An extension of Tasaki’s flat-band Hubbard model

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Abstract

We present a new class of flat-band Hubbard models which have saturated ferromagnetic ground states at two distinct electron numbers for different values of parameters. The models are extensions of Tasaki’s flat-band models.

1 Introduction

It is widely believed that the spin-independent Coulomb interaction and the Pauli exclusion principle can generate ferromagnetism in itinerant electron systems. One of the motivations to study the Hubbard model has been to establish and understand the generation of ferromagnetism in simplified situations taking account of these effects [1]. Mielke [2] and Tasaki [3], independently, presented Hubbard models which exhibit saturated ferromagnetism for certain electron numbers when the Coulomb interaction $U$ is positive. These models have a common feature that the single electron spectra contain dispersionless bands, and are called flat-band models. In [4] and [5], Tasaki also discovered Hubbard models exhibiting ferromagnetism which models are nonsingular in the sense that both the density of states and the Coulomb interaction are finite. Recently Tanaka and Ueda succeeded in proving the existence of saturated ferromagnetism in a Hubbard model obtained by adding extra hopping terms to Mielke’s flat-band model on the kagomé lattice [6].

Although the flat band Hubbard models are singular and not physically realistic, their study can be a basis of more realistic results about ferromagnetism. It is therefore important to find out which flat-band models exhibit ferromagnetism. Although an abstract criterion was presented by Mielke [2], we still do not know precise class of models which satisfy the criterion.

In this paper, we follow Tasaki’s construction of his flat band models, and construct a new class of Hubbard models in arbitrary dimensions with finite $U$ and finite-range hopping. We prove that the models exhibit ferromagnetism in their ground states at two distinct electron numbers. The difference between Tasaki’s original model and ours can easily be seen from Fig.1 where the simplest one-dimensional versions of the models are illustrated. Tasaki’s model has one “internal site” (gray dot in the figure) in each unit cell, while ours has two. This difference in lattice structure makes our model to have different “exchange mechanism” where a single-electron state localized at each pair of internal sites play an important role. See section 4 for more details.
Figure 1: The lattice structure and the hopping amplitude in the one dimensional flat band models of (a) Tasaki’s and (b) ours. The black dots are the external sites (in $E$) and the gray dots are the internal sites (in $I$). Tasaki’s model has one internal cite in each cell while our has two.

We have thus found that a extension of Tasaki’s construction lead to a new class of models exhibiting ferromagnetism. We hope this study will shed light on general structure of flat-band ferromagnetism.

2 The model and main results

2.1 Construction of the lattice

In the original flat-band models by Tasaki [3], the basic cell in the lattice $\Lambda$ consists of a single internal site and some external sites. In our new models, the basic cell consists of two internal sites and some external sites. More precisely we let the basic cell be

$$C = \{u, v, x_1, x_2, \ldots, x_n\}. \quad (2.1)$$

We call $u$ and $v$ the internal sites of $C$, and $x_1, x_2, \ldots, x_n$ the external sites.

To form the lattice $\Lambda$, we assemble $M$ identical copies $C_1, C_2, \ldots, C_M$ of the basic cell $C$, and identify external sites from $m$ distinct cells and regard them as a single site. In other words, an external site in $\Lambda$ is shared by $m$ distinct cells. We denote by $|\Lambda|$ the number of sites in $\Lambda$. See Fig.2 for an example of a cell and a resulting lattice.

The lattice is naturally decomposed as

$$\Lambda = I \cup E \quad (2.2)$$

where $I$ and $E$ are the sets of internal sites and external sites, respectively. We also denote by $J$ the assembly $\{1, 2, \ldots, M\}$ of the indices of cells. From the above construction, we see that the numbers of sites in these sublattices are $|I| = 2M$, $|E| = nM/m$. By using $|\Lambda|$, we can write $|I| = 2m|\Lambda|/(2m + n)$, $|E| = n|\Lambda|/(2m + n)$ and $|J| = m|\Lambda|/(2m + n)$. 
In what follows we always regard $C_j$ as a subset of $\Lambda$. We denote the two internal sites in $C_j$ as $u_j$ and $v_j$. For an external site $x \in E$, we denote by $J_x$ the collection of indices $j$ such that $x \in C_j$. We also define $\Lambda_x \subset \Lambda$ to be the union of $m$ cells which contain the site $x$.

