

Gapless Excitation above a Domain Wall Ground State in a Flat-Band Hubbard Model

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We construct a set of exact ground states with a localized ferromagnetic domain wall and with an extended spiral structure in a deformed flat-band Hubbard model in arbitrary dimensions. We show the uniqueness of the ground state for the half-filled lowest band in a fixed magnetization subspace. The ground states with these structures are degenerate with all-spin-up or all-spin-down states under the open boundary condition. We present a spin one-point function in terms of local electron number density, and find the domain wall structure in our model. We show the existence of gapless excitations above a domain wall ground state in dimensions higher than one. On the other hand, under the periodic boundary condition, the ground state is the all-spin-up or all-spin-down state. We show that the spin-wave excitation above the all-spin-up or -down state has an energy gap because of the anisotropy.

KEY WORDS: ferromagnetic domain wall; spiral state; flat-band Hubbard model; exact solution; quantum effect; spin-wave; gapless excitation.

1. INTRODUCTION

Domain structures are observed universally in many ferromagnetic systems. If a system has a translational symmetry, this symmetry is broken spontaneously by domains. In classical spin systems, universal properties of the domain wall have been studied extensively. For example in the Ising model on the cubic lattice, Dobrushin proved that a horizontal domain wall is stable against the thermal fluctuations at sufficiently low temperatures.⁽¹⁾ This structure in the Ising model is also preserved under quantum perturbations. Borgs, Chayes and Fröhlich proved that the horizontal domain wall on the d -dimensional hyper cubic lattice is stable also

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against weak quantum perturbations at sufficiently low temperatures for $d \geq 3$.⁽²⁾ On the other hand, a diagonal domain wall structure is unstable in the Ising model, since some local operators can deform the diagonal domain wall state to many other ground states without loss of energy. In the ferromagnetic XXZ model in dimensions higher than one, however, no local operator can deform the diagonal domain wall ground state to other ground states by the exchange interaction. This fact suggests that the diagonal domain structures are stable at sufficiently low temperatures in sufficiently high dimensions, even though there is no proof. Alcaraz, Salinas and Wreszinski construct a set of ground state with diagonal domain wall structure in the XXZ model with a critical boundary field in arbitrary dimensions for an arbitrary spin.⁽³⁾ Gottstein and Werner clarified the structure of ground states in the one-dimensional XXZ model with an infinite-volume.⁽⁴⁾ Koma and Nachtergaele proved that there is an energy gap above any ground states in the one-dimensional XXZ model.⁽⁵⁾ They also showed an interesting result that there exists a gapless excitation above the domain wall ground state in the XXZ model in two dimensions.⁽⁶⁾ Matsui extended this theorem to the XXZ model in arbitrary dimensions higher than one.⁽⁷⁾ Bolina, Contucci, Nachtergaele and Starr gave more precise bound for the gapless excitation above the diagonal domain wall ground state in the XXZ model.⁽⁸⁾ Bach and Macris evaluate a spin one-point function in the domain wall state of the one-dimensional XXZ model by a rigorous perturbation method.⁽⁹⁾ Datta and Kennedy also discussed the existence of a domain wall in one-dimensional XXZ models by another rigorous perturbation method.⁽¹⁰⁾ They show that the exchange interaction destroys the domain wall in the antiferromagnetic model, while the domain wall exists in the ferromagnetic model at zero temperature. The role of the quantum effects should be studied more in many other models.

Recently, a deformed flat-band Hubbard model with an exact domain wall ground state was proposed.^(11,12) The purpose of this paper is to study excitations above the domain wall ground state in this model and clarify whether or not, this model has the same spectra as in the XXZ model. The flat-band Hubbard model was proposed as a lattice electron model with a ferromagnetic ground state. Some remarkable results for ferromagnetic ground states have been obtained in this class of models. Mielke and Tasaki have independently shown that the ground state gives saturated ferromagnetism in a class of many-electron models on a lattice, which are called flat-band Hubbard models.^(13,14) Nishino, Goda and Kusakabe extended their result to more general models.⁽¹⁵⁾ Tasaki proved also the stability of the saturated ferromagnetism against a perturbation which bends the electron band.⁽¹⁶⁾ Tanaka and Ueda have shown the stability of the saturated ferromagnetism in a more complicated two-dimensional

model in Mielke's class.⁽¹⁷⁾ Tasaki has studied the energy of the spin-wave excitations in the flat-band Hubbard model.⁽¹⁸⁾ He has shown that the dispersion of the one-magnon excitation is non-singular in the flat-band Hubbard model, contrary to the Nagaoka ferromagnetism. The flat-band ferromagnetism is believed to be stable against a small perturbation or the change of the electron number density.⁽¹⁹⁾ Unlike the ferromagnetic quantum spin model, we expect strong quantum effects in the ferromagnetic ground state of the electrons on the lattice. The fermion statistics and fully polarized spin configuration imply that this state is microscopically entangled with respect to the electron site configuration. Therefore, the calculations of the ground state expectation value become more complicated than those in the XXZ model in which the ground state can be written in a product state.

