Stability of Ferromagnetism in the Hubbard Model on the Kagome Lattice

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The Hubbard model on the kagome lattice has highly degenerate ground states (the flat lowest band) in the corresponding single-electron problem and exhibits the so-called flat-band ferromagnetism in the many-electron ground states as was found by Mielke [J. Phys. A **24**, L73 (1991)]. Here we study the model obtained by adding extra hopping terms to the above model. The lowest single-electron band becomes dispersive, and there is no band gap between the lowest band and the other band. We prove that, at half filling of the lowest band, the ground states of this perturbed model remain saturated ferromagnetic if the lowest band is nearly flat.

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Numerous studies have been made on the Hubbard model, a tight-binding model of electrons with on-site interactions, to understand mechanisms for itinerant-electron ferromagnetism [1–4]. Recently, a significant breakthrough was brought by Mielke [5] and by Tasaki [6] who proved that certain classes of Hubbard models have ferromagnetic ground states. These models in common have multi single-electron bands containing dispersionless bands and are called flat-band Hubbard models.

Although these flat-band Hubbard models shed light on the role of the Coulomb interaction in ferromagnetism, the models with completely flat bands are still singular. Since the bands supporting ferromagnetism are flat, the ferromagnetic states are already among the ground states of these models in the noninteracting case. This implies that the flat-band models do not describe true competition between the kinetic energy and the Coulomb interaction. The next important step is thus to clarify whether the flat-band ferromagnetism is stable against perturbations which turn the flat bands into dispersive bands. As for Tasaki's version of flat-band Hubbard models, local stability of the ferromagnetic ground state in perturbed nearly flat-band models was proved [7]. Tasaki also gave a concrete example of nearly flat-band Hubbard models in which he could prove that the ground states are ferromagnetic [8,9]. See [10,11] for related results.

As for Mielke's version of flat-band Hubbard models, on the other hand, there have been no rigorous results about stability (or instability) of ferromagnetism in perturbed nearly flat-band models. Here we note the following essential difference between Mielke's and Tasaki's models: there are no band gaps in Mielke's models while there are finite band gaps in Tasaki's models. We stress that the problem of stability of ferromagnetism is much more subtle and difficult in Mielke's models, where one might encounter various low energy excitation modes which reflect the gapless nature of the band structures.

In this Letter, we treat the model obtained by adding hopping terms to the Hubbard model on the kagome lattice, a typical example of Mielke's models [12]. The added terms change the flat lowest band into a dispersive band of a cosine type, but the band structure remains gapless. We prove that our model has saturated ferromagnetic ground states at half filling of the lowest band, provided that the lowest band is nearly flat.

Although the added terms considered here are special, this is the first time, to our knowledge, that a nonsingular Hubbard model with gapless dispersive bands and a simple lattice structure (where all the lattice sites are identical) is proved to exhibit ferromagnetism for finite on-site interactions. We hope that our result will open a route to a better understanding of itinerant-electron ferromagnetism. Very recently, a possibility of (nearly) flat-band ferromagnetism in quantum dot arrays was proposed [13]. We also hope that our result will stimulate research in this field.

Definition.—We first define the reference lattice $\mathcal{L}$ as

$$\mathcal{L} = \left\{ n_1\nu_1 + n_2\nu_2 \;\middle|\; \begin{array}{ll} n_i \in \mathbb{Z} & \text{and} \quad 0 \le \\ n_i < L & \text{for } i = 1, 2 \end{array} \right\}, \tag{1}$$

where $\nu_1 = (1, 0)$, $\nu_2 = (\frac{1}{2}, \sqrt{3}/2)$, and L is a positive integer. For each $\alpha \in \mathcal{L}$ we define [14]

$$C_\alpha^1 = \left\{ x = n_1 \frac{\nu_1}{2} + n_2 \frac{\nu_2}{2} | n_1, n_2 \in \mathbb{Z}, |x - \alpha| = \frac{1}{2} \right\}, \tag{2}$$

$$C_\alpha^2 = \left\{ x = n_1 \frac{\nu_1}{2} + n_2 \frac{\nu_2}{2} | n_1, n_2 \in \mathbb{Z}, |x - \alpha| = \sqrt{3}/2 \right\}, \tag{3}$$

