Existence of Saturated Ferromagnetic and Spiral States in 1D Lieb-Ferrimagnetic Models away from Half-Filling

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In order to study conditions for the appearance of ferromagnetism in a wide filling region, we investigate numerically three types of one-dimensional Lieb-ferrimagnetic Hubbard models: a periodic diamond (PD) chain, a periodic alternately-attached leg (PAAL) chain and an open diamond (OD) chain. All of these models have a flat band (or equivalently, degenerate single-electron eigenvalues). The PD and OD chains commonly have a local-loop structure. Nagaoka’s theorem holds only in the PD chain. At half-filling, it has been rigorously proven that all of these models are ferrimagnet. Away from half-filling, however, quite different magnetic properties are found. In the fillings $1/3 < \rho < 1/2$, the ground state of the PD chain for a infinitely-large $U$ is the extended ferromagnetic state, that is, the saturated ferromagnetic state or the spiral state for odd or even number of electrons, respectively. In the PAAL chain, on the other hand, there is no magnetic order. Thus, the flat band is found to be not a sufficient condition of the extended ferromagnetic state. We find, moreover, that the saturated ferromagnetism appears in the OD chain, although the Nagaoka theorem does not hold on this chain. This indicates that the local-loop structure plays an important role on the appearance of the extended ferromagnetic state.

KEYWORDS: Hubbard Model, Flat Band, Nagaoka’s Theorem, Saturated Ferromagnetism, Spiral State, Ferromagnetic State in an Extended Sense, Numerical Diagonalization

§1. Introduction

Ferromagnetism in strongly correlated electron systems has attracted great interests. Since ferromagnetism is a purely many-body phenomenon and appears for sufficiently strong interactions and high electron fillings in general, we have to investigate properties of the ferromagnetism by non-perturbative methods. The important question whether the Coulomb interaction is enough to realize ferromagnetism is still far from completely understanding.

Up to recent, two rigorous results concerning with the existence of saturated ferromagnetism have been known on the Hubbard-type models which consist of the hopping term and the on-site Coulomb interaction term. They are Nagaoka’s theorem and (nearly-)flat-band ferromagnetism.

Nagaoka’s theorem holds only for the system with just one hole added to the half-filling. Therefore, after Nagaoka’s theorem was found, it has been repeatedly studied from various points of view whether Nagaoka’s theorem holds or not for more than one hole. In the two dimensional square lattice, many authors show that the saturated ferromagnetic state is no longer the ground state for the two-hole case. Kusakabe and Aoki, however, showed that the ground state of the two-hole system is not the ordinary singlet state but the spiral state. The definition of the spiral state is that its spin structure factor $S(Q)$ takes its peak at $Q = 2\pi/L$ ($L$: system size).

On the contrary, the flat-band ferromagnetism is realized at the half-filling of the lowest-energy flat band, for example, the quarter-filling in the one-dimensional Mielke-Tasaki model.

Between the one hole added to the half-filling (Nagaoka’s ferromagnetism) and the quarter-filling (flat-band ferromagnetism), a new type of ferromagnetism has been found in a one-dimensional Mielke-Tasaki model. The ground state in this filling region has been shown to be the saturated ferromagnetic state or the spiral state corresponding to the odd or even number of holes, respectively. The spins in the spiral state have a ferromagnetic correlation up to half of the system size. Therefore, we regard both states, the saturated ferromagnetic state and the spiral state, as a ferromagnetic state in an extended sense. Hereafter, we call them the extended ferromagnetic state.

In this paper, to study conditions to realize the extended ferromagnetic state in high electron fillings, we investigate three categories of models, (A), (B) and (C). To classify the these categories, we take notice of the following three characteristics: existence of the flat band (or equivalently, existence of the degenerate eigenvalues in the single-electron state), existence of local loops (triangles or squares) and holding of Nagaoka’s theorem. Although the existence of the flat band is a common characteristic in the categories (A), (B) and (C), the local-loop structure exists in (A) and (C), and Nagaoka’s theorem holds only for (A). Here, we note that all the three characteristics are satisfied in the flat-band ferromagnetic models which was previously studied. In
this paper, therefore, we would treat other Hubbard-type models.

