Ferromagnetic transition of the Kondo lattice with Coulomb repulsion: Exact results

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The Coulomb interaction among conduction electrons is introduced in the Kondo-lattice Hamiltonian. According to the Perron-Frobenius theorem, we exactly show that the ground state of the Kondo lattice in one dimension with the open boundary condition is ferromagnetic and has the total spin $S=(N-N_c)/2$ in the limit $U\rightarrow\infty$, where N is the number of sites and N_c is the number of conduction electrons. Exact-diagonalization calculations clearly indicate that the ferromagnetic state appears for a wide range of Coulomb strength. Our theory predicts that antiferromagnetic correlations of localized spins change into ferromagnetic ones with the increase of Coulomb interactions.

Strongly correlated electron systems have been studied for many years with considerable efforts. The Nagaoka theorem[1] and the Lieb's theorem[2] are examples of the few known exact results for these systems. Recently exact results were obtained in heavy fermions in the strong-coupling limit[3] and with low carrier densities.[4,5] These models indicate an example of the itinerant ferromagnetism of two-carrier systems. The purpose of this paper is to show some rigorous results on the Kondo-lattice systems. The Hamiltonian is the Kondo-lattice model with Coulomb interactions:

$$H=-t\sum_{\langle ij\rangle\sigma}c_{i\sigma}^{\dagger}c_{j\sigma}+U\sum_{i}n_{i\uparrow}n_{i\downarrow}+J\sum_{i}\sigma_i\cdot\mathbf{S}_i\ , \tag{1}$$

where $\langle ij\rangle$ indicates a nearest-neighbor pair of sites and we denote $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$. σ_i and $\mathbf{S}_i$ are spin operators of conduction electrons and localized spins, respectively. The third term of the exchange interaction may be either ferromagnetic or antiferromagnetic. The second term represents the on-site Coulomb interaction among conduction electrons. In this paper we assume that the lattice is one dimensional and we denote the number of lattice sites as N and the number of conduction electrons as N_c.

In recent works, a ferromagnetic ground state of the one-dimensional Kondo lattice has been investigated where two limits are shown to exhibit the ferromagnetism. One is the low-carrier limit $n_c\rightarrow 0$ (Ref. 4) and the other is the strong-coupling case $J\rightarrow\infty$.[3] We show the third candidate to show a ferromagnetic ground state. We believe that the Coulomb repulsions between d electrons in heavy fermions cannot be easily neglected although this issue has never been investigated well until now. First we show the following proposition.

Let us assume that U is very large and $N_c<N$. Then the ground state of the one-dimensional Kondo-lattice model in Eq. (1) has the total spin $S=(N-N_c)/2$ for $J>0$ (antiferromagnetic case) and $S=(N+N_c)/2$ for $J<0$ (ferromagnetic case), where we set the open boundary condition.

As is well known, the lower-order perturbation theories predict the oscillating effective interaction between two localized spins.[6-9] According to numerical studies, there are strong antiferromagnetic correlations between nearest-neighbor spins in the one-dimensional model with the half-filled conduction band.[10,11] When we take account of the Coulomb interaction U among conduction electrons, we should change our picture because exchange process of conduction electrons are much reduced by U. A proof of the proposition is the following.

Let us denote the operators of localized electrons as $f_{i\sigma}$ and $f_{i\sigma}^{\dagger}$. Our basis states are written as

$$\psi_{\{x_i\},\{\sigma_i\};\{s_i\}}=\prod_{j=1}^{N_c}c_{x_j\sigma_j}^{\dagger}\prod_{j=1}^{N}f_{js_j}^{\dagger}|0\rangle\ , \tag{2}$$