and $C_\alpha = C_\alpha^1 \cup C_\alpha^2$ [Fig. 1(a)]. Then, the kagome lattice Λ can be constructed as $\Lambda = \cup_{\alpha \in \mathcal{L}} C_\alpha$, where a site $x \in \Lambda$ is generally counted 4 times in different C_α [Fig. 1(b)]. Our lattice has open boundaries. Periodic lattices can be also treated with extra technical complication. We denote by Φ_0 the state with no electrons and denote by $c_{x,\sigma}$ and $c_{x,\sigma}^\dagger$ the annihilation and the creation operators, respectively, of an electron with spin σ at site x in Λ. These operators satisfy the usual fermion anticommutation relations. The number operator is defined as $n_{x,\sigma} = c_{x,\sigma}^\dagger c_{x,\sigma}$. The total spin operators $\boldsymbol{S}_{\text{tot}} = [S_{\text{tot}}^{(1)}, S_{\text{tot}}^{(2)}, S_{\text{tot}}^{(3)}]$ are defined

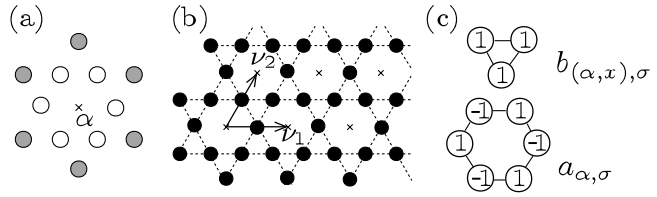

FIG. 1. (a) Local lattice $C_\alpha = C_\alpha^1 \cup C_\alpha^2$. The open and the gray circles represent sites in C_α^1 and C_α^2, respectively. (b) Lattice Λ. (c) The operators $b_{(\alpha,x),\sigma}$ and $a_{\alpha,\sigma}$ are supported on the triangle and the hexagon, respectively. The number in a circle is the coefficient of $c_{x,\sigma}$ for the site.

as $S_{\rm tot}^{(i)} = \frac{1}{2}\sum_{x\in\Lambda}\sum_{\sigma,\tau=\uparrow,\downarrow} c_{x,\sigma}^\dagger p_{\sigma\tau}^{(i)} c_{x,\tau}$ for $i = 1, 2, 3$, where $p^{(i)} = [p^{(i)}]_{\sigma,\tau=\uparrow,\downarrow}$ are the Pauli matrices. We denote by $S_{\rm tot}(S_{\rm tot}+1)$ the eigenvalue of $(\boldsymbol{S}_{\rm tot})^2$.

Let us define our Hubbard Hamiltonian. First, for each $x \in C_\alpha^2$ we define $b_{(\alpha,x),\sigma} = c_{x,\sigma} + \sum_{y\in C_\alpha^1;|y-x|=\frac{1}{2}} c_{y,\sigma}$. We also define $a_{\alpha,\sigma} = \sum_{y\in C_\alpha^1} \mu[\alpha, y] c_{y,\sigma}$ for $\alpha \in \mathcal{L}$, where we pick $\mu[\alpha, y]$ to be alternately $+1$ and -1 when going around a hexagon. [See Fig. 1(c).] To each C_α we associate the local Hamiltonian

$$\mathcal{H}_\alpha = -s\sum_{\sigma=\uparrow,\downarrow} a_{\alpha,\sigma}^\dagger a_{\alpha,\sigma} + \frac{t}{3}\sum_{\sigma=\uparrow,\downarrow}\sum_{x\in C_\alpha^2} b_{(\alpha,x),\sigma}^\dagger b_{(\alpha,x),\sigma} + \frac{U}{4}\sum_{x\in C_\alpha} n_{x,\uparrow} n_{x,\downarrow}, \tag{4}$$

where s, t, and U are positive parameters. Then, the Hubbard Hamiltonian on the whole lattice Λ is defined as $\mathcal{H} = \sum_{\alpha\in\mathcal{L}} \mathcal{H}_\alpha$.

