Spin-reflection positivity of the Kondo lattice at half-filling

1,2Takashi Yanagisawa and 1Yukihiro Shimoi

1Fundamental Physics Section, Electrotechnical Laboratory
1-1-4, Umezono, Tsukuba, Ibaraki 305, Japan

2Max Planck Institute for Physics of Complex Systems
Bayreuther Str.40, Haus 16, 01187 Dresden, Germany

Abstract

We examine the spin-reflection positivity of the ground state of the Kondo lattice model at half-filling with the antiferromagnetic and ferromagnetic exchange couplings $J \neq 0$. For every positive $U > 0$, where $U$ is the Coulomb interaction between the conduction electrons, we can show that the ground state is unique.

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I. INTRODUCTION

Strongly-correlated electrons have been studied with considerable effort. Their complete understanding is now still difficult. Among the various models the Kondo lattice model is important as a fundamental model for heavy-fermion systems which are typical strongly-correlated-electron systems. In strongly-correlated electrons, rigorous results are still rare although they will provide us valuable information as benchmarks. Recently, exact results were obtained in some limiting cases for the Kondo lattice. \cite{1,2} Recently, an idea of the spin-reflection positivity was introduced, proving its validity for the strongly-correlated electrons at half-filling. \cite{4,5} This idea was first successfully applied to the Hubbard model for $U > 0$ at half-filling and $U < 0$ at every filling. \cite{5} Later it was shown that this method is valid for the symmetric-periodic Anderson model. \cite{6} The purpose of this paper is to investigate the spin-reflection positivity for the Kondo lattice following the method in Ref. \cite{7}. We show that the ground state of the Kondo lattice ($J \neq 0$) has the property of spin-reflection positivity at half-filling for $U > 0$ where $U$ is the Coulomb interaction between the conduction electrons. In our method, the Coulomb interactions between the conduction electrons are crucial in deriving an energy inequality such as $E(C) \geq E(P)$ where $C$ is a coefficient matrix of the eigenstates of Hamiltonian and $P$ is a semipositive definite matrix defined by $P = (C^\dagger C)^{1/2}$. As we have pointed out first in Ref. \cite{7}, we can apply the Schwarz inequality by using fermions in dealing with the local-spin operators, where we investigated $J < 0$ and $U > |J|/4$. In this paper we discuss this method in more details and show that it is straightforward to generalize our method for any non-zero $J$ and $U > 0$. 

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II. THE SPIN-REFLECTION PROPERTY OF THE KONDO LATTICE

A. Antiferromagnetic Kondo lattice

Let us consider the Kondo lattice model given as

\[
H = - \sum_{\sigma, \langle i,j \rangle} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} - \frac{U}{2} \sum_{i\sigma} n_{ci\sigma} + U \sum_{i} n_{ci\uparrow} n_{ci\downarrow} + J \sum_{i} \sigma_i \cdot S_i, \tag{1}
\]

where \(\sigma_i\) and \(S_i\) denote spin operators of the conduction electrons and the localized spins, respectively. \(c_{i\sigma}(c_{i\sigma}^\dagger)\) denote annihilation (creation) operators of the conduction electrons and we write \(n_{ci\sigma} = c_{i\sigma}^\dagger c_{i\sigma}\). The second term indicates the chemical potential so that we consider the half-filling case. What we will consider is the following statement.

**Proposition A** We assume that the lattice is bipartite. \(\langle i,j \rangle\) in eq.(1) denotes a pair of sites where one is on the sublattice A and the other is on the B sublattice. The number of the lattice is finite and the lattice is connected which means that there is a connected path of bonds between every pair of sites. Then the ground state of the Kondo lattice in eq.(1) for the antiferromagnetic-coupling \(J > 0\) and \(U > 0\) at half-filling is unique.

**Remarks** We show several remarks before going into a proof. We have introduced the Coulomb interaction \(U\) on each site to show a uniqueness of the ground state. We write the Kondo lattice model in the following form,

\[
H = - \sum_{\langle i,j \rangle\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \frac{1}{2} J_{\perp} \left( c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger f_{i\uparrow}^\dagger f_{i\uparrow} + c_{i\downarrow}^\dagger c_{i\uparrow}^\dagger f_{i\downarrow}^\dagger f_{i\downarrow} \right) + \frac{1}{4} J_z (n_{ci\uparrow} - n_{ci\downarrow})(n_{fi\uparrow} - n_{fi\downarrow}) + U \sum_{i} n_{ci\uparrow} n_{ci\downarrow} - \frac{U}{2} \sum_{\sigma} n_{ci\sigma}, \tag{2}
\]