where $\{x_i\}$ represent positions of conduction electrons: $x_1<x_2<\cdots<x_{Nc}$. $\{\sigma_i\}$ and $\{s_i\}$ denote spin configurations of the conduction and localized electrons, respectively. We can show that every off-diagonal matrix element is negative with appropriate choice of the phase factors of basis states. We start from states $\psi_{\{x_i\},\{\sigma_i\};\{s_i\}}$ with fixed $\{\sigma_i\}$ and $\{s_i\}$, and then applying the Hamiltonian to $\psi_{\{x_i\},\{\sigma_i\};\{s_i\}}$. We obtain new basis states where one pair of conduction and localized spins with opposite spins are exchanged. For example, if $x_i=k$ and $\sigma_i=-s_k$, $H\psi_{\{x_i\},\{\sigma_i\};\{s_i\}}$ contains the following state:

$$\psi_{\{x_i\},\{\sigma_1,\ldots,\sigma_{i-1},-\sigma_i,\sigma_{i+1},\ldots,\sigma_{Nc}\};\{s_i,\ldots,s_{k-1},-s_k,s_{k+1},\ldots,s_N\}}=c_{x_1\sigma_1}^{\dagger}\cdots c_{x_i,-\sigma_i}^{\dagger}\cdots c_{x_{N_c},-\sigma_{N_c}}^{\dagger}f_{1s_1}^{\dagger}\cdots f_{k,-s_k}^{\dagger}\cdots f_{Ns_N}^{\dagger}|0\rangle\ . \tag{3}$$

This basis state should have a factor $(-)$ so that the off-diagonal matrix element $J/2$ is negative for $J>0$. Third vectors obtained by applying the Hamiltonian twice have the same factors $(+)$ as starting vectors. In this way we can consistently assign phase factors to basis states with the assumption that U is infinitely large. In real-space representation, any configurations can be obtained starting from an aribitrary state by applying H successively as similar to the strong coupling Kondo lattice.[3] Then according to the Perron-Frobenius theorem,[12,13] the ground state is unique and every element of the eigenvector is positive. It is easy to show that the ground state has the total spin $S=(N-N_c)/2$ for $J>0$ (antiferromagnetic). A trial state of the type

$$\psi_{\mathrm{tr}}=\prod_{j=1}^{N_c}(c_{j\uparrow}^\dagger f_{j\downarrow}^\dagger - c_{j\downarrow}^\dagger f_{j\uparrow}^\dagger)(S^-)^n \prod_{i=N_c+1}^{N} f_{i\uparrow}^\dagger|0\rangle , \qquad (4)$$

has nonzero inner product with the ground state. Therefore, $S=(N-N_c)/2$. Similarly the total spin of the ground state is $S=(N+N_c)/2$ for $J<0$ (ferromagnetic *s-d* interaction).

Our theorem indicates an example of the ferromagnetism induced by the Coulomb repulsion. In particular, the complete ferromagnetic state is realized for $J<0$. When the Hund coupling works between conduction and f electrons, the complete ferromagnetic state of itinerant electrons can be the ground state if U is large.

The mechanism of the ferromagnetism for large U resembles the situations of other two limits $n_c \to 0$ and $J\to\infty$. The double-exchange processes[13] give rise to ferromagnetic interactions between two localized spins. However, the large-U model is never reduced to a "*t-J* model," which is different from the strong-coupling model where the Hamiltonian is effectively approximated by the *t-J* model.

Now let us turn to investigate the phase diagram. We calculate the critical values U_c of U; for $U>U_c$ the ground state is ferromagnetic with the total spin $S=(N-N_c)/2$ or $S=(N+N_c)/2$. It is not an easy way to estimate U_c even in the one-dimensional space. We have done it by exact numerical diagonalizations for small clusters. In our calculations the number of lattice sites N is 4, 5, 6, 7, and 8. In Table I, we show ground-state energies for $N=6$ and $U=0$ and ∞. The ferromagnetic ground states are really observed for large U. Critical values of U for the antiferromagnetic J are shown in Fig. 1 for $J=0.5$ ($t=1$) where we impose the open boundary condition. Apparently U_c is an increasing function of n_c ($=N_c/N$) and U_c becomes 0 for $n_c \ll 1$ because the ground state is rigorously shown to be ferromagnetic for $N_c=1$.[4,5] Our evaluations indicate that $U_c\to\infty$ near half-filling for $J>0$ and that the paramagnetic state is very much stable against magnetic orderings at half-filling $N_c=1$. At very low densities of the carriers it is expected that the ground state has the finite total spin