Remarks.—It is possible to rewrite $\mathcal{H}$ into the standard form as $\mathcal{H} = \sum_\sigma \sum_{x,y\in\Lambda} t_{xy} c_{x,\sigma}^\dagger c_{y,\sigma} + \sum_{x\in\Lambda} U_x n_{x,\uparrow} n_{x,\downarrow}$, where the model parameters are given by $U_x = U$, and $t_{xy} = 2(t-s)$ if $x = y$, $t_{xy} = t + s$ if $|x-y| = 1/2$, $t_{xy} = -s$ if $|x-y| = \sqrt{3}/2$, $t_{xy} = s$ if $|x-y| = 1$, and $x, y \in C_\alpha^1$ with some α, and $t_{xy} = 0$ otherwise, except for the sites close to the boundary. The single-electron dispersion relations (calculated in the model with periodic boundary conditions) are given by $E_1(k) = -2s[3 - e(k)]$, $E_2(k) = t[3 - \sqrt{3 + 2e(k)}]$, and $E_3(k) = t[3 + \sqrt{3 + 2e(k)}]$ with $e(k) = \cos k_1 + \cos k_2 + \cos(k_1 - k_2)$, where $k = k_1\nu_1^* + k_2\nu_2^*$ is the wave vector expanded in terms of reciprocal-lattice vectors $\nu_1^* = (1, -1/\sqrt{3})$ and $\nu_2^* = (0, 2/\sqrt{3})$. Note that $E_1(0) = E_2(0) = 0$, which means that there is no gap between the lowest and the second lowest bands.

One readily finds that $\{a_{\alpha,\sigma}, b_{(\beta,x),\sigma}^\dagger\} = 0$ for any $\alpha, \beta \in \mathcal{L}$ and $x \in C_\beta^2$. This implies that $\{a_{\alpha,\sigma}^\dagger \Phi_0\}_{\alpha\in\mathcal{L}}$ spans the space corresponding to the lowest band.

If we set $s = 0$, our model has highly degenerate single-electron ground states and becomes essentially the flat-band model of Mielke's (although there is a difference in boundary conditions). In this case, the model exhibits flat-band ferromagnetism for all positive values of U. In the model with $s > 0$, the situation is quite different because double occupancies of lower energy states, which destroy the ferromagnetic order, may reduce the total energy of the system. It is indeed easy to prove that the ground states of our model have $S_{\rm tot} = 0$ (or $\frac{1}{2}$) for $U = 0$ and cannot exhibit saturated ferromagnetism for sufficiently small U. (See, for example, Sec. 3.3 of [4].) The following theorem establishes that the ferromagnetic ground states are stable for sufficiently large t and U when the electron number is $|\mathcal{L}|$.

Main theorem: *Consider the Hubbard model defined as above with the electron number $|\mathcal{L}|$. Then, there exist critical values $(t/s)_{\rm c}$ and $(U/s)_{\rm c}$, independent of the lattice size, such that, if both $t/s > (t/s)_{\rm c}$ and $U/s > (U/s)_{\rm c}$ are satisfied, the ground states of the model have $S_{\rm tot} = |\mathcal{L}|/2$. Furthermore, the ground state is unique up to the degeneracy due to the rotational symmetry.*

In Tasaki's models, the stability of ferromagnetism may be, at least at a heuristic level, understood as a consequence of the band gap separating the lowest nearly flat band from other bands. The band gap enforces the electrons to occupy the lowest band while the interaction rules out double occupancies of sites. Then the situation is almost as in the flat-band models, and the systems exhibit ferromagnetism. To Mielke's models, which have no band gaps, the above argument does not apply, and the origin of the stability of ferromagnetism seems more subtle. Nevertheless, our proof is based on essentially the same philosophy as that of Tasaki's proof in [8]. Namely, we first establish ferromagnetism in a local model described by $\mathcal{H}_\alpha$ and then show that this local ferromagnetism can be "connected," which results in macroscopic ferromagnetism in the whole system. The results of the analysis of $\mathcal{H}_\alpha$ are summarized in the following lemma.

Lemma: *If t/s and U/s are sufficiently large, the minimum eigenvalue of $\mathcal{H}_\alpha$ is $-6s$ and any eigenstate Φ belonging to this eigenvalue is written as*

$$\Phi = a_{\alpha,\uparrow}^\dagger \Phi_\uparrow + a_{\alpha,\downarrow}^\dagger \Phi_\downarrow, \tag{5}$$

with suitable states $\Phi_\uparrow$ and $\Phi_\downarrow$. Furthermore, it satisfies

$$c_{x,\downarrow} c_{x,\uparrow} \Phi = 0 \tag{6}$$

for all $x \in C_\alpha$.