where \(f_{i\sigma}(f_{i\sigma}^\dagger)\) denote annihilation (creation) operators of localized spins. \(n_{ci\sigma}\) and \(n_{fi\sigma}\) indicate the number operators of the conduction electrons and the localized spins, respectively. We should work in the subspace where the condition \(n_{fi\uparrow} + n_{fi\downarrow} = 1\) holds. In Ref. [7] we introduced the Lagrange multipliers in the Hamiltonian. Of course, we do not necessarily need to introduce the Lagrange multiplier to restrict the Hilbert space. This is only a matter of taste. We have written the perpendicular- and z-component of exchange interaction as
$J_\perp$ and $J_z$, respectively. Let us assume that $J = J_\perp = J_z$. We make the electron-hole transformation for the up spins: $c_{i\uparrow} \rightarrow c_{i\uparrow}^\dagger$, $c_{i\uparrow}^\dagger \rightarrow c_{i\uparrow}$ for $i \in A$, $f_{i\uparrow} \rightarrow -f_{i\uparrow}^\dagger$, $f_{i\uparrow}^\dagger \rightarrow f_{i\uparrow}$ for $i \in A$ and $c_{i\uparrow} \rightarrow -c_{i\uparrow}^\dagger$, $c_{i\uparrow}^\dagger \rightarrow -c_{i\uparrow}$ for $i \in B$, $f_{i\uparrow} \rightarrow f_{i\uparrow}^\dagger$, $f_{i\uparrow}^\dagger \rightarrow f_{i\uparrow}$ for $i \in B$ where we have assumed that the lattice is bipartite-divided into two disjoint sets $A$ and $B$. The spin-down electrons are unaltered, $c_{i\downarrow} \rightarrow c_{i\downarrow}$ and $f_{i\downarrow} \rightarrow f_{i\downarrow}$. In this transformation the $z$-component of the total spin is invariant at half-filling: $S_z = 0 \rightarrow S_z = 0$. Then $H$ is transformed into

$$\tilde{H} = - \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} - U \sum_i n_{ci\uparrow} n_{ci\downarrow} + \frac{U}{2} \sum_{i\sigma} n_{ci\sigma} + \frac{1}{2} \sum_i \left[ -\frac{1}{2} J_\perp (c_{i\downarrow} f_{i\uparrow}^\dagger f_{i\uparrow} + c_{i\uparrow}^\dagger f_{i\uparrow} f_{i\downarrow}^\dagger) + \frac{1}{4} J_z (1 - n_{ci\uparrow} - n_{ci\downarrow})(1 - n_{fi\uparrow} - n_{fi\downarrow}) \right]. \quad (3)$$

We work in the $S_z = 0$ subspace since $S_z$ and $S_z$ are conserved and every energy eigenvalue has a corresponding eigenfunction in this subspace. For $\tilde{H}$ the constraint should read $n_{fi\uparrow} = n_{fi\downarrow}$. Here let us comment on this constraint. We set $Q_i \equiv n_{fi\uparrow} - n_{fi\downarrow}$. It is easy to see that $Q_i$ commutes with $\tilde{H}$ and $Q_j$ (for any $j$):

$$[Q_i, \tilde{H}] = 0; [Q_i, Q_j] = 0 (\forall i, j). \quad (4)$$

Therefore the total space is divided into disjoint subspaces which are specified by eigenvalues of $Q_i$. The physical space is given by $S_0 = \{ \psi(\neq 0)|Q_i \psi = 0 (\forall i) \}$. In this subspace, the wave function satisfies

$$\tilde{H}\psi = E\psi, \quad (5)$$

$$Q_i \psi = 0 (\forall i), \quad (6)$$

which are basic equations in our discussion.