Here, we deform a flat-band Hubbard model by a complex anisotropy parameter q . The SU(2) spin rotation symmetry in the original flat-band model is reduced to U(1) symmetry in our deformed model. First, we study our model under an open boundary condition. The anisotropy $|q| \neq 1$ leads to a localized domain wall with finite width. The domain structure is characterized in terms of the local order parameter $\langle S_x^{(3)} \rangle$, which represents the third component of the localized spin at site x . This local order parameter takes the same sign within one domain. The domain wall center is a set of sites x defined by zeros of the local order parameter $\langle S_x^{(3)} \rangle = 0$. We show the uniqueness of the ground state with a fixed magnetization in a half-filled electron number in the lowest energy band. We represent $\langle S_x^{(3)} \rangle$ in terms of the local electron density $\langle n_x \rangle$, and show the profile of the ferromagnetic domain wall. We study the low energy excitations in this model. We show that there exists a gapless excitation above the domain wall ground state. This excited state is constructed by acting a local operator near the domain wall on the ground state. We discuss reliability of our results in the infinite-volume limit, although we present our result with a finite system size. This property of the domain wall ground state is similar to the gapless excitation above the domain wall ground state in the XXZ model as well. Next, we study the model under the periodic boundary condition. In this case, either all-spin-up or all-spin-down state is allowed as a ground state. We show that a spin-wave excitation above the all-spin-up ground state has an energy gap because of the anisotropy. This property is similar to the Ising gap in the ferromagnetic XXZ model.

This paper is organized as follows. In Section 2, we define a deformed flat-band Hubbard model on a decorated d -dimensional integer lattice. In Section 3, we construct a set of ground states and prove the uniqueness of the ground state in a subspace with each fixed magnetization. The domain

wall structure is shown in terms of the spin one-point function. We also obtain a representation for the spin correlation function. In Section 4, we show the existence of gapless excitation above the domain wall ground state in a sufficiently large system size. An upper bound on the excitation energy is given in Theorem 4.1 and Corollary 4.1. In Section 5, we consider our model under the periodic boundary condition. We estimate an energy gap of the spin-wave excitation above the all-spin-up ground state. Finally, we summarize our results in Section 6.

2. DEFINITION OF THE MODEL

The Hubbard model is a model which represents a many-electron system on an arbitrary lattice. In this section, we define a d -dimensional deformed flat-band Hubbard model illustrating its physical meaning. Our model is a generalization of the Tasaki model given in ref. 14.

2.1. Lattice

The lattice Λ on which our deformed Hubbard model is defined is decomposed into two sublattices

$$\Lambda = \Lambda_o \cup \Lambda'. \quad (1)$$

Λ_o is d -dimensional integer lattice with linear size L , which is defined

$$\Lambda_o := \left\{ x = (x_1, x_2, \dots, x_d) \in \mathbb{Z}^d \mid |x_j| \leq \frac{L-1}{2} \quad j = 1, 2, \dots, d \right\}. \quad (2)$$

Λ' can be further decomposed to Λ_j ($j = 1, 2, \dots, d$), i.e.

$$\Lambda' = \bigcup_{j=1}^d \Lambda_j. \quad (3)$$

Λ_j is obtained as a half integer translation of Λ_o to j th direction,

$$\Lambda_j := \left\{ x + e^{(j)} \mid x \in \Lambda_o \right\} \cup \left\{ x - e^{(j)} \mid x \in \Lambda_o \right\}, \quad (4)$$

where $e^{(j)}$ is defined

$$e^{(j)} := (0, \dots, 0, \underbrace{\frac{1}{2}}_{j\text{th}}, 0, \dots, 0). \quad (5)$$

We show the lattice in the two-dimensional case in Fig. 1 as an example.

2.2. Electron Operators and the Fock Space

The creation and annihilation operators for an electron are denoted by $c_{x,\sigma}^\dagger$ and $c_{x,\sigma}$. They obey the standard anticommutation relations

$$\{c_{x,\sigma}, c_{y,\tau}^\dagger\} = \delta_{x,y} \delta_{\sigma,\tau}, \quad \{c_{x,\sigma}, c_{y,\tau}\} = 0 = \{c_{x,\sigma}^\dagger, c_{y,\tau}^\dagger\}, \tag{6}$$

where $\{A, B\} = AB + BA$, for sites $x, y \in \Lambda$ and spin coordinates $\sigma, \tau = \uparrow, \downarrow$. We define no-electron state Φ_{vac} by

$$c_{x,\sigma} \Phi_{\text{vac}} = 0 \tag{7}$$

for all $x \in \Lambda$ and $\sigma = \uparrow, \downarrow$. We construct a Fock space spanned by a basis

$$\left\{ \left(\prod_{x \in A} c_{x,\uparrow}^\dagger \right) \left(\prod_{x \in B} c_{x,\downarrow}^\dagger \right) \Phi_{\text{vac}} \mid A, B \subset \Lambda \right\}. \tag{8}$$