Proof of Lemma: Since all the local Hamiltonians are the translated copies of $\mathcal{H}_0$, it suffices to prove the lemma for $\alpha = 0$. From now on, for convenience, we identify C_0^1 and C_0^2 with $\{0, 2, \ldots, 10\}$ and $\{1, 3, \ldots, 11\}$, respectively [we first label $(\frac{1}{2}, 0)$ as 0, then label the rest of the sites as $1, \ldots, 11$ in the clockwise order].

We start by solving a single-electron problem for $\mathcal{H}_0$. Let $I = \{0, \pm\frac{\pi}{3}, \pm\frac{2\pi}{3}, \pi\}$. The eigenvalues are given by

$$\varepsilon_1(p) = \begin{cases} 0 & \text{if } p \in I\backslash\{\pi\}; \\ -6s & \text{if } p = \pi, \end{cases} \tag{7}$$

and $\varepsilon_2(p) = \frac{t}{3}(3 + 2\cos p)$ with $p \in I$. The eigenstate corresponding to $\varepsilon_1(p)$ is expressed as $d_{p,\sigma}^\dagger \Phi_0$ with

$$d_{p,\sigma} = 1/\sqrt{6(3 + 2\cos p)} \sum_{l=0}^{5} e^{ipl}(c_{2l,\sigma} - c_{2l-1,\sigma} - c_{2l+1,\sigma}) \tag{8}$$

(where $c_{-1,\sigma}$ is regarded as $c_{11,\sigma}$). Note that the set $\{d^\dagger_{p,\sigma}\Phi_0\}_{p\in I}$ is orthonormal since $\{d_{p,\sigma}, d^\dagger_{p',\sigma}\} = \delta_{p,p'}$.

We consider the many-electron problem for $\mathcal{H}_0$, first in the limit $t, U \to \infty$. Let Φ be a state on C_0 which has a finite energy in this limit. Since all $\varepsilon_2(p)$ are infinite in the limit $t \to \infty$, Φ must be expanded as

$$\Phi = \sum_{I_\uparrow, I_\downarrow \subset I} g(I_\uparrow; I_\downarrow)\Phi(I_\uparrow; I_\downarrow) \tag{9}$$

with complex coefficients $g(I_\uparrow; I_\downarrow)$, where

$$\Phi(I_\uparrow; I_\downarrow) = \prod_{p\in I_\uparrow} d^\dagger_{p,\uparrow} \prod_{p'\in I_\downarrow} d^\dagger_{p',\downarrow}\Phi_0. \tag{10}$$

Here, and throughout the present Letter, the products are ordered in such a way that $d^\dagger_{p,\uparrow}$ (respectively, $d^\dagger_{p,\downarrow}$) is always on the left of $d^\dagger_{p',\uparrow}$ (respectively, $d^\dagger_{p',\downarrow}$) if $p < p'$.

Since the on-site interaction $n_{x,\uparrow}n_{x,\downarrow} = c^\dagger_{x,\uparrow}c^\dagger_{x,\downarrow}c_{x,\downarrow}c_{x,\uparrow}$ is positive semidefinite, the state Φ in the form of (9) must further satisfy

$$\sum_{I_\uparrow, I_\downarrow \subset I} g(I_\uparrow; I_\downarrow)c_{x,\downarrow}c_{x,\uparrow}\Phi(I_\uparrow; I_\downarrow) = 0 \tag{11}$$

for any $x \in C_0$ in order to have finite energy in the limit $U \to \infty$. From (7), (9), and (10), one finds that the expectation value of $\mathcal{H}_0$ for the state Φ is $E_\Phi = (\Phi, \mathcal{H}_0\Phi)/(\Phi, \Phi) = -6s + 6sF\|\Phi\|^{-2}$, with $F = \sum_{I_\uparrow, I_\downarrow \subset I\setminus\{\pi\}}[|g(I_\uparrow; I_\downarrow)|^2 - |g(I^\pi_\uparrow; I^\pi_\downarrow)|^2]$ and $\|\Phi\|^2 = [\sum_{I_\uparrow, I_\downarrow \subset I} |g(I_\uparrow; I_\downarrow)|^2]$ [15], where coefficients g should satisfy the condition (11). Here, and in what follows, we abbreviate $I_\sigma \cup \{p\}$ as I^p_σ for $p \in I$. In the following, we show $F \geq 0$. This implies $E_\Phi \geq -6s$ since $s > 0$.