First, we compare two models of (A) and (B). As we will see in §2, at high (from more than 1/3 to less than 1/2) electron fillings, we find that the extended ferromagnetism (not ferrimagnetism) appears in a model of (A) while all the ground states at less than half-filling are singlet or (disconnected) paramagnet in a model of (B). Thus, we conclude that the existence of the flat band is not a sufficient condition for the appearance of the extended ferromagnetic state. Furthermore, we find that in a model of (C), the saturated ferromagnetic state appears at high electron fillings in spite that the model does not satisfy the condition for Nagaoka’s theorem to hold. This indicates that the existence of the local-loop structure plays an important role for the appearance of the extended ferromagnetic state. We would stress that this is the first result about the appearance of the saturated ferromagnetic state in such a wide range of fillings on a system to which Nagaoka’s theorem is not applicable.

The rest of this paper is organized as following. In the next section, models and some definitions are presented. Rigorous results related to the present problem are also reviewed. In §3, numerical results for models of (A) and of (B) are presented. The result for model of (C) is obtained in §4, along with the discussion about the relation between the local-loop structure and the connectivity condition. Summary and further discussions are given in §5.

§2. Models and Related Statements

First, we define the models and some basic definitions treated in this paper. The Hamiltonian on a lattice \( \Lambda \) is

\[
H = H_{\text{hop}} + H_{\text{int}}
\]

\[
= -t \sum_{\langle i, j \rangle \in \Lambda} \sum_{\sigma = \uparrow, \downarrow} c_{i, \sigma}^\dagger c_{j, \sigma} + U \sum_{i \in \Lambda} n_{i, \uparrow} n_{i, \downarrow},
\]

where \( U > 0 \) is the on-site Coulomb repulsion energy, \( \langle i, j \rangle \) denotes the nearest-neighbor pair in the lattice \( \Lambda \) and \( c_{i, \sigma}^\dagger, c_{i, \sigma} \) and \( n_{i, \sigma} \) are the creation, the annihilation and the number operators of the electron on site \( i \) with spin \( \sigma \), respectively. We assign the hopping term \(-t < 0\) to each bond. \( N_e, N_h \) and \( \rho_e \) denote the number of electrons, the number of holes and the electron filling, respectively. Here, \( N_h = 0 \) when the whole system is half-filled. We consider the following models as examples for the categories, model(A), model(B) and model(C):

(A) PD chain: diamond chain with the periodic boundary condition.

(B) PAAL chain: alternately-attached leg chain with the periodic boundary condition.

(C) OD chain: diamond chain with the open boundary condition.

The diamond chain and the alternately-attached leg chain are shown in Figs. 1(a) and 1(b), respectively. The PD chain has been studied as a possible model for an experiment of polymer chain ferromagnetism by Macêdo et al. [1].

The band structures of the PD and PAAL chains are seen in Figs. 2(a) and 2(b), respectively. Here, “band” means a dispersion relation of the single-electron state. The PD and PAAL chains have a flat-band, namely, a completely-degenerate dispersion relation. Although the band cannot be defined on the OD chain because of the absence of periodicity, an equivalent degeneracy exists in the single-electron energy spectrum of the OD chain.

Nagaoka’s theorem holds only in the PD chain since this model satisfies the connectivity condition for \( N_h = 1 \). The connectivity condition means that the Hamiltonian matrix is irreducible, namely, in a physical picture, all of states in a subspace with a fixed magnetization can be produced from any state by permitted motions of electrons. In the PAAL and OD chains, the connectivity is not satisfied for \( N_h = 1 \).

The PD and OD chains have a common characteristic that they have a local-loop structure. Here, the local loop means a loop with three or four sites (a triangle or a square, respectively). It should be noted that the local loop itself always satisfies the connectivity condition for \( N_h = 1 \) while loops with more than four sites do not satisfy the condition.

At half-filling, it is also noted that all these models have the ferrimagnetic ground state because of the difference of the numbers of sites in the two sublattices, which has been rigorously proven by Lieb [2].

§3. Role of the Flat Band

In the following two sections, we present numerical results obtained by the numerical diagonalization technique (Lanczos method). We consider, hereafter, the case that \( U = \infty \) as a limit of strong correlation.