We also define a number operator $n_{x,\sigma}$ by $n_{x,\sigma} = c_{x,\sigma}^\dagger c_{x,\sigma}$ whose eigenvalue represents a number of electrons at site x with spin σ . Note anticommutation relations $\{c_{x,\sigma}^\dagger, c_{x,\sigma}^\dagger\} = 0$ i.e. $c_{x,\sigma}^\dagger c_{x,\sigma}^\dagger = 0$. This relation implies the

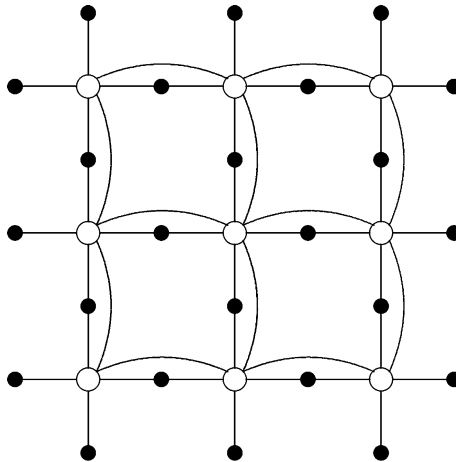


Fig. 1. Two-dimensional lattice (with $L=3$). The white circles are sites in Λ_o and the black dots are sites in Λ' . Electrons at a site can hop to another site if this site is connected to the original site with a line or a curve.

Pauli principle. We employ the open boundary condition, when we consider domain wall ground states. This is realized by $c_{x,\sigma} = 0$ if $|x_j| > L/2$ for some $j = 1, 2, \dots, d$ with $x = (x_l)_{l=1}^d$. We employ the periodic boundary condition, when we consider the spin-wave excitation above the all-spin-up ground state.

2.3. Deformed Flat-Band Hubbard Model

Before we define the Hamiltonian, we introduce new operators $\tilde{a}_{x,\sigma}^\dagger$ and $d_{x,\sigma}$ defined by

$$\tilde{a}_{x,\sigma}^\dagger = \begin{cases} -q^{p(\sigma)/4} \sum_{j=1}^d c_{x-e^{(j)},\sigma}^\dagger + \lambda c_{x,\sigma}^\dagger - q^{-p(\sigma)/4} \sum_{j=1}^d c_{x+e^{(j)},\sigma}^\dagger & \text{if } x \in \Lambda_o, \\ \lambda^{-1} c_{x,\sigma}^\dagger & \text{if } x \in \Lambda', \end{cases} \quad (9)$$

and

$$d_{x,\sigma} = \begin{cases} \lambda^{-1} c_{x,\sigma} & \text{if } x \in \Lambda_o, \\ q^{-p(\sigma)/4} c_{x-e^{(j)},\sigma} + \lambda c_{x,\sigma} + q^{p(\sigma)/4} c_{x+e^{(j)},\sigma} & \text{if } x \in \Lambda_j, \end{cases} \quad (10)$$

where q is a complex parameter, λ is a positive parameter and $p(\sigma)$ takes $+1$ if $\sigma = \uparrow$ and -1 if $\sigma = \downarrow$. And we formally define $\tilde{a}_{x,\sigma}^\dagger = 0$ and $d_{x,\sigma} = 0$ if $|x_j| > L/2$ for some $j = 1, 2, \dots, d$ with $x = (x_l)_{l=1}^d$. This definitions correspond to the open boundary condition for the original electron operators. Note that these $\tilde{a}_{x,\sigma}^\dagger$ and $d_{x,\sigma}$ satisfy the anticommutation relations,

$$\{\tilde{a}_{x,\sigma}^\dagger, d_{y,\tau}\} = \delta_{x,y} \delta_{\sigma,\tau}, \quad \{\tilde{a}_{x,\sigma}^\dagger, \tilde{a}_{y,\tau}\} = 0 = \{d_{x,\sigma}, d_{y,\tau}\}. \quad (11)$$

