Rigorous Results for the One-Electron Kondo-Lattice Model

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(Received 16 July 1991)

The ground state of the Kondo-lattice model with one conduction electron is analyzed. A rigorous proof is given that this system forms an incomplete ferromagnetic order with $S_{\rm tot}=(N-1)/2$ for antiferromagnetic exchange coupling. The wave function of the ground state is derived and some of its properties are discussed.

PACS numbers: 75.30.Mb

In recent years the Kondo-lattice model has attracted much interest as a model to describe the so-called heavy-fermion systems and also as one of the typical models of strongly correlated electron systems [1]. This model consists of a lattice of N localized spins ($S_i=\frac{1}{2}$) interacting with extended electron states in a single conduction band (with second quantization operators $c_{is}^{\dagger}$ and c_{is}). In its simplest version the Hamiltonian is given by

$$\mathcal{H}=-t\sum_{i,j}\sum_{s}c_{is}^{\dagger}c_{js}-\tfrac{1}{2}J\sum_{i}[S_i^z(c_{i\uparrow}^{\dagger}c_{i\uparrow}-c_{i\downarrow}^{\dagger}c_{i\downarrow}) +S_i^{+}c_{i\downarrow}^{\dagger}c_{i\uparrow}+S_i^{-}c_{i\uparrow}^{\dagger}c_{i\downarrow}]. \quad (1)$$

The first term denotes the hopping of the conduction electrons between nearest-neighbor sites with a hopping matrix element $-t$. The interaction between electrons and localized spins is given by the second term as an exchange coupling ($J<0$ for antiferromagnetic and $J>0$ for ferromagnetic coupling). This model is based on the more fundamental periodic Anderson model and can be derived from its strong-coupling limit [2].

Much effort has been invested to study this model. Various approaches, like the $1/N_f$ expansion [3] or the Gutzwiller variational method [4], have led to a good understanding of the formation of a coherent electron band with a heavy mass. Concerning, however, magnetic properties or the microscopic mechanism for unconventional superconductivity found in some heavy-fermion compounds, these descriptions are still rather poor and rigorous results obtained so far are rare. Very recently, several groups studied the finite-size 1D system with numerical methods such as the quantum Monte Carlo method (for a half-filled conduction band) [5] or Lanczos' exact diagonalization method (for various electron concentrations) [6]. In these studies it was found that for the half-filled band the ground state is antiferromagnetic, a total spin singlet. However, lowering the number of electrons, the system develops a ferromagnetic correlation at very low concentrations [6]. In this Letter we shall consider the limit of low electron concentration. By concentrating on the special case of just one conduction electron we will derive some rigorous results for the system with antiferromagnetic coupling ($J<0$).

To find the ground state of the one-electron system we start from a simplified Hamiltonian whose transversal exchange coupling is omitted, keeping only Ising-like coupling. Obviously, the ground state of this system has the energy $E=\varepsilon(\mathbf{k}=0)-|J|/4$, where $\varepsilon(\mathbf{k})=-t\sum_{\mathbf{a}}\exp(i\mathbf{k}\cdot\mathbf{a})$ with the sum over all nearest-neighbor vectors $\mathbf{a}$ and $\varepsilon(0)=-zt$ (z is the lattice coordination number). This state corresponds to a complete alignment of all localized spins and an electron described by a plane-wave state. In this way no scattering occurs for the electron and a maximal gain of kinetic energy is possible. The electron spin is parallel to the localized spins for $J>0$ [$S_{\rm tot}^z=(N+1)/2$] and antiparallel for $J<0$ [$S_{\rm tot}^z=(N-1)/2$].

