Ferromagnetism in the Hubbard Model with a Gapless Nearly-Flat Band

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Abstract We present a version of the Hubbard model with a gapless nearly-flat lowest band which exhibits ferromagnetism in two or more dimensions. The model is defined on a lattice obtained by placing a site on each edge of the hypercubic lattice, and electron hopping is assumed to be only between nearest and next nearest neighbor sites. The lattice, where all the sites are identical, is simple, and the corresponding single-electron band structure, where two cosine-type bands touch without an energy gap, is also simple. We prove that the ground state of the model is unique and ferromagnetic at half-filling of the lower band, if the lower band is nearly flat and the strength of on-site repulsion is larger than a certain value which is independent of the lattice size. This is the first example of ferromagnetism in three dimensional non-singular models with a gapless band structure.

Keywords Hubbard model · Ferromagnetism · Gapless band structure · Nearly-flat band

1 Introduction

Since the Hubbard model, a simple tight-binding model with on-site repulsion, was formulated in the early 1960s, numerous attempts have been made on it to understand mechanisms for itinerant-electron ferromagnetism [1–3]. To date, some rigorous examples of ferromagnetism [4], ferromagnetism [5–15] and metallic ferromagnetism [16,17] in the Hubbard model have been proposed, and it is well recognized that an interplay between the quantum mechanical motion of electrons and repulsive interaction between electrons does generate ferromagnetism.

Among the others, flat-band models proposed by Mielke and Tasaki provided a significant breakthrough in understanding of itinerant-electron ferromagnetism [6–11]. The flat-band models in common have multi single-electron bands including a flat (highly degenerate) lowest band. In these models, one finds that electrons occupy the flat band in order to minimize...
the kinetic energy and then the spins of electrons occupying the flat band align parallel to each other, i.e., align ferromagnetically, in order to avoid an increase of energy due to on-site repulsion. The next important step was also taken by Tasaki, who proved that the ferromagnetism in flat-band models on lattices constructed by the cell-construction method is stable against perturbations which turn flat bands into dispersive ones provided that the on-site repulsion is sufficiently large [12,13]. Note that an electron has a tendency to occupy a lower kinetic energy state when the repulsion is small. Tasaki’s models which have dispersive bands thus exhibit the Pauli paramagnetism when the on-site repulsion is vanishing, and remain nonferromagnetic when the on-site repulsion is small. Tasaki’s models could describe the true competition between the kinetic energy and the on-site repulsion, and established that the spin-independent repulsion can cause the itinerant-electron ferromagnetism.

Although the stability of ferromagnetism in Tasaki’s models is shown in rather general settings, as for Mielke’s flat-band models on line graphs, less is known about stability or instability of ferromagnetism in perturbed nearly-flat-band models. Here we note that there are no band gaps above flat lowest bands in Mielke’s flat-band models, whereas there are finite band gaps in Tasaki’s models and corresponding (unperturbed) flat-band models. This is an essential difference. The occurrence of ferromagnetism in Tasaki’s models, at least at a heuristic level, can be understood as a consequence of the band gap as follows. The band gap enforces the electrons to occupy the lowest nearly-flat band while the on-site repulsion forbids double occupancy of sites. Then, despite that the lowest band is dispersive, the situation is almost as in the flat-band models, and the system exhibits ferromagnetism. In fact, a certain parameter in hopping amplitudes which controls the energy gap in the band structure plays an important role in the rigorous proof of ferromagnetism in Tasaki’s models. On the other hand, it is more subtle and difficult to show the stability of ferromagnetism against a perturbation in Mielke’s flat-band models since there might be various low energy excitation modes reflecting a gapless nature of the band structure. Some examples of nearly-flat-band models related to Mielke’s flat-band models in two dimensions, such as models on the kagome lattice and on the regular lattice of corner sharing tetrahedra [14,15], have been proposed and proved to have ferromagnetic ground states; as far as we know, however, there are no examples in three or more dimensions.

In this paper, we propose a version of the Hubbard model which has a gapless nearly-flat lowest band and exhibits ferromagnetism in the ground state in two or more dimensions. Our model is defined on a lattice obtained by placing a site on each edge of the hypercubic lattice. In a certain case, it is reduced to a gapless flat-band model. In two dimensions the corresponding flat-band model is Mielke’s flat-band model on the regular lattice of corner sharing tetrahedra. In three or more dimensions, the corresponding flat-band model is slightly different from Mielke’s one, but they are closely related. Although the perturbative hopping term considered in this paper is rather special, our model is simple such that all the lattice sites are identical and electron hopping is assumed to be only between nearest and next nearest neighbor sites. We believe that our model is helpful for a better understanding of ferromagnetism in the Hubbard model.

2 Definition of the Model and the Main Result

2.1 Definition of the Lattice

We start by describing the lattice $\Lambda$ on which our Hubbard Hamiltonian is defined. Let $G = (V, E)$ be a graph, where $V$ is a set of vertices and $E$ is a set of edges. The vertex set $V$ is assumed to be a subset of $\mathbb{Z}^\nu$ with $\nu \geq 2$. 

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Fig. 1 The lattice structure for $\nu = 2$. Thin lines represent edges in $E$ and filled circles represent lattice sites. For example, the subsets $\mathcal{P}(x)$ and $\mathcal{P}_{x}$ of $\mathcal{P}$ are given by $\mathcal{P}(x) = \{p_1, p_2\}$ and $\mathcal{P}_{x} = \{p_1, p_2, p_3, p_4\}$, respectively. The subset $\mathcal{C}_{x}$ of the lattice sites is $\{w, x, y, z\}$.

\[
\mathcal{V} = \left\{ \alpha = (\alpha_1, \ldots, \alpha_\nu) \mid \alpha_l \in \mathbb{Z}, -\frac{L-1}{2} \leq \alpha_l \leq \frac{L-1}{2} \text{ for } l = 1, \ldots, \nu \right\},
\]

where $L$ is an odd integer.\(^1\) We impose periodic boundary conditions in all directions.\(^2\)

Let $e(\alpha, \beta)$ be a line segment between nearest neighbor vertices $\alpha$ and $\beta$ in $\mathcal{V}$. The edge set $E$ is a collection of these line segments,\(^3\)

\[
E = \{e(\alpha, \beta) \mid \alpha, \beta \in \mathcal{V}, |\alpha - \beta| = 1\}.
\]

For each edge $e(\alpha, \beta)$ in $E$, we denote by $m(\alpha, \beta)$ the point taken in the middle of $\alpha$ and $\beta$. Then we define the lattice $\Lambda$ as a collection of these mid-points

\[
\Lambda = \{x = m(\alpha, \beta) \mid e(\alpha, \beta) \in \mathcal{E}\}.
\]

Before proceeding to the definition of our Hubbard Hamiltonian, let us introduce some more notation. Let $\mathcal{P}$ be the set of all regular squares with side-length 1 whose corners are located at vertices in $\mathcal{V}$. For four edges of a regular square $p$ in $\mathcal{P}$, we find the corresponding mid-points, sites in $\Lambda$, which we denote by $x_i(p)$ with $i = 1, 2, 3, 4$. For convenience, we assume that $x_3(p)$ denotes the site opposite to that denoted by $x_1(p)$. Each edge whose mid-point is $x$ is shared by $2(\nu - 1)$ regular squares in $\mathcal{P}$; we denote by $\mathcal{P}(x)$ the collection of these regular squares. Each vertex $\alpha$ in $\mathcal{V}$ is shared by $2\nu(\nu - 1)$ regular squares in $\mathcal{P}$; we denote by $\mathcal{P}_{\alpha}$ the collection of these regular squares. Each vertex $\alpha$ in $\mathcal{V}$ is shared by $2\nu$ edges, $e(\alpha, \alpha + \delta_l)$ and $e(\alpha, \alpha - \delta_l)$ with $l = 1, \ldots, \nu$, where $\delta_l$ denotes the unit vector along the $l$-axis. We define $\mathcal{C}_{\alpha}$ as the collection of the mid-points of these edges

\[
\mathcal{C}_{\alpha} = \{x = m(\alpha, y) \mid y = \alpha \pm \delta_l, l = 1, \ldots, \nu\}.
\]

The lattice structure for $\nu = 2$ is shown in Fig. 1.

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\(^1\) The reason why we choose $L$ to be an odd integer is only technical. We can treat the case of even $L$ with a slight modification.

\(^2\) This condition is also imposed to simplify the argument. It is easy to apply the present method to the model with open boundary conditions.

\(^3\) For $\alpha$ in $\mathcal{V}$ or $x$ in $\Lambda$ defined by (3), $|\alpha|$ or $|x|$ denotes the usual Euclidean distance. For a set $X$, we use the same symbol $|X|$ to denote the number of elements in $X$. 
2.2 Definition of the Hamiltonian and the Main Result

Let $c_{x,\sigma}$ and $c_{x,\sigma}^\dagger$ be annihilation and creation operators, respectively, of an electron with spin $\sigma$ at a site $x$ in $\Lambda$. These operators satisfy the anticommutation relations

$$\{c_{x,\sigma}, c_{y,\tau}\} = \{c_{x,\sigma}^\dagger, c_{y,\tau}^\dagger\} = 0$$

and

$$\{c_{x,\sigma}^\dagger, c_{y,\tau}\} = \delta_{x,y}\delta_{\sigma,\tau}$$

for $x, y \in \Lambda$ and $\sigma, \tau = \uparrow, \downarrow$. The number operator is defined by

$$n_{x,\sigma} = c_{x,\sigma}^\dagger c_{x,\sigma}.$$

The total spin operators $S_{\text{tot}} = (S_{\text{tot}}^{(1)}, S_{\text{tot}}^{(2)}, S_{\text{tot}}^{(3)})$ of the system are defined by

$$S_{\text{tot}}^{(i)} = \frac{1}{2} \sum_{x \in \Lambda} \sum_{\sigma, \tau = \uparrow, \downarrow} c_{x,\sigma}^\dagger \mathbf{p}^{(i)}_{\sigma\tau} c_{x,\tau}$$

for $i = 1, 2, 3$, where $\mathbf{p}^{(i)} = [\mathbf{p}^{(i)}_{\sigma\tau}]_{\sigma, \tau = \uparrow, \downarrow}$ are the Pauli matrices

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

We also define the raising and lowering operators on the eigenvalues of $S_{\text{tot}}^{(3)}$ by $S_{\text{tot}}^{+} = S_{\text{tot}}^{(1)} + i S_{\text{tot}}^{(2)}$ and $S_{\text{tot}}^{-} = S_{\text{tot}}^{(1)} - i S_{\text{tot}}^{(2)}$, respectively. We denote by $S_{\text{tot}}(S_{\text{tot}} + 1)$ the eigenvalue of $(S_{\text{tot}})^2$.

