In the small J region below the dashed lines, S_{tot} has its minimum value. As seen clearly in the figures, the L dependence of the these phase boundaries is small: even the smallest 8 site system shows very similar boundaries as $L = 14$. Therefore, we may conclude that the FM phase boundary in the infinite system is close to the results shown in the figure. Of course, this conclusion means that the FM phase exists in the KLM at *finite* J, at least when the mapping to H_{eff} is valid (roughly, $J \gtrsim 4t$).

Now we determine the phase boundary of the KLM. Figure 2(a) shows S_{tot} of the ground state for $L = 8$. Again, open BC have been used. As for H_{eff}, the region where $S_{\text{tot}} = \frac{1}{2}N = \frac{1}{2}(L - N_c)$ extends in the large and intermediate J regions for all ρ_c. This FM phase corresponds to the one discussed before, in which N_c localized spins are compensated by the c electrons and all the other unpaired spins align in the same direc-

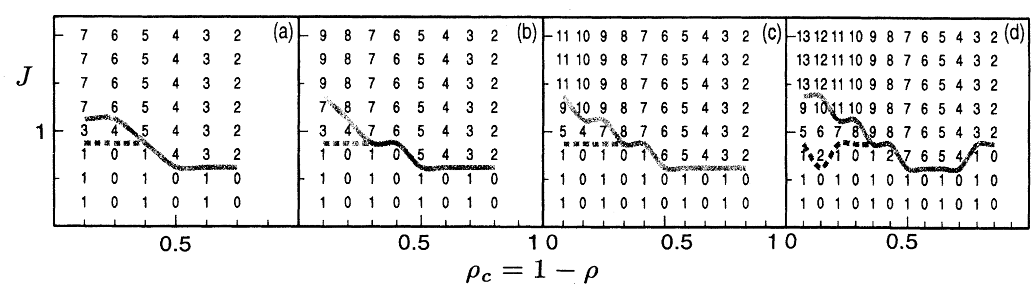

FIG. 1. The total spin $2S_{\text{tot}}$ of the effective model. (a) $L = 8$, (b) $L = 10$, (c) $L = 12$, (d) $L = 14$.

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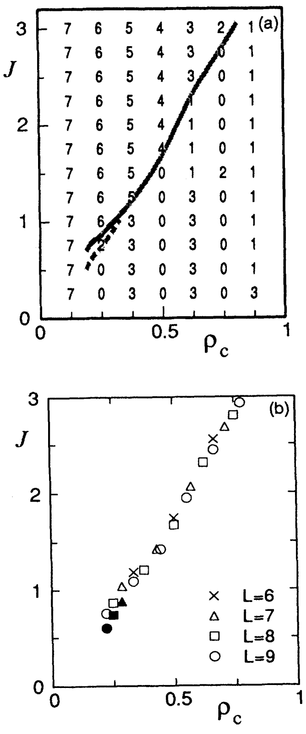

FIG. 2. (a) The total spin $2S_{\rm tot}$ of the Kondo lattice model with $L = 8$. (b) The FM-PM phase boundary below which $S_{\rm tot}$ takes the minimum value. Open symbols and ×: the boundary of $S_{\rm tot} = \frac{1}{2}(L - N_c)$. Solid symbols: the boundary of intermediate $S_{\rm tot}$.

tion. Large spins are found in some cases in the small J region. However this does not indicate FM but is rather due to finite-size effects as will be discussed later. (For example, at $N_c = 3$, there is a narrow region with $2S_{\rm tot} = 1$ between $J = 1.0$ and 1.25. The spin $2S_{\rm tot} = 3$ at smaller J is a finite-size effect.) Thus we may draw the FM phase boundary as in Fig. 2(a) neglecting these finite-size effects. The solid line denotes the boundary of $S_{\rm tot} = \frac{1}{2}(L - N_c)$ and the dashed one is for intermediate $S_{\rm tot}$. This FM phase boundary agrees quite well with the MC result for system sizes up to $L = 24$ and therefore should be close to the infinite system size phase boundary.

We comment here on the large spins seen in Fig. 2(a) which are not intrinsic. One is the triplet at $N_c = 6$ and $J = 1.5$ and the other is for odd N_c and for very small J. The former case becomes a singlet under different BC and the latter case is explained by the following argument. In the $J = 0$ limit, the ground state for odd N_c has an open shell in the c-electron configuration. When J is finite but smaller than the charge excitation energies, only the partially filled orbital interacts with the localized spins. This subsystem would be well approximated by a charge excited state of the $N_c = 1$ case. Because this excited state has the same $S_{\rm tot}$ as the ground state, the ground state for odd N_c and for $J \sim 0$ has $S_{\rm tot} = \frac{1}{2}(L-1)$, rather than the minimum. As L increases, the charge excitation energies decrease and this large-spin region vanishes.

This FM-PM phase boundary is confirmed by systematic calculations done for different system sizes. We have calculated the critical J below which the total spin $S_{\rm tot}$ takes its minimum value. The results for the systems of L=6, 7, 8, and 9 with open BC are plotted in Fig. 2(b). Here again we neglect large spins at smaller J for odd N_c, because they are due to finite-size effects as discussed above. Except in the small ρ_c region, $S_{\rm tot}$ changes from $\frac{1}{2}(L - N_c)$ to its minimal possible value with decreasing J. At small ρ_c ($N_c = 2$ for $L = 7$, 8, 9), we have observed a region with intermediate $S_{\rm tot}$ between the "maximum" $[S_{\rm tot} = \frac{1}{2}(L - N_c)]$ and minimum spin regions. However, from this calculation it is premature to draw a conclusion of whether there is an intermediate FM region with $\langle S_j^z \rangle < \frac{1}{2}(1 - \rho_c)$ and whether the FM-PM transition is first or second order. The order of critical J of the FM-PM boundary is the same for the KLM and its effective model $H_{\rm eff}$. However, ρ_c dependence of the boundary shows different behaviors for these two models. This is due to higher-order terms neglected in $H_{\rm eff}$, which become important for $J \lesssim 4t$. The higher-order corrections are more important in the large ρ_c region, because the density of local singlets is higher there and the contribution of their polarization becomes more significant. This is the reason that the difference in the phase boundary between these two models is larger near half filling. It is worth noting that the FM region extends down to weaker coupling for smaller concentration. This is consistent with the rigorous results of the $\rho_c = 0$ and $\rho_c = 1$ limits mentioned before. Considering this fact together with the small finite-size effects seen in Fig. 2(b), we may conclude that the FM-PM phase boundary in the 1D KLM should be close to the one obtained here.