We now include the transversal part of the exchange interaction (spin flip). No modification of the ground state happens for the case $J>0$, since it has maximal $S_{\rm tot}$, so that the transverse coupling is ineffective. Therefore, let us further concentrate on the more interesting case $J<0$ whose state including spin-flip processes can be written as

$$|\Psi\rangle=\sum_{i=1}^{N}\left[\Gamma^i c_{i\downarrow}^{\dagger}+\sum_{j=1}^{N}\Gamma_j^i c_{i\uparrow}^{\dagger}S_j^{-}\right]|\mathrm{FM}\rangle, \quad (2)$$

where $|\mathrm{FM}\rangle$ denotes the electron vacuum and the aligned localized spins, all spins up. This state has the spin quantum numbers $S_{\rm tot}=S_{\rm tot}^z=(N-1)/2$ in the case $\Gamma^i+\sum_j\Gamma_j^i=0$ for all i. The Schrödinger equations for the coefficients Γ^i and Γ_j^i are

$$\begin{aligned}&-t\sum_a\Gamma^{i+a}+\tfrac{1}{4}J\Gamma^i-\tfrac{1}{2}J\Gamma_i^i=E\Gamma^i,\\ &-t\sum_a\Gamma_j^{i+a}-\tfrac{1}{2}J\Gamma^i\delta_{ij}+\tfrac{1}{4}J\Gamma_j^i(2\delta_{ij}-1)=E\Gamma_j^i.\end{aligned} \quad (3)$$

These equations are easily solved by Fourier transformation, leading to the eigenvalue equation

$$\varepsilon(\mathbf{k})+\frac{J}{4}+\left(\frac{J}{2}\right)^2\frac{F(E)}{1-(J/2)F(E)}=E, \quad (4)$$

where

$$F(E)=\frac{1}{N}\sum_{\mathbf{q}}\frac{1}{E+J/4-\varepsilon(\mathbf{q})}. \quad (5)$$

The form of the wave function is given by

$$\tilde{\Gamma}^{\mathbf{k}}=\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}\Gamma^{i}e^{-i\mathbf{k}\cdot\mathbf{r}_i},$$
$$\tilde{\Gamma}^{\mathbf{k}}_{\mathbf{q}}=\frac{1}{N}\sum_{i,j}\Gamma^{i}_{j}e^{-i\mathbf{k}\cdot\mathbf{r}_i}e^{-i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)}=-\frac{1}{\sqrt{N}}\tilde{\Gamma}^{\mathbf{k}}\frac{E+J/4-\varepsilon(\mathbf{k})}{E+J/4-\varepsilon(\mathbf{k}+\mathbf{q})}, \tag{6}$$

and the normalization condition $N(|\tilde{\Gamma}^{\mathbf{k}}|^2+\sum_{\mathbf{q}}|\tilde{\Gamma}^{\mathbf{k}}_{\mathbf{q}}|^2)=1$. Note that the state with the lowest energy has the momentum $\mathbf{k}=0$.

Before considering properties of this state we give here a rigorous proof that this state found is the ground state.

Theorem.—The ground state of the Kondo-lattice model with one conduction electron has the total spin quantum number $S_{\mathrm{tot}}=(N-1)/2$ and is unique apart from the $(2S_{\mathrm{tot}}+1)$-fold spin degeneracy, if the hopping matrix element $(-t)$ is negative and the exchange-coupling constant is negative (antiferromagnetic coupling).

Proof.—We use the following site representation for the basis states in the Hilbert space:

$$|js;s_1,\ldots,s_N\rangle=sc^{\dagger}_{js}|\text{electron vacuum}\rangle\otimes|s_1,\ldots,s_N\rangle \tag{7}$$

($|s_1,\ldots,s_N\rangle$ is the localized spin configuration), where we introduce the phase convention that a negative sign is attached to wave functions with a spin-down electron ($s,s_n=\pm1$ and $\hat{S}^z_n|js;s_1,\ldots,s_N\rangle=\frac{1}{2}s_n|js;s_1,\ldots,s_N\rangle$). The Schrödinger equation in this representation has the form

$$\mathcal{H}|js;s_1,\ldots,s_N\rangle=-t\sum_{i,j}|is;s_1,\ldots,s_N\rangle-\tfrac{1}{4}Jss_j|js;s_1,\ldots,s_N\rangle$$
$$+\tfrac{1}{4}J(1-ss_j)|j-s;s_1,\ldots,s_{j-1},-s_j,s_{j+1},\ldots,s_N\rangle. \tag{8}$$

It is essential for this proof that none of the off-diagonal elements of the Hamiltonian matrix is positive for $J<0$ and $-t<0$.