![Figure 2: An example of a cell and a lattice. From the quadrangular cell with four sites (a), one can form (b) a decorated square lattice by identifying four external sites. This defines flat-band Hubbard model in two dimensions. For the precise definition see (2.19) and (2.20) (where one should set $n = 2$, $m = 4$). When $N_e = |\Lambda|/5$, the model exhibits saturated ferromagnetism for any $t > 0$, $s' > 0$ and $U > 0$. The model also exhibits saturated ferromagnetism for any $t > 0$, $U > 0$ when $N_e = 3|\Lambda|/5$ and $s' = 0$. See Theorem 2.1 and Theorem 2.2.](image)

2.2 Fermion operators

We consider an electron system on the lattice $\Lambda$. For each site $r \in \Lambda$ and $\sigma = \uparrow, \downarrow$, we define the creation and the annihilation operators $c_{r,\sigma}^\dagger$ and $c_{r,\sigma}$ for an electron at site $r$ with spin $\sigma$. These operators satisfy the canonical anticommutation relations

$$\{c_{r,\sigma}^\dagger, c_{s,\tau}\} = \delta_{r,s}\delta_{\sigma,\tau}, \quad (2.3)$$

and

$$\{c_{r,\sigma}^\dagger, c_{s,\tau}^\dagger\} = \{c_{r,\sigma}, c_{s,\tau}\} = 0, \quad (2.4)$$

for any $r, s \in \Lambda$ and $\sigma, \tau = \uparrow, \downarrow$, where $\{A, B\} = AB + BA$. We denote by $\Phi_{\text{vac}}$ a normalized vector state which satisfies $c_{r,\sigma}\Phi_{\text{vac}} = 0$ for any $r \in \Lambda$ and $\sigma = \uparrow, \downarrow$. Then for arbitrary subsets
Λ↑, Λ↓ ⊂ Λ, we define a state

\[
\left( \prod_{r \in \Lambda^\uparrow} c_{r,\uparrow}^\dagger \right) \left( \prod_{r \in \Lambda^\downarrow} c_{r,\downarrow}^\dagger \right) \Phi_{\text{vac}}
\]

(2.5)
in which sites in Λ↑ are occupied by up-spin electrons and sites in Λ↓ by down-spin electrons.

Next we define total spin operator \( \hat{S}_{\text{tot}} = (\hat{S}_{\text{tot}}^{(1)}, \hat{S}_{\text{tot}}^{(2)}, \hat{S}_{\text{tot}}^{(3)}) \) by

\[
\hat{S}_{\text{tot}}^{(\alpha)} = \frac{1}{2} \sum_{r \in \Lambda} c_{r,\sigma}^\dagger (p^{(\alpha)})_{\sigma,\tau} c_{r,\tau}
\]

(2.6)
for \( \alpha = 1, 2, \) and 3. Here \( p^{(\alpha)} \) are the Pauli matrices defined by

\[
p^{(1)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad p^{(2)} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad p^{(3)} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\]

(2.7)

We finally define special fermion operators as in [3]. Let \( \nu > 0 \) be a constant. For \( x \in \mathcal{E} \), let

\[
a_{x,\sigma} = c_{x,\sigma} - \frac{\nu}{2} \sum_{j \in J_x} (c_{uj,\sigma} + c_{vj,\sigma}),
\]

(2.8)
where the sum is over \( m \) sites adjacent to \( x \). For \( j \in \mathcal{J} \), let

\[
b_{j,\sigma} = c_{uj,\sigma} + c_{vj,\sigma} + \nu \sum_{x \in C_j \cap \mathcal{E}} c_{x,\sigma},
\]

(2.9)
where the sum is over the \( n \) external sites in the cell \( C_j \), and

\[
d_{j,\sigma} = c_{uj,\sigma} - c_{vj,\sigma}.
\]

(2.10)

From the anticommutation relations for the basic \( c \) operators, one can easily verify that

\[
\{a_{x,\sigma}^\dagger, b_{j,\tau}\} = \{a_{x,\sigma}^\dagger, d_{j,\tau}\} = \{b_{j,\sigma}^\dagger, d_{k,\tau}\} = 0
\]

(2.11)
for any \( x \in \mathcal{E}, j, k \in \mathcal{J}, \) and \( \sigma, \tau = \uparrow, \downarrow \).