**Proof** There are two kinds of electrons with spin up and spin down. Let $\psi_\alpha^\sigma$ be an orthonormal basis set which is composed solely of spin-$\sigma$ $c$ and $f$ electrons. We assume that basis states are real. We follow the method of Ref. [5] and the ground-state wave function in the space $S_z = 0$ is written as $\psi = \sum_{\alpha\beta} C_{\alpha\beta} \psi_\alpha^\uparrow \otimes \psi_\beta^\downarrow$. $C = (C_{\alpha\beta})$ is called the coefficient matrix of $\psi$. Now the expectation value of $\tilde{H}$ is given by:
\[ F = \text{Tr}(C^\dagger H_0^c C + C H_0^c C^\dagger) - J_\perp \sum_i \frac{1}{2} \text{Tr}(M_{f^i}^\dagger C M_{c^i}^\dagger C^\dagger + M_{f^i}^\dagger C M_{c^i}^\dagger C) \]
\[ + \frac{1}{4} \sum_i \left[ \frac{1}{4} \text{Tr}(C^{\dagger} N_{c^i}^{f^i} C + C N_{c^i}^{f^i} C^{\dagger}) \right] - \frac{1}{4} \text{Tr}(C^{\dagger} N_{c^i}^{f^i} C + C^{\dagger} N_{c^i}^{f^i} C) \]
\[ + \frac{1}{4} \text{Tr}(N_{c^i}^{f^i} C^{\dagger} N_{c^i}^{f^i} C + N_{f^i}^{f^i} C N_{c^i}^{f^i} C^{\dagger}) \]
\[ - U \sum_i \text{Tr}(N_{c^i}^{f^i} C N_{c^i}^{f^i} C^{\dagger}) + \frac{U}{2} \sum_i \text{Tr}(C^{\dagger} N_{c^i}^{f^i} C + C N_{c^i}^{f^i} C^{\dagger}). \] (7)

The matrices are defined by the following,

\[ (H_0^c)_{\alpha\alpha'} = <\psi^{\sigma}_{\alpha}| - \sum_{<i,j>} t_{ij} c_{i\sigma} c_{j\sigma}|\psi^{\sigma}_{\alpha'}>, \] (8a)

\[ (M_{f^i}^c)_{\alpha\alpha'} = <\psi^{\sigma}_{\alpha}| f_{i\sigma} c_{i\sigma}|\psi^{\sigma}_{\alpha'}>, \] (8b)

\[ (M_{c^i}^f)_{\alpha\alpha'} = <\psi^{\sigma}_{\alpha}| f_{i\sigma} c_{i\sigma}|\psi^{\sigma}_{\alpha'}>, \] (8c)

\[ (N_{c^i}^{f^i})_{\alpha\alpha'} = <\psi^{\sigma}_{\alpha}| n_{c\sigma} n_{f\sigma}|\psi^{\sigma}_{\alpha'}>, \] (8d)

\[ (N_{c^i}^{c^i})_{\alpha\alpha'} = <\psi^{\sigma}_{\alpha}| n_{c\sigma}|\psi^{\sigma}_{\alpha'}>, \] (8e)

\[ (N_{f^i}^{f^i})_{\alpha\alpha'} = <\psi^{\sigma}_{\alpha}| n_{f\sigma}|\psi^{\sigma}_{\alpha'}>. \] (8f)

Please note that these matrices are real ones. From the definition, \((N_{c^i}^{f^i})_{\alpha\alpha'} = \sum_\beta <\psi^{\sigma}_{\alpha}| n_{c\sigma}|\psi^{\sigma}_{\beta} <\psi^{\sigma}_{\beta}| n_{f\sigma}|\psi^{\sigma}_{\alpha} > = (N_{c^i}^{c^i})_{\alpha\alpha'}\). We have the up-down symmetry: \(N_{c^i}^{f^i} = N_{c^i}^{c^i}\), \(N_{f^i}^{f^i} = N_{f^i}^{c^i}\), \(H_0^c = H_0^{c^i}\) and \(M_{c^i}^{f^i} = M_{f^i}^{c^i}\). Variation of the functional \(F\) with respect to \(C\) leads to the following equation,

\[ EC = CH_0^c + H_0^c C - J_\perp \sum_i \frac{1}{2} (M_{f^i}^c C M_{c^i}^c + M_{f^i}^c C M_{f^i}^c C^\dagger) + J_z \sum_i \frac{1}{4} (N_{c^i}^c C + C N_{c^i}^c) \]
\[ - \frac{1}{4} (C N_{c^i}^f + N_{f^i}^f C) - \frac{1}{4} (C N_{c^i}^c + N_{c^i}^f C) + \frac{1}{4} (N_{c^i}^c C N_{c^i}^f + N_{f^i}^f C N_{c^i}^c) \]
\[ - U \sum_i N_{c^i}^c C N_{c^i}^c + \frac{U}{2} \sum_i (C N_{c^i}^c + N_{c^i}^c C). \] (9)

