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Ferromagnetic ground state in the Kondo lattice model

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Abstract. We present a series of rigorous examples of the Kondo lattice model that exhibit full ferromagnetism in the ground state. The models are defined in one-, two- and three-dimensional lattices, and are characterized by a range of hopping terms, specific electron filling, and large ferromagnetic coupling. Our examples show that a sufficient strong but finite exchange coupling between conduction electrons and localized spins could overcome the competition from mobility of a finite density of electrons and drive the system from a paramagnetic phase to a ferromagnetic phase. We also establish a relation of ferromagnetism between the Hubbard model and Kondo lattice model. Meanwhile some rigorous results on ferromagnetism in the corresponding Hubbard model are presented.

PACS. 75.10.Lp Band and itinerant models – 75.50.-y Studies of specific magnetic materials

1 Introduction and the main result

The Kondo lattice model has been of considerable interest due to its relevance to magnetism in strongly correlated electron systems, such as transition metal oxides (See Ref. [1]). The model is defined on a discrete lattice $\wedge$ with $N_\wedge$ lattice sites. Except for itinerant electrons, every site is occupied by one localized spin $\mathbf{S}_i$ with spin S. The simplest version of the Hamiltonian is given by

$$\mathrm{H} = \sum_{ij} t_{ij} \mathrm{c}^\dagger_{i,\sigma} \mathrm{c}_{j,\sigma} - J \sum_{i\in\wedge} \mathbf{S}_i \cdot \mathbf{S}_{ic} \qquad (1)$$

where $\mathrm{c}^\dagger_{i,\sigma}$ and $\mathrm{c}_{i,\sigma}$ are the creation and annihilation operators of the conduction electron at site i with spin $\sigma(=\uparrow,\downarrow)$. $(\mathbf{S}_{ic})_\alpha = \sum_{\sigma,\sigma'} \mathrm{c}^\dagger_{i,\sigma}(\sigma_\alpha)_{\sigma\sigma'}\mathrm{c}_{i,\sigma'}/2$ where σ_α $(\alpha = x, y, z)$ are the Pauli matrices. In this paper, we restrict our discussion in the case of $J > 0$, *i.e.*, the ferromagnetic Hund coupling. The origin of the Hund coupling is the Coulomb interaction. The antiferromagnetic coupling $J < 0$ only appears in some restricted spaces, for example, the case of half filling of electrons.

One of the basic physical problems in this model is whether a paramagnetic phase could evolve to a fully saturated ferromagnetic phase when the exchange coupling between electrons and localized spins becomes much larger. In the strong Hund coupling limit $(J \to +\infty)$, the spin of conduction electron is parallel to the localized spin on the same site, and a conduction electron prefers to hop between two sites on which two localized spins are parallel to each other. The property favors to form a ferromagnetic state, and lead to the double exchange mechanism for ferromagnetism proposed by Zener [2] and subsequently studied extensively [3–6]. This picture was confirmed rigorously in a single-electron case and other limits by Kubo [7] and by Sigrist *et al.*[8]. However, the case of two electrons on a closed ring has a spin singlet ground state [7,9], and the case of a half filled band on a bipartite lattice has an anti-ferromagnetic or ferri-magnetic state instead of a ferromagnetic one [10]. For a finite density of electrons, the kinetic energy does not favor to form a ferromagnetic state rather than a paramagnetic one. Thus a physically interested problem is whether the strong exchange coupling could overcome the kinetic energy of a finite density of electrons to form a ferromagnetic state. As far as we know, there are no rigorous examples that the double exchange ferromagnetism exists in the case of a finite density of electrons, and finite exchange coupling. In this paper we present a series of rigorous examples which exhibit fully saturated ferromagnetism in the ground state.

In order to establish a rigorous result on ferromagnetism, we define the model on the lattices $\wedge$ as shown in Figure 1. The lattice sites are decomposed into two subsets: A and B. Each A site has n_a $(= 2, 3, 4, \cdots)$ nearest neighbor B sites, and each B site has $n_\mathrm{b} = 2$ nearest neighbor A sites so that each B site is located in the middle point of a bond between two A sites. The hopping terms are defined such that they can be rewritten in a compact form,

$$\mathrm{H} = \sum_{i\in\mathrm{A}} \mathrm{h}_{i0} - J \sum_{i\in\wedge} \mathbf{S}_i \cdot \mathbf{S}_{ic} \qquad (2)$$