To prove $F \geq 0$, we first derive conditions on g imposed by (11). If we denote $(\varphi^{(p)}_x)^* = \{c_{x,\sigma}, d^\dagger_{p,\sigma}\}$, the left-hand side of (11) becomes

$$\sum_{I_\uparrow, I_\downarrow \subset I; |I_\uparrow|\geq 1, |I_\downarrow|\geq 1} g(I_\uparrow; I_\downarrow) \sum_{p\in I_\uparrow} \sum_{p'\in I_\downarrow} (-1)^{|I_\uparrow|-1} \mathsf{S}^p_{I_\uparrow} \mathsf{S}^{p'}_{I_\downarrow} (\varphi^{(p)}_x)^* (\varphi^{(p')}_x)^* \Phi(I_\uparrow\setminus\{p\}; I_\downarrow\setminus\{p'\})$$

$$= \sum_{p,p'\in I} (\varphi^{(p)}_x)^* (\varphi^{(p')}_x)^* \sum_{I_\uparrow \subset I\setminus\{p\}} \sum_{I_\downarrow \subset I\setminus\{p'\}} (-1)^{|I_\uparrow|} \mathsf{S}^p_{I_\uparrow} \mathsf{S}^{p'}_{I_\downarrow} g(I^p_\uparrow; I^{p'}_\downarrow)\Phi(I_\uparrow; I_\downarrow) = \sum_{I_\uparrow, I_\downarrow \subset I} \sum_{p,p'\in I} (\varphi^{(p)}_x)^* (\varphi^{(p')}_x)^* \tilde{g}(I^p_\uparrow; I^{p'}_\downarrow)\Phi(I_\uparrow; I_\downarrow), \tag{12}$$

where $\mathsf{S}^p_{I_\sigma}$, which corresponds to a sign factor coming from exchange of the fermion operators, equals 1 if $\sum_{p'\in I_\sigma; p'<p} 1$ is even and -1 otherwise. In the final expression of (12), we introduced subsidiary coefficients $\tilde{g}$ defined as $\tilde{g}(I^p_\uparrow; I^{p'}_\downarrow) = 0$ if $p \in I_\uparrow$ or $p' \in I_\downarrow$ and $\tilde{g}(I^p_\uparrow; I^{p'}_\downarrow) = (-1)^{|I_\uparrow|}\mathsf{S}^p_{I_\uparrow}\mathsf{S}^{p'}_{I_\downarrow} g(I^p_\uparrow; I^{p'}_\downarrow)$ otherwise. Therefore, $c_{x,\downarrow}c_{x,\uparrow}\Phi = 0$ holds if and only if $\sum_{p,p'\in I}(\varphi^{(p)}_x)^*(\varphi^{(p')}_x)^*\tilde{g}(I^p_\uparrow; I^{p'}_\downarrow) = 0$ for any $I_\uparrow, I_\downarrow \subset I$. Taking the sum of this equation over $x \in C^1_0$, we find that $\sum_{p\in I} \frac{1}{(3+2\cos p)} \tilde{g}(I^p_\uparrow; I^{-p}_\downarrow) = 0$ and similarly taking the sum over $x \in C^2_0$, we find that $\sum_{p\in I} \frac{(1+\cos p)}{(3+2\cos p)} \tilde{g}(I^p_\uparrow; I^{-p}_\downarrow) = 0$ (where we identified $-\pi$ with π). By eliminating $\tilde{g}(I^0_\uparrow; I^0_\downarrow)$ from these two equations, we obtain

$$\tilde{g}(I^\pi_\uparrow; I^\pi_\downarrow) = -\tfrac{1}{16}\tilde{g}(I^{\pi/3}_\uparrow; I^{-\pi/3}_\downarrow) - \tfrac{1}{16}\tilde{g}(I^{-\pi/3}_\uparrow; I^{\pi/3}_\downarrow) - \tfrac{3}{8}\tilde{g}(I^{2\pi/3}_\uparrow; I^{-2\pi/3}_\downarrow) - \tfrac{3}{8}\tilde{g}(I^{-2\pi/3}_\uparrow; I^{2\pi/3}_\downarrow). \tag{13}$$

Our analysis below relies heavily on this condition.