From the constraint equations \(Q_i \psi = 0\), \(C\) must satisfy
We can easily show that this equation is equivalent to the constraint, \( n_{fi^\uparrow} = n_{fi^\downarrow} \) which indicates that we have no singly-occupied f-electron sites. From the equation in eq.(10), we obtain \( <n_{fi^\uparrow}(1-n_{fi^\downarrow})> = TrC^\dagger N_{fi^\downarrow}^\dagger (1-N_{fi^\downarrow}) = TrC^\dagger N_{fi^\downarrow}^\dagger (1-N_{fi^\downarrow})C = 0 \) because \( N_{fi^\downarrow}^\dagger \) is a diagonal matrix diag\( (\sigma_1, \sigma_2, \cdots) \) where the diagonal elements are 0 or 1: \( \sigma_i = 0 \) or 1. Inversely, we set that \( <n_{fi^\uparrow}(1-n_{fi^\downarrow})> = 0 \). Then \( 0 = TrC^\dagger N_{fi^\downarrow}^\dagger C(1-N_{fi^\downarrow}) = TrC^\dagger(N_{fi^\downarrow}^\dagger)^2 C(1-N_{fi^\downarrow})^2 = Tr(1-N_{fi^\downarrow})C^\dagger N_{fi^\downarrow}^\dagger N_{fi^\downarrow}^\dagger C(1-N_{fi^\downarrow}) = ||N_{fi^\downarrow}^\dagger C(1-N_{fi^\downarrow})||^2 \), where the norm \( || \cdot || \) is defined by \( ||A||^2 = TrA^\dagger A \). This means that \( N_{fi^\downarrow}^\dagger C(1-N_{fi^\downarrow}) = 0 \). Similarly, we have \( (1-N_{fi^\downarrow}^\dagger)CN_{fi^\downarrow}^\dagger = 0 \). Hence eq.(10) is followed. More directly, we can show eq.(10) by calculating \( n_{fi^\uparrow} = \Sigma_{\alpha\beta} C_{\alpha\beta} \psi_{\alpha}^\dagger \psi_{\beta} = \Sigma_{\alpha\beta} \Sigma_{\alpha'\beta'} C_{\alpha\beta} |\psi_{\alpha'}| <\psi_{\alpha'}|n_{fi^\uparrow}|\psi_{\beta} = \Sigma_{\alpha\beta\alpha'} C_{\alpha\beta} \psi_{\alpha'}^\dagger \psi_{\alpha}\psi_{\beta} = \Sigma_{\alpha\beta\alpha'} C_{\alpha\beta} \psi_{\alpha'}^\dagger \psi_{\alpha}\psi_{\beta} = \Sigma_{\alpha\beta}(N_{fi^\dagger}^\dagger C)_{\alpha\beta} \psi_{\alpha} \psi_{\beta} \), where we denote the basis as \( \psi_{\alpha} = \psi_{\alpha}^\uparrow \otimes \psi_{\beta}^\downarrow \).

We can obtain similarly \( n_{fi^\downarrow} = \Sigma_{\alpha\beta}(CN_{fi^\uparrow}^\dagger)_{\alpha\beta} \psi_{\alpha} \psi_{\beta} \) and eq.(10) is also followed.

Then we can obtain the energy \( E(C) \) given by the right-hand side in eq.(7) with two equations (9) and (10). Now, the identity below is useful in the following discussion.

\[
J_z Tr(C^\dagger N_{ci^\dagger}^\dagger CN_{fi^\dagger}^\dagger + C^\dagger N_{fi^\dagger}^\dagger CN_{ci^\dagger}^\dagger) \\
= -J_z \frac{1}{z} TrC^\dagger (z N_{ci^\dagger}^\dagger - N_{fi^\dagger}^\dagger) C(z N_{ci^\dagger}^\dagger - N_{fi^\dagger}^\dagger) \\
+ z J_z TrC^\dagger N_{ci^\dagger}^\dagger CN_{fi^\dagger}^\dagger + \frac{1}{z} J_z TrC^\dagger N_{fi^\dagger}^\dagger CN_{ci^\dagger}^\dagger \\
= -J_z \frac{1}{z} TrC^\dagger (z N_{ci^\dagger}^\dagger - N_{fi^\dagger}^\dagger) C(z N_{ci^\dagger}^\dagger - N_{fi^\dagger}^\dagger) \\
+ z J_z TrC^\dagger N_{ci^\dagger}^\dagger CN_{fi^\dagger}^\dagger + \frac{1}{2z} J_z Tr(C^\dagger N_{fi^\dagger}^\dagger C + CN_{fi^\dagger}^\dagger C^\dagger), \tag{11}
\]

where \( z \) is a positive real number \( z > 0 \) and we have used the relation in eq.(10) to derive the second equality. Then the energy \( E(C) \) is written as