The Kondo-lattice model has the full rotational symmetry in the spin space, so that the total spin S_{tot} as well as its z component S^z_{tot} are good quantum numbers. It is easily seen that in the given basis the Hamiltonian is decoupled into $N+2$ subspaces labeled by $S^z_{\mathrm{tot}}=M$, since all basis states are eigenstates of $\hat{S}^z_{\mathrm{tot}}$. Furthermore, for finite J inside these M subspaces, no additional decoupling occurs; i.e., for two arbitrary basis states α and β with the same S^z_{tot} there always exists an integer n with $\langle\alpha|\mathcal{H}^n|\beta\rangle\neq0$. Because each M subspace is connected and all off-diagonal matrix elements of the Hamiltonian are not positive, the Perron-Frobenius theorem states that the lowest eigenvalue is unique and all components of its eigenvector have the same sign, say positive. Therefore the ground state $|\psi_g(M)\rangle$ in each subspace is nondegenerate and has a positive wave function.

The next step is to show that this eigenstate has the total spin $S_{\mathrm{tot}}=\frac{1}{2}(N-1)$. Since this eigenstate is nondegenerate in the M subspace, it also must be an eigenstate of the Casimir operator $\hat{S}^2_{\mathrm{tot}}$. Therefore it is enough to construct a state $|\phi\rangle$, with $S_{\mathrm{tot}}=\frac{1}{2}(N-1)$, $S^z_{\mathrm{tot}}=M$ such that $\langle\phi|\psi_g(M)\rangle\neq0$, because states with different S_{tot} are orthogonal to each other [7]. For this construction we start with a state in the subspace $S^z_{\mathrm{tot}}=\frac{1}{2}(N-1)$ which has the electron localized at the site j forming a spin singlet with one of the localized spins, say S_1:

$$|\phi(\tfrac{1}{2}(N-1))\rangle=|j,+1;-1,+1,+1,\ldots,+1\rangle+|j,-1;+1,+1,+1,\ldots,+1\rangle. \tag{9}$$

Note that the relative plus sign in this singlet combination results from our phase convention for the basis states. Obviously, this is a state with $S_{\mathrm{tot}}=\frac{1}{2}(N-1)$. By the application of the total spin lowering operator S^-_{tot} we change S^z_{tot}, but keep S_{tot} fixed. Thus, a state with $S^z_{\mathrm{tot}}=M$ is obtained by

$$|\phi(M)\rangle=(S^-_{\mathrm{tot}})^{(N-1)/2-M}|\phi(\tfrac{1}{2}(N-1))\rangle. \tag{10}$$

Because the electron spin and the localized spin at the site 1 are coupled to a singlet $|\phi(M)\rangle$ is given by

$$|\phi(M)\rangle=(c^{\dagger}_{j\downarrow}c_{j\uparrow}+S_1^-+S_2^-+\cdots+S_N^-)^{(N-1)/2-M}|\phi(\tfrac{1}{2}(N-1))\rangle$$
$$=(S_2^-+\cdots+S_N^-)^{(N-1)/2-M}|\phi(\tfrac{1}{2}(N-1))\rangle$$
$$=[\tfrac{1}{2}(N+1)-M]!\sum_{s_2,\ldots,s_N}{}'[|j,+1;-1,s_2,\ldots,s_N\rangle+|j,-1;+1,s_2,\ldots,s_N\rangle], \tag{11}$$

where $\sum'$ denotes the summation under the constraint $s_2+\cdots+s_N=2M$. Obviously, $|\phi(M)\rangle$ is a non-negative vector in our basis. Consequently, $\langle\phi(M)|\psi_g(M)\rangle\neq0$, since $|\psi_g(M)\rangle$ has only positive components. Thus, the theorem is proved. It is clear that in the complete Hilbert space the ground state has the spin degeneracy $2S_{\mathrm{tot}}+1=N$.