We consider the Hubbard Hamiltonian on the lattice $\Lambda$ given by

$$H = H_{\text{hop}} + H_{\text{int}},$$

where the first term in the right-hand side,

$$H_{\text{hop}} = \sum_{\sigma = \uparrow, \downarrow} \sum_{x, y \in \Lambda} t_{x,y} c_{x,\sigma}^\dagger c_{y,\sigma},$$

with real parameters $t_{x,y}$, which we will specify below, represents energy associated with the quantum mechanical motion of electrons, and the second term,

$$H_{\text{int}} = U \sum_{x \in \Lambda} n_{x,\uparrow} n_{x,\downarrow},$$

with $U > 0$, represents a repulsive interaction between electrons with up- and down-spin at the same site.

The parameter $t_{x,y}$, which is called the hopping amplitude, is defined as follows. First we introduce new fermion operators. For each vertex $\alpha$ in $\mathcal{V}$, let

$$a_{\alpha,\sigma} = \sum_{x \in C_{\alpha}} c_{x,\sigma},$$

and for each regular square $p$ in $\mathcal{P}$, let

$$b_{p,\sigma} = \sum_{i=1}^{4} (-1)^i c_{x_i(p),\sigma},$$

(see Fig. 2). We note that the following anticommutation relations are satisfied:
Fig. 2 The states corresponding to \( a \)- and \( b \)-operators. Thin lines represent edges in \( \mathcal{E} \). a \( \nu = 2 \). b \( \nu = 3 \)

\[
\{ a_{\alpha, \sigma}^\dagger, a_{\beta, \sigma} \} = \begin{cases} 
2\nu & \text{if } \alpha = \beta; \\
1 & \text{if } |\alpha - \beta| = 1; \\
0 & \text{otherwise}, 
\end{cases}
\]  

(14)

and

\[
\{ b_{p, \sigma}^\dagger, b_{q, \sigma} \} = \begin{cases} 
4 & \text{if } p = q; \\
\mu[p, q] & \text{if } p \text{ and } q \text{ share a common edge}; \\
0 & \text{otherwise}, 
\end{cases}
\]  

(15)

where \( \mu[p, q] = (-1)^{i+j} \) when the mid-point of the common edge corresponds to \( x_i(p) \) as well as \( x_j(q) \). We also note that the anticommutation relation

\[
\{ a_{\alpha, \sigma}^\dagger, b_{p, \tau} \} = 0
\]

(16)

holds for any \( \alpha \in \mathcal{V} \), any \( p \in \mathcal{P} \) and \( \sigma, \tau = \uparrow, \downarrow \). Then we define the hopping amplitudes \( t_{x, y} \) so that the hopping term \( H_{\text{hop}} \) can be written as

\[
H_{\text{hop}} = -s \sum_{\sigma = \uparrow, \downarrow} \sum_{\alpha \in \mathcal{V}} a_{\alpha, \sigma}^\dagger a_{\alpha, \sigma} + t \sum_{\sigma = \uparrow, \downarrow} \sum_{p \in \mathcal{P}} b_{p, \sigma}^\dagger b_{p, \sigma}
\]

(17)
The hopping amplitudes for $\nu = 2$. Filled circles represent lattice sites with parameters $s \geq 0$ and $t > 0$. Explicitly the hopping amplitudes are given by

$$t_{x,y} = \begin{cases} 
-2s + 2(\nu - 1)t & \text{if } x = y; \\
-s & \text{if } |x - y| = 1 \text{ and } m(x, y) \in \mathcal{V} \\
t & \text{if } |x - y| = 1 \text{ and } m(x, y) \notin \mathcal{V}; \\
-(s + t) & \text{if } |x - y| = \sqrt{2}; \\
0 & \text{otherwise},
\end{cases}$$

(18)

where $m(x, y)$ is defined to be the point taken in the middle of sites $x$ and $y$ in $\Lambda$, as in the case of $m(\alpha, \beta)$ for $\alpha, \beta \in \mathcal{V}$ (see Fig. 3).

The main result of this paper is the occurrence of ferromagnetism in the model defined above at zero temperature:

**Theorem 1** Consider the Hubbard Hamiltonian $H$ with the hopping matrix given by (18), and suppose that the number $N_e$ of electrons is $|\mathcal{V}|$. Then, for each value of $s$ there exist $t_c$ and $U_c$ which are independent of the lattice size $|\mathcal{V}|$ such that for $t > t_c$ and $U > U_c$, the following are valid:

1. the ground state energy is $-2\nu s|\mathcal{V}|$,
2. the ground states have the maximal total spin $S_{\text{tot}} = N_e/2$,
3. the ground state is unique apart from $(2S_{\text{tot}} + 1)$-fold degeneracy due to the spin rotation symmetry.

In the case $s = 0$, the single-electron ground state energy is zero and $|\mathcal{V}|$-fold degenerate, as we will see in the next section. In this case, the model corresponds to the flat-band Hubbard model and the ground state exhibits saturated ferromagnetism for all positive values of $t$ and $U$ ($t_c = 0$, $U_c = 0$). In particular, in the case $\nu = 2$, our model with $s = 0$ is equivalent to the flat-band Hubbard model on the line graph of the square lattice, and the occurrence of saturated ferromagnetism in the model was proved by Mielke [6,7]. Our model in three or more dimensions, however, does not belong to the flat-band models on line graphs. It is also noted that our model does not belong to the class of flat-band models discussed in detail by Mielke and Tasaki [11]. We will give the proof of Theorem 1 for $s = 0$ in Appendix.

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4 One finds that our model with $s = 0$ is unitary equivalent to Mielke’s flat-band model by performing a gauge transformation $c_{x,\sigma} \rightarrow -c_{x,\sigma}$ at all sites in one of the two sublattices, say, $\{x = m(\alpha, \alpha + \delta_1) | \alpha \in \mathcal{V}\}$. 
On the other hand, the lowest band of the model is dispersive for $s > 0$, and the proof for such cases is quite different from that for the flat-band case. Here we adopt the same idea which is used for proving the occurrence of ferromagnetism in Tasaki’s models [12,13]. We first decompose the Hamiltonian $H$ into local Hamiltonians, and investigate their properties, in particular, conditions for states to attain the local minimum energy in detail. Then the ferromagnetic state is shown to attain the minimum energy simultaneously for all the local Hamiltonians for $t > t_c$ and $U > U_c$. That is, the model is “frustration free” when the lower band supporting the ferromagnetism is almost flat and the on-site repulsion is sufficiently large. It is noted that, compared with Tasaki’s nearly-flat band case, we need more lengthy discussion about local properties because of the gapless nature of our model. We will devote ourselves to such discussion in Sect. 4 and complete the proof for the case $s > 0$ in Sect. 5.

3 Single-Electron Dispersion Relations and Basis States of the $N_e$-Electron Space

Let us consider the single-electron Schrödinger equation for our Hubbard Hamiltonian. Let $\Phi_{1,\sigma}$ be a single-electron state

$$\Phi_{1,\sigma} = \sum_{x \in A} \phi_x c_{x,\sigma}^\dagger \Phi_0,$$

where $\phi_x$ is a complex coefficient and $\Phi_0$ is the state with no electron in $A$. Applying $H$ to $\Phi_{1,\sigma}$, we obtain the eigenvalue equation

$$\sum_{y \in A} t_{x,y} \phi_y = \varepsilon \phi_x,$$

where $\varepsilon$ denotes a single-electron energy eigenvalue.

Because of the translation invariance of the Hamiltonian, we can write an eigenstate $(\phi_x)_{x \in A}$ in the form of the Bloch state as $\phi_x = e^{ik \cdot x} v_x(k)$, where $v_x(k)$ satisfies $v_x(k) = v_{x+z}(k)$ for any $z \in \mathbb{Z}^\nu$ and $k$ is an element in $\mathcal{K}$ defined by

$$\mathcal{K} = \left\{ k = (k_1, \ldots, k_\nu) \mid k_l = \frac{2\pi}{L} n_l, \ n_l = 0, \pm 1, \ldots, \pm \frac{L-1}{2} \text{ for } l = 1, \ldots, \nu \right\}.$$

Then the eigenvalue equation is reduced to

$$\begin{pmatrix} -4s \cos^2 \frac{k_l}{2} + 4t \sum_{m=1 \atop m \neq l}^\nu \cos^2 \frac{k_m}{2} \end{pmatrix} v_l - 4(s + t) \sum_{m=1 \atop m \neq l}^\nu \left( \cos \frac{k_m}{2} \right) v_m = \varepsilon v_l$$

with $l = 1, \ldots, \nu$, where we write $v_l$ for $v_{k_l/2}(k)$ for notational simplicity.