The anticommutation relations for the \( a \) operators are

\[
\{a_{x,\sigma}^\dagger, a_{y,\tau}\} = \begin{cases} 1 + \frac{m\nu^2}{2} & \text{if } x = y, \sigma = \tau; \\ \frac{\ell_{x,y}\nu^2}{4} & \text{if } x \neq y, \sigma = \tau; \\ 0, & \text{otherwise}. \end{cases}
\]

(2.12)
For \( x, y \in \mathcal{E} \), we defined
\[
\ell_{x,y} = |\Lambda_x \cap \Lambda_y \cap \mathcal{I}|,
\] (2.13)
which is the number of the internal sites directly connected both to \( x \) and \( y \). For the \( b \) operators, we similarly have
\[
\{ b_{j,\sigma}^\dagger, b_{k,\tau} \} = \begin{cases} 2 + n\nu^2, & \text{if } j = k, \sigma = \tau; \\ \ell_{j,k} \nu^2, & \text{if } j \neq k, \sigma = \tau; \\ 0, & \text{otherwise}. \end{cases}
\] (2.14)
For \( j, k \in \mathcal{J} \), we defined
\[
\ell_{j,k} = |C_j \cap C_k \cap \mathcal{E}|,
\] (2.15)
which is the number of external sites which are included in both \( C_j \) and \( C_k \). For the \( d \) operators, we have
\[
\{ d_{j,\sigma}^\dagger, d_{k,\tau} \} = \begin{cases} 2, & \text{if } j = k, \sigma = \tau; \\ 0, & \text{otherwise}. \end{cases}
\] (2.16)
Since the states \( a_{x,\sigma}^\dagger \Phi_{\text{vac}}, b_{j,\sigma}^\dagger \Phi_{\text{vac}} \) and \( d_{j,\sigma}^\dagger \Phi_{\text{vac}} \) are linearly independent and the number of these states are \( 2|\Lambda| \), an arbitrary many-electron state of the system can be represented as a linear combination of the basis states
\[
\Psi_0(E_\uparrow, E_\downarrow, J_\uparrow, J_\downarrow, J'_\uparrow, J'_\downarrow) = \left( \prod_{x \in E_\uparrow} a_{x,\uparrow}^\dagger \right) \left( \prod_{x \in E_\downarrow} a_{x,\downarrow}^\dagger \right) \left( \prod_{j \in J_\uparrow} b_{j,\uparrow}^\dagger \right) \left( \prod_{j \in J_\downarrow} b_{j,\downarrow}^\dagger \right) \left( \prod_{j \in J'_\uparrow} d_{j,\uparrow}^\dagger \right) \left( \prod_{j \in J'_\downarrow} d_{j,\downarrow}^\dagger \right) \Phi_{\text{vac}} \] (2.17)
with arbitrary subsets \( E_\uparrow, E_\downarrow \subset \mathcal{E}, J_\uparrow, J_\downarrow, J'_\uparrow, J'_\downarrow \subset \mathcal{J} \). Here \( |E_\uparrow| + |E_\downarrow| + |J_\uparrow| + |J_\downarrow| + |J'_\uparrow| + |J'_\downarrow| = N_e \) is the total electron number.

### 2.3 An extension of Tasaki’s flat-band model

We study a Hubbard model with the Hamiltonian
\[
H = t \sum_{j=1}^{M} \sum_{\sigma=\uparrow,\downarrow} b_{j,\sigma}^\dagger b_{j,\sigma} + s' \sum_{j=1}^{M} \sum_{\sigma=\uparrow,\downarrow} d_{j,\sigma}^\dagger d_{j,\sigma} + U \sum_{r \in \Lambda} n_{r,\uparrow} n_{r,\downarrow}
\] (2.18)
where \( t > 0, s' \) and \( U \geq 0 \) are real, and \( n_{r,\sigma} = c_{r,\sigma}^\dagger c_{r,\sigma} \) is the number operator. We can rewrite the same Hamiltonian in the more standard form as
\[
H = \sum_{r,s,\sigma \in \Lambda} t_{r,s} c_{r,\sigma}^\dagger c_{s,\sigma} + U \sum_{r \in \Lambda} n_{r,\uparrow} n_{r,\downarrow}
\] (2.19)
where $t_{r,s}$ are the hopping amplitudes given by