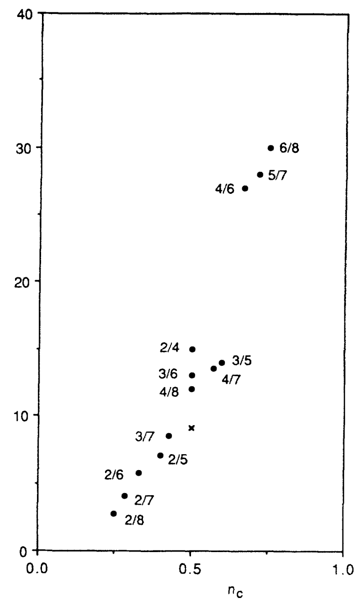

FIG. 1. U_c vs n_c for the antiferromagnetic J ($J=0.5$) with the open boundary condition. Numbers in the figure indicate N_c/N. The cross indicates the extrapolated value at $n_c=\frac{1}{2}$ in the limit $N\to\infty$.

TABLE I. Lowest energies of the Kondo lattice for $N=6$ and $J=0.5$ as a function of the electron number N_c and the total spin S. The ground-state energy for fixed N_c is underlined. Top: $U=0$; bottom: $U=\infty$.

$S \backslash N_c$	1	2	3	4	5
0		$\underline{-3.735\,42}$		$\underline{-6.224\,02}$	
$\frac{1}{2}$	$-1.995\,56$		$\underline{-5.111\,37}$		$\underline{-6.816\,5}$
1		$-3.728\,20$		$-6.213\,59$	
$\frac{3}{2}$	$-2.007\,26$		$-5.105\,10$		$-6.806\,35$
2		$-3.708\,55$		$-6.185\,55$	
$\frac{5}{2}$	$\underline{-2.014\,51}$		$-5.088\,31$		$-6.792\,00$
3		$-3.634\,32$		$-6.138\,45$	
$\frac{7}{2}$	$-1.676\,94$		$-4.742\,80$		$-6.441\,95$
0		$-3.500\,91$		$-4.219\,65$	
$\frac{1}{2}$	$-1.995\,56$		$-4.263\,78$		$\underline{-3.452\,95}$
1		$-3.509\,16$		$\underline{-4.226\,85}$	
$\frac{3}{2}$	$-2.007\,26$		$\underline{-4.272\,79}$		$-3.045\,24$
2		$\underline{-3.519\,16}$		$-3.838\,13$	
$\frac{5}{2}$	$\underline{-2.014\,51}$		$-3.903\,26$		$-2.602\,36$
3		$-3.164\,00$		$-3.428\,72$	
$\frac{7}{2}$	$-1.676\,94$		$-3.514\,80$		$-2.146\,66$

$S>0$ even for the noninteracting band according to the discussions in Refs. 4 and 5. In Fig. 2, we show the ferromagnetic region in the U-n_c plane for the ferromagnetic interaction $J<0$. When we have one conduction electron $N_c=1$, we can rigorously show that the ground state is ferromagnetically ordered and has the total spin $S=(N+1)/2$ even for $U=0$.[4] We expect that the ferromagnetic region exists for finite $n_c>0$ for the noninteracting conduction band due to a similar discussion for the antiferromagnetic case. Since large $|J|$ favors a formation of local triplet, the ordered state is the most favorable to gain the kinetic energy and exchange energy. Our picture is that local triplets are moving around with forming a high-spin state. U_c is an increasing function of n_c and may be infinite at half-filling $n_c=1$. At the half-filling case, the paramagnetic state is also the ground state for the ferromagnetic $J<0$ because this phase is connected with the Haldane state[14,15] and it may be scaled to the Haldane state for the half-filled band even for large U. However, for less than half-filling, the ground state is quite a different state with gapless excitations. This issue may have some close relation with the one-dimensional spin-1 chain with hole doping. In Fig. 3 we show the phase diagrams which we expect from numerical exact diagonalizations. U_c is dependent on the magnitude of J. For large $|J|$ the paramagnetic state is unstable for small perturbations of Coulomb interactions as shown in Fig. 4.