Setting $A_{l,m} = \cos(k_l/2) \cos(k_m/2)$ and

$$\varepsilon' = -\frac{1}{s + t} \left( \frac{\varepsilon}{4} - t \sum_{l=1}^\nu \cos^2 \frac{k_l}{2} \right),$$
we can further rewrite (22) as
\[
\sum_{m=1}^{\nu} A_{l,m} v_m = \varepsilon' v_l.
\]
(24)

It is easy to see that the rank of matrix \( A = [A_{l,m}]_{1 \leq l, m \leq \nu} \) is 1, and therefore \( \varepsilon' = 0 \) is the \((\nu - 1)\)-fold degenerate eigenvalue of \( A \). It is also easy to see that the vector \((v_m)_{m=1}^{\nu} = (\cos(k_1/2), \cos(k_2/2), \ldots, \cos(k_{\nu}/2))\) is an eigenstate of \( A \) and its eigenvalue is given by
\[
\varepsilon' = \sum_{l=1}^{\nu} \cos^2 \frac{k_l}{2}.
\]
(25)

As a result we obtain the single-electron energy eigenvalues which are characterized by the dispersion relations
\[
\varepsilon_0(k) = -4s \sum_{l=1}^{\nu} \cos^2 \frac{k_l}{2} = -2s \sum_{l=1}^{\nu} (1 + \cos k_l)
\]
(26)

and
\[
\varepsilon_1(k) = 4t \sum_{l=1}^{\nu} \cos^2 \frac{k_l}{2} = 2t \sum_{l=1}^{\nu} (1 + \cos k_l).
\]
(27)

The eigenvalue \( \varepsilon_1(k) \) is \((\nu - 1)\)-fold degenerate for each \( k \). See Fig. 4 for the dispersion relations for \( \nu = 2 \).

In the case of \( s = 0 \), \( \varepsilon_0(k) = 0 \) for all \( k \in \mathcal{K} \), i.e., the single-electron ground state energy is zero and \(|\mathcal{V}|\)-fold degenerate.

In the rest of this section we comment on a construction of \( N_e \)-electron states.

Let us denote by \( f_{(0,k),\sigma} \) a fermion operator corresponding to the eigenstate with the eigenvalue \( \varepsilon_0(k) \). We also denote by \( f_{(l,k),\sigma} \) with \( l = 1, \ldots, \nu - 1 \) fermion operators corresponding to linearly independent \( \nu - 1 \) eigenstates with the eigenvalue \( \varepsilon_1(k) \). Then, owing to linear independence of the energy eigenstates, any \( N_e \)-electron state can be represented as a linear combination of the states.
\[
\left( \prod_{i \in A_{\uparrow}} f_{i,\uparrow}^\dagger \right) \left( \prod_{i \in A_{\downarrow}} f_{i,\downarrow}^\dagger \right) \Phi_0
\]
with \(|A_{\uparrow}| + |A_{\downarrow}| = N_e\), where \(A_{\uparrow}\) and \(A_{\downarrow}\) are arbitrary subsets of \(\{i = (l, k) \mid l = 0, \ldots, \nu - 1, k \in \mathcal{K}\}\).

(28)

It is crucial to find that the fermion operators \(f_{(0,k),\sigma}\) can be expanded as a linear combination of \(a_{\alpha,\sigma}\). This is observed as follows. First we note that \(\sum_{\alpha \in \mathcal{V}} u_{\alpha} a_{\alpha,\sigma} \Phi_0\) is zero if and only if \(u_{\alpha} = 0\) for all \(\alpha \in \mathcal{V}\), i.e., the states \(a_{\alpha,\sigma} \Phi_0\) are linearly independent. Next consider the single-electron Schrödinger equation

\[ H \sum_{\beta \in \mathcal{V}} \phi_{\beta} a_{\beta,\sigma} \Phi_0 = \varepsilon \sum_{\beta \in \mathcal{V}} \phi_{\beta} a_{\beta,\sigma} \Phi_0, \]

(30)

where \(\phi_{\beta}\) are complex coefficients and \(\varepsilon\) is real. By using the anticommutation relations (14) and (16), we reduce the left-hand side of the above equation to a linear combination of \(a_{\beta,\sigma} \Phi_0\). Then, comparing the coefficients of \(a_{\beta,\sigma} \Phi_0\) in the left- and the right-hand sides, we obtain

\[ -2\nu s \phi_{\beta} - s \sum_{\alpha \in \mathcal{V}} \phi_{\alpha} = \varepsilon \phi_{\beta}. \]

(31)

By solving the above equation we obtain the eigenvalue \(\varepsilon_0(k)\) with \(k \in \mathcal{K}\). Therefore the sets \(\{f_{(0,k),\sigma}\}_{k \in \mathcal{K}}\) and \(\{a_{\alpha,\sigma} \Phi_0\}_{\alpha \in \mathcal{V}}\) span the same space. This also indicates the fact that any \(N_e\)-electron state can be represented as a linear combination of the states

\[
\Phi \left( V_{\uparrow}, B_{\uparrow}; V_{\downarrow}, B_{\downarrow} \right) = \left( \prod_{\alpha \in V_{\uparrow}} a_{\alpha,\uparrow}^\dagger \right) \left( \prod_{i \in B_{\uparrow}} f_{i,\uparrow}^\dagger \right) \left( \prod_{\alpha \in V_{\downarrow}} a_{\alpha,\downarrow}^\dagger \right) \left( \prod_{i \in B_{\downarrow}} f_{i,\downarrow}^\dagger \right) \Phi_0
\]

with \(|V_{\uparrow}| + |V_{\downarrow}| + |B_{\uparrow}| + |B_{\downarrow}| = N_e\), where \(V_{\uparrow}\) and \(V_{\downarrow}\) are arbitrary subsets of \(\mathcal{V}\), and \(B_{\uparrow}\) and \(B_{\downarrow}\) are arbitrary subsets of \(\{i = (l, k) \mid l = 1, \ldots, \nu - 1, k \in \mathcal{K}\}\).

(32)

\(4\) Local Properties of the Model

In this section we represent the Hamiltonian (9) as a sum of local Hamiltonians and investigate properties of the local Hamiltonians. As a consequence we will obtain a lemma which will play a central role in the proof of Theorem 1 for \(s > 0\).

4.1 Decomposition of the Hamiltonian

For each vertex \(\alpha \in \mathcal{V}\), we define the sublattice \(A_\alpha\) as

\[ A_\alpha = \{ x = x_i(p) \mid i = 1, \ldots, 4, \ p \in \mathcal{P}_\alpha \}, \]

(34)

which is the collection of the sites on the edges of the regular squares which share vertex \(\alpha\). (In the case \(\nu = 2\), \(A_\alpha\) consists of 12 filled circles depicted in Fig. 3.) Then we define the local Hamiltonian \(h_\alpha\) on the lattice \(A_\alpha\) by
\[ h_\alpha = -s \sum_{\sigma=\uparrow,\downarrow} a_{\alpha,\sigma}^\dagger a_{\alpha,\sigma} + \frac{t}{4} \sum_{\sigma=\uparrow,\downarrow} \sum_{p \in P} b_{p,\sigma}^\dagger b_{p,\sigma} + \frac{U}{2(2\nu-1)} \sum_{x \in \Lambda_\alpha} n_{x,\uparrow} n_{x,\downarrow}. \]  

By using \( h_\alpha \), the Hamiltonian \( H \) is decomposed as

\[ H = \sum_{\alpha \in V} h_\alpha. \]

It is noted that the local Hamiltonians do not commute with one another, and it is thus not trivial to find out something about the whole system, such as the energy and magnetic properties of the ground state, by using these local Hamiltonians.

The properties of the local Hamiltonian \( h_\alpha \) for sufficiently large values of \( U/s \) and \( t/s \) are summarized in the following lemma.

**Lemma 1** Consider the local Hamiltonian \( h_\alpha \) on the Hilbert space where the electron number on the local lattice \( \Lambda_\alpha \) is not fixed. Suppose that \( t/s \) and \( U/s \) are sufficiently large. Then the minimum eigenvalue of \( h_\alpha \) is \(-2\nu s\) and any eigenstate \( \Phi \) with this eigenvalue can be expressed as

\[ \Phi = a_{\alpha,\uparrow}^\dagger \Phi_\uparrow + a_{\alpha,\downarrow}^\dagger \Phi_\downarrow, \]  

by using some states \( \Phi_\uparrow \) with \( a_{\alpha,\downarrow} \Phi_\uparrow = 0 \) and \( \Phi_\downarrow \) with \( a_{\alpha,\uparrow} \Phi_\downarrow = 0 \). Furthermore, \( \Phi \) satisfies

\[ c_{x,\downarrow} c_{x,\uparrow} \Phi = 0 \]  

for all \( x \in \Lambda_\alpha \).

The above lemma claims that electrons do not doubly occupy the localized states corresponding to \( a_{\alpha,\sigma} \) when the strength of the repulsive interaction is sufficiently large and the high-energy part of local single-electron energy eigenvalues is well separated from the lower levels.

It is remarked that a similar lemma is proved for Tasaki’s models and the proof of our lemma proceeds in almost the same way as in [12, 13]. However, the proof for our case is much more involved. The difference is due to the following reason. The localized states corresponding to \( a \)-operators in Tasaki’s models contain a parameter which controls a band gap or hopping amplitudes. By taking a certain limit of this parameter, the local Hamiltonians of Tasaki’s models are reduced to “atomic Hamiltonians”, which have no hoppings of electrons. This fact makes it somewhat easier to treat the local Hamiltonians. On the other hand, our model does not contain such a parameter, and we have to prove the lemma by directly using eigenstates of \( h_\alpha \).

It is also remarked that the local Hamiltonian \( h_\alpha \) is supported on the sublattice consisting of \( 2\nu(2\nu-1) \) sites, which becomes a 12-site lattice even in two dimensions, and the decomposition with smaller sublattices probably does not work. It is a non-trivial task to analytically solve a problem of interacting electrons on this lattice size.\(^5\)

### 4.2 Single-Electron Problem for the Local Hamiltonian

Because of the translation invariance, it suffices to investigate \( h_0 \), the local Hamiltonian associated with the origin \( 0 = (0, \ldots, 0) \) of \( V \), in order to prove Lemma 1. Since \( h_0 \) is

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\(^5\) In Ref. [15], a similar lemma is proved relying on numerical calculations.
defined only on $\Lambda_0$, we consider the space constructed by using fermion operators $c_{x,\sigma}$ with $x \in \Lambda_0$, $\sigma = \uparrow, \downarrow$.