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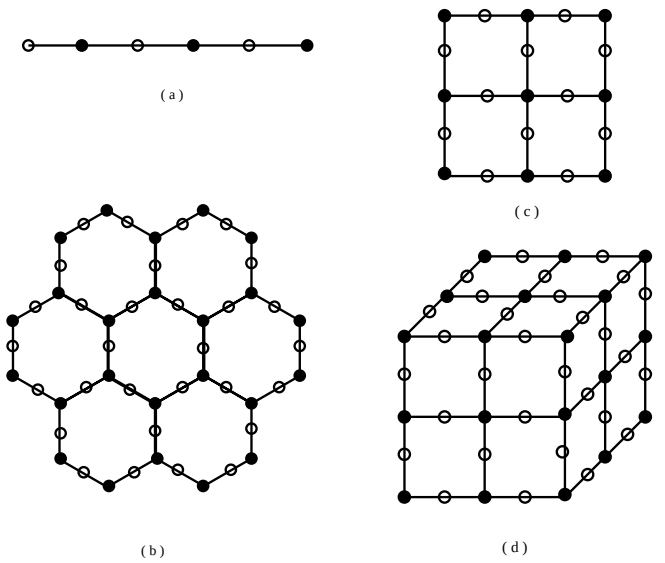

Fig. 1. Several examples of the lattices with $n_{\rm a}=2$ (a), 3 (b), 4 (c), 6 (d), and $n_{\rm b}=2$. Other lattices are also possible. For example the diamond structure lattice has $n_{\rm a}=4$ as the lattice (c) and is three-dimensional, the Kagome lattice also has $n_{\rm a}=4$ and is two-dimensional, and the triangular lattice has $n_{\rm a}=6$ as the lattice (d) and is two-dimensional. The filled points stand for lattice sites belonging to A, and the open points for lattice sites belonging to B.

where

$$\mathrm{h}_{i0}=-t'\sum_{\sigma}\mathrm{a}^{\dagger}_{i,\sigma}\mathrm{a}_{i,\sigma}+\frac{t}{2}\sum_{\delta,\sigma}\mathrm{a}^{\dagger}_{i+\delta,\sigma}\mathrm{a}_{i+\delta,\sigma}, \tag{3}$$

$$\mathrm{a}^{\dagger}_{i,\sigma}=\lambda\mathrm{c}^{\dagger}_{i,\sigma}-\sum_{\delta}\mathrm{c}^{\dagger}_{i+\delta,\sigma},\ \text{if } i\in\mathrm{A}, \tag{4}$$

$$\mathrm{a}^{\dagger}_{i,\sigma}=\lambda\mathrm{c}^{\dagger}_{i,\sigma}+\sum_{\delta}\mathrm{c}^{\dagger}_{i+\delta,\sigma},\ \text{if } i\in\mathrm{B}, \tag{5}$$

where the summation δ runs over all the nearest neighbor sites of i. $\{\mathrm{a}^{\dagger}_{i,\sigma},\mathrm{a}_{i,\sigma}\}=\lambda^2+n_{\mathrm{a(b)}}$ if $i\in$ A(B), $\{\mathrm{a}^{\dagger}_{i,\sigma},\mathrm{a}_{j,\sigma}\}=1$ if i and j are a pair of the nearest neighbor A and B sites, and the other anti-commutators vanish. In this case, $t_{ij}=t_{ji}=t$ if i and j are a pair of the nearest neighbor A sites; $t_{ij}=-t'$ if i and j are a pair of the nearest neighbor B sites; $t_{ij}=\lambda(t+t')$ if i and j are a pair of the nearest neighbor sites; $t_{ii}=n_{\rm a}t-t'\lambda^2$ if $i\in$ A; $t_{ii}=t\lambda^2-n_{\rm b}t'$ if $i\in$ B; and $t_{ij}=0$ otherwise. $t,t'\geq 0$ and λ is a non-zero constant. The total spin operator $\mathbf{S}_{\rm tot}=\sum_{i\in\wedge}(\mathbf{S}_i+\mathbf{S}_{ic})$ commutes with the Hamiltonian and is a good quantum number. Denote by $N_\wedge$ the number of the lattice sites. The maximum value of the total spin is $S_{\rm tot}=SN_\wedge+N_{\rm e}/2$ if the number of electrons $N_{\rm e}<N_\wedge$, and $S_{\rm tot}=SN_\wedge+(2N_\wedge-N_{\rm e})/2$ if the number of electrons $N_{\rm e}>N_\wedge$.

The main result in this paper is summarized as follows

Theorem I: Define the Kondo lattice model (Eq. (2)) with the hopping matrix $\{t_{ij}\}$. Take $t=1$ the energy unit. $t_{\rm c}(\lambda)$ as shown in Figure 2 and $f_{\rm c}(\lambda,t')$ as shown in Figures 3 and 4 are two functions obtained numerically.