For a subset $I_\downarrow$ of I, we define $\bar{I}_\downarrow = \{-p | p \in I_\downarrow\}$ and denote by $N(I_\uparrow; I_\downarrow)$ the number of elements in $I_\uparrow \cap \bar{I}_\downarrow \cap (I\setminus\{0, \pi\})$. Condition (13) relates $\tilde{g}(I_\uparrow; I_\downarrow)$ with $I_\uparrow, I_\downarrow$ such that $N(I_\uparrow; I_\downarrow) = r$ and $\tilde{g}(I'_\uparrow; I'_\downarrow)$ with $I'_\uparrow, I'_\downarrow$ such that $N(I'_\uparrow; I'_\downarrow) = r + 1$. This motivates us to decompose F as $F = F' + \sum_{r=0}^4 F_r$, where

$$F_r = \sum_{\substack{I_\uparrow, I_\downarrow \subset I\setminus\{\pi\}; \\ N(I_\uparrow; I_\downarrow) = r+1}} |g(I_\uparrow; I_\downarrow)|^2 - \sum_{\substack{I_\uparrow, I_\downarrow \subset I\setminus\{\pi\}; \\ N(I_\uparrow; I_\downarrow) = r}} |g(I^\pi_\uparrow; I^\pi_\downarrow)|^2, \tag{14}$$

$$F' = \sum_{I_\uparrow, I_\downarrow \subset I\setminus\{\pi\}; N(I_\uparrow; I_\downarrow) = 0} |g(I_\uparrow; I_\downarrow)|^2. \tag{15}$$

Since the term F' is apparently non-negative, $F \geq 0$ is implied by $F_r \geq 0$ for $r = 0, \ldots, 4$.

We shall prove that $F_r \geq 0$ by using (13). For a pair of $I^\pi_\uparrow$ and $I^\pi_\downarrow$ such that $N(I^\pi_\uparrow; I^\pi_\downarrow) = r$, the number of nonzero $\tilde{g}$ on the right-hand side of (13) is, by the definition, at most $4 - r$, and thus for such a pair we have [16]

$$|\tilde{g}(I^\pi_\uparrow; I^\pi_\downarrow)|^2 \leq \frac{9}{64}(4 - r) \sum_{p\in I\setminus\{0,\pi\}} |\tilde{g}(I^p_\uparrow; I^{-p}_\downarrow)|^2. \tag{16}$$

Then, we find that

$$\sum_{\substack{I_\uparrow, I_\downarrow \subset I\setminus\{\pi\}; \\ N(I_\uparrow; I_\downarrow) = r}} |g(I^\pi_\uparrow; I^\pi_\downarrow)|^2 = \sum_{\substack{I_\uparrow, I_\downarrow \subset I\setminus\{\pi\}; \\ N(I_\uparrow; I_\downarrow) = r}} |\tilde{g}(I^\pi_\uparrow; I^\pi_\downarrow)|^2 \leq \frac{9}{64}(4 - r) \sum_{\substack{I_\uparrow, I_\downarrow \subset I\setminus\{\pi\}; \\ N(I_\uparrow; I_\downarrow) = r}} \sum_{p\in I\setminus\{0,\pi\}} |\tilde{g}(I^p_\uparrow; I^{-p}_\downarrow)|^2$$

$$= \frac{9}{64}(4 - r)(r + 1) \sum_{\substack{I_\uparrow, I_\downarrow \subset I\setminus\{\pi\}; \\ N(I_\uparrow; I_\downarrow) = r+1}} |g(I_\uparrow; I_\downarrow)|^2 \leq \frac{27}{32} \sum_{I_\uparrow, I_\downarrow \subset I\setminus\{\pi\}; N(I_\uparrow; I_\downarrow) = r+1} |g(I_\uparrow; I_\downarrow)|^2. \tag{17}$$