Now we investigate the spin correlations of localized spins. In Fig. 5, the typical behavior of the nearest-neighbor spin correlation is shown as a function of U, where $N=6$ and $J=0.5$. This figure indicates that the antiferromagnetic correlations really change into the ferromagnetic ones with the increase of U. We observe a sharp increase due to the level crossing at U_c, which indicates that the ferromagnetic transition is a first-order transition. At moderate values of U localized spins

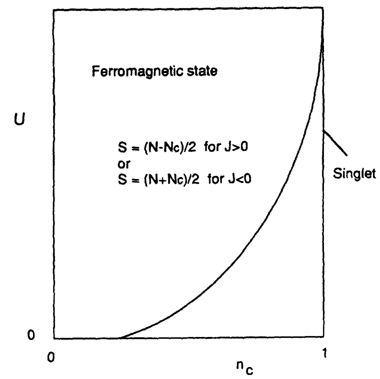

FIG. 3. Schematic phase diagram in the U-n_c plane. The boundary curve meets the line $U=0$ at finite n_c.

behave as though they are independent spins with very small correlations. This may be what we call the dense Kondo state. For large U the spins of localized electrons are set in the almost same direction.

In the following we consider a theoretical design of ferromagnets in the conduction-rich case which means the model that the number of localized spins is less than the number of lattice sites. In fact we can show the following statement.

Let us consider the one-dimensional s-d model with two localized spins. We set the open boundary condition for $N_c<N$ and we assume that the Coulomb repulsion between the conduction electrons is very large. Then among the ground states there is one where localized spins show a parallel correlation $0<\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle \leq \frac{1}{4}$.

This conclusion is independent of the distance of two spins and is also valid for the antiperiodic boundary condition if N_c and N are even numbers. A proof is due to the generalized Perron-Frobenius theorem.[16] We can show that among the ground states there is one state with

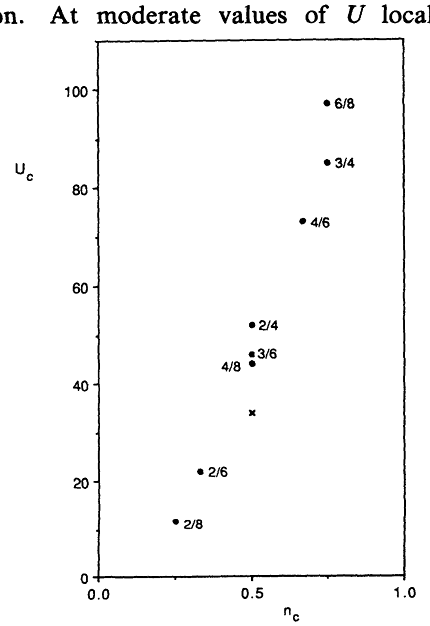

FIG. 2. U_c vs n_c for the ferromagnetic J ($J=-0.5$) with the open boundary condition. Numbers in the figure indicate N_c/N. The cross indicates the extrapolated value at $n_c=\frac{1}{2}$ in the limit $N\rightarrow\infty$.