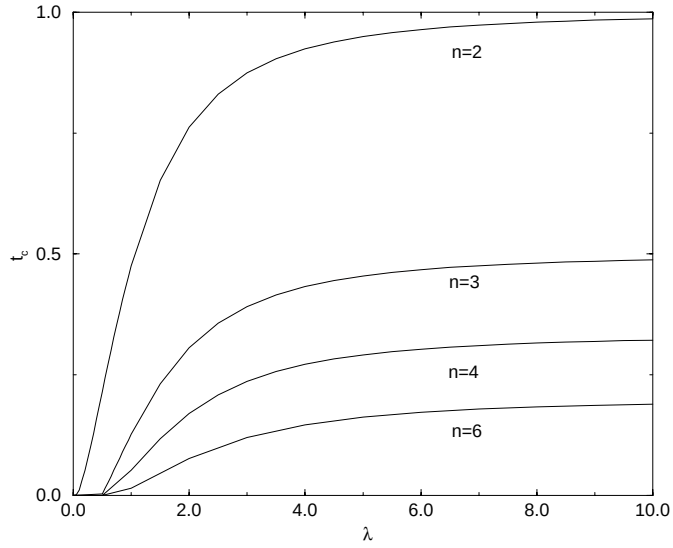

Fig. 2. λ-dependence of $t'_{\rm c}$ calculated for the case of $f=+\infty$. $t_{\rm c}(\lambda)\to 1,1/2,1/3,1/5$ for $n_{\rm a}=2,3,4,6$ as $\lambda\gg 1$.

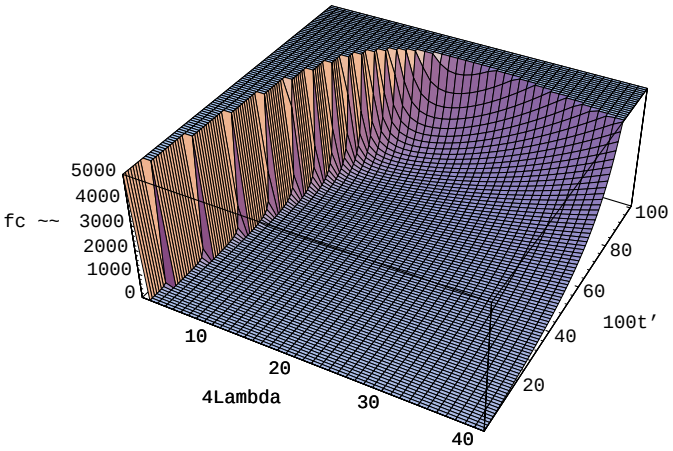

Fig. 3. λ- and t'-dependence of $f_{\rm c}$ calculated for the case of $n_{\rm a}=2$.

Assume $t'\leq t_{\rm c}(\lambda)$ and $JS\geq f_{\rm c}(\lambda,t')$. When the density of electrons is $n_{\rm e}=n_{\rm b}/(n_{\rm a}+n_{\rm b})$, the ground state exhibits the maximum of the total spin $S_{\rm max}$ and is non-degenerate.

Three remarks or corollaries are made:

1) $+\lambda$ and $-\lambda$ give the same result, *i.e.*, $t_{\rm c}(\lambda)=t_{\rm c}(-\lambda)$ and $f_{\rm c}(\lambda,t')=f_{\rm c}(-\lambda,t')$. This is shown by utilizing the gauge transformation: $\mathrm{c}_{i\sigma}\to\epsilon(i)\mathrm{c}_{i\sigma}$ where $\epsilon(i)=1$ if $i\in$ A, and -1 if $i\in$ B. Under this transformation, $\lambda\to-\lambda$ and all other terms remain invariant in equation (1).

2) When $n_{\rm e}=1+n_{\rm a}/(n_{\rm a}+n_{\rm b})$ and $t\to-t$ and $t'\to-t'$, the ground state exhibits (not fully saturated) ferromagnetism. It is shown by utilizing the transformation: $\mathrm{c}_{i\sigma}\to\mathrm{c}^{\dagger}_{i\sigma}$ and $\{\mathbf{S}^{+}_i,\mathbf{S}^{-}_i,\mathbf{S}^{z}_i\}\to\{-\mathbf{S}^{-}_i,-\mathbf{S}^{+}_i,-\mathbf{S}^{z}_i\}$.

3) The model in equation (2) contains the next nearest neighbor hopping and is a multi-band one. When the density of electron is $n_{\rm b}/(n_{\rm a}+n_{\rm b})$, the lowest energy band is fully filled. Due to existence of the energy gap between

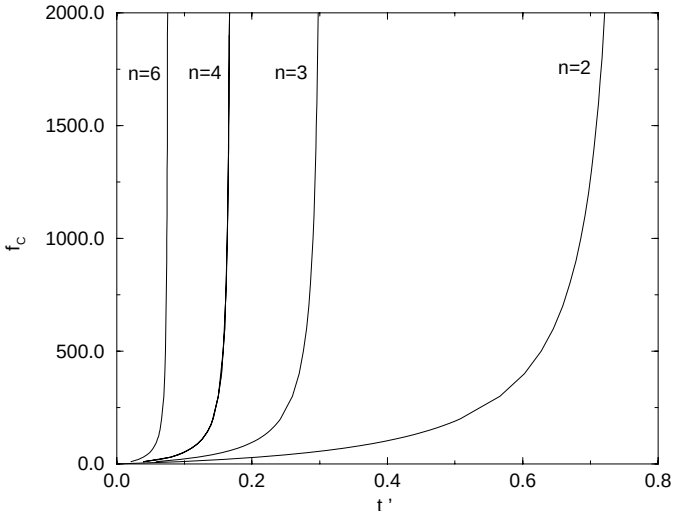

Fig. 4. t'-dependence of $f_{\rm c}$ calculated for the case of $\lambda = 2$ and $n_{\rm a} = 2$, 3, 4, 6.

the lowest energy bands, the ferromagnetic state should be insulating.