In this subsection we will solve the single-electron problem for $h_0$. As usual we can solve it by using basis states $\{c_{x,\sigma}\}_{x \in \Lambda_0}$ of the single-electron Hilbert space $\mathcal{H}$ on $\Lambda_0$, but we adopt a slightly different method here.

To prove Lemma 1, we will consider finite energy states in the limit $t \to \infty$. So let us firstly characterize single-electron states which have infinitely large energy in the limit $t \to \infty$. Let $\mathcal{H}_b$ be the single-electron Hilbert space spanned by the states $b_{p,\sigma}^\dagger \Phi_0$ with $p \in \mathcal{P}_0$, which are linearly independent. Since all the creation operators $b_{p,\sigma}^\dagger$ anticommute with $a_{0,\sigma}$, we find that $h_0 \Phi_{1,\sigma} \in \mathcal{H}_b$ for any $\Phi_{1,\sigma} \in \mathcal{H}_b$. This implies that it is possible to obtain eigenstates of $h_0$ within $\mathcal{H}_b$. Since the operator $\sum_{p \in \mathcal{P}_0} b_{p,\sigma}^\dagger b_{p,\sigma}$ restricted on $\mathcal{H}_b$ is positive definite, corresponding energy eigenvalues are proportional to $t$, and thus $\mathcal{H}_b$ consists of high energy states.

Let $\mathcal{H}_b^\perp$ be the orthogonal complement of $\mathcal{H}_b$ within $\mathcal{H}$. In the following, we solve the single-electron problem for $h_0$ within $\mathcal{H}_b^\perp$, by constructing states orthogonal to those in $\mathcal{H}_b$ (or equivalently by constructing local fermion operators anticommuting with $b_{p,\sigma}^\dagger$).

Let $\partial \Lambda_0$ be the collection of the “boundary” sites in $\Lambda_0$

$$\partial \Lambda_0 = \Lambda_0 \setminus \mathcal{C}_0.$$ (39)

Without loss of generality, we can assume that $x_3(p), x_4(p) \in \partial \Lambda_0$ for all $p \in \mathcal{P}_0$. Then, we define

$$d_{p,\sigma} = \frac{1}{\sqrt{2}} \left( c_{x_3(p)} + c_{x_4(p)} \right)$$ (40)

for each $p \in \mathcal{P}_0$ and

$$\tilde{a}_{x,\sigma} = 2c_{x,\sigma} + \sum_{p \in \mathcal{P}(x)} \mu[x, p] \left( c_{x_3(p),\sigma} - c_{x_4(p),\sigma} \right),$$ (41)

for each $x \in \mathcal{C}_0$, where $\mu[x, p]$ takes $-1$ if $x$ corresponds to $x_1(p)$ and $1$ if $x$ corresponds to $x_2(p)$. By a straightforward calculation, we can check that

$$\{b_{p,\sigma}^\dagger, d_{q,\tau}\} = \{b_{p,\sigma}^\dagger, \tilde{a}_{x,\sigma}\} = 0$$ (42)

for any $p, q \in \mathcal{P}_0$ and $x \in \mathcal{C}_0$. It is also not difficult to check that $|\mathcal{P}_0| + |\mathcal{C}_0|$ states, $d_{p,\sigma}^\dagger \Phi_0$ with $p \in \mathcal{P}_0$ and $\tilde{a}_{x,\sigma} \Phi_0$ with $x \in \mathcal{C}_0$, are linearly independent. Noting that the dimension of $\mathcal{H}_b$ is $|\mathcal{P}_0|$, and $|\mathcal{P}_0| + (|\mathcal{P}_0| + |\mathcal{C}_0|) = |\Lambda_0|$, we find that these states span the orthogonal complement $\mathcal{H}_b^\perp$ of $\mathcal{H}_b$.

Since the operator $s a_{0,\sigma}^\dagger a_{0,\sigma}$ restricted to $\mathcal{H}$ is a projection onto the space spanned by the single state $a_{0,\sigma}^\dagger \Phi_0$, $h_0$ restricted to $\mathcal{H}_b^\perp$ has exactly two eigenvalue; one is $0$ and the other is $-2\nu s$ to which $a_{0,\sigma}^\dagger \Phi_0$ belongs.

One easily finds that all $d_{p,\sigma}^\dagger$ with $p \in \mathcal{P}_0$, which are supported only on the sites in $\partial \Lambda_0$, anticommute with not only $b_{p,\sigma}$ but also $a_{0,\sigma}$, so that the states $d_{p,\sigma}^\dagger \Phi$ are the eigenstates of $h_0$ with eigenvalue $0$. Furthermore, it follows from $\{d_{p,\sigma}^\dagger, d_{q,\sigma}\} = \delta_{p,q}$ that the set of states $\{d_{p,\sigma}^\dagger \Phi_0\}_{p \in \mathcal{P}_0}$ is orthonormal.

Let us determine the rest of eigenstates with eigenvalue $0$. Since the anticommutation relation

$$\{d_{p,\sigma}^\dagger, \tilde{a}_{x,\sigma}\} = 0$$ (43)
holds for $p \in \mathcal{P}_0$ and $x \in C_0$, our task is to construct fermion operators which anticommute with $a_{0,\sigma}^\dagger$, by using $\tilde{d}_{x,\sigma}$ with $x \in C_0$. In the following, we write $x_l$ for $m(0, \delta_l)$ and $x_{-l}$ for $m(0, -\delta_l)$ with $l = 1, \ldots, v$. We note that

$$C_0 = \{ x_l \mid l = \pm 1, \ldots, \pm v \}.$$  \hfill (44)

By using $\tilde{d}_{x,\sigma}$, we form fermion operators which anticommute with one another. We write again $d_{i,\sigma}$ for these fermion operators. To label new $d$-operators which we will define below, we introduce a set $\mathcal{D} = \{ 1, \ldots, v \}$, and also

$$\mathcal{J} = \left\{ 0, \pm \frac{2\pi}{v}, \ldots, \pm \frac{2\pi}{v} \frac{(v - 1)}{2} \right\}$$  \hfill (45)

for odd $v$, and

$$\mathcal{J} = \left\{ 0, \pm \frac{2\pi}{v}, \ldots, \pm \frac{2\pi}{v} \frac{v - 2}{2}, \pi \right\}$$  \hfill (46)

for even $v$.

Now, for $l \in \mathcal{D}$, let us define

$$d_{l,\sigma} = \frac{1}{2\sqrt{2v}} (\tilde{d}_{x_l,\sigma} - \tilde{d}_{x_{-l},\sigma}).$$  \hfill (47)

We also define

$$d_{k,\sigma} = \frac{1}{2\sqrt{2v(\nu + 1 - \nu \delta_{k,0})}} \sum_{l=1}^{\nu} e^{i\nu l} (\tilde{d}_{x_l,\sigma} + \tilde{d}_{x_{-l},\sigma})$$  \hfill (48)

for $k \in \mathcal{J}$. We note that $d_{k,\sigma}$ with $k = 0$ is equal to $(1/\sqrt{2v}) a_{0,\sigma}$. Furthermore, as we will see below, we have the anticommutation relations

$$\left\{ d_{i,\sigma}, d_{j,\sigma} \right\} = \delta_{i,j}$$  \hfill (49)

for any $i, j \in \mathcal{D} \cup \mathcal{J}$. Therefore, the single-electron states $d_{i,\sigma}^\dagger \Phi_0$ with $i \in \mathcal{D} \cup \mathcal{J}\setminus\{0\}$ in $\mathcal{H}_b^\perp$ are orthonormal eigenstates of $h_0$ with eigenvalue 0.

To prove (49), let us first calculate the anticommutation relations for $\tilde{d}_{x,\sigma}$ and $\tilde{d}_{y,\sigma}$ with $x, y \in C_0$. Noting that $|\mathcal{P}(x_l)| = 2(\nu - 1)$ and $|\mathcal{P}(x_l) \cap \mathcal{P}(x_{-l})| = \emptyset$ for $l = \pm 1, \ldots, \pm v$, we find

$$\left\{ \tilde{d}_{x_l,\sigma}^\dagger, \tilde{d}_{x_{l},\sigma} \right\} = 4 + 2 |\mathcal{P}(x_l)| = 4\nu,$$  \hfill (50)

and

$$\left\{ d_{x_l,\sigma}^\dagger, d_{x_{-l},\sigma} \right\} = 0.$$  \hfill (51)

Next, noting that, for $l, l' = \pm 1, \ldots, \pm v$ and $l \neq \pm l'$, $\mathcal{P}(x_l) \cap \mathcal{P}(x_{l'})$ always has only one element, say $p$, such that either $x_l = x_1(p)$, $x_{l'} = x_2(p)$ or $x_l = x_2(p)$, $x_{l'} = x_1(p)$ holds, we have

$$\left\{ \tilde{d}_{x_l,\sigma}^\dagger, \tilde{d}_{x_{l'},\sigma} \right\} = 2\mu[x_l, p] \mu[x_{l'}, p] = -2.$$  \hfill (52)

Then, by using anticommutation relations (50)–(52), we obtain

$$\left\{ (\tilde{d}_{x_l,\sigma} - \tilde{d}_{x_{-l},\sigma}), (\tilde{d}_{x_{l'},\sigma} - \tilde{d}_{x_{-l'},\sigma}) \right\} = 8\nu \delta_{l,l'},$$  \hfill (53)

$^6$ The regular square $p$ is in the plane including the $l$-axis and the $l'$-axis.
\[
\left\{ (\tilde{a}_{xi,\sigma} + \tilde{a}_{x-i,\sigma}^\dagger), (\tilde{a}_{xj,\sigma} + \tilde{a}_{x-j,\sigma}^\dagger) \right\} = 8\nu \delta_{i,j'} - 8(1 - \delta_{i,j'}) ,
\]
and
\[
\left\{ (\tilde{a}_{xi,\sigma}^\dagger + \tilde{a}_{x-i,\sigma}^\dagger), (\tilde{a}_{xj,\sigma} - \tilde{a}_{x-j,\sigma}^\dagger) \right\} = 0
\]
for \( i, j' \in \mathcal{D} \). From, (53)–(55), we obtain the desired relations (49).