This theorem holds for all dimensions if $J<0$ is finite. Furthermore, it is valid also if the electron hopping goes beyond nearest-neighbor hopping, as long as all matrix elements are negative. Even if some hopping matrix elements are positive, the theorem is still valid if they can be transformed into negative ones by assigning appropriate phase factors to the basis functions. The proof is not based on the translational symmetry of the system. Therefore, it is also true for systems which have a certain disorder: The hopping matrix elements may depend on the position as long as they are negative. In the same way J may be site dependent, but must always be negative. Even long-range exchange interaction J_{ij} between the localized spin at the site i and the electron at the site j does not affect the theorem.

A remark is necessary here for the case $J=-\infty$ with the translational-symmetric Kondo lattice. For this extreme exchange coupling the electron forms a complete singlet with the localized spin at the site it is occupying. As shown in Ref. [8] this system can be mapped to one which obeys the Nagaoka theorem [9]. Therefore, in a strict sense the theorem is only valid in the two- and three-dimensional lattices. However, in the case of a 1D system the ground states with different $S_{\rm tot}$ are degenerate.

Since we have derived one of the N degenerate ground-state wave functions, we can discuss here some of its properties. One important point is the coherence among the localized spins given by

$$\delta K_{SS}(\mathbf{r}_i-\mathbf{r}_j)=\langle\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j\rangle-\langle\mathbf{S}_i\rangle\cdot\langle\mathbf{S}_j\rangle$$
$$=\sum_{\mathbf{q}}|\tilde{\Gamma}^0_{\mathbf{q}}|^2\cos[\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)]\,, \qquad (12)$$

where $\langle S_i^x\rangle=\langle S_i^y\rangle=0$ and $\langle S_i^z\rangle=\frac{1}{2}-(1/N)\sum_{\mathbf{q}}|\Gamma^0_{\mathbf{q}}|^2$. In the limit $|J|\ll zt$ the long-range behavior of $\delta K_{SS}(\mathbf{r})$ is essentially exponential as obtained by approximating the energy $E\approx\varepsilon(0)+J/4$. For $|\mathbf{r}|$ much larger than the lattice spacing Eq. (12) can be replaced by an integral (3D),

$$\delta K_{SS}(\mathbf{r})=|\tilde{\Gamma}^0|^2\left(\frac{J}{2}\right)^2\frac{1}{(2\pi)^3}\int d^3q\frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{(tq^2-J/2)^2}$$
$$=|\tilde{\Gamma}^0|^2\left(\frac{J}{2t}\right)^{3/2}\frac{1}{8\pi}e^{-r/\xi}\,, \qquad (13)$$

with the coherence length $\xi=\sqrt{2t/|J|}$. As $|J|$ increases the coherence length decreases. Thus, turning to large $|J|$ ($\gg zt$), the lattice spacing becomes a natural cutoff for the coherence and the correlation function tends to the form

$$\delta K_{SS}(\mathbf{r})=|\tilde{\Gamma}^0|^2\frac{1}{N}\sum_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{r}}\,, \qquad (14)$$

where we used that $E\approx 3J/4$ for $J\to-\infty$. This sum is the lattice δ function, so that there is no correlation for finite $\mathbf{r}$.

The electron moving in the lattice of localized spins is a magnetic polaron, accompanied by a spin-polarization cloud. This cloud is described by the correlation function between electron and localized spins:

$$K_{eS}(\mathbf{r}_i-\mathbf{r}_j)=N\langle\hat{\mathbf{S}}_{ei}\cdot\hat{\mathbf{S}}_j\rangle$$
$$=\frac{1}{4}-\frac{N}{2}\left|\tilde{\Gamma}^0-\frac{1}{\sqrt{N}}\sum_{\mathbf{q}}\tilde{\Gamma}^0_{\mathbf{q}}e^{i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)}\right|^2, \qquad (15)$$

where for simplicity the constant $\langle\hat{\mathbf{S}}_{ei}\rangle\cdot\langle\hat{\mathbf{S}}_j\rangle$ is not subtracted. For small $|J|$ the $K_{eS}(\mathbf{r})$ is obtained in a similar way as $\delta K_{SS}(\mathbf{r})$,

$$K_{eS}(r)=\frac{1}{4}-\frac{N}{2}|\tilde{\Gamma}^0|^2\left(1+\frac{1}{4\pi\xi^2}\frac{e^{-r/\xi}}{r}\right)^2, \qquad (16)$$

where the coherence length is the same as in $K_{SS}(r)$ [Eq. (13)]. Thus ξ is also the length scale of the extension of the spin-polarization cloud. For large $|J|$ this extension also shrinks down to on-site correlation only, for $J\to-\infty$.