The proof of Theorem I is divided into two steps: In Section 2, we introduce a lemma which establishes a relationship on ferromagnetism between the Kondo lattice model and the Hubbard model; in Section 3, we introduce a theorem on ferromagnetism in the Hubbard model, which was first proved in one-dimensional case by Tasaki [11]. We improve and generalize the result to higher dimensional cases. Combining the lemma in Section 2 and the theorem in Section 3 will prove Theorem I. Finally we make some discussions on ferromagnetism in the Kondo lattice model.

2 Lemma on the ferromagnetism in the Hubbard model and Kondo lattice model

The proof of Theorem I will make use of rigorous results for the Hubbard model. A general form of the Hubbard model is

$$\mathrm{H_H} = \sum_{ij} t_{ij} \mathrm{c}^{\dagger}_{i,\sigma} \mathrm{c}_{j,\sigma} + U \sum_{i} \mathrm{n}_{i,\uparrow} \mathrm{n}_{i,\downarrow}, \tag{6}$$

where $\mathrm{c}^{\dagger}_{i,\sigma}$ and $\mathrm{c}_{i,\sigma}$ are the creation and annihilation operators for conduction electron with spin σ at site i, respectively. $\mathrm{n}_{i,\sigma} = \mathrm{c}^{\dagger}_{i,\sigma}\mathrm{c}_{i,\sigma}$. It is believed that the Hubbard model is more difficult to form ferromagnetism. However the model contains less degrees of freedom than the Kondo lattice model. On ferromagnetism, these two models are related to each other. Here we first introduce a lemma that establishes the relation.

Lemma: Assume the Kondo lattice model (Eq. (1)) and the Hubbard model (Eq. (6)) have the same hopping terms for conduction electrons, and have the same number of conduction electrons. The ground state of the Hubbard model exhibits the maximum of the total spin of conduction electrons. When $JS \geq U$, the ground state of the Kondo lattice model is also fully saturated ferromagnetic. If the ground state of the Hubbard model is non-degenerate, so is the ground state of the corresponding Kondo lattice model.

Remark: it is worth pointing out that this lemma holds for any hopping matrix, and is not limited in the case of equation (2). The condition of $JS \geq U$ is a sufficient, not necessary one.

Proof of the lemma: the proof of the theorem is based on the variational principle. The Kondo lattice model can be rewritten as

$$\mathrm{H_K} = \mathrm{H_H} + \sum_{i} \mathrm{V}_i. \tag{7}$$

The first term is the Hamiltonian for the Hubbard model as in equation (6), and the second term is the summation for the local interaction,

$$\mathrm{V}_i = -J\mathbf{S}_i \cdot \mathbf{S}_{i\mathrm{c}} - U \mathrm{n}_{i,\uparrow}\mathrm{n}_{i,\downarrow}. \tag{8}$$

Let first us consider the local Hamiltonian of the interaction V_i at site i. The total spin and the number of electron(s) are good quantum numbers. On each site, there are four configurations for conduction electron(s) and localized spin: an empty state, single occupancy, and double occupancy, in which single occupancy contains two states with total spin $S + 1/2$ and $S - 1/2$. The corresponding energies for V_i are: $-JS/2$ for the single occupancy with $S + 1$, $-U$ for the double occupancy, 0 for empty, and $J(S + 1)/2$ for the single occupancy with $S - 1$.

When the ground state of the Hubbard model exhibits the maximum of the total spin, one of them consists of all electrons with spin up, denoted by $|\Psi_{\rm c}\rangle$,

$$\mathrm{H_H}|\Psi_{\rm c}\rangle = \epsilon_{\rm c}|\Psi_{\rm c}\rangle, \tag{9}$$

where $\epsilon_{\rm c}$ is the lowest energy of $\mathrm{H_H}$. The state for the Kondo lattice model consists of localized spins as well as the itinerant electrons. Construct the state as

$$|\Psi_{\rm F}\rangle = |\Psi_{\rm c}\rangle \otimes |\Psi_{\rm s}\rangle, \tag{10}$$

where $|\Psi_{\rm s}\rangle = |\uparrow\uparrow\cdots\uparrow\rangle$ consists of all localized spins aligning up. The state $|\Psi_{\rm F}\rangle$ exhibits the maximum of both the total spin and its z component. On this state, we obtain

$$\mathrm{H_H}|\Psi_{\rm F}\rangle = \epsilon_{\rm c}|\Psi_{\rm F}\rangle \tag{11}$$

and

$$\sum_{i} \mathrm{V}_i|\Psi_{\rm F}\rangle = -\frac{1}{2}N_{\rm e}JS|\Psi_{\rm F}\rangle. \tag{12}$$