The results in this subsection are summarized as follows. Let \( \mathcal{I} = \mathcal{P}_0 \cup \mathcal{D} \cup \mathcal{J} \). The fermion operators defined by (40), (47) and (48) satisfy the anticommutation relation
\[
\left\{ d_{i,\sigma}^\dagger, d_{j,\sigma} \right\} = \delta_{i,j}
\]
for any \( i, j \in \mathcal{I} \). The single-electron states \( d_{i,\sigma}^\dagger \Phi_0 \) with \( i \in \mathcal{I} \) satisfy
\[
h_0 d_{i,\sigma}^\dagger \Phi_0 = \varepsilon_i d_{i,\sigma}^\dagger \Phi_0 ,
\]
where \( \varepsilon_i \) are given by
\[
\varepsilon_i = \begin{cases} -2\nu s & \text{if } i = 0; \\ 0 & \text{otherwise}, \end{cases}
\]
and they form an orthonormal basis\(^7\) for subspace \( \mathcal{H}_b^\perp \).

### 4.3 Proof of Lemma 1

By using the local fermion operators introduced in the previous section, we solve a many-electron problem for \( h_0 \). First, we will consider the problem in the limit \( t, U \to \infty \), where it will be proved that the minimum expectation value of \( h_0 \) is equal to or greater than \(-2\nu s\) and that any state which attains the minimum expectation value is an eigenstate of \( h_0 \).

Let \( \Phi \) be a state on \( \Lambda_0 \) with a finite energy in the limit \( t, U \to \infty \). Consider representing \( \Phi \) by using the fermion operators \( \{d_{i,\sigma}^\dagger\}_{i \in \mathcal{I}} \) and \( \{b_{p,\sigma}^\dagger\}_{p \in \mathcal{P}_0} \). In the limit \( t \to \infty \), since the terms \( tb_{p,\sigma}^\dagger b_{p,\sigma} \) in \( h_0 \) are positive semidefinite, \( \Phi \) with a finite energy must satisfy \( b_{p,\sigma} \Phi = 0 \) for all \( p \in \mathcal{P}_0 \) and \( \sigma = \uparrow, \downarrow \). This means that a finite energy state \( \Phi \) is written as
\[
\Phi = \sum_{I_\uparrow, I_\downarrow \subset \mathcal{I}} g(I_\uparrow; I_\downarrow) \Phi(I_\uparrow; I_\downarrow)
\]
with complex coefficients \( g(I_\uparrow; I_\downarrow) \), where
\[
\Phi(I_\uparrow; I_\downarrow) = \left( \prod_{i \in I_\uparrow} d_{i,\uparrow}^\dagger \right) \left( \prod_{j \in I_\downarrow} d_{j,\downarrow}^\dagger \right) \Phi_0 .
\]

Here, to avoid an ambiguity which may arise due to the exchange of fermion operators, we adopt the following rule for the product of fermion operators. Let \( \theta \) be a one-to-one mapping from \( \mathcal{I} \) to \( \mathbb{Z} \). Then, we assume that the products of the fermion operators in \( \Phi(I_\uparrow; I_\downarrow) \) are ordered in such a way that \( d_{i,\uparrow}^\dagger \) (respectively, \( d_{i,\downarrow}^\dagger \)) is always on the left of \( d_{j,\uparrow}^\dagger \) (respectively, \( d_{j,\downarrow}^\dagger \)) if \( \theta(i) < \theta(j) \). For later use, we also define
\[
S_i^j = \prod_{j \in I_\uparrow; \theta(j) < \theta(i)} (-1).
\]

\(^7\) Note that \( |\mathcal{I}| = |\mathcal{P}_0| + |\mathcal{D}| + |\mathcal{J}| = |\mathcal{P}_0| + |\mathcal{S}_0| \) which equals the dimension of \( \mathcal{H}_b^\perp \).
For example, we have
\[
\left( \prod_{j \in I} d_{j,\sigma}^\dagger \right) = S_{i_\sigma}^I d_{i,\sigma}^\dagger \left( \prod_{j \in I \setminus \{i\}} d_{j,\sigma}^\dagger \right).
\]

(62)

Let us consider furthermore the limit \( U \to \infty \). Since the on-site interaction \( U n_{x,\uparrow} n_{x,\downarrow} = U c_{x,\uparrow}^c c_{x,\downarrow} c_{x,\uparrow} c_{x,\downarrow} \) is positive semidefinite, a state \( \Phi \) with finite energy satisfies \( c_{x,\downarrow} c_{x,\uparrow} \Phi = 0 \) for any \( x \in \Lambda_0 \). Substituting (59) into this equation, we find that the coefficients \( g(I_{\uparrow}; I_{\downarrow}) \) must be chosen so that
\[
\sum_{I_{\uparrow}, I_{\downarrow} \subset \mathcal{I}} g(I_{\uparrow}; I_{\downarrow}) c_{x,\downarrow} c_{x,\uparrow} \Phi(I_{\uparrow}; I_{\downarrow}) = 0
\]

(63)

will always hold for any \( x \in \Lambda_0 \).

By using the coefficients \( g(I_{\uparrow}; I_{\downarrow}) \) which satisfy the condition (63), let us now express an expectation value \( E[\Phi] \) of \( h_0 \) for \( \Phi \) in the limit of \( t, U \to \infty \). Since the eigenvalues of \( -s \sum_\sigma a_{0,\sigma}^\dagger a_{0,\sigma} \) for \( \Phi(I_{\uparrow}; I_{\downarrow}) \) are simply given by
\[
\begin{cases}
-4\nu s & \text{if } 0 \in I_{\uparrow} \cap I_{\downarrow}; \\
-2\nu s & \text{if } 0 \in I_{\uparrow} \cup I_{\downarrow} \text{ and } 0 \not\in I_{\uparrow} \cap I_{\downarrow}; \\
0 & \text{otherwise,}
\end{cases}
\]

(64)

and the set of all states \( \Phi(I_{\uparrow}; I_{\downarrow}) \) is orthonormal, we have
\[
E[\Phi] = \frac{\langle \Phi, h_0 \Phi \rangle}{\langle \Phi, \Phi \rangle} = \left( -4\nu s \sum_{I_{\uparrow}, I_{\downarrow} \subset \mathcal{I}} |g(I_{\uparrow}; I_{\downarrow})|^2 - 2\nu s \sum_{I_{\uparrow}, I_{\downarrow} \subset \mathcal{I}} |g(I_{\uparrow}; I_{\downarrow})|^2 \right) \|\Phi\|^{-2}
\]

(65)

(66)

with
\[
\|\Phi\| = \sqrt{\langle \Phi, \Phi \rangle} = \left( \sum_{I_{\uparrow}, I_{\downarrow} \subset \mathcal{I}} |g(I_{\uparrow}; I_{\downarrow})|^2 \right)^{1/2}.
\]

(67)

By noting that
\[
\sum_{I_{\uparrow}, I_{\downarrow} \subset \mathcal{I}} + \sum_{I_{\uparrow}, I_{\downarrow} \subset \mathcal{I}} + \sum_{I_{\uparrow}, I_{\downarrow} \subset \mathcal{I}} = \sum_{I_{\uparrow}, I_{\downarrow} \subset \mathcal{I}},
\]

(68)

we rewrite \( E[\Phi] \) as
\[
E[\Phi] = -2\nu s + 2\nu s F[\Phi]|\Phi|^2
\]

(69)
where
\[
F[\Phi] = \sum_{I_\uparrow, I_\downarrow \in \mathcal{I}} |g(I_\uparrow; I_\downarrow)|^2 - \sum_{0 \notin I_\uparrow \cup I_\downarrow} |g(I_\uparrow; I_\downarrow)|^2
\]
\[
= \sum_{I_\uparrow, I_\downarrow \in \mathcal{I} \setminus \{0\}} |g(I_\uparrow; I_\downarrow)|^2 - \sum_{I_\uparrow, I_\downarrow \in \mathcal{I} \setminus \{0\}} |g(\{0\} \cup I_\uparrow; \{0\} \cup I_\downarrow)|^2. \tag{70}
\]

In the following, we show \( F[\Phi] \geq 0 \). This implies \( E[\Phi] \geq -2\nu s \) since \( s > 0 \).

In order to prove \( F[\Phi] \geq 0 \) we investigate in detail the conditions on \( g(I_\uparrow; I_\downarrow) \) imposed by (63). The left-hand side of (63) is calculated as
\[
\sum_{I_\uparrow, I_\downarrow \in \mathcal{I}} \sum_{n \in I_\uparrow} \sum_{m \in I_\downarrow} (-1)^{|I_\uparrow|-1} S_{I_\uparrow}^n S_{I_\downarrow}^m (\varphi_x^{(n)})^* (\varphi_x^{(m)})^* \Phi(I_\uparrow \setminus \{n\}; I_\downarrow \setminus \{m\}),
\]

where \((\varphi_x^{(i)})^* = \{d_{i,\sigma}^\dagger, c_{x,\sigma}\}\). The expression (71) is further calculated as
\[
\sum_{n,m \in \mathcal{I}} (\varphi_x^{(n)})^* (\varphi_x^{(m)})^* \sum_{I_\uparrow, I_\downarrow \in \mathcal{I}} \sum_{|I_\uparrow| \geq 1, |I_\downarrow| \geq 1} (-1)^{|I_\uparrow|-1} S_{I_\uparrow}^n S_{I_\downarrow}^m \chi[n \in I_\uparrow] \chi[m \in I_\downarrow]
\times g(I_\uparrow; I_\downarrow) \Phi(I_\uparrow \setminus \{n\}; I_\downarrow \setminus \{m\})
\]
\[
= \sum_{n,m \in \mathcal{I}} (\varphi_x^{(n)})^* (\varphi_x^{(m)})^* \sum_{I_\uparrow \in \mathcal{I} \setminus \{n\}} \sum_{I_\downarrow \in \mathcal{I} \setminus \{m\}} (-1)^{|I_\uparrow|} S_{I_\uparrow}^n S_{I_\downarrow}^m
\times g([n] \cup I_\uparrow; \{m\} \cup I_\downarrow) \Phi(I_\uparrow; I_\downarrow)
\]
\[
= \sum_{I_\uparrow, I_\downarrow \in \mathcal{I}} \sum_{n,m \in \mathcal{I}} (\varphi_x^{(n)})^* (\varphi_x^{(m)})^* \tilde{g}(n, I_\uparrow; m, I_\downarrow) \Phi(I_\uparrow; I_\downarrow), \tag{72}
\]

where \(\chi[\text{event}]\) is the indicator function which takes 1 if event is true and 0 otherwise, and we have introduced the subsidiary coefficients defined as
\[
\tilde{g}(n, I_\uparrow; m, I_\downarrow) = \begin{cases} 0 & \text{if } n \in I_\uparrow \text{ or } m \in I_\downarrow; \\ (-1)^{|I_\uparrow|} S_{I_\uparrow}^n S_{I_\downarrow}^m \tilde{g}([n] \cup I_\uparrow; \{m\} \cup I_\downarrow) & \text{otherwise.} \end{cases} \tag{73}
\]