We can easily obtain the following inverse relations of (9) and (10)

$$c_{x,\sigma}^\dagger = \begin{cases} q^{p(\sigma)/4} \sum_{j=1}^d \tilde{a}_{x-e^{(j)},\sigma}^\dagger + \frac{1}{\lambda} \tilde{a}_{x,\sigma}^\dagger + q^{-p(\sigma)/4} \sum_{j=1}^d \tilde{a}_{x+e^{(j)},\sigma}^\dagger & \text{if } x \in \Lambda_o, \\ \lambda \tilde{a}_{x,\sigma}^\dagger & \text{if } x \in \Lambda', \end{cases} \quad (12)$$

and

$$c_{x,\sigma} = \begin{cases} \lambda d_{x,\sigma} & \text{if } x \in \Lambda_o, \\ -q^{-p(\sigma)/4} d_{x-e^{(j)},\sigma} + \frac{1}{\lambda} d_{x,\sigma} - q^{p(\sigma)/4} d_{x+e^{(j)},\sigma} & \text{if } x \in \Lambda_j. \end{cases} \quad (13)$$

The existence of inverse relations implies that the Fock space is also spanned by another basis

$$\left\{ \left(\prod_{x \in A} \tilde{a}_{x,\uparrow}^\dagger \right) \left(\prod_{x \in B} \tilde{a}_{x,\downarrow}^\dagger \right) \Phi_{\text{vac}} \middle| A, B \subset \Lambda \right\}. \quad (14)$$

This fact is useful to obtain the ground states.

The definition of our Hubbard Hamiltonian is given by

$$H := H_{\text{hop}} + H_{\text{int}}, \quad (15)$$

where H_{hop} and H_{int} defined

$$H_{\text{hop}} = t \sum_{\sigma=\uparrow,\downarrow} \sum_{x \in \Lambda'} d_{x,\sigma}^\dagger d_{x,\sigma} \quad (16)$$

and

$$H_{\text{int}} = U \sum_{x \in \Lambda} n_{x,\uparrow} n_{x,\downarrow} \quad (17)$$

with $t, U > 0$. The hopping Hamiltonian H_{hop} can be written in the following form:

$$H_{\text{hop}} = \sum_{x,y \in \Lambda} t_{x,y}^{(\sigma)} c_{x,\sigma}^\dagger c_{y,\sigma}, \quad (18)$$

where

$$t_{x,y}^{(\sigma)} = (t_{y,x}^{(\sigma)})^* = \begin{cases} td(|q|^{1/2} + |q|^{-1/2}) & \text{if } x = y \in \Lambda_o, \\ t\lambda^2 & \text{if } x = y \in \Lambda', \\ t\lambda q^{p(\sigma)/4} & \text{if } x \in \Lambda', y \in \Lambda_o, \text{ with} \\ & [x] < [y] \text{ and } |x - y| = \frac{1}{2}, \\ t\lambda q^{-p(\sigma)/4} & \text{if } x \in \Lambda', y \in \Lambda_o, \text{ with} \\ & [x] > [y] \text{ and } |x - y| = \frac{1}{2}, \\ te^{-ip(\sigma)\theta/2} & \text{if } x, y \in \Lambda_o \text{ with} \\ & [x] > [y] \text{ and } |x - y| = 1, \\ 0 & \text{otherwise} \end{cases} \quad (19)$$

with a definition $[x] = \sum_{j=1}^d x_j$. We parametrize² $q = |q|e^{i\theta}$ by $0 \leq \theta < 2\pi$. Each term $t_{x,y}^{(\sigma)\dagger} c_{x,\sigma} c_{y,\sigma}$ in the hopping Hamiltonian represents that an electron with spin σ hops from site x to site y with a probability proportional to $|t_{x,y}^{(\sigma)}|^2$.

Since the interaction Hamiltonian H_{int} represents an on-site repulsive interaction, this Hamiltonian can be regarded as a simplification of the Coulomb interaction between two electrons.

Note that this system conserves the number of electron. The total electron number operator \hat{N}_e is defined by

$$\hat{N}_e := \sum_{x \in \Lambda} \sum_{\sigma = \uparrow, \downarrow} n_{x,\sigma}. \quad (20)$$

Since the Hamiltonian commutes with this operator, we can set the electron number to an arbitrary filling. In the present paper, we only consider that the electron number is equal to $|\Lambda_o|$, namely, only the Hilbert space \mathcal{H} is spanned by the following basis²

$$\left\{ \left(\prod_{x \in A} c_{x,\uparrow}^\dagger \right) \left(\prod_{x \in B} c_{x,\downarrow}^\dagger \right) \Phi_{\text{vac}} \mid A, B \subset \Lambda \text{ with } |A| + |B| = |\Lambda_o| \right\}, \quad (21)$$

or

$$\left\{ \left(\prod_{x \in A} \tilde{a}_{x,\uparrow}^\dagger \right) \left(\prod_{x \in B} \tilde{a}_{x,\downarrow}^\dagger \right) \Phi_{\text{vac}} \mid A, B \subset \Lambda \text{ with } |A| + |B| = |\Lambda_o| \right\}. \quad (22)$$