$$
\begin{align*}
&\begin{cases}
  t_{x,x} = m t v^2, & x \in \mathcal{E}; \\
  t_{u_i,u_i} = t_{v_i,v_i} = t + s', & i \in \mathcal{J}; \\
  t_{u_i,v_i} = t_{v_i,u_i} = t - s', & i \in \mathcal{J}; \\
  t_{x,u_i} = t_{u_i,x} = t_{x,v_i} = t_{v_i,x} = \begin{cases}
    t v, & x \in \mathcal{C}_i \\
    0, & x \notin \mathcal{C}_i
  \end{cases}, & x \in \mathcal{E}, i \in \mathcal{J}; \\
  t_{x,y} = \ell_{x,y} t v^2, & x,y \in \mathcal{E}, x \neq y; \\
  t_{u_i,u_j} = t_{v_i,v_j} = t_{u_i,v_j} = 0, & i,j \in \mathcal{J}, i \neq j.
\end{cases}
\end{align*}
$$

(2.20)

From the anticommutation relations (2.11) and (2.16), one easily find that the single-electron Schrödinger equation corresponding to (2.18) has $|\mathcal{E}|$-fold degenerate eigenstates $a_{x,\sigma}^\dagger \Phi_{\text{vac}}$ with energy 0 and $M$-fold degenerate eigenstates $d_{j,\sigma}^\dagger \Phi_{\text{vac}}$ with energy $2s'$. It is also easy to see that the remaining eigenvalues are positive. We have thus defined a new class of flat-band Hubbard models. The models exhibit ferromagnetism as the following two theorems state.

**Theorem 2.1** Consider the above Hubbard model with $N_e = |\mathcal{E}| = n|\Lambda|/(2m+n)$ and $s' > 0$. For any $U > 0$, the ground states have total spin $S_{\text{tot}} = S_{\text{max}} (= N_e/2)$, and are non-degenerate apart from the trivial $(2S_{\text{max}} + 1)$-fold degeneracy.

**Theorem 2.2** Consider the above Hubbard model with $N_e = |\mathcal{E}| + |\mathcal{J}| = (n+m)|\Lambda|/(2m+n)$ and $s' = 0$. For any $U > 0$, the ground states have total spin $S_{\text{tot}} = S_{\text{max}} (= N_e/2)$, and are non-degenerate apart from the trivial $(2S_{\text{max}} + 1)$-fold degeneracy.

It is remarkable that the new models show saturated ferromagnetism at two distinct electron numbers for different values of the parameters. This is a unique property of our models.

### 3 Proof

We define the states $\Phi_{1\uparrow}, \Phi_{2\uparrow}$ as

$$
\Phi_{1\uparrow} = \left( \prod_{x \in \mathcal{E}} a_{x,\uparrow}^\dagger \right) \Phi_{\text{vac}}, \quad \Phi_{2\uparrow} = \left( \prod_{x \in \mathcal{E}} a_{x,\uparrow}^\dagger \right) \left( \prod_{j \in \mathcal{J}} d_{j,\uparrow}^\dagger \right) \Phi_{\text{vac}}.
$$

(3.1)

We decompose the Hamiltonian as $H = H_{\text{hop}} + H_{\text{int}}$ where

$$
H_{\text{hop}} = t \sum_{j=1}^{M} \sum_{\sigma=\uparrow,\downarrow} b_{j,\sigma}^\dagger b_{j,\sigma} + s' \sum_{j=1}^{M} \sum_{\sigma=\uparrow,\downarrow} d_{j,\sigma}^\dagger d_{j,\sigma},
$$

(3.2)
\[ H_{\text{int}} = U \sum_{r \in \Lambda} n_{r,\uparrow}^\dagger n_{r,\downarrow}. \] (3.3)

Note that both \( H_{\text{hop}} \) and \( H_{\text{int}} \) are positive semidefinite.

### 3.1 Proof of Theorem 2.1

We consider the case with \( N_e = |\mathcal{E}| \) and \( s' > 0 \), and prove Theorem 2.1. Since the proof is essentially the same as that found in [2, 3], we shall be brief. Since \( H \geq 0 \) and \( H \Psi_{1\uparrow} = 0 \), we see that an arbitrary ground state \( \Phi_{\text{GS}} \) satisfies

\[ H_{\text{hop}} \Phi_{\text{GS}} = 0, \quad H_{\text{int}} \Phi_{\text{GS}} = 0. \] (3.4)

From the second relation in (3.4), we further find that \( \Phi_{\text{GS}} \) must satisfy

\[ c_{r,\uparrow} c_{r,\downarrow} \Phi_{\text{GS}} = 0 \] (3.5)

for any \( r \in \Lambda \).