First of all, we calculate the total spin of the ground state in the 12 sites system of the PD chain and the PAAL chain with the infinitely-large \( U \) for \( N_e = 7, 8, 9, 10 \) and 11. Results are shown in Table 1. In the

| Table 1. The total spin of the 12 sites PD and PAAL chains and their anti-periodic versions. |
| --- |
| PD chain, the ground states for high (more than 1/3) electron fillings are the saturated ferromagnetic state for odd numbers of electrons and the spiral state for even numbers. The spin-spin correlation function, as an example, for \( N_e = 10 \) is plotted in Fig. 3. In fact, we see that the spins within a half of system size are aligned ferromagnetically. We note here that for \( N_e \leq 6 \), the ground state is always singlet state and not the spiral state. The dependence of \( S_{\text{tot}} \) on \( N_e \) is shown in Fig. 4. These results show that the ground states for these fillings are the extended ferromagnetic state. For the anti-periodic chain, the even-odd property of electron
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numbers reverses. This is the same as the spiral state in the other models. We would stress that ferromagnetism, but not ferrimagnetism, appears in the PD chain. This observation is not intuitively understandable from the naive picture of the spin alignment due to the flat band for a sufficiently-small $U$. This shows that the extended ferromagnetism is realized by a true many-body effect that electrons in all the bands correlate each other. We also study the 18 sites PD chain. Although the calculation is limited in subspaces with large magnetization, the results are consistent with the results in the 12 sites chain.

On the other hand, the ground state of the PAAL chain is (disconnected) paramagnetic or singlet state, neither ferromagnetic nor ferrimagnetic. Moreover, the singlet state is not the spiral state. These results do not change for the anti-periodic boundary condition. These are also summarized in Table I. The results show that the spins even in the flat band do not align, at least, in the strongly interacting case except for the half-filled. The same assertion has been pointed out in the other model by Arita et al. These results also deny the following naive picture: when $U$ is large, only up (or down) spins are filled in the flat band and thus a ferrimagnetism may appear $\rho_e \leq 1/3$.

These results for the PD chain and the PAAL chain show that the existence of the flat band is not a sufficient condition for the appearance of the extended ferromagnetic state while the condition for Nagaoka’s theorem to hold is important for it.

§4. Ferromagnetism without Nagaoka’s Theorem

Next, we further study a model where Nagaoka’s ferromagnetism does not appear but the extended ferromagnetic state appears for $N_h \geq 2$. As an example of such a model, we investigate the OD chain which does not satisfy the connectivity condition at one hole. We calculate the OD chains with 10 and 16 sites. The results are summarized in Table II. For two holes in 10 sites chain

| Table II | The total spin of the ground state for the OD chain. |

and $2 \leq N_h \leq 4$ in 16 sites chain, the ground state is found to be the saturated ferromagnetic state. We note here that this is the first result about the appearance of the saturated ferromagnetism in such a wide range of fillings on the system to which Nagaoka’s theorem does not apply as far as we know. It is reasonable that the spiral state does not exist in the OD chain since the spiral state only exists for periodic systems as seen in other models.

The result of the OD chain shows that the local-loop structure plays an important role to realize the extended ferromagnetic state. Noting that when $N_h \geq 2$, the connectivity condition is satisfied even in the OD chain, we can obtain the following picture about the realization mechanism of the extended ferromagnetic state. The local loop creates a local ferromagnetic moment by local hopping since the local loop itself satisfies the connectivity condition as stated in §2. The global ferromagnetic moment, that is, the extended ferromagnetism is created by global hopping of electrons which is permitted if the connectivity condition is satisfied. The fact that the ground state is singlet (not the spiral state) for $\rho_e \leq 1/3$ suggests that the electron hopping is independent in each local loop when the electron filling is sufficiently low. Thus, we confirm that the high electron filling condition is another important factor to realize the extended ferromagnetic state. In the above picture, we can understand why the ground state of the PAAL chain is not ferromagnetic in spite that the PAAL chain also satisfies the connectivity condition when $N_h \geq 2$. Because, the PAAL chain, in the first place, cannot create the local moment for the absence of the local-loop structure. This picture is consistent with the observations ferromagnetic state in other Hubbard-type models, for example, the existence of the spiral state for two holes in the single band Hubbard model on the square lattice and so on.