\[
E(C) = Tr(C^\dagger H_0^C + CH_0^C C^\dagger) + J_\perp \sum_i \frac{1}{2} Tr(M_{fi^\downarrow} C M_{fi^\uparrow} C^\dagger + M_{fi^\uparrow} C M_{fi^\downarrow} C^\dagger) \\
+ J_z \sum_i \frac{1}{4} Tr(C^\dagger N_{fi^\dagger}^\dagger C + CN_{fi^\dagger}^\dagger C^\dagger) - \frac{1}{4} Tr(CN_{fi^\dagger}^\dagger C^\dagger + C^\dagger N_{fi^\dagger}^\dagger C) - \frac{1}{4} Tr(CN_{ci^\dagger}^\dagger C^\dagger + C^\dagger N_{ci^\dagger}^\dagger C) \\
+ \sum_i \frac{-1}{4z J_z} TrC^\dagger (z N_{ci^\dagger}^\dagger - N_{fi^\dagger}^\dagger) C(z N_{ci^\dagger}^\dagger - N_{fi^\dagger}^\dagger)
\]
\[
+ \frac{1}{4} z |J_z| \text{Tr} C^\dagger N_{ei}^k C N_{ei}^l + \frac{1}{8z} |J_z| \text{Tr}(C^\dagger N_{f_i}^i C + C N_{f_i}^i C^\dagger) ,
- U \sum_i \text{Tr} C_i^\dagger N_{ei}^i C N_{ei}^l + \frac{U}{2} \sum_i \text{Tr}(C_i^\dagger N_{ei}^i C + C N_{ei}^i C^\dagger) .
\]

(12)

Since the energy \( E(C) \) is symmetric with respect to the spin, we can set that \( C \) is hermitian: \( C = C^\dagger \). It is also easy to see that \( C \) and \( C^\dagger \) satisfy the same Schrödinger equation. There is a hermitian positive semidefinite matrix \( P \) which satisfies \( CC^\dagger = P^2 \), where \( P \) is determined uniquely. \[9\] According to the Schwarz inequality for a square matrix \( M \),

\[
|\text{Tr} CM C^\dagger M^\dagger| \leq \text{Tr} P M P^\dagger,
\]

(13)

we obtain an inequality \( E(C) \geq E(P) \) for \( J > 0 \) and \( U > z |J_z|/4 \). Since \( z \) is an arbitrary positive real number, we can choose \( z \) so that \( U > z |J_z|/4 \) holds for any positive \( U \). Therefore we have \( E(C) \geq E(P) \) for every \( U > 0 \). Since we have assumed that \( C \) is the coefficient matrix of the ground state, we obtain \( E(C) = E(P) \). This indicates that there is a state with \( C = P \) or \( C = -P \) among the ground states. Here we will show that the new matrix \( P \) also satisfies the constraint \( n_{fi\uparrow} = n_{fi\downarrow} \), i.e. \( N_i P = P N_i \) where we set \( N_i \equiv N_{f_i}^\dagger = N_{f_i}^\downarrow \).

Due to the Schwarz inequality \( \text{Tr} CN_i C N_i \leq \text{Tr} P N_i P N_i \), we have \( 0 \leq \text{Tr} P N_i P(1 - N_i) = \text{Tr} P N_i P - \text{Tr} P N_i P N_i \leq \text{Tr} C N_i C - \text{Tr} C N_i C N_i = \text{Tr} C N_i C(1 - N_i) = 0 \).

Then \( \text{Tr} P N_i P(1 - N_i) = 0 \) is followed, which indicates that \( \text{Tr} P N_i P(1 - N_i) = \text{Tr} P N_i^2 P(1 - N_i)^2 = \text{Tr}(1 - N_i) P N_i N_i P(1 - N_i) = \| N_i P(1 - N_i) \|^2 = 0 \). Hence \( N_i P(1 - N_i) = 0 \), i.e. \( N_i P = N_i P N_i \) holds. Similarly we have \( P N_i = N_i P N_i \). Therefore we have obtained the constraint equation for \( P \) given by,

\[
N_{f_i}^\dagger P = P N_{f_i}^\dagger.
\]

(14)

This result shows that the equality \( E(C) = E(P) \) has its meaning.

Now we will show that the ground state is unique following the argument of Ref. \[4\].