Let us discuss the symmetry of the model. First important symmetry is a U(1) symmetry. We define spin operators at site x by

$$S_x^{(l)} := \sum_{\sigma, \tau = \uparrow, \downarrow} c_{x,\sigma}^\dagger \frac{\mathcal{P}_{\sigma,\tau}^{(l)}}{2} c_{x,\tau}, \quad (23)$$

where $\mathcal{P}^{(l)}$ ($l = 1, 2, 3$) denote Pauli matrices

$$\mathcal{P}^{(1)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mathcal{P}^{(2)} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \mathcal{P}^{(3)} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (24)$$

²Throughout the present paper, we denote a complex conjugate of $\alpha \in \mathbb{C}$ by α^* and its absolute value by $|\alpha|$. We also denote $|v|$ to represent a norm of a vector v in d -dimensional Euclidean space and $|A|$ to represent the cardinality of a set A .

The Hamiltonian commutes with the third component of total spin operator

$$[H, S_{\text{tot}}^{(3)}] = H S_{\text{tot}}^{(3)} - S_{\text{tot}}^{(3)} H = 0 \tag{25}$$

with

$$S_{\text{tot}}^{(l)} = \sum_{x \in \Lambda} S_x^{(l)}. \tag{26}$$

We call the eigenvalue of $S_{\text{tot}}^{(3)}$ magnetization. We can classify energy eigenstate by the magnetization. Note that this U(1) symmetry generated by $S_{\text{tot}}^{(3)}$ is enhanced to an SU(2) symmetry in the case of $q = 1$ i.e. Hamiltonian commutes with any component of total spin operator. In this case, this model becomes the original flat-band Hubbard model given by Tasaki ^(14,16). Another important symmetry is generated by a product of parity and spin rotation defined by

$$\Pi = \Pi^{-1} = P \exp\left(i\pi S_{\text{tot}}^{(1)}\right), \tag{27}$$

where P is a parity operator defined by $P c_{x,\sigma} P = c_{-x,\sigma}$ and $P c_{x,\sigma}^\dagger P = c_{-x,\sigma}^\dagger$. Π transforms $c_{x,\sigma}$ and $c_{x,\sigma}^\dagger$ to $c_{-x,\bar{\sigma}}$ and $c_{-x,\bar{\sigma}}^\dagger$, where $\bar{\sigma} = \downarrow$ if $\sigma = \uparrow$ or $\bar{\sigma} = \uparrow$ if $\sigma = \downarrow$. Note the following transformation of the total magnetization $\Pi S_{\text{tot}}^{(3)} \Pi = -S_{\text{tot}}^{(3)}$. An energy eigenstate with the total magnetization M is transformed by Π into another eigenstate with the total magnetization $-M$, which belongs to the same energy eigenvalue. Note that the Hamiltonian of the XXZ model with a boundary field h

$$-J \sum_{x \in \Lambda_o} \sum_{j=1}^d \left[S_x^{(1)} S_{x+2e^{(j)}}^{(1)} + S_x^{(2)} S_{x+2e^{(j)}}^{(2)} + \frac{q+q^{-1}}{2} S_x^{(3)} S_{x+2e^{(j)}}^{(3)} + h S_x^{(3)} - h S_{x+2e^{(j)}}^{(3)} \right], \tag{28}$$

has these two symmetries as well. Our deformation of the hopping Hamiltonian in the flat-band Hubbard model is one of the simplest way which preserves these two symmetries. If one does not want to add the XXZ Hamiltonian which leads to the ferromagnetism trivially, one reaches to our model naturally.

3. GROUND STATES

In this section, we obtain ground states of the model with the fixed electron number $N_e = |\Lambda_o|$ on the basis of Tasaki's construction method.⁽¹⁴⁾

3.1. Construction of Ground States

The representation of the hopping Hamiltonian in terms of $d_{x,\sigma}$,

$$H_{\text{hop}} = t \sum_{\sigma=\uparrow,\downarrow} \sum_{x \in \Lambda'} d_{x,\sigma}^\dagger d_{x,\sigma} \quad (29)$$

indicates the positive semi-definiteness $H_{\text{hop}} \geq 0$. The positive semi-definiteness of the interaction Hamiltonian $H_{\text{int}} \geq 0$ is also clear because $n_{x,\sigma} = c_{x,\sigma}^\dagger c_{x,\sigma} \geq 0$, then the total Hamiltonian is also positive semi-definite

$$H = H_{\text{hop}} + H_{\text{int}} \geq 0. \quad (30)$$

First, we consider a fully polarized state Φ_\uparrow defined by

$$\Phi_\uparrow = \left(\prod_{x \in \Lambda_o} \tilde{a}_{x,\uparrow}^\dagger \right) \Phi_{\text{vac}}. \quad (31)$$

We easily verify $H\Phi_\uparrow = 0$ from the anticommutativity (11), and therefore Φ_\uparrow is a ground state of H . Next, we determine all other ground states.