In the first equality of (72) we have used \( S_{I_\uparrow \cup \{i\}}^n \). Since all the states \( \Phi(I_\uparrow; I_\downarrow) \) are linearly independent, we find that the condition (63) becomes
\[
\sum_{n,m \in \mathcal{I}} (\varphi_x^{(n)})^* (\varphi_x^{(m)})^* \tilde{g}(n, I_\uparrow; m, I_\downarrow) = 0 \tag{74}
\]
for any \( I_\uparrow, I_\downarrow \subseteq \mathcal{I} \) and for any \( x \in \mathcal{A}_0 \).

By choosing the sites in \( C_0 \) as \( x \), we rewrite condition (74) more concretely. Take \( x_i = m(0, \delta_i) \in C_0 \) as \( x \) in condition (74). Noting that \( \varphi_x^{(i)} \) is vanishing if \( i \in \mathcal{P}_0 \) or \( i \in \mathcal{D} \setminus \{l\} \),

we obtain

\[
\text{We calculate the coefficients } \varphi_x^{(i)} = \{d_{i,\sigma}^\dagger, c_{x,\sigma}\} \text{ by using (40), (41), (47) and (48).}
\]
\[ g(l; l) + \tilde{g}(0; 0) + \frac{1}{\nu + 1} \sum_{k, k' \in \mathcal{J} \setminus \{0\}} e^{-ikl}e^{-ik'l} \tilde{g}(k; k') \\
+ (\tilde{g}(l; 0) + \tilde{g}(0; l)) + \frac{1}{\sqrt{\nu + 1}} \sum_{k \in \mathcal{J} \setminus \{0\}} e^{-ikl}(\tilde{g}(l; k) + \tilde{g}(k; l)) \\
+ \frac{1}{\sqrt{\nu + 1}} \sum_{k \in \mathcal{J} \setminus \{0\}} e^{-ikl}(\tilde{g}(0; k) + \tilde{g}(k; 0)) = 0, \quad (75) \]

where we write \( \tilde{g}(n; m) \) for \( \tilde{g}(n, I_\uparrow; m, I_\downarrow) \). Similarly, for \( x_\downarrow = m(0, -\delta_l) \in \mathcal{C}_0 \), we obtain

\[ g(l; l) + \tilde{g}(0; 0) + \frac{1}{\nu + 1} \sum_{k, k' \in \mathcal{J} \setminus \{0\}} e^{-ikl}e^{-ik'l} \tilde{g}(k; k') \\
- (\tilde{g}(l; 0) + \tilde{g}(0; l)) - \frac{1}{\sqrt{\nu + 1}} \sum_{k \in \mathcal{J} \setminus \{0\}} e^{-ikl}(\tilde{g}(l; k) + \tilde{g}(k; l)) \\
+ \frac{1}{\sqrt{\nu + 1}} \sum_{k \in \mathcal{J} \setminus \{0\}} e^{-ikl}(\tilde{g}(0; k) + \tilde{g}(k; 0)) = 0. \quad (76) \]

Then, summing the above two equations over \( l \in \mathcal{D} \) we obtain the condition

\[ \tilde{g}(0, I_\uparrow; 0, I_\downarrow) = -\frac{1}{\nu} \sum_{l \in \mathcal{D}} \tilde{g}(l, I_\uparrow; l, I_\downarrow) - \frac{1}{(\nu + 1)} \sum_{k \in \mathcal{J} \setminus \{0\}} \tilde{g}(k, I_\uparrow; -k, I_\downarrow). \quad (77) \]

Our analysis below highly relies on the above relation.

Let \( I_\downarrow \) be the set defined by

\[ I_\downarrow = \{i \mid i \in I_\downarrow \cap (\mathcal{P}_0 \cup \mathcal{D})\} \cup \{-i \mid i \in I_\uparrow \cap \mathcal{J}\}, \quad (78) \]

and let \( N(I_\uparrow; I_\downarrow) \) be the number of elements in \( I_\uparrow \cap I_\downarrow \cap (\mathcal{D} \cup \mathcal{J} \setminus \{0\}) \). Condition (77) relates \( g([0] \cup I_\uparrow; [0] \cup I_\downarrow) \) with \( N(I_\uparrow; I_\downarrow) = r \) and \( g(I_\uparrow'; I_\downarrow') \) with \( N(I_\uparrow'; I_\downarrow') = r + 1 \). This motivates us to decompose \( F[\Phi] \) as

\[ F[\Phi] = F'[\Phi] + \sum_{r=0}^{2\nu-1} F_r[\Phi], \quad (79) \]

where

\[ F_r[\Phi] = \sum_{I_\uparrow, I_\downarrow \subseteq \mathcal{I} \setminus \{0\}} |g(I_\uparrow; I_\downarrow)|^2 - \sum_{I_\uparrow, I_\downarrow \subseteq \mathcal{I} \setminus \{0\}} \sum_{N(I_\uparrow; I_\downarrow) = r+1} |g([0] \cup I_\uparrow; [0] \cup I_\downarrow)|^2, \quad (80) \]

and

\[ F'[\Phi] = \sum_{I_\uparrow, I_\downarrow \subseteq \mathcal{I} \setminus \{0\}} \sum_{N(I_\uparrow; I_\downarrow) = r} |g(I_\uparrow; I_\downarrow)|^2. \quad (81) \]

The term \( F'[\Phi] \) is apparently non-negative, and therefore \( F[\Phi] \geq 0 \) is implied by \( F_r[\Phi] \geq 0 \) for \( r = 0, \ldots, 2\nu - 1 \).

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9 We think of \(-\pi\) as \(\pi\) when \(\nu\) is even (\(\pi\) is in \(\mathcal{J}\)).
We will prove $F_r[\Phi] \geq 0$ by using (77). First we note that, for a pair of $I_\uparrow$ and $I_\downarrow$ such that $N(I_\uparrow; I_\downarrow) = r$, the number of non-zero $\tilde{g}$ in the right-hand side of (77) is at most $2\nu - r - 1$ (see the definition (73) of $\tilde{g}$). For such a pair of $I_\uparrow$ and $I_\downarrow$, using the Schwarz inequality, we have

$$|\tilde{g}(0, I_\uparrow; 0, I_\downarrow)|^2 \leq \frac{2\nu - r - 1}{\nu^2} \sum_{l \in \mathcal{D}} |\tilde{g}(l, I_\uparrow; l, I_\downarrow)|^2 + \frac{2\nu - r - 1}{(\nu + 1)^2} \sum_{k \in \mathcal{J}\setminus\{0\}} |\tilde{g}(k, I_\uparrow; -k, I_\downarrow)|^2. \quad (82)$$

Then, noting that $0 \leq \frac{2\nu - r - 1}{(\nu + 1)^2} \leq \frac{2\nu - r - 1}{\nu^2}$, we find that

$$\sum_{I_\uparrow, I_\downarrow \subseteq \mathcal{I}\setminus\{0\}} \sum_{N(I_\uparrow; I_\downarrow) = r} |g(\{0\} \cup I_\uparrow; \{0\} \cup I_\downarrow)|^2$$

$$\leq \frac{2\nu - r - 1}{\nu^2} \sum_{I_\uparrow, I_\downarrow \subseteq \mathcal{I}\setminus\{0\}} \sum_{l \in \mathcal{D}} |\tilde{g}(l, I_\uparrow; l, I_\downarrow)|^2 + \frac{2\nu - r - 1}{(\nu + 1)^2} \sum_{I_\uparrow, I_\downarrow \subseteq \mathcal{I}\setminus\{0\}} \sum_{k \in \mathcal{J}\setminus\{0\}} |\tilde{g}(k, I_\uparrow; -k, I_\downarrow)|^2$$

$$\leq \frac{(2\nu - r - 1)(\nu + 1)}{\nu^2} \sum_{I_\uparrow, I_\downarrow \subseteq \mathcal{I}\setminus\{0\}} |g(I_\uparrow; I_\downarrow)|^2. \quad (83)$$

To get the final line, we have used the fact that, for a pair of $I_\uparrow$ and $I_\downarrow$ with $N(I_\uparrow; I_\downarrow) = r + 1$, there are $(r + 1)$ elements $n$ in $\mathcal{D} \cup (\mathcal{J}\setminus\{0\})$ for which we can find a suitable pair $I_\prime_\uparrow$ and $I_\prime_\downarrow$ with $N(I_\prime_\uparrow; I_\prime_\downarrow) = r$ such that either $\{n\} \cup I_\prime_\uparrow = I_\uparrow$ and $\{n\} \cup I_\prime_\downarrow = I_\downarrow$ or $\{n\} \cup I_\prime_\uparrow = I_\uparrow$ and $\{\neg n\} \cup I_\prime_\downarrow = I_\downarrow$ holds. Therefore we obtain

$$F_r[\Phi] \geq 1 - \frac{(2\nu - r - 1)(\nu + 1)}{\nu^2} \sum_{I_\uparrow, I_\downarrow \subseteq \mathcal{I}\setminus\{0\}} |g(I_\uparrow; I_\downarrow)|^2. \quad (84)$$

Since $\frac{(2\nu - r - 1)(\nu + 1)}{\nu^2} \leq 1$, we conclude that $F_r[\Phi] \geq 0$.