The Schrödinger equation reads

\[
EC = C H_0^\dagger + H_0^\dagger C - J_z \sum_i \frac{1}{2} ( M_{fci}^\dagger C M_{cfi}^i + M_{cfi}^\dagger C M_{fci}^i ) + J_z \sum_i \frac{1}{4} ( N_{cfi}^\dagger C + N_{cfi}^i C )
\]

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\[ -\frac{1}{4}(CN_{fi}^2 + N_{fi}^2) - \frac{1}{4}(CN_{ci}^2 + N_{ci}^2) \]
\[ -\frac{1}{4z}|J_z| \sum_i (zN_{ci}^\dagger - N_{fi}^\dagger)C(zN_{ci}^\dagger - N_{fi}^\dagger) \]
\[ + \frac{1}{8z}|J_z| \sum_i (N_{ci}^\dagger C + CN_{fi}^\dagger) - (U - \frac{z}{4}|J_z|) \sum_i N_{ci}^\dagger C N_{ci}^\dagger + \frac{U}{2} \sum_i (CN_{ci}^\dagger + N_{ci}^\dagger C). \]  

(15)

Let \( R = P - C \); then \( R \) is positive semidefinite and satisfies eq.(14). Let us define \( K \) as a kernel of \( R \), i.e. \( K = \{ v|Rv = 0 \} \). \( C \) and \( P \) are diagonalized by a unitary matrix \( U \):
\( C = U^\dagger \text{diag}(\sigma_1, \ldots, \sigma_r)U \) and \( P = U^\dagger \text{diag}(||\sigma_1||, \ldots, ||\sigma_r||)U \) where \( \sigma_1, \ldots, \sigma_r \) are eigenvalues of \( C \). At least there is one positive \( \sigma_i \), such that \( \sigma_i = ||\sigma_i|| \); otherwise we have \( C = -P \). Thus \( R = P - C \) has at least one zero eigenvalue, which indicates that there is a vector \( v \) satisfying \( Rv = 0 \). Then we obtain:
\[ 0 = RH_0^i v - J_z \sum_i \frac{1}{2}(M_{fi}^\dagger RM_{fi}^\dagger + M_{ci}^\dagger RM_{ci}^\dagger) v + J_z \sum_i \frac{1}{4} R N_{ci}^\dagger N_{fi}^\dagger v \]
\[ - \frac{1}{4} R N_{fi}^\dagger v - \frac{1}{4} R N_{ci}^\dagger v - \frac{1}{4z}|J_z| \sum_i (zN_{ci}^\dagger - N_{fi}^\dagger)R(zN_{ci}^\dagger - N_{fi}^\dagger)v \]
\[ - (U - z|J_z|/4) \sum_i N_{ci}^\dagger R N_{fi}^\dagger v + \frac{1}{8z}|J_z| \sum_i R N_{fi}^\dagger v + \frac{U}{2} \sum_i R N_{ci}^\dagger v. \]  

(16)

Since \( v^\dagger R = 0 \), \( \sum_i [J_z v^\dagger(M_{fi}^\dagger RM_{fi}^\dagger + M_{ci}^\dagger RM_{ci}^\dagger)]v + (1/2z)J_z v^\dagger(zN_{ci}^\dagger - N_{fi}^\dagger)R(zN_{ci}^\dagger - N_{fi}^\dagger)v + 2(U - zJ_z/4)v^\dagger R N_{ci}^\dagger R N_{fi}^\dagger v = 0 \). holds. Because \( R \) is positive semidefinite and \( N_{ci}^\sigma = N_{ci}^{-\sigma} \), \( N_{fi}^\sigma = N_{fi}^{-\sigma} \) and \( M_{ci}^\sigma = M_{ci}^{-\sigma} \), we have \( v^\dagger M_{fi}^\dagger RM_{fi}^\dagger v = v^\dagger M_{fi}^\dagger RM_{fi}^\dagger v = v^\dagger N_{ci}^\dagger R N_{ci}^\dagger = v^\dagger N_{fi}^\dagger R N_{fi}^\dagger = 0 \) and then \( R M_{fi}^\dagger v = R N_{fi}^\dagger v = R N_{ci}^\dagger v = 0 \) is followed. If we substitute \( N_{fi}^\dagger v = 0 \) for v, we obtain \( R N_{ci}^\dagger N_{fi}^\dagger v = 0 \). As a result, \( RH_0v = 0 \) follows. Now, by successive application of \( H_0, M \) and \( N \), we can construct all the basis states by virtue of the connectivity. Thus, every vector is in \( K \). This proves the uniqueness of the lowest energy state for \( J > 0 \) and \( U > 0 \) because we can easily reach a contradiction if we assume that there are two ground states [3]. Since the energy-expectation value is continuous with respect to parameters involved in the Hamiltonian there is no level crossing with respect to \( J \).(q.e.d.)

In the large-\( U \) limit, \( H \) is mapped onto a spin-1/2 antiferromagnetic Heisenberg model. Then we can say that
Corollary: We assume the same conditions in the Proposition A. Then for the Kondo lattice with $J > 0$ and $U > 0$ at half-filling, the ground state has $S = 0$.