Hence the state is an eigenstate of $\mathrm{H_K}$. Considering the second term in equation (7), we compare the energy of two single occupancies with spin $S + 1/2$ with one empty and one double occupancy. In this case the number of electrons is conserved. The energy difference is $U - JS$. If $JS > U$, the configuration of the two single occupancies has a lower energy than the configuration with one empty

and one double occupancy. Thus $-\frac{1}{2}N_{\rm e}JS$ is the minimum of the total energy for $\sum_i {\rm V}_i$ when $JS > U$ and the number of electrons is $N_{\rm e}$. As both $\rm H_H$ and $\sum_i {\rm V}_i$ have the minimum of energy on the state $|\Psi_{\rm F}\rangle$, according to the variational principle, the state must be the ground state or one of the ground states (if degenerate) of the Kondo lattice model in equation (1).

If $|\Psi_{\rm c}\rangle$ is the unique ground state of $\rm H_H$, then $|\Psi_{\rm F}\rangle$ is the unique ground state of $\rm H_K$. Both $\epsilon_{\rm c}$ and $-N_{\rm e}JS/2$ are the lowest energies of $\rm H_H$ and $\sum_i {\rm V}_i$, respectively, and their summation $\epsilon_{\rm c}-N_{\rm e}JS/2$ is the ground state energy of $\rm H_K$. If $\rm H_K$ has another ground state assuming $|\Psi_{\rm a}\rangle$, then

$$ {\rm H_K}|\Psi_{\rm a}\rangle = (\epsilon_{\rm c} - \frac{1}{2}N_{\rm e}JS)|\Psi_{\rm a}\rangle. \tag{13} $$

In the variational principle, we obtain

$$ \langle\Psi_{\rm a}|{\rm H_H}|\Psi_{\rm a}\rangle \geq \epsilon_{\rm c}; \tag{14} $$

$$ \langle\Psi_{\rm a}|\sum_i {\rm V}_i|\Psi_{\rm a}\rangle \geq -\frac{1}{2}N_{\rm e}JS. \tag{15} $$

Combining the two inequalities (Eqs. (14, 15)) and equation (13), we conclude that only equality holds in the two inequality, *i.e.* $|\Psi_{\rm a}\rangle$ is also a ground state of $\rm H_H$ and $\sum_i {\rm V}_i$. As $-N_{\rm e}JS/2$ is the minimal of $\sum_i {\rm V}_i$, it indicates that the spins of $N_{\rm e}$ electrons must be parallel to the localized spins. Consider the unique ground state of $\rm H_H$ possesses the maximal of total spins.All spins in $\Psi_{\rm a}$ must be parallel to each other. Hence $|\Psi_{\rm a}\rangle$ is the unique state $|\Psi_{\rm F}\rangle$. Q.E.D.

3 Ferromagnetism in the Hubbard model

Let us now introduce a theorem on ferromagnetism in the Hubbard model on the lattices in Figure 1. We take the Hamiltonian in the form,

$$ {\rm H_H} = \sum_{i\in {\rm A}} {\rm h}_{i0} + U\sum_i {\rm n}_{i\uparrow}{\rm n}_{i\downarrow}, \tag{16} $$

in which the hopping matrix is as the same as equation (2) for the conduction electrons. In his letter [11], Tasaki presented a theorem in the one-dimensional case. Here we make a little improvement of his result to a larger regime in a one-dimensional case and generalize it to higher dimensional cases. A revised and improved theorem states

Theorem II: Define the Hubbard model (Eq. (16)) on the lattices (See Fig. 1) with the hopping matrix $\{t_{ij}\}$ as in the Kondo lattice model (Eq. (2)). Take $t = 1$ the energy unit. $t_{\rm c}(\lambda)$ as shown in Figure 2 and $f_{\rm c}(\lambda, t')$ as shown in Figures 3 and 4 are two functions obtained numerically. Assume $t' \leq t_{\rm c}(\lambda)$ and $U \geq f_{\rm c}(\lambda, t')$. When the density of electrons is $n_{\rm e} = n_{\rm b}/(n_{\rm a} + n_{\rm b})$, the ground state exhibits the maximum of the total spin $S_{\max}$ and is non-degenerate.