To get the second line, we have used the fact that, for $I_\uparrow$ and $I_\downarrow$ such that $N(I_\uparrow; I_\downarrow) = r + 1$, there are $r + 1$ elements p in $I\setminus\{0, \pi\}$ for which we can find suitable subsets $I'_\uparrow$ and $I'_\downarrow$ such that $\{p\} \cup I'_\uparrow = I_\uparrow$ and $\{-p\} \cup I'_\downarrow = I_\downarrow$. To obtain the final inequality, we have used $(4 - r)(r + 1) \leq 6$ for $0 \leq r \leq 4$. By using (17) we obtain

$$F_r \geq \frac{5}{32} \sum_{I_\uparrow, I_\downarrow \subset I \setminus \{\pi\}; N(I_\uparrow; I_\downarrow) = r+1} |g(I_\uparrow; I_\downarrow)|^2 \geq 0. \qquad (18)$$

We therefore conclude that $F \geq 0$. The above analysis also shows that the equality $F = 0$ holds only when F' and F_r are vanishing, i.e., $g(I_\uparrow; I_\downarrow) = 0$ for any pair of $I_\uparrow$ and $I_\downarrow$ such that $\pi \in I_\uparrow \cap I_\downarrow$ or $\pi \notin I_\uparrow \cup I_\downarrow$.

In other words, we have shown that $E_\Phi \geq -6s$ for any Φ and that any Φ attaining the minimum expectation value $-6s$ is written as

$$\Phi = \sum_{I_\uparrow, I_\downarrow \subset I; \pi \in I_\uparrow \cup I_\downarrow, \pi \notin I_\uparrow \cap I_\downarrow} g(I_\uparrow; I_\downarrow) \Phi(I_\uparrow; I_\downarrow) \qquad (19)$$

and further satisfies the finite energy condition (11). One finds that such minimizing Φ indeed exists by testing $d^\dagger_{\pi,\uparrow}\Phi_0$ or $\prod_{p \in I} d^\dagger_{p,\uparrow}\Phi_0$. By construction such Φ is an eigenstate of $\mathcal{H}_0$ as well as $-s\sum_\sigma a^\dagger_{0,\sigma}a_{0,\sigma}$. Since it is known to be the lowest energy state of $\mathcal{H}_0$ in the limit $t, U \to \infty$, the continuity of energy implies that such Φ is the lowest energy state of $\mathcal{H}_0$ for sufficiently large t/s and U/s. It is also easy to check that such Φ has the properties stated in the lemma. [Note that $d_{\pi,\sigma} = (\mu[0,0]/\sqrt{6})a_{0,\sigma}$.] This completes the proof of the lemma. ■

Proof of Theorem: We assume that the values of t/s and U/s are large enough for the statement in the lemma to hold. We note that how large t/s and U/s should be is independent of the size of Λ, because the lemma is concerned with the local Hamiltonian.

From the lemma we find that the lowest energy E_G of $\mathcal{H}$ is bounded below by $-6s|\mathcal{L}|$, while, by taking $\Phi_f = \prod_{\alpha \in \mathcal{L}} a^\dagger_{\alpha,\uparrow}\Phi_0$ as a variational state, we find that $-6s|\mathcal{L}|$ is an upper bound on E_G [17]. Therefore, $E_G = -6s|\mathcal{L}|$, and Φ_f and its SU(2) rotations are among the ground states. Apparently these states have $S_{tot} = |\mathcal{L}|/2$.

The remaining task is to prove the uniqueness. Let Φ_G be an arbitrary ground state. The lemma implies that E_G is attained if and only if $\mathcal{H}_\alpha\Phi_G = -6s\Phi_G$ for all $\alpha \in \mathcal{L}$. Thus Φ_G must satisfy the conditions stated in the lemma.

The condition (5) implies that Φ_G is expressed as [18]

$$\Phi_G = \sum_{\{\sigma\}} \varphi(\{\sigma\}) \prod_{\alpha \in \mathcal{L}} a^\dagger_{\alpha,\sigma_\alpha}\Phi_0, \qquad (20)$$

where $\{\sigma\}$ is a shorthand for a spin configuration $\{\sigma_\alpha\}_{\alpha \in \mathcal{L}}$, the summation is over $\sigma_\alpha = \uparrow, \downarrow$ for all $\alpha \in \mathcal{L}$, and $\varphi(\{\sigma\})$ is a complex coefficient.