By using (2.17) and the first condition in (3.4), \( \Phi_{\text{GS}} \) can be represented as a linear combination of the basis states

\[ \Psi_1(E_\uparrow, E_\downarrow, J_\uparrow, J_\downarrow) = \left( \prod_{x \in E_\uparrow} a_{x,\uparrow}^\dagger \right) \left( \prod_{x \in E_\downarrow} a_{x,\downarrow}^\dagger \right) \Phi_{\text{vac}}. \] (3.6)

By using the anticommutation relations \( \{ c_{x,\sigma}, a_{y,\tau}^\dagger \} = \delta_{\sigma,\tau} \delta_{x,y} \), we see that

\[ a_{x,\uparrow}^\dagger a_{x,\downarrow}^\dagger c_{x,\uparrow} c_{x,\downarrow} \Psi_1^{(\nu)}(E_\uparrow, E_\downarrow, J_\uparrow, J_\downarrow) = \begin{cases} \Psi_1^{(\nu)}(E_\uparrow, E_\downarrow, J_\uparrow, J_\downarrow), & \text{if } x \in E_\uparrow \cap E_\downarrow; \\ 0, & \text{otherwise}, \end{cases} \] (3.7)

for any \( x \in \mathcal{E} \). By using (3.5) for \( r \in \mathcal{E} \) we find that only the basis states satisfying \( E_\uparrow \cap E_\downarrow = \emptyset \), contribute to \( \Phi_{\text{GS}} \).

In this way, \( \Phi_{\text{GS}} \) can be written as

\[ \Phi_{\text{GS}} = \sum_{\sigma} g[\sigma] \left( \prod_{x \in \mathcal{E}} a_{x,\sigma(x)}^\dagger \right) \Phi_{\text{vac}} \] (3.8)

where the sum is over all the spin configuration \( \sigma = (\sigma_x)_{x \in \mathcal{E}} \) on \( \mathcal{E} \) and \( g[\sigma] \) is a coefficient.

By using (3.8) and the anticommutation relations \( \{ c_{u_{j,\sigma}, a_{y,\tau}^\dagger} \} = -(\nu/2) \delta_{\sigma,\tau} \chi[x \in \mathcal{E} \cap C_j] \) for any \( x \in \mathcal{E} \), where \( \chi[\text{true}] = 1, \chi[\text{false}] = 0 \), we get

\[ c_{u_{j,\uparrow}^\dagger} c_{u_{j,\downarrow}} \Phi_{\text{GS}} = \frac{\nu^2}{4} \sum_{\alpha,\beta} \sum_{\sigma} \text{sgn}[\alpha,\beta] (g[\sigma] - g[\sigma_{\alpha\leftrightarrow\beta}]) \left( \prod_{x \in \mathcal{E} \setminus \{\alpha,\beta\}} a_{x,\sigma(x)}^\dagger \right) \Phi_{\text{vac}} \] (3.9)
where we have introduced an arbitrary ordering in $\mathcal{E}$ to avoid double counting and the factor $\text{sgn}[\alpha, \beta]$ comes from the exchange of fermion operators. The spin configuration $\sigma_{\alpha \leftrightarrow \beta}$ is obtained from $\sigma = (\sigma_\alpha)_{\alpha \in \mathcal{E}}$ by switching $\sigma_\alpha$ and $\sigma_\beta$. Since the basis states in (3.9) are all linearly independent, we find from the property (3.5) that

$$g[\sigma] = g[\sigma_{\alpha \leftrightarrow \beta}] \quad (3.10)$$

for the sites $\alpha, \beta$ which belong to $\mathcal{E} \cap C_j$. Since the entire lattice is connected, (3.10) ensures that the lowest energy is unique in each sector with a fixed $S_{\text{tot}}^{(3)}$. Therefore $\Phi_{1 \uparrow}$ is the unique ground state apart from the degeneracy for rotational invariance. This completes the proof of Theorem 2.1.