The conditions that a state Φ is a ground state are obviously $H_{\text{hop}}\Phi = 0$ and $H_{\text{int}}\Phi = 0$. In other words,

$$\tilde{a}_{x,\sigma}\Phi = 0 \quad \text{for all } x \in \Lambda' \quad \text{with } \sigma = \uparrow, \downarrow \quad (32)$$

and

$$c_{y,\uparrow}c_{y,\downarrow}\Phi = 0 \quad \text{for all } y \in \Lambda. \quad (33)$$

We expand Φ into the following series:

$$\Phi = \sum_{A,B} \psi(A,B) \left(\prod_{x \in A} \tilde{a}_{x,\uparrow}^\dagger \right) \left(\prod_{y \in B} \tilde{a}_{y,\downarrow}^\dagger \right) \Phi_{\text{vac}}, \quad (34)$$

where the summation is taken over all $A, B \subset \Lambda$ with $|A| + |B| = |\Lambda_o|$. The first condition (32) implies that $\psi(A, B)$ does not vanish only for

$A, B \subset \Lambda_o$. The second condition (33) for $y \in \Lambda_o$ means $\psi(A, B)$ takes 0 for $A \cap B \neq \emptyset$ with $A, B \subset \Lambda_o$. Then we obtain the following form:

$$\Phi = \sum_{\sigma} \phi(\sigma) \left(\prod_{x \in \Lambda_o} \tilde{a}_{x, \sigma_x}^{\dagger} \right) \Phi_{\text{vac}}, \tag{35}$$

where the summation is taken over all possible spin configurations $\sigma = (\sigma_x)_{x \in \Lambda_o}$. To satisfy the second condition (33) for $y \in \Lambda_j$ ($j = 1, 2, \dots, d$), the coefficient holds

$$\phi(\sigma) = q^{[p(\sigma_{y-e(j)}) - p(\sigma_{y+e(j)})]/2} \phi(\sigma_{y-e(j), y+e(j)}), \tag{36}$$

where $\sigma_{x,y}$ is spin configuration obtained by the exchange σ_x and σ_y in the original configuration σ . This relation implies the uniqueness of the ground state with a fixed total magnetization, since two arbitrary spin configurations with same total magnetization can be related by successive exchanges of two nearest neighbour spins. Therefore the degeneracy of these ground states is exactly the same as that in the SU(2) symmetric model. This degeneracy is also the same as the ground states in the XXZ model.⁽³⁾

Note that we can find the ‘‘shift operator’’ S_q^- which makes the ground state with magnetization M from fully polarized ground state Φ_{\uparrow} by acting certain times

$$\Phi_M = (S_q^-)^{L^d - 2M} \Phi_{\uparrow}, \tag{37}$$

where Φ_M is the ground state with magnetization M . And S_q^- can be written as

$$S_q^- = \sum_{x \in \Lambda} q^{[x]} \tilde{a}_{x, \downarrow}^{\dagger} d_{x, \uparrow}. \tag{38}$$

3.2. Another Representation of Ground States

To explore the nature of the ground state, we write the ground state in a more explicit way as obtained by Gottstein and Werner in ref. 4. We define the following electron operator creating a superposed state

$$\alpha_x^{\dagger}(\zeta) = \sum_{\sigma = \uparrow, \downarrow} \eta_{x, \sigma} \tilde{a}_{x, \sigma}^{\dagger}, \tag{39}$$

where we define a function of $x \in \Lambda$ and spin σ

$$\eta_{x,\sigma} = \zeta^{-p(\sigma)/2} q^{-p(\sigma)[x]/2}$$

with $[x] = \sum_{j=1}^d x_j$. We define a ground state $\Psi(\zeta)$ for an arbitrary complex number ζ by

$$\Psi(\zeta) = \sum_{n=0}^{L^d} \zeta^n (S_q^-)^n \Phi_{\uparrow} = \left(\prod_{x \in \Lambda_0} \alpha_x^{\dagger}(\zeta) \right) \Phi_{\text{vac}}. \quad (40)$$

One can see the localization property of the electrons in this representation $\Psi(\zeta)$. The spin state of an electron at each site is completely determined. Unlike the ground state with a fixed total magnetization, one knows the conditional probability of the electron spin at site x . In principle, one can check whether this ground state is realized or not by local observations. From this fact, the state $\Psi(\zeta)$ is expected to be healthy even in the infinite-volume limit. We expect that the corresponding ground state to $\Psi(\zeta)$ is also a pure state in the infinite-volume limit, as in the XXZ model. Note that the expectation value of an arbitrary local operator in the corresponding ground state $\Psi(\zeta)$ in the XXZ model is asymptotically equal to that in Φ_M for $|\zeta|, |M| = O(1)$.⁽⁸⁾ We expect that the ground state $\Psi(\zeta)$ in our Hubbard model has many properties which are the same as the domain wall ground state in XXZ model. In our Hubbard model, however, these are difficult to be shown, since the state $\Psi(\zeta)$ defined here in the Hubbard model is not a product state unlike the ground state in the XXZ model.