Finally, we examine the condition for equality $F[\Phi] = 0$. Since $F'[\Phi] \geq 0$ by the definition and we have shown $F_r[\Phi] \geq 0$, $F[\Phi] = 0$ holds only when $F'[\Phi]$ and $F_r[\Phi]$ are vanishing. Here it is easy to see that $F'[\Phi] = 0$ holds only if all the coefficients appearing in the sum in the right-hand side of (81), i.e., coefficients $g(I_\uparrow; I_\downarrow)$ for $I_\uparrow$ and $I_\downarrow$ such that $0 \not\in I_\uparrow \cup I_\downarrow$ and $N(I_\uparrow; I_\downarrow) = 0$, are identically zero.

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10 We could easily find the condition for this equality in the case of the kagome lattice [14], but we have to consider this carefully in the present model. The condition for the equality depends on the form of the finite energy condition (74). This point should be kept in mind in applying the present method to other models.
To see when $F_r[\Phi] = 0$ holds, let us look into the inequality (84). The factor $(\frac{(2v-r-1)(r+1)}{v^2})$ in (84) is equal to 1 if $r = v - 1$ and is less than 1 otherwise. Therefore we find that $F_r[\Phi]$ with $r \neq v - 1$ is vanishing only if all the coefficients $g(I_1; I_\perp)$ in the sum in the right-hand side of (80) are zero. On the other hand, we need further consideration for $r = v - 1$. By using the inequality (82) with $r = v - 1$, we obtain

$$
\sum_{I_1, I_\perp \subset I \setminus \{0\}} \left| g(\{0\} \cup I_1; \{0\} \cup I_\perp) \right|^2
\leq \frac{1}{v} \sum_{I_1, I_\perp \subset I \setminus \{0\}} \sum_{l \in \mathcal{D}} \left| \tilde{g}(l, I_1; l, I_\perp) \right|^2
+ \frac{v}{(v+1)^2} \sum_{I_1, I_\perp \subset I \setminus \{0\}} \sum_{k \in \mathcal{J} \setminus \{0\}} \left| \tilde{g}(k, I_1; -k, I_\perp) \right|^2.
$$

(85)

The right-hand side is rewritten as

$$
\sum_{n=0}^v \sum_{I_1, I_\perp \subset I \setminus \{0\}} R_n \left| g(I_1; I_\perp) \right|^2
$$

with $R_n = n/v + (v - n)v/(v + 1)^2$. Noting that $R_v = 1$ we obtain

$$
F_{v-1}[\Phi] \geq \sum_{n=0}^{v-1} (1 - R_n) \sum_{I_1, I_\perp \subset I \setminus \{0\}} \left| g(I_1; I_\perp) \right|^2.
$$

(87)

Now suppose that $F_{v-1}[\Phi] = 0$. Since $R_n < 1$ for $n = 0, \ldots, v - 1$, we find that all the coefficients $g(I_1; I_\perp)$ in the sum in the right-hand side of the above inequality should be zero. We thus have $\tilde{g}(k, I_1; -k, I_\perp) = 0$ with $k \in \mathcal{J} \setminus \{0\}$ for any $I_1, I_\perp \subset I \setminus \{0\}$ such that $N(I_1; I_\perp) = v - 1$. Then, (77) becomes

$$
\tilde{g}(0, I_1; 0, I_\perp) = -\frac{1}{v} \sum_{l \in \mathcal{D}} \tilde{g}(l, I_1; l, I_\perp)
$$

(88)

for $N(I_1; I_\perp) = v - 1$. Note that the number of non-zero $\tilde{g}$ in the right-hand side of (88) is at most one. Repeating the same argument as above with the relation (88), we find that $F_{v-1}[\Phi] = 0$ only when all the coefficients in the sum in the right-hand side of (80) are zero.

---

11 Note that $|I_1 \cap I_\perp \cap \mathcal{D}| = n$ implies $|I_1 \cap I_\perp \cap (\mathcal{J} \setminus \{0\})| = v - n$ when $N(I_1; I_\perp) = v$. Then, considering in a similar way below (83), we obtain $R_n$.

12 Put $I'_1 = \{k\} \cup I_1$ and $I'_\perp = \{-k\} \cup I_\perp$. If $k \in I_1$ or $-k \in I_\perp$, we have $\tilde{g}(k, I_1; -k, I_\perp) = 0$ by the definition; otherwise, since $N(I'_1; I'_\perp) = v$ and $|I'_1 \cap I'_\perp \cap \mathcal{D}| \neq v$, we have $g(I'_1; I'_\perp) = 0$, which implies $\tilde{g}(k, I_1; -k, I_\perp) = 0$.

13 Put $I'_1 = \{l\} \cup I_1$ and $I'_\perp = \{l\} \cup I_\perp$. If $I'_1 \cap I'_\perp \cap \mathcal{D} \neq \mathcal{D}$, we have $\tilde{g}(l, I_1; l, I_\perp) = 0$ (see also footnote 12). If $I'_1 \cap I'_\perp \cap \mathcal{D} = \mathcal{D}$, $|I_1 \cap I_\perp \cap \mathcal{D}| = v - 1$ and there is only one element $l$ in $\mathcal{D}$ for which $\tilde{g}(l, I_1; l, I_\perp)$ can be non-zero.
zero. Therefore, we conclude that $F[\Phi] = 0$ holds only if $g(I \uparrow; I \downarrow) = 0$ for any pair of $I \uparrow$ and $I \downarrow$ such that $0 \in I \uparrow \cap I \downarrow$ and $0 \notin I \uparrow \cup I \downarrow$.

So far we have proved that $E[\Phi] \geq -2v\nu s$ and that the minimum expectation value $-2v\nu s$ is attained by states $\Phi$ which satisfy finite energy state condition (74) and can be expanded as

$$\Phi = \sum_{I \uparrow, I \downarrow \subset \mathcal{I}} g(I \uparrow; I \downarrow) \Phi(I \uparrow; I \downarrow).$$

(89)

It follows from the above expression that any state which attains the minimum expectation value $-2v\nu s$ is an eigenstate of $h_0$ as well as $-s \sum_{\sigma} a_{0,\sigma}^\dagger a_{0,\sigma}$. It is noted that there really exist such eigenstates under condition (74); $d_0^\dagger \Phi_0$ and $\left( \prod_{I \in \mathcal{I}} d_i^\dagger \right) \Phi_0$ are examples.

By the continuity of eigenvalues we conclude that $-2v\nu s$ is the minimum eigenvalue of $h_0$ for sufficiently large values of $t/s$ and $U/s$, and that the corresponding eigenstates are the same as those which give the minimum expectation value of $h_0$ in the limit $t/s, U/s \rightarrow \infty$. It is easy to check that such eigenstates have the properties stated in Lemma 1. Because of the translation invariance, the same holds for all $h_\alpha$ and this completes the proof of Lemma 1.

5 Proof of Theorem 1 for $s > 0$; Nearly-Flat-Band Ferromagnetism

Suppose that the number $N_c$ of electrons is $|\mathcal{V}|$ and that the values of $t/s$ and $U/s$ are so large that Lemma 1 holds. We note that Lemma 1 is associated only with the local Hamiltonians and that how large $t/s$ and $U/s$ should be is independent of the size of the whole lattice.

Since the minimum eigenvalue of the local Hamiltonians $h_\alpha$ is $-2v\nu s$, as claimed in Lemma 1, the eigenvalue of the Hamiltonian $H = \sum_{\alpha \in \mathcal{V}} h_\alpha$ is bounded from below by $-2v\nu s|\mathcal{V}|$. On the other hand, taking the fully saturated ferromagnetic state

$$\Phi_{\text{ferro}} = \left( \prod_{\alpha \in \mathcal{V}} a_{\alpha, \uparrow}^\dagger \right) \Phi_0$$

(90)

as a variational state for $H$ and noting that

$$-s a_{\beta, \downarrow}^\dagger a_{\beta, \downarrow} \Phi_{\text{ferro}} = 0$$

(91)

and

$$-s a_{\beta, \downarrow}^\dagger a_{\beta, \uparrow} \Phi_{\text{ferro}} = -s \left( 2v - a_{\beta, \uparrow}^\dagger a_{\beta, \uparrow}^\dagger \right) \Phi_{\text{ferro}} = -2v\nu s \Phi_{\text{ferro}}$$

(92)

for all $\beta \in \mathcal{V}$, we find that the upper bound on the ground state energy is also given by $-2v\nu s|\mathcal{V}|$. Therefore, the ground state energy is exactly $-2v\nu s|\mathcal{V}|$. It is easy to see that the state $\Phi_{\text{ferro}}$ has the maximal total spin $S_{\text{tot}} = N_c/2$. Our remaining task is to prove the uniqueness of the ground state up to $(N_c + 1)$-fold degeneracy due to the spin rotation symmetry.

Let $\Phi_G$ be a ground state, and assume that $\Phi_G$ is expanded in terms of the basis states $\Phi(V \uparrow, B \uparrow; V \downarrow, B \downarrow)$ in (32) with $N_c = |\mathcal{V}|$. Since $H \Phi_G = -2v\nu s|\mathcal{V}| \Phi_G$, $\Phi_G$ must satisfy $h_\alpha \Phi_G = -2v\nu s \Phi_G$ for all $\alpha \in \mathcal{V}$. Thus $\Phi_G$ must satisfy the properties stated in Lemma 1.