The spin-correlation function is another useful source of information for magnetic properties. Figure 3 shows the structure factor of the f-f spin correlation, $S(q)$, of the KLM with $N_c = 4$ for several J. We use the antiperiodic BC to have translational invariance.[10] We can see the competition of the FM and PM phases in $S(q)$. For small J, $S(q)$ has a prominent peak at $q = \frac{1}{2}\pi$, corresponding to $2k_F = \rho_c\pi$ of the c electrons. This strong spin correlation comes from the RKKY mechanism. As J increases, the $2k_F$ peak becomes weak and another peak appears at $q = 0$. This can be understood by the Kondo screening, which squeezes the localized spins. An important point is that the interaction among the unpaired

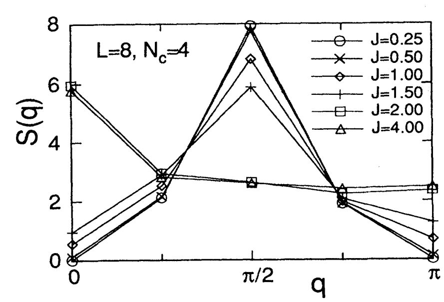

FIG. 3. The f-f spin structure factor of the KLM.

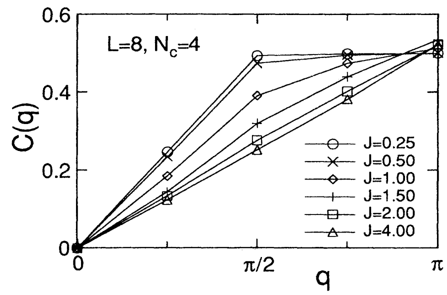

FIG. 4. The charge structure factor of the KLM.

spins is ferromagnetic. Thus, with increasing J, the FM tendency is gradually enhanced, so that it competes with the RKKY mechanism.

It is also important to determine the nature of the PM phase. In this phase the c electrons have a strong $2k_F$ spin correlation, similar to the localized spins. In this sense, we may call this phase a Luttinger liquid.[11] This conclusion is supported by our results for the charge correlation function. Figure 4 shows the c-electron structure factor $C(q)$. It is easily seen that $C(q)$ has a "cusp" at $q = \frac{1}{2}\pi$ for small J and this singularity moves to $q = \pi$ with increasing J. Therefore, the charge correlation in the PM phase has also a Luttinger liquid behavior characterized by $2k_F$ of the c electron. On the other hand, $q = \pi$ corresponds to $4\tilde{k}_F$ of the f electrons in H_{eff}, $4\tilde{k}_F = 2\rho\pi$. The reason why $4\tilde{k}_F$ becomes dominant rather than $2\tilde{k}_F$ is that the ground state of H_{eff} is ferromagnetic. Therefore, this crossover reflects the locking of the c electrons with the localized spins. At least for this system size, there is no evidence that the localized spins cooperate to make a large Fermi surface, but whether this occurs for $L = \infty$ is an open question. Further study is also necessary to confirm the Luttinger-liquid behaviors of the correlation functions and to obtain their critical exponents, since the system size studied here is not large enough to draw a definitive conclusion. The superconducting correlations are also calculated for on-site, nearest-neighbor singlet and triplet pairs, but no enhancement is found for any J.

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[1] Earlier numerical studies of the KLM are R. M. Fye and D. J. Scalapino, Phys. Rev. B **44**, 7486 (1991); K. Yamamoto and K. Ueda, J. Phys. Soc. Jpn. **59**, 3284 (1990).

[2] M. Sigrist, H. Tsunetsugu, and K. Ueda, Phys. Rev. Lett. **67**, 2211 (1991).

[3] H. Tsunetsugu *et al.*, Phys. Rev. B **46**, 3175 (1992); J. A. White (unpublished); R. Hirsch (private communication).

[4] M. Troyer and D. Würtz, Phys. Rev. B **47**, 2886 (1993).

[5] P. Fazekas and E. Müler-Hartmann, Z. Phys. B **85**, 285 (1991), and references therein.

[6] M. Sigrist *et al.*, Phys. Rev. B **46**, 13 838 (1992).

[7] The proof of nonexistence of ferromagnetism in 1D [E. Lieb and D. Mattis, Phys. Rev. **125**, 164 (1962)] does not hold for the KLM and its effective model.

[8] H. Shiba and M. Ogata, Int. J. Mod. Phys. B **5**, 31 (1991).

[9] Some of these terms were first given in J. E. Hirsch, Phys. Rev. B **30**, 5383 (1984).

[10] When periodic BC are used, the ground state is always spin singlet in this case. However, the FM tendency in the large J region is seen as a peak of $S(q)$ at the smallest momentum $q_{\min} = 2\pi/L$. This momentum approaches zero with increasing L, which is consistent with the results under the open BC.

[11] F. D. M. Haldane, J. Phys. C **14**, 2585 (1981).