Let us impose the condition (6) on Φ_G in the form of (20). Let β and γ be nearest neighbor points in $\mathcal{L}$, i.e., $|\beta - \gamma| = 1$, and let $m(\beta, \gamma) \in \Lambda$ be the site located at the midpoint between β and γ. It is easy to see that $\{c_{m(\beta,\gamma),\sigma}, a^\dagger_{\alpha,\sigma}\}$ is nonvanishing if $\alpha = \beta$ or γ, and is vanishing otherwise. Then, 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 $\{\tau\}$ satisfying that $\sigma_\beta = \tau_\gamma$, $\sigma_\gamma = \tau_\beta$, and $\sigma_\alpha = \tau_\alpha$ for $\alpha \neq \beta, \gamma$. Examining $c_{m(\beta,\gamma),\downarrow}c_{m(\beta,\gamma),\uparrow}\Phi_G = 0$ for all the pairs of nearest neighbor points in $\mathcal{L}$, we find that $\varphi(\{\sigma\}) = \varphi(\{\tau\})$ whenever $\sum_\alpha \sigma_\alpha = \sum_\alpha \tau_\alpha$. Therefore Φ_G is written as $\Phi_G = \sum_{M=0}^{|\mathcal{L}|} \varphi_M (S^-_{tot})^M \Phi_f, ,$ where φ_M are new coefficients and the spin lowering operator S^-_{tot} is defined by $S^-_{tot} = \sum_{x \in \Lambda} c^\dagger_{x,\downarrow}c_{x,\uparrow}$. This completes the proof. ■

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[12] It is possible to prove the stability of ferromagnetism in Mielke's models on other lattices such as a regular lattice of corner-sharing tetrahedra. The details will appear elsewhere.
[13] H. Tamura, K. Shiraishi, T. Kimura, and H. Takayanagi, Phys. Rev. B **65**, 085324 (2002).
[14] Here $|\cdot|$ denotes the Euclidean norm. We use the same symbol $|X|$ to denote the number of elements in a set X.
[15] Note that $\Phi(I_\uparrow; I_\downarrow)$ are the eigenstates of $-s\sum_\sigma a^\dagger_{0,\sigma}a_{0,\sigma}$ and the set of these states is orthonormal.
[16] We have used inequality $|\sum_{i=1}^N z_i|^2 \leq N\sum_{i=1}^N |z_i|^2$ which follows from the Schwarz inequality.
[17] Note that $-sa^\dagger_{\alpha,\uparrow}a_{\alpha,\uparrow}\Phi_f = -s(6 - a_{\alpha,\uparrow}a^\dagger_{\alpha,\uparrow})\Phi_f = -6s\Phi_f$ since $\{a_{\alpha,\sigma}, a^\dagger_{\alpha,\sigma}\} = 6$ and $(a^\dagger_{\alpha,\sigma})^2 = 0$, which follow from straightforward calculations.
[18] Proof: Since all $a^\dagger_{\alpha,\sigma}\Phi_0$ with $\alpha \in \mathcal{L}$ are linearly independent, we can form a basis of the single-electron Hilbert space on Λ by adding $|\Lambda| - |\mathcal{L}|$ linearly independent states. We denote these states by $f^\dagger_{i,\sigma}\Phi_0$ with $i \in \mathcal{I}$, where $\mathcal{I}$ is some index set with $|\mathcal{I}| = |\Lambda| - |\mathcal{L}|$. Then, the set of states $(\prod_{\alpha \in \mathcal{L}_\uparrow} a^\dagger_{\alpha,\uparrow})(\prod_{\beta \in \mathcal{L}_\downarrow} a^\dagger_{\beta,\downarrow})(\prod_{i \in I_\uparrow} f^\dagger_{i,\uparrow}) \times (\prod_{j \in I_\downarrow} f^\dagger_{j,\downarrow})\Phi_0$ with $\mathcal{L}_\uparrow, \mathcal{L}_\downarrow \subset \mathcal{L}$ and $I_\uparrow, I_\downarrow \subset \mathcal{I}$ satisfying $\sum_\sigma(|\mathcal{L}_\sigma| + |I_\sigma|) = N_e$ is a basis of N_e-electron Hilbert space. We suppose that Φ_G is expanded with respect to this basis and then use condition (5).