B. Ferromagnetic Kondo lattice

Let us turn to investigate the Kondo lattice model $H$ with the ferromagnetic coupling $J = J_\perp = J_z < 0$ for the half-filled band. We again assume that $\Lambda$ is bipartite and we make the electron-hole transformaton for the up spins: $c_{i \uparrow} \rightarrow c_{i \uparrow}^\dagger$, $c_{i \uparrow}^\dagger \rightarrow c_{i \uparrow}$ for $i \in A$, $f_{i \uparrow} \rightarrow f_{i \uparrow}^\dagger$, $f_{i \uparrow}^\dagger \rightarrow f_{i \uparrow}$ for $i \in A$ and $c_{i \uparrow} \rightarrow -c_{i \uparrow}^\dagger$, $c_{i \uparrow}^\dagger \rightarrow -c_{i \uparrow}$ for $i \in B$, $f_{i \uparrow} \rightarrow -f_{i \uparrow}^\dagger$, $f_{i \uparrow}^\dagger \rightarrow -f_{i \uparrow}$ for $i \in B$ where we have assumed that the lattice $\Lambda$ is bipartite-divided into two disjoint sets $A$ and $B$. Note that the signs in front of $f$-electron operators are different from those for the case $J > 0$.

The spin-down electrons are unaltered, $c_{i \downarrow} \rightarrow c_{i \downarrow}$ and $f_{i \downarrow} \rightarrow f_{i \downarrow}$. In this transformation the $z$-component of the total spin is invariant: $S_z = 0 \rightarrow S_z = 0$. Then $H$ is transformed into

$$
\tilde{H} = -\sum_{<i,j>} t_{ij} c_{i\sigma} c_{j\sigma} - U \sum_i n_{c_{i\uparrow}} n_{c_{i\downarrow}} + \frac{U}{2} \sum_{i\sigma} n_{c_{i\sigma}} + \frac{1}{2} J_\perp (c_{i\uparrow} c_{i\downarrow} f_{i\uparrow}^\dagger f_{i\downarrow}^\dagger + c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger f_{i\uparrow} f_{i\downarrow}^\dagger) + \frac{1}{4} J_z (1 - n_{c_{i\uparrow}} - n_{c_{i\downarrow}})(1 - n_{f_{i\uparrow}} - n_{f_{i\downarrow}}). \quad (17)
$$

Clearly we can apply the method in the previous section and then we obtain the inequality $E(C) \geq E(P)$ for $J < 0$ and $U > 0$. A similar identity to eq.(11) is easy to derive for $J < 0$:

$$
J_z Tr(C^\dagger N_{ci}^\dagger C N_{fi}^\dagger + C^\dagger N_{fi}^\dagger C N_{ci}^\dagger)
= -|J_z| \frac{1}{z} Tr C^\dagger (z N_{ci}^\dagger + N_{fi}^\dagger) C (z N_{ci}^\dagger + N_{fi}^\dagger) + \frac{1}{z} J_z Tr C^\dagger N_{ci}^\dagger C N_{fi}^\dagger. \quad (18)
$$

We can prove that $C = P$ (or $C = -P$) is a unique solution of $E(C) = E(P)$. Thus we have shown that the lowest-energy state is unique. Therefore

Proposition B: If we assume the same conditions mentioned in Proposition A for the Hamiltonian in eq.(17), then the ground state at half-filling is unique for $J < 0$ and $U > 0$.

Remarks: If we assume that the A and B sublattices have the same number of lattice sites, then the ground state of the Kondo lattice has $S = 0$ since in the large-$|J|$ limit, $H$
is mapped onto the spin-1 Heisenberg model. In general, we may be able to consider the lattices where the number of sites in the A sublattice $|A|$ is greater than that of the B sublattice $|B|$. In this case, the ground state may have a high spin $S = |A| - |B|$, which is proved by the Perron-Frobenius theorem. For example, the 1D odd-site model with the open boundary condition has $S = 1$ ground state, while if we impose the periodic boundary condition, the ground state has $S = 0$ for small clusters according to a diagonalization method.