This can be illustrated also by considering the on-site correlation $K_{eS}(\mathbf{r}=0)$ as a combination of a spin-singlet and a spin-triplet configuration: $K_{eS}(\mathbf{r}=0)=(-3|\psi_s|^2+|\psi_t|^2)/4$ with $|\psi_s|^2+|\psi_t|^2=1$. For very small $|J|$ the distribution is $|\psi_s|^2=|\psi_t|^2=\frac{1}{2}$ (note that the symmetry of the system is broken for every finite J). With increasing $|J|$ the weight shifts towards the singlet configuration in order to gain exchange energy, leading finally to $|\psi_s|^2=1$ at $J=-\infty$ (Fig. 1). In the case that the on-site coupling is completely singlet there is no correlation with neighboring sites and the spin-polarization cloud has no extension.

Carrying a spin cloud the electron must have an enhanced effective mass compared with the bare electron mass. This mass m^* characterizes the charge excitation of the system whose spectrum is given by the $\mathbf{k}$-dependent energy $E_{\mathbf{k}}$ defined by the eigenvalue equation, Eq. (4). Considering a simple cubic lattice the effective mass is

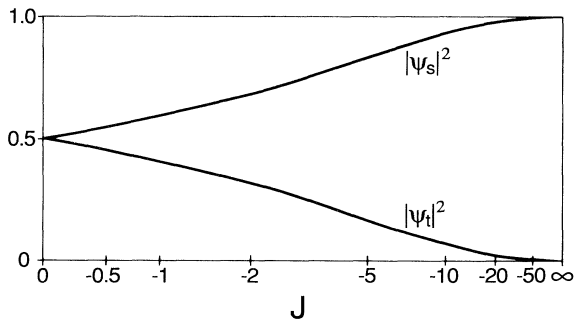

FIG. 1. On-site electron-spin–localized-spin correlation subdivided in singlet ($|\psi_s|^2$) and triplet ($|\psi_t|^2$) contributions for a 3D system. The nonlinear scale of J corresponds to $J/(-zt/2+J)$.

given by

$$\frac{m^*}{m_0}=\frac{1}{m}\left(\frac{\partial^2 E_{\mathbf{k}}}{\partial k_i^2}\right)^{-1}=1-\frac{J^2}{2}\frac{F'(E_0)}{[1-(J/2)F(E_0)]^2}, \tag{17}$$

where $\varepsilon(\mathbf{k})$ is taken as $\mathbf{k}^2/2m_0$ for small $\mathbf{k}$. This mass ratio changes continuously from 1 at $J=0$ to 2 at $J=-\infty$. This latter ratio 2 is due to the fact that the electron is combined into an on-site singlet with the localized spin. The overlap integral between two neighboring singlets renormalizes the effective hopping term by just a factor of $\frac{1}{2}$.

We have demonstrated that the one-electron Kondo-lattice system with antiferromagnetic coupling has a ground state which is incompletely ferromagnetic. Obviously, in the case of ferromagnetic coupling the complete ferromagnetic state has the lowest energy. These results may have importance for the future study of the Kondo-lattice problem as a well understood limit of this model. The exact solution for the ground state also represents a rigorous description of a magnetic polaron in a system without exchange coupling between the localized spins.

As we indicated above there exists a certain relationship with the system analyzed by Nagaoka (for $J=-\infty$ even the two systems are completely equivalent) [9]. In the one-hole Hubbard model the Nagaoka theorem is rigorously applicable only in the limit of infinite on-site correlation. On the other hand, the results discussed here are valid for the whole range of the exchange-coupling constant J in the one-electron Kondo-lattice system. They also cover realistic values of J in all dimensions and, therefore, we may expect that this type of ferromagnetism could be realized in some rare-earth compounds.

This work is supported by a Grant-in-Aid for Scientific Research from the Ministry of Education, Science and Culture of Japan.

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