Proof of Theorem II: I first consider the part of hopping terms. The local Hamiltonian $\rm h_{i0}$ contains $2n_{\rm a} + 1$ sites. The t- and t'-terms commute with each other,

$$ [-t'\sum_\sigma {\rm a}^\dagger_{i,\sigma}{\rm a}_{i,\sigma}, \frac{t}{2}\sum_{\delta\in {\rm NNA},\sigma} {\rm a}^\dagger_{i+\delta,\sigma}{\rm a}_{i+\delta,\sigma}] = 0. \tag{17} $$

It indicates that these two terms can be diagonalized simultaneously. For the first term, its lowest energy is $-(\lambda^2+n_{\rm a})t'$ ($t' \geq 0$), and the state is $\rm a^\dagger_{i,\sigma}|0\rangle$ and is nondegenerate. The other $2n_{\rm a}$ eigenstates are degenerate with eigenvalue zero. For the second term, it is positive semidefinite, and its eigenvalues must be non-negative. Using the operators $\rm a^\dagger_{i+\delta,\sigma}$, the second term can be expressed as a $n_{\rm a} \times n_{\rm a}$ matrix, and has $(n_{\rm a} - 1)$-fold degenerate eigenstates with eigenvalue $(\lambda^2 + 1)t/2$, and an eigenstate with eigenvalue $(\lambda^2+n_{\rm a}+1)t/2$. The other $n_{\rm a}+1$ hidden eigenstates are degenerate with eigenvalue zero. Therefore in the single electron case, the ground state of $\rm h_{i0}$ is $\rm a^\dagger_{i,\sigma}|0\rangle$ with lowest energy $-(\lambda^2 + n_{\rm a})t'$. It has other $n_{\rm a}$ degenerate eigenstates with zero and $n_{\rm a}$ eigenvalues with positive eigenvalues. Denote the eigenvalues by ϵ_n. I have

$$ \begin{aligned} \epsilon_0 &= -(\lambda^2 + n_{\rm a})t'; \\ \epsilon_n &= 0, \quad \text{for } n = 1, \cdots, n_{\rm a}; \\ \epsilon_n &= (\lambda^2 + 1)t/2, \quad \text{for } n = n_{\rm a} + 1, \cdots, 2n_{\rm a} - 1; \\ \epsilon_{2n_{\rm a}} &= (\lambda^2 + n_{\rm a} + 1)t/2. \end{aligned} \tag{18} $$

Construct the state $|\Psi_{\rm c}\rangle = \prod_{i\in {\rm A}} {\rm a}^\dagger_{i,\uparrow}|0\rangle$ for $N_{\rm e} = N_{\rm A}$ electrons ($N_{\rm A}$ is the number of A sites). It is crucial that this state is an eigenstate for all $\rm h_{i0}$, although $[{\rm h}_{i0}, {\rm h}_{j0}] \neq 0$ when i and j are a pair of the nearest neighbor sites.

$$ {\rm h}_{i0}|\Psi_{\rm c}\rangle = \epsilon_0|\Psi_{\rm c}\rangle \tag{19} $$

for all $i \in$ A. When $t' = 0$, ϵ_0 is equal to zero. This is the lowest energy of $\rm h_{i0}$ for any n electrons based on equations (18). In other words, it is the global lowest energy of $\rm h_{i0}$ in terms of different electrons. In this case, we conclude that $|\Psi_{\rm c}\rangle$ is the lowest energy state of $\sum_{i\in {\rm A}} {\rm h}_{i0}$ with the density of electrons $n_{\rm e} = n_{\rm b}/(n_{\rm a} + n_{\rm b})$ since each local Hamiltonian $\rm h_{i0}$ has its lowest energy on the state. This is a flat-band ferromagnet [12,13].

When $t' \neq 0$, ϵ_0 is no longer the global lowest energy of $\rm h_{i0}$, although $|\Psi_{\rm c}\rangle$ is still an eigenstate of $\rm h_{i0}$. For example the ground state of two electrons has the energy $2\epsilon_0$ which is less than ϵ_0. In fact the state $|\Psi_{\rm c}\rangle$ is apparently not the ground state in the case of $U = 0$ or very small U in the variational principle. In the case, the ground state is a paramagnetic state. To overcome this difficulty, we rewrite $\rm H_H$ (Eq. (16)) as

$$ {\rm H_H} = \sum_{i\in {\rm A}} {\rm h}_i \tag{20} $$

where

$$ {\rm h}_i = {\rm h}_{i0} + \sum_\delta \alpha_{i+\delta} f {\rm n}_{i+\delta\uparrow}{\rm n}_{i+\delta\downarrow}. \tag{21} $$