§5. Summary and Discussions

We have investigated three models, the periodic diamond (PD) chain, the periodic alternately-attached leg (PAAL) chain and the open diamond (OD) chain. These models belong to different categories classified by the following three characteristics: the flat-band, the local-loop structure and Nagaoka’s theorem. Although the flat band (or the equivalent degeneracy of eigenvalues) exists in all of the chains, the local-loop structure exists in the PD and OD chains and Nagaoka’s theorem hold only in the PD chain.

First, we calculated the PD and PAAL chains by the exact diagonalization technique. The result for the PD chain is that the ground state for the infinitely-large $U$ is the extended ferromagnetic state for $1/3 < \rho_e < 1/2$. The result for the PAAL chain, which is contrary to the PD chain, the spins do not align except $\rho_e = 1/2$, at least for the infinitely-large $U$. Comparing the results of the PD and PAAL chains, it is concluded that the existence of flat band does not necessarily cause ferromagnetism. That is, it is shown that the extended ferromagnetic state is not realized by the flat-band. Moreover, we stress that the extended ferromagnetism is realized by a true many-body effect which can not be understood from the single-electron picture like the spin-alignment mechanism of flat band for a sufficiently-small $U$ case.

Next, calculating the OD chain, we found that the saturated ferromagnetic state, remarkably, appears in the wide range of electron fillings in spite of the absence of the condition for Nagaoka’s theorem to hold. The result shows that the existence of the local-loop structure is essentially important for the appearance of the extended ferromagnetism. We, therefore, obtain the following picture to realize the extended ferromagnetic state. Once
the local ferromagnetic moments are generated by electron hopping in a local loop, the extended ferromagnetic state are realized by global hopping of electrons if the connectivity condition are satisfied and the electron filling is sufficiently high. This picture shows again that the extended ferromagnetism appears due to a purely many-body effect.

Here, let us consider the case of half-filling. We point out that the existence (or absence) of the extended ferromagnetic state seems independent on the property at half-filling from the present results where the ground state at half-filling is commonly ferrimagnetic. The result in the 1D Mielke-Tasaki model also supports this statement since in the model, the ground state for half-filling is singlet while the ground state for \(1/4 < N_e < 1/2\) is the extended ferromagnetic state.\(^{[18]}\)

We note, at last, that the above picture to realize the extended ferromagnetic state can be easily generalized to non-Hubbard-type models in which the extended ferromagnetic state appears: the double-exchange model,\(^{[19]}\) the Kondo-lattice model,\(^{[20]}\) the two-band model,\(^{[21]}\) and the ferromagnetic \(t-J\) model.\(^{[22]}\) In these models, the spin-exchange interaction, instead of the local-loop structure, generates the local ferromagnetic moment. We think that the picture obtained in the present paper also give the essential insight for those models in the above sense.

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Fig. 1. The diamond chain (a) and the alternately-attached leg chain (b).

Fig. 2. The energy bands of the PD chain (a) and the PAAL chain (b).

Fig. 3. The spin-spin correlation function for $N_0 = 10$.

Fig. 4. The change of total spins of the 12 sites PD chain in high electron fillings.
Fig. 1(a): Diamond chain.

Fig. 1(b): Alternately-attached leg chain
Fig. 2: Y. Watanabe and S. Miyashita
Fig. 3: Y. Watanabe and S. Miyashita
Fig. 4: Y. Watanabe and S. Miyashita
| $L = 12$ | The PD chain | The PAAL chain |
|---------|---------------|----------------|
| $N_c$   | peridc        | periodic       | unit-peridic   |
| 11      | Nagaoka Ferro.| Spiral State   | Para (disconnect) | Para (disconnect) |
| 10      | Spiral State  | Saturated Ferro.| Singlet       | Singlet         |
| 9       | Saturated Ferro.| Spiral State | Singlet       | Singlet         |
| 8       | Singlet      | Singlet        | Singlet       | Singlet         |
| 7       | Singlet      | Singlet        | Singlet       | Singlet         |

Table I. Y. Watanabe and S. Miyashita.
| holes | 10 sites         | 16 sites        |
|-------|----------------|----------------|
| 1     | Disconnect     | Disconnect     |
| 2     | Saturated Ferro.| Saturated Ferro.|
| 3     | singlet        | Saturated Ferro.|
| 4     | singlet        | Saturated Ferro.|
| 5     | singlet        | singlet        |

**Table II.** Y. Watanabe and S. Miyashita.