### 3.2 Proof of Theorem 2.2

We treat the case with $N_e = |\mathcal{E}| + |\mathcal{J}|$ and $s' = 0$, and prove Theorem 2.2. By using $\Phi_{2 \uparrow}$ instead of $\Phi_{1 \uparrow}$, we find that the conditions (3.4) and (3.5) are still valid. By using (2.17) and the first condition in (3.4), we find that an arbitrary ground state $\Phi_{\text{GS}}$ can be represented as a linear combination of the basis states

$$\Psi_2(E_\uparrow, E_\downarrow, J_\uparrow, J_\downarrow) = \left( \prod_{x \in E_\uparrow} a_{x, \uparrow}^\dagger \right) \left( \prod_{x \in E_\downarrow} a_{x, \downarrow}^\dagger \right) \left( \prod_{j \in J_\uparrow} d_{j, \uparrow}^\dagger \right) \left( \prod_{j \in J_\downarrow} d_{j, \downarrow}^\dagger \right) \Phi_{\text{vac}}. \quad (3.11)$$

As before, (3.5) and (3.7) imply that only the basis states with $E_\uparrow \cap E_\downarrow = \emptyset$ contribute to $\Phi_{\text{GS}}$. We will also prove that the basis states should satisfy $J_\uparrow \cap J_\downarrow = \emptyset$ in order to contribute to $\Phi_{\text{GS}}$. In other words, $d$ states cannot be doubly occupied in a ground state. We prove Theorem 2.2 assuming this claim.

From (3.11) and the above mentioned constraints, we have

$$\Phi_{\text{GS}} = \sum_\sigma g[\sigma] \left( \prod_{x \in \mathcal{E}} a_{x, \sigma(x)}^\dagger \right) \left( \prod_{j \in \mathcal{J}} d_{j, \sigma(u_j)}^\dagger \right) \Phi_{\text{vac}} \quad (3.12)$$

where the sum is over all the spin configurations $\sigma = (\sigma_r)_{r \in \mathcal{E} \cup \mathcal{J}}$ and $g[\sigma]$ is a coefficient. Here, for notational simplicity, we identified the index set $\mathcal{J}$ with the set of sites $\{u_j\}_{j \in \mathcal{J}}$.

By using (3.12) and the anticommutation relations $\{c_{u_j, \sigma}, a_{x, \tau}^\dagger\} = -(\nu/2)\delta_{\sigma, \tau} \chi[x \in \mathcal{E} \cap C_j]$, $\{c_{u_j, \sigma}, d_{k, \tau}^\dagger\} = \delta_{\sigma, \tau} \chi[u_k \in C_j]$ for any $x \in \mathcal{E}$, $j, k \in \mathcal{J}$, we get

$$c_{u_j, \uparrow} c_{u_j, \downarrow} \Phi_{\text{GS}} = \frac{\nu^2}{4} \sum_{\alpha, \beta \in \mathcal{E} \cap C_j} \sum_{s.t. \alpha > \beta} \text{sgn}(\alpha, \beta) (g[\sigma] - g[\sigma_{\alpha \leftrightarrow \beta}])$$
\[
-\frac{\nu}{2} \sum_{\alpha \in \mathcal{E}} \sum_{\beta \in \mathcal{C}} \sum_{\begin{array}{c}
\sigma \\
\begin{array}{c}
s.t. \sigma_\alpha = \uparrow \\
\sigma_\beta = \downarrow
\end{array}
\end{array}} \text{sgn}(\alpha, \beta)(g[\sigma] - g[\sigma_{\alpha \rightarrow \beta}])
\]

\[
\times \left( \prod_{x \in \mathcal{E}} a^\dagger_{x, \sigma(x)} \right) \left( \prod_{j \in \mathcal{J}} d^\dagger_{j, \sigma(u_j)} \right) \Phi_{\text{vac}}.
\] (3.13)

Since this quantity vanishes for all \( j \in \mathcal{J} \), we finally find that
\[
g[\sigma] = g[\sigma_{\alpha \rightarrow \beta}].
\] (3.14)

Since the entire lattice is connected, (3.14) ensures that the lowest energy state is unique in each sector with a fixed \( S_{\text{tot}}^{(3)} \). Therefore \( \Phi_{2\uparrow} \) is the unique ground state apart from the degeneracy for rotational invariance. This completes the proof of Theorem 2.2.