$\alpha_{i+\delta} = \alpha$ if $\delta = 0$, 1/2 if $\delta = 1$, and $(1 - \alpha)/n_{\rm a}$ if $\delta = 2$ ($0 \leq \alpha \leq 1$). Due to introducing the Hubbard term in $\rm h_i$, the situation has changed: $\langle\Psi_{\rm c}|{\rm h}_i|\Psi_{\rm c}\rangle$ may be its minimum when U is sufficiently large, for example in the one-dimensional case [11]. In the one-dimensional case $\rm h_i$ contains five sites, and can be solved exactly. Part of

the results was obtained numerically in [11]. In the case of two electrons there are twenty five states for the finite f case. Ten of them are spin triplet, which have the lowest energy ϵ_0. Another fifteen states are spin singlet. Expanding the singlet state in terms of the singlet pair operator $(c^\dagger_{i,\uparrow}c^\dagger_{j\downarrow}-c^\dagger_{i,\downarrow}c^\dagger_{j\uparrow})$, the characteristic polynomial for the Hamiltonian can be calculated exactly. At $U=+\infty$, there are only ten singlet states due to exclusion of the double occupancy. When $t'<t_c(\lambda)$, the lowest energy of the singlet states is higher than ϵ_0 and when $t'>t_c(\lambda)$, it is lower than ϵ_0. $t_c(\lambda)$ is calculated in the case of $U=+\infty$ by solving two fourth-order and sixth-order polynomial equations numerically (see Fig. 2). This indicates that in the case of $t'>t_c(\lambda)$ and any finite U the singlet state has a lower energy than the triplet state and the single electron state. When $t'<t_c(\lambda)$, I have a f_c so that the singlet state has a higher energy than ϵ_0 when $U>f_c(\lambda,t')$. f_c is calculated by solving the characteristic polynomial equation numerically (I take $\alpha=1/2$) as shown in Figure 3.

The other $(2n_a+1)$-site problems ($n_a=3,4,6$) are solved numerically by exact diagonalization. The similar results on $t_c(\lambda)$ and $f_c(\lambda,t')$ with different n_a are obtained. I have $t_c(\lambda)\to 1/(n_a-1)$ when $\lambda\gg 0$. For example in $n_a=2$ or one-dimensional case, $t_c(\lambda)\to 1$. When $t'<t_c(\lambda)$, the larger n_a is, the larger f_c is so that the lowest energy of the singlet state is higher than ϵ_0. I just present numerical results of $\lambda=2$ for $n_a=2,3,4,6$ in Figure 4.

The uniqueness of the ground state is proved by Tasaki in the one-dimensional case [11]. His proof also holds for the higher dimensional case. Assume $|\Psi\rangle$ is a ground state of H_H. Since ϵ_c is the lowest energy of h_i, using the variational principle, the state must satisfy

$$h_{i0}|\Psi\rangle=\epsilon_c|\Psi\rangle \tag{22}$$

for all sites $i\in A$ and

$$n_{i\uparrow}n_{i\downarrow}|\Psi\rangle=0 \tag{23}$$

for all sites on the lattice. According to Tasaki's lemma, $|\Psi\rangle$ must be written in the form

$$|\Psi\rangle=a^\dagger_{i\uparrow}|\Psi_1\rangle+a^\dagger_{i\downarrow}|\Psi_2\rangle \tag{24}$$

with some state $|\Psi_1\rangle$ and $|\Psi_2\rangle$ if it is a ground state of $h_{i,0}$ ($i\in A$). As $|\Psi\rangle$ is also a ground state of $h_{i+a,0}$ where $i+a$ is one of the nearest neighbor sites belonging to A, applying Tasaki's lemma once again, we obtain

$$\begin{aligned}|\Psi\rangle=&a^\dagger_{i,\uparrow}a^\dagger_{i+a,\uparrow}|\psi'_1\rangle\\&+(a^\dagger_{i,\uparrow}a^\dagger_{i+a,\downarrow}+a^\dagger_{i,\downarrow}a^\dagger_{i+a,\uparrow})|\psi'_2\rangle\\&+a^\dagger_{i,\downarrow}a^\dagger_{i+a,\downarrow}|\psi'_3\rangle\end{aligned} \tag{25}$$

with some states $|\psi'_n\rangle$ ($n=1,2,3$). The operators $a^\dagger_{i,\sigma}$ and $a^\dagger_{i+a,\sigma}$ form a spin triplet state. Successively applying Tasaki's lemma, one obtain

$$\begin{aligned}|\Psi\rangle&=\sum_{M=0}^{N_A}C_M\delta(\sum_i\sigma(i)-N_A+M)\prod_i a^\dagger_{i,\sigma(i)}|0\rangle\\&=\sum_{M=0}^{N_A}C_M(\sum_i S^-_{ic})^{N_A-M}|\Psi_c\rangle\end{aligned} \tag{26}$$

with N_A+1 coefficients C_M. Therefore the state ground state is unique except for N_A+1 spin SU(2) degeneracy.