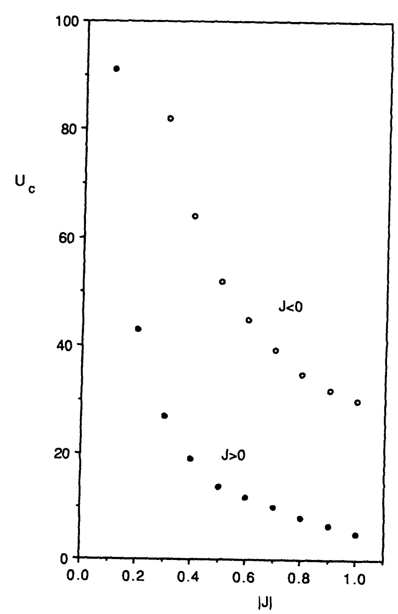

FIG. 4. U as a function of $|J|$ for $N=4$ and $N_c=2$ with the open boundary condition. Solid circles are for the antiferromagnetic interactions and open circles are for the ferromagnetic ones.

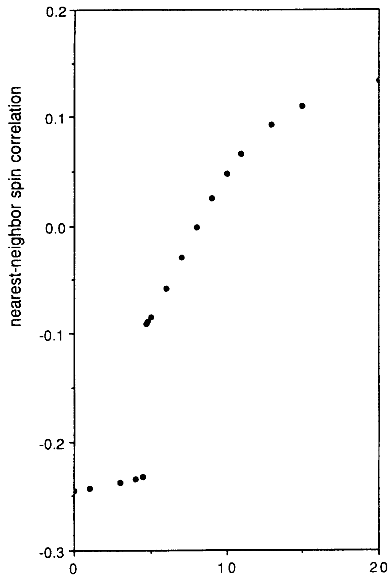

FIG. 5. Nearest-neighbor spin correlation $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle$ vs U for $N=6$ and $N_c=4$ with the antiperiodic boundary condition.

a non-negative eigenvector which shows ferromagnetism. Since in this case the Hamiltonian is not necessarily connected, the uniqueness is not proved. This proposition indicates a possibility of the ferromagnetic interaction of spins induced by Coulomb interactions in the diluted Kondo lattice. Let us point out that an interaction between the spins separated by a distance $R \equiv 2na$ can be ferromagnetic even for the noninteracting case $U=0$, where a is the lattice constant and n is an integer. A numerical evidence is shown in Table II where the spin correlation functions are evaluated for the two-impurity Kondo model. For the half-filled conduction band, spin correlations are oscillating functions of the distance R between two spins. For less than half-filling exact diagonalization calculations clearly indicate the appearance of the high-spin state for the Kondo systems with dilutions of localized spins.

TABLE II. $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ for the two-impurity Kondo model. R denotes the distance between two spins and bc denotes the boundary condition of the conduction electron chain.

N	N_c	bc	U	R	$\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$
10	10	P	0	1	−0.731 37
				2	0.246 38
				3	−0.730 44
				4	0.245 62
8	8	AP	0	1	−0.733 10
				2	0.246 61
				3	−0.732 24
	4	AP	0	1	−0.734 65
				2	−0.720 96
			∞	1	0.170 23
				2	0.100 35

In this paper we have shown rigorously that the ground state of the one-dimensional Kondo lattice with large Coulomb repulsion is ferromagnetic and has the total spin $S=(N-N_c)/2$ for $J>0$ (antiferromagnetic) and or $S=(N+N_c)/2$ for $J<0$ (ferromagnetic exchange interaction) where $N_c<N$. Exact diagonalization calculations predict the appearance of the ferromagnetic phase for a wide range of Coulomb strength in the $U-n_c$ plane. Our results indicate a singlet ground state for the half-filled case ($N_c=N$) for all the values of U. We have also shown the possibility of ferromagnets for diluted Kondo-lattice systems. In particular, the spins of localized electrons separated by a distance of $2na$ are easily set in the same direction for the half-filled conduction band (where n is an integer). Our results should be kept in mind as rules of the theoretical or experimental design of ferromagnets.

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[16]The generalized Perron-Frobenius theorem is the following. Let A be a nonpositive square matrix. A has nonpositive eigenvalues. Let α be the smallest eigenvalue. Then there is a non-negative eigenvector having α as eigenvalue. It is noteworthy that uniqueness of the ground-state vector is not guaranteed in this theorem because A can be a block diagonal matrix.