It remains to prove that \( d \) states cannot be doubly occupied. Since \( a \) states cannot be doubly occupied, the ground state can be expanded in the basis states (3.11) as
\[
\Phi_{\text{GS}} = \sum_{E_\uparrow, E_\downarrow, J_\uparrow, J_\downarrow} f(E_\uparrow, E_\downarrow, J_\uparrow, J_\downarrow) \Psi_2(E_\uparrow \setminus \{x\}, E_\downarrow \setminus \{y\}, J_\uparrow, J_\downarrow).
\] (3.15)

Let \( u_j \) and \( v_j \) be the internal sites which belong to a cell \( C_j \). By using (3.15) and the anticommutation relations \( \{c_{u_j, \sigma}, a^\dagger_{x, \tau}\} = -(\nu/2)\delta_{\sigma, \tau} \chi[x \in \mathcal{E} \cap C_j], \{c_{v_j, \sigma}, d^\dagger_{k, \tau}\} = \delta_{\sigma, \tau} \chi[u_k \in C_j], \{c_{v_j, \sigma}, d^\dagger_{k, \tau}\} = -\delta_{\sigma, \tau} \chi[u_k \in C_j] \) for any \( x \in \mathcal{E}, j, k \in \mathcal{J} \), we get
\[
c_{\gamma_j, \uparrow} c_{\gamma_j, \downarrow} \Phi_{\text{GS}} = \frac{\nu^2}{4} \sum_{x, y \in C_j} \sum_{E_\uparrow, E_\downarrow, J_\uparrow, J_\downarrow} \sum_{\begin{array}{c}
s.t. x \in E_\uparrow, y \in E_\downarrow \\
E_\uparrow \cap E_\downarrow = \emptyset
\end{array}} f(E_\uparrow, E_\downarrow, J_\uparrow, J_\downarrow) \text{sgn}(x, y) \Psi_2(E_\uparrow \setminus \{x\}, E_\downarrow \setminus \{y\}, J_\uparrow, J_\downarrow)
\]
\[
\pm \frac{\nu}{2} \sum_{x \in C_j} \sum_{E_\uparrow, E_\downarrow, J_\uparrow, J_\downarrow} \sum_{\begin{array}{c}
s.t. x \in E_\uparrow, y \in E_\downarrow \\
E_\uparrow \cap E_\downarrow = \emptyset
\end{array}} f(E_\uparrow, E_\downarrow, J_\uparrow, J_\downarrow) \text{sgn}(x, u_j) \Psi_2(E_\uparrow \setminus \{x\}, E_\downarrow, J_\uparrow, J_\downarrow \setminus \{j\})
\]
\[
\pm \frac{\nu}{2} \sum_{y \in C_j} \sum_{E_\uparrow, E_\downarrow, J_\uparrow, J_\downarrow} \sum_{\begin{array}{c}
s.t. y \in E_\downarrow, x \in E_\uparrow \\
E_\uparrow \cap E_\downarrow = \emptyset
\end{array}} f(E_\uparrow, E_\downarrow, J_\uparrow, J_\downarrow) \text{sgn}(u_j, y) \Psi_2(E_\uparrow, E_\downarrow \setminus \{y\}, J_\uparrow \setminus \{j\}, J_\downarrow)
\]
\[ + \sum_{E', E_1, J_1 \in J_1 \atop s.t. E' \cap E_1 = \emptyset} \sum_{j \in J_1} f(E_1, E_1', J_1', J_1) \text{sgn}(u_j, u_j) \Psi_2(E_1, E_1, J_1' \{j\}, J_1' \{j\}) \] (3.16)

where \( \mp \) is \(-\) for \( \gamma = u \) and \(+\) for \( \gamma = v \), and \( \text{sgn}(x, y) \) depend on the sites \( x, y \) and \( E_1, E_1', J_1, J_1' \).