3.3. Spin One-Point Functions

Let us now consider expectation values of the spin operators in the ground state $\Psi(\zeta)$. We denote an expectation value of an operator A in the ground state $\Psi(\zeta)$ by $\langle A \rangle_{\zeta}$. The expectation value of a localized spin at site x is written

$$\begin{aligned} \langle S_x^{(j)} \rangle_{\zeta} &= \frac{1}{2} \sum_{\sigma, \tau = \uparrow, \downarrow} \mathcal{P}_{\sigma, \tau}^{(j)} \frac{\langle \Psi(\zeta), c_{x, \sigma}^{\dagger} c_{x, \tau} \Psi(\zeta) \rangle}{\|\Psi(\zeta)\|^2} \\ &= \frac{1}{2} \sum_{\sigma, \tau = \uparrow, \downarrow} \mathcal{P}_{\sigma, \tau}^{(j)} \frac{\langle c_{x, \sigma} \Psi(\zeta), c_{x, \tau} \Psi(\zeta) \rangle}{\|\Psi(\zeta)\|^2}. \end{aligned} \quad (41)$$

The following anticommutation relations

$$\{c_{x, \sigma}, \alpha_y^{\dagger}(\zeta)\} = \lambda \eta_{x, \sigma} \delta_{x, y} \quad (42)$$

for $x, y \in \Lambda_o$, and

$$\{c_{x,\sigma}, \alpha_y^\dagger(\zeta)\} = -\eta_{x,\sigma} \left(q^{-1/4} \delta_{x-e^{(j)},y} + q^{1/4} \delta_{x+e^{(j)},y} \right) \quad (43)$$

for $x \in \Lambda_j$ and $y \in \Lambda_o$ are useful to calculate the expectation value. These anticommutation relations (42) and (43) yield an equation

$$c_{x,\sigma} \Psi(\zeta) = \eta_{x,\sigma} \Psi_x(\zeta). \quad (44)$$

Here, the state $\Psi_x(\zeta)$ is defined by

$$\Psi_x(\zeta) = \begin{cases} \operatorname{sgn}(x) \lambda \left(\prod_{y \neq x} \alpha_y^\dagger(\zeta) \right) \Phi_{\text{vac}} & \text{if } x \in \Lambda_o, \\ \left(\operatorname{sgn}(x - e^{(j)}) q^{-1/4} \prod_{y \neq x - e^{(j)}} \alpha_y^\dagger(\zeta) \right. \\ \left. + \operatorname{sgn}(x + e^{(j)}) q^{1/4} \prod_{y \neq x + e^{(j)}} \alpha_y^\dagger(\zeta) \right) \Phi_{\text{vac}} & \text{if } x \in \Lambda_j, \end{cases} \quad (45)$$

where $\operatorname{sgn}(x)$ takes ± 1 . Then, the expectation value of $c_{x,\sigma}^\dagger c_{x,\tau}$ for all $x \in \Lambda$ in the ground state $\Psi(\zeta)$ can be written in terms of $\Psi_x(\zeta)$,

$$\langle c_{x,\sigma}^\dagger c_{x,\tau} \rangle_\zeta = \eta_{x,\sigma}^* \eta_{x,\tau} \frac{\|\Psi_x(\zeta)\|^2}{\|\Psi(\zeta)\|^2}. \quad (46)$$

Thus we obtain the representations of spin one-point functions at site $x \in \Lambda$ in terms of an electron number density $\langle n_x \rangle_\zeta$ ($n_x := n_{x,\uparrow} + n_{x,\downarrow}$),

$$\langle S_x^{(1)} \rangle_\zeta = \frac{\langle n_x \rangle_\zeta}{2} \frac{\zeta q^{[x]} + (\zeta q^{[x]})^*}{1 + |\zeta q^x|^2}, \quad (47)$$

$$\langle S_x^{(2)} \rangle_\zeta = \frac{\langle n_x \rangle_\zeta}{2i} \frac{\zeta q^{[x]} - (\zeta q^{[x]})^*}{1 + |\zeta q^x|^2}, \quad (48)$$

$$\langle S_x^{(3)} \rangle_\zeta = \frac{\langle n_x \rangle_\zeta}{2} \frac{1 - |\zeta q^{[x]}|^2}{1 + |\zeta q^{[x]}|^2}. \quad (49)$$