### C. Spin-correlation functions

Our theorem for the Kondo lattice model may have many implications. Let us consider the spin-correlation functions given as $S_{fc}(i) \equiv \langle S_i^+ \sigma_i^- \rangle$, $S_{ff}(i,j) \equiv \langle S_i^+ S_j^- \rangle$ and $S_{cc}(i,j) \equiv \langle \sigma_i^+ \sigma_j^- \rangle$. The spin-reflection positivity implies that these correlation functions have definite signs for every $J (\neq 0)$. After making the electron-hole transformation for $J > 0$, $S_{fc}(i)$ is written as

$$S_{fc}(i) = -c_i^\dagger f^\dagger f_{i\uparrow} c_i^\dagger f_{i\downarrow} = -\text{Tr} C^\dagger M^\dagger C M_f^\dagger C \leq 0.$$  \hspace{1cm} (19)

In a similar manner, it is easy to obtain

$$S_{ff}(i,j) \leq 0; i \in A, j \in B,$$  \hspace{1cm} (20)

$$S_{cc}(i,j) \leq 0; i \in A, j \in B,$$  \hspace{1cm} (21)

$$S_{ff}(i,j) \geq 0; i \in A, j \in A,$$  \hspace{1cm} (22)

$$S_{cc}(i,j) \geq 0; i \in A, j \in A.$$  \hspace{1cm} (23)

Thus antiferromagnetic orderings are found for nearest-neighbor spins and for c and f electrons on each site. The RKKY interactions between localized spins are oscillating functions. Instead, for the ferromagnetic coupling $J < 0$, $S_{fc}(i)$ shows a ferromagnetic order.
\[ S_{fc}(i) = Tr C^\dagger M^\dagger_{cf} C M^\dagger_{fc} \geq 0. \] (24)

Note that we have chosen the different signs for f electrons in the electron-hole transformation for \( J < 0 \). \( S_{ff}(i, j) \) and \( S_{cc}(i, j) \) have same structures as the case for \( J > 0 \).
III. DISCUSSION

In this paper we have applied the method of spin-reflection positivity to the Kondo lattice model by writing the exchange interaction with fermion operators of localized electrons. We have shown that the Kondo lattice with the non-zero exchange couplings $J \neq 0$ and $U > 0$ at half-filling has a unique ground state and the total spin is 0 where we have assumed that the A and B sublattices have the same number of lattice sites. Our theory depends on the Schwarz inequality to derive the equation $E(C) = E(P)$ where $C$ is the coefficient matrix of the ground state and $P$ is the semipositive definite matrix given by $P = (C^\dagger C)^{1/2}$. It is important that the constraint equation $N_i C = CN_i$, which represents $n_{fi\uparrow} = n_{fi\downarrow}$, is conserved for $P$: $N_i P = P N_i$. This is a highly non-trivial result. Our results can be generalized to more general models where the number of the f-electron sites is less than that of the conduction electrons. For example, the two-impurity Kondo model has a unique ground state which is continuous with respect to $J > 0$ and $J < 0$ as far as $U > 0$. A characteristic structure of the two-impurity problem may be observed as a sharp crossover between the RKKY regime and the on-site Kondo regime. The spin-reflection positivity implies the antiferromagnetic orderings between the f and conduction electrons within each site as well as the nearest-neighbor antiferromagnetic RKKY interactions for $J > 0$. The RKKY interaction shows an oscillating behavior with a period which is precisely equal to the lattice constant($\times 2$) for the half-filled conduction band.

From a technical point of view, the fact that $Q_i$ commutes with Hamiltonian $\tilde{H}$ and $Q_j$ is important because an eigenfunction of $\tilde{H}$ is also an eigenfunction of $Q_i$. The total space is divided into disjoint subspaces according to eigenvalues of $Q_i$. Let us comment here about the Lagrange-multiplier method in Ref. [7]. We define $H_{\text{eff}} = \tilde{H} + \sum_i \lambda_i Q_i$. Then basic equations in each subspace are written as

$$H_{\text{eff}}\psi = E\psi,$$  \hspace{1cm} (25)$$

and
\[ Q_i \psi = q_i \psi (\forall i), \] (26)

where \( q_i \) takes 0, -1 and 1. The variational condition for \( F \equiv \langle H_{eff} \rangle = \langle \tilde{H} \rangle + \sum_i \lambda_i < Q_i \rangle \) reads \( \partial F/\partial \lambda_i = \langle \psi | Q_i | \psi \rangle = 0 \) which indicates \( q_i = 0 (\forall i) \). Therefore we obtain the same equations as eqs.(5) and (6). The conditions \( < Q_i > = 0 \) project out the physical subspace \( S_0 \). If we start from a state which does not belong to \( S_0 \), we cannot obtain a correct solution in a diagonalization since they have different (discrete) quantum numbers.
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[8] This is basically due to identities $2xy = -(x-y)^2 + x^2 + y^2$ or $2xy = (x+y)^2 - (x^2+y^2)$.

Then we shift $x$ to $xz (z > 0)$.

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