These quantities vanish for all \( j \in J \) because of (3.15). By adding these two relations thus obtained, we find that

\[ \sum_{E_1, E_1', J_1, J_1' \in J_1 \atop s.t. E_1 \cap E_1' = \emptyset} \sum_{J_1 \cap J_1' = \emptyset} f(E_1, E_1, J_1, J_1') \text{sgn}(x, y) \Psi_2(E_1 \{x\}, E_1' \{y\}, J_1, J_1') = 0 \] (3.17)

The linear independence of \( \Psi_2 \) implies that each coefficient of \( \Psi_2 \) in (3.17) is vanishing. This means that

\[ f(E_1, E_1, J_1, J_1) \text{sgn}(u_j, u_j) = \]

\[ -\frac{\nu^2}{4} \sum_{x, y \in C_j} \sum_{E_1', E_1', J_1', J_1' \in J_1 \atop E_1' \cap E_1' = \emptyset} \sum_{s.t. E_1 \{x\}, E_1' \{y\}, J_1' \{j\} = \emptyset} f(E_1', E_1', J_1', J_1') \text{sgn}(x, y) \] (3.18)

for any \( E_1, E_1' \subset E \) and \( J_1, J_1' \subset J \) with \( E_1 \cap E_1' = \emptyset \). Note that the two electrons occupying the same \( d \) state in \( \{E_1, E_1', J_1, J_1'\} \) are removed and added to \( E \) in the new configuration \( \{E_1', E_1', J_1', J_1'\} \).

Now suppose that \( d \) state is doubly occupied in \( r \) different cells. More precisely we assume that there is a configuration \( \{E_1, E_1', J_1, J_1'\} \) with \( f(E_1, E_1', J_1, J_1') \neq 0 \) such that \( |J_1 \cap J_1'| = r \). We use the relation (3.18) to this configuration by setting \( j \in J_1 \cap J_1' \). Then one finds that the summation in the right-hand side of (3.18) is over configurations \( \{E_1', E_1', J_1', J_1'\} \) where the \( d \) state in \( C_j \) is not occupied and there are two more occupied \( a \) states compared with the original configuration. Thus \( \{E_1', E_1', J_1', J_1'\} \) has \( (r - 1) \) cells with doubly occupied \( d \) states and at least one cell with the empty \( d \) state. Because of (3.18), there is at least one such
configuration with non-vanishing $f(E'_\uparrow, E'_\downarrow, J'_\uparrow, J'_\downarrow)$. Repeating the argument $r$ times, one concludes that there is at least one configuration $\{E'_\uparrow, E'_\downarrow, J'_\uparrow, J'_\downarrow\}$ with $f(E'_\uparrow, E'_\downarrow, J'_\uparrow, J'_\downarrow) \neq 0$ which has no cells with doubly occupied $d$ states and at least $r$ cells with no $d$ states. But this is a contradiction since the maximum possible electron number for such a configuration is $|E| + |J| - r < |E| + |J| = N_e$. This proves the desired claim that $r$ is always 0.

4 Discussions

Let us make two remarks about our model.

First we discuss the mechanisms that generate ferromagnetism in the present and Tasaki’s models. In Tasaki’s models, electrons in the lowest flat-band may be regarded (in the basis corresponding to the $a$ operators) as almost localized at external sites. Roughly speaking, a small overlap of the wave functions at an internal site generates “exchange interaction” which leads to ferromagnetism as in Fig. 3 (a). In the situation of Theorem 2.1, the picture is almost the same in our models. The electrons are almost localized at external sites and overlap at intermediate sites as in Fig. 3 (b). In the situation of Theorem 2.2, however, the picture is essentially different from that in Tasaki’s model. Each electron in the lowest flat bands is either almost localized at an external site or localized at a pair of internal sites. The basic “exchange interaction” involves three electrons as in the Fig. 3 (c). This is why the proof of Theorem 2.2 required a new technique.

Secondly let us discuss the possibility of further extending Tasaki’s construction. A natural question is whether one can treat models with three or more internal sites. As for results corresponding to Theorem 2.1, it is obvious that our proof (and Tasaki’s original proof) automatically extends to such models. But results corresponding to Theorem 2.2

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{exchange_mechanisms.png}
\caption{Exchange mechanisms in the one dimensional models. (a) An almost localized state for electrons in the lowest flat-band (a state). (b) In the case of Theorem 2.1, overlap of two states almost localized at neighboring external sites generate ferromagnetism just as in Tasaki’s flat-band model. (c) In the case of Theorem 2.2, the exchange interaction also involves a state localized at two internal sites.}
\end{figure}
which involves a new exchange mechanism, are much more delicate. We suspect that a new idea is required to cover the general cases.

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