We expect that the electron number density in the ground state $\Psi(\zeta)$ is almost constant on Λ_o or on Λ' respectively, from the definition of $\Psi(\zeta)$. Indeed, in the one-dimensional model, we can check this conjecture by the exact bounds.⁽¹²⁾

As in the domain wall ground state of the XXZ model discussed in refs. 5, 7, 20, the two domains are distinguished by the sign of the local order parameter $\langle S_x^{(3)} \rangle_\zeta$. The domain wall center is defined by zeros of $\langle S_x^{(3)} \rangle_\zeta$ which is located at x with $[x] = -\log_{|q|} |\zeta|$. The function $\frac{1}{2} \langle n_x \rangle_\zeta - |\langle S_x^{(3)} \rangle_\zeta|$ decays exponentially as x is far away from the center. This decay length defines the domain wall width $1/\log|q|$. If the number density is almost constant on each sublattice Λ_o or Λ' as we conjectured, the behaviors of the spin one-point functions are not controlled by the number density. In large λ limit for real $q > 1$, electrons are completely localized at integer sites, and the spin one-point functions are exactly the same as those obtained in the XXZ model defined on Λ_o .

For a complex $q = |q|e^{i\theta}$, one can see the spiral structure with a pitch angle θ . The vector $\langle \vec{S}_x \rangle_\zeta := (\langle S_x^{(j)} \rangle_\zeta)_{j=1}^3$ is rotated with the angle $[x]\theta$ around the third spin axis depending on the site x . Note that this spiral structure of the ground state does not exist in the XXZ model, though the complex anisotropy parameter $q = e^{i\theta}$ is possible in the XXZ Hamiltonian. The corresponding model is described in the Tomonaga-Luttinger liquid without ferromagnetic order in one dimension.

The translational symmetry in the infinite-volume limit is broken by the domain wall or the spiral structure for finite $\log|\zeta|$. Both symmetries generated by $S^{(3)}$ and Π are broken spontaneously as well.

3.4. Spin Correlation Functions

The spin correlation function can be also represented in terms of the correlation function of the local electron number operators

$$\langle S_x^{(j)} S_y^{(l)} \rangle_\zeta = \frac{1}{4} \sum_{\sigma, \tau, \sigma', \tau'} \frac{\eta_{x, \sigma}^* \mathcal{P}_{\sigma, \tau}^{(j)} \eta_{x, \tau}}{|\zeta q^{[x]}| + |\zeta q^{[x]}|^{-1}} \frac{\eta_{y, \sigma'}^* \mathcal{P}_{\sigma', \tau'}^{(l)} \eta_{y, \tau'}}{|\zeta q^{[x]}| + |\zeta q^{[x]}|^{-1}} \langle n_x n_y \rangle_\zeta. \quad (50)$$

We can rewrite

$$\langle S_x^{(j)} S_y^{(l)} \rangle_\zeta = \langle S_x^{(j)} \rangle_\zeta \langle S_y^{(l)} \rangle_\zeta \frac{\langle n_x n_y \rangle_\zeta}{\langle n_x \rangle_\zeta \langle n_y \rangle_\zeta}. \quad (51)$$

if $\lambda < \infty$. If one estimates the correlation function of the local electron number operators, one can check the cluster property of the ground state. Actually this can be done for the one-dimensional model.⁽¹²⁾

4. EXISTENCE OF GAPLESS EXCITATIONS

Here, we show an upper bound of excitation energy in $d \geq 2$ for sufficiently large finite volume under the open boundary condition. We generalize some parts of Matsui’s argument for the product ground state in the XXZ model in ref. 7 to those for the non-product ground state in the flat-band Hubbard model. We estimate the energy in a trial state constructed by acting a local operator on a domain wall ground state $\Psi(\zeta)$.

4.1. Low Energy Excitations

Here, we show two results for low energy excitations in our model.

Theorem 4.1. (“Local gapless excitation” above the ground state $\Psi(\zeta)$). In the d -dimensional Hubbard model defined by the Hamiltonian (15) with $d \geq 2$ and the system volume $|\Lambda_o| = L^d$, for an arbitrary $\zeta \in \mathbb{C}$ with $|\log_{|q_l|} |\zeta| | < d(L - 1)/2$ and an arbitrary l with $1 < l \leq L + 2|\log_{|q_l|} |\zeta| | / d$, there exists a local operator O_l defined on a compact support with a linear size l and a constant $F_1 > 0$ independent of the system size such that

$$\frac{(O_l \Psi(\zeta), H O_l \Psi(\zeta))}{\|O_l \Psi(\zeta)\|^2} < F_1 U l^{-1} \tag{52}$$

and $(\Psi(\zeta), O_l \Psi(\zeta)) = 0$. Moreover, there is an upper bound on the norm of a projected state $P_0 O_l \Psi(\zeta)$, where P_0 is the projection operator onto the space of ground states. There exist constants $L_1 > 0$, $R > 1