The condition (37) implies that

$$a_{\alpha, \uparrow}^\dagger a_{\alpha, \downarrow}^\dagger \Phi_G = 0$$

(93)
for any $\alpha \in \mathcal{V}$. Since $a_{\alpha, \uparrow}^+ a_{\alpha, \downarrow}^+ \Phi(V_\uparrow, B_\downarrow; V_\downarrow, B_\uparrow) \neq 0$ if $\alpha \notin V_\uparrow \cup V_\downarrow$ and the states of the form $a_{\alpha, \uparrow}^+ a_{\alpha, \downarrow}^+ \Phi(V_\uparrow, B_\downarrow; V_\downarrow, B_\uparrow)$ are linearly independent with each other, $\Phi$ is expanded only in terms of the basis states $\Phi(V_\uparrow, B_\downarrow; V_\downarrow, B_\uparrow)$ with $V_\uparrow \cup V_\downarrow = \mathcal{V}$. Then, taking into account $N_e = |\mathcal{V}|$, we find that $\Phi_G$ is written as

$$\Phi_G = \sum_{\{\sigma\}} \varphi(\{\sigma\}) \left( \prod_{\alpha \in \mathcal{V}} a_{\alpha, \sigma_\alpha}^+ \right) \Phi_0, \quad (94)$$

where $\{\sigma\}$ is a shorthand for a spin configuration $\{\sigma_\alpha\}_{\alpha \in \mathcal{V}}$ of electrons each of which is singly occupying a state corresponding to $a_{\alpha, \sigma_\alpha}$, the summation is taken over all spin configurations, and $\varphi(\{\sigma\})$ is a new complex coefficient. As for the product of fermion operators, we adopt the same rule as in (60) with another one-to-one mapping $\theta'$ from $\mathcal{V}$ to $\mathbb{Z}$.

Let us impose the condition (38) on $\Phi_G$ in the form of (94). Note that (38) must hold for sites in all $A_\alpha$, i.e., for all sites in $\Lambda$. Choose site $x = m(\beta, \gamma)$. By the definition of $a_{\alpha, \sigma}$, one finds that $\{c_{m(\beta, \gamma)}, a_{\alpha, \sigma}^+\}$ is 1 if $\alpha$ is either $\beta$ or $\gamma$, and zero otherwise. Then, we have

$$c_{m(\beta, \gamma)}, \downarrow c_{m(\beta, \gamma)}, \uparrow \Phi_G$$

$$= \sum_{\{\sigma\}} S^{\beta}_{\gamma, \mathcal{V}\setminus\{\beta\}} \varphi(\{\sigma\}) c_{m(\beta, \gamma)}, \downarrow c_{m(\beta, \gamma)}, \uparrow a_{\beta, \sigma_\beta}^+ a_{\gamma, \sigma_\gamma}^+ \prod_{\alpha \in \mathcal{V}\setminus\{\beta, \gamma\}} a_{\alpha, \sigma_\alpha}^+ \Phi_0$$

$$= \sum_{\{\sigma\}} S^{\beta}_{\gamma, \mathcal{V}\setminus\{\beta\}} \varphi(\{\sigma\}) \chi[\sigma_\beta = \uparrow, \sigma_\gamma = \downarrow] - \chi[\sigma_\beta = \downarrow, \sigma_\gamma = \uparrow]$$

$$\times \left( \prod_{\alpha \in \mathcal{V}\setminus\{\beta, \gamma\}} a_{\alpha, \sigma_\alpha}^+ \right) \Phi_0, \quad (95)$$

where $S^{\beta}_{\gamma, \mathcal{V}\setminus\{\beta\}}$ and $S^{\beta}_{\gamma, \mathcal{V}\setminus\{\beta\}}$ are defined similarly as in (61) with $\theta$ replaced by $\theta'$. Since all the states $\left( \prod_{\alpha \in \mathcal{V}\setminus\{\beta, \gamma\}} a_{\alpha, \sigma_\alpha}^+ \right) \Phi_0$ in the last line are linearly independent, it follows from the condition $c_{m(\beta, \gamma)}, \downarrow c_{m(\beta, \gamma)}, \uparrow \Phi_G = 0$ that $\varphi(\{\sigma\}) = \varphi(\{\tau\})$ for any pair of spin configurations $\{\sigma\}$ and $\{\tau\}$ such that $\sigma_\beta = \tau_\beta$, $\sigma_\gamma = \tau_\gamma$, and $\sigma_\alpha = \tau_\alpha$ for $\alpha \neq \beta$, $\gamma$.

Repeating the same argument for all sites in $\Lambda$, we find that

$$\varphi(\{\sigma\}) = \varphi(\{\tau\})$$

(96)

if $\sum_{\alpha \in \mathcal{V}} \sigma_\alpha = \sum_{\alpha \in \mathcal{V}} \tau_\alpha$ (we regard $\uparrow$ as +1 and $\downarrow$ as −1 in the sum). Therefore $\Phi_G$ is always expanded as

$$\Phi_G = \sum_{M=\frac{N_e}{2}}^{N_e} \varphi_M \left( S^{t}_{\text{tot}} \right)^{N_e-M} \Phi_{\text{ferro}} \quad (97)$$

with complex coefficients $\varphi_M$. This completes the proof of Theorem 1 for $s > 0$.

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Appendix: Proof of Theorem 1 for $s = 0$; Flat-Band Ferromagnetism

Throughout this section, we assume that $s = 0$ and the other parameters $t$ and $U$ take arbitrary positive values.
As we have seen in Sect. 3, the single-electron ground state energy is zero and $|\mathcal{V}|$-fold degenerate for $s = 0$, and the single-electron ground states are given by $a_\alpha^\dagger \Phi_0$ with $\alpha \in \mathcal{V}$. Since both $H\text{hop}$ with $s = 0$ and $H\text{int}$ are positive semidefinite, we find that the energy eigenvalue of $H$ is bounded from below by zero. Taking a state $\Phi_{\text{ferro}}$ in (90) as a variational state, we conclude that the ground state energy of $H$ for $N_e = |\mathcal{V}|$ is exactly zero.

To show the uniqueness of the ground state, we will use the following property which was pointed out by Mielke [10]. Consider Hubbard models with $M$-fold degenerate single-electron ground state energy. Then, we can construct a set of $M$-fold degenerate single-electron ground states which satisfy the following condition. Let $\Phi_{1, \sigma}^{(i)}$ with $i = 1, 2, \ldots, M$ be linearly independent single-electron ground states with spin $\sigma$. For each $i$, there exists site $x_i$ such that $c_{x_i, \sigma} \Phi_{1, \sigma}^{(i)} \neq 0$ and $c_{x_i, \sigma} \Phi_{1, \sigma}^{(j)} = 0$ for $j \neq i$.

In our model, we can construct single-electron ground states which possess the above property in the following manner. For each $\alpha \in \mathcal{V}$, let us define a new fermion operator by

$$
\tilde{a}_\alpha, \sigma = a_\alpha, \sigma - \sum_{n=1}^{L-1} (-1)^n a_{\alpha + n \delta, \sigma}
$$

(recall that $\mathcal{V}$ is periodic). Since $\tilde{a}_\alpha, \sigma$ is a linear combination of $a_\beta, \sigma$ with $\beta \in \mathcal{V}$, the single-electron states $\tilde{a}_\alpha^\dagger, \sigma \Phi_0$ apparently have energy 0. Furthermore, we have

$$
\left\{ \tilde{a}_\beta, \sigma, \ c_{m(\alpha, \alpha + \delta), \sigma} \right\} = \begin{cases} 2 & \text{if } \beta = \alpha; \\ 0 & \text{otherwise}. \end{cases}
$$

These anticommutation relations imply that the single-electron states $\tilde{a}_\alpha^\dagger, \sigma \Phi_0$ with $\alpha \in \mathcal{V}$ have the desired property. We note that (99) also implies the linear independence of these single-electron states.

Let us prove the uniqueness of the ground state by using $\{\tilde{a}_\alpha, \sigma\}_{\alpha \in \mathcal{V}}$ introduced as above. Let $\Phi_G$ be a ground state, which must be a zero energy state for both $H\text{hop}$ and $H\text{int}$. Since $\Phi_G$ is a zero energy state for $H\text{hop}$, we expand it as

$$
\Phi_G = \sum_{V_\uparrow, V_\downarrow \subset \mathcal{V}} \varphi'(V_\uparrow; V_\downarrow) \left( \prod_{\alpha \in V_\uparrow} \tilde{a}_\alpha^\dagger, \uparrow \right) \left( \prod_{\alpha \in V_\downarrow} \tilde{a}_\alpha^\dagger, \downarrow \right) \Phi_0
$$

with complex coefficients $\varphi'(V_\uparrow; V_\downarrow)$. To be a zero energy state of the on-site interaction, $\Phi_G$ in the form of (100) must further satisfy the condition $c_{x, \downarrow} c_{x, \uparrow} \Phi_G = 0$ for all $x$ in $\Lambda$. We examine this condition for sites $x = m(\alpha, \alpha + \delta, \nu)$ with $\alpha \in \mathcal{V}$. Then, taking account of (99), we find that $\varphi'(V_\uparrow; V_\downarrow)$ is vanishing if $V_\uparrow \cap V_\downarrow \neq \emptyset$. A ground state $\Phi_G$ is thus rewritten as

$$
\Phi_G = \sum_{[\sigma]} \varphi'([\sigma]) \left( \prod_{\alpha \in \mathcal{V}} \tilde{a}_\alpha^\dagger, [\sigma] \right) \Phi_0
$$

with new coefficients $\varphi'([\sigma])$. Now we have expressed $\Phi_G$ in the same fashion as in (94). Examining repeatedly the condition $c_{x, \downarrow} c_{x, \uparrow} \Phi_G = 0$ for sites $x = m(\beta, \beta + \delta_l)$ with $l \neq \nu$, we obtain the same relation for $\varphi'([\sigma])$ as that in (96). Therefore, we conclude that the ground state is unique apart from the degeneracy due to the spin rotation symmetry. This completes the proof of Theorem 1 for $s = 0$.  

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