In short, we conclude that when $t'\le t_c(\lambda)$ and $J\ge f_c(\lambda,t')$, the ground states of h_i with $n=1,\cdots,n_a+1$ electrons has the global lowest energy ϵ_0, and those of $n=n_a+2,\cdots,2(2n_a+1)$ has higher energies. Under these conditions each $h_i|\Psi_c\rangle=\epsilon_0|\Psi_c\rangle$ and ϵ_0 is the global lowest energy of h_i. In the variational principle $|\Psi_c\rangle$ is the lowest energy state of $\sum_i h_i$. Therefore I conclude that $|\Psi_c\rangle$ is the ground state of equation (6) when $t'<t_c(\lambda)$, $U>f_c(\lambda,t')$ and the density of electrons is $n_b/(n_a+n_b)$. Due to spin SU(2) symmetry other $2S_{tot}$ ground states are constructed by $(\sum_i S^-_{ic})^m|\Psi_c\rangle$ ($m=1,2,\cdots,2S_{tot}$) and $S_{tot}=N_\wedge/2$ Q.E.D.

Combining this theorem and the lemma, we prove Theorem I. From the proof of Theorem II we have to make use of the variational principle to reduce the ferromagnetic problem on the lattice $\wedge$ to that on a $2n_a+1$-site cluster. Numerical calculations on these small clusters are needed to determine the functions t_c and f_c. A direct application of the method used in the Hubbard to the Kondo model is not successful, since the Kondo lattice model contains localized spins as well as conduction electrons. On the other hand exact diagonalization is only available for very few-site and low spin problem. Physically we believe the Kondo lattice model is easier to form a ferromagnetic state than the Hubbard model, and our lemma also proves this point. However technically it is not so easy to extract some exact results from the Kondo lattice model. Our lemma provides an efficient way to understand ferromagnetism in the Kondo lattice model by utilizing some results of the Hubbard model.

Theorem II is valid at the electron filling $n_e=n_b/(n_a+n_b)$. After introducing the next nearest neighbor hopping in H_H, the band of electrons is divided into two or more subbands. For instance, in the one-dimensional case the single electron spectra are $\epsilon_1(k)=-2t'\cos 2k-2(t+t')$ and $\epsilon_2(k)=+2t\cos 2k+\lambda^2(t+t')$ with $|k|\le\pi/2$. The filling n_e means the lower band is fully filled. In this case the ground state is insulating [11]. However Penc *et al.* found that the ferromagnetism survives when the system deviates from the fully filling of the lower band [14]. In this case the ferromagnetic state is metallic.

4 Discussions

The mechanism of ferromagnetism in the Kondo model is usually summarized as the double exchange mechanism in the strong coupling limit. Sometimes the physical picture of double exchange mechanism is also true in the case

of finite coupling. In the case of one-electron, the ground state of Kondo lattice model is always fully saturated ferromagnetic, which is proved by using of the lemma and the fact that the ground state of the Hubbard model with one electron has always the maximum of total spin 1/2. In the case of two electrons, the result depends on the boundary condition. For example the ground state is a spin singlet on a ring even in the strong Hund coupling limit. Essentially the mechanism is a one-particle picture. The motion of electrons, or the kinetical energy tends to form a paramagnetic state. To form a ferromagnet, the exchange coupling has to overcome the competition from the kinetical energy. On the lattices in Figure 1 when $t' = 0$ the spectrum of single electron is completely flat, and there is no competition from the kinetical energy. Thus even a small coupling will lead to electrons to form a ferromagnetic state when the flat-band is fully filled. The true competition comes from the case of $t' \neq 0$. From the numerical results in Figures 3 and 4, we find that f_c is much larger than t and t'. We use the variational approach to obtain f_c. Hence it is a sufficient condition. At least it tells us that we need a strong exchange coupling to reach a ferromagnetic state. Hence to flatten the band structure of electrons and to increase the exchange coupling and electron-electron interaction are two of the basic routines to look for ferromagnetism in the Kondo lattice model.

Another route to ferromagnetism in the Hubbard model was proposed by Müller-Hartmann [15]. On a one-dimensional chain, let take the nearest-neighbor hopping term $-t$ and the next nearest neighbor hopping term t' (both t and t' are positive). The single electron spectrum is

$$\epsilon(k) = -2t\cos k + 2t'\cos 2k. \tag{27}$$

At the bottom of the band there appear two degenerate minima around $\cos k_0 = t/4t'$ when $t' > t/4$. In the large U limit, Muller-Hartmann showed that the mode is equivalent to a system with two one-dimensional chains coupled ferromagnetically in a low density limit of electrons. The resulting Hamiltonian has a ferromagnetic ground state. Numerical calculation confirmed Müller-Hartmann's idea and show that the ferromagnetism exists in the case of a finite density of electrons and finite U [16]. This mechanism can be also realized in the $t-t'$ Kondo lattice model. Using the results of the Hubbard model, we conclude that the ground state of the Kondo lattice model is ferromagnetic when the electron band has several degenerate minima and exchange coupling is sufficiently large at least in the one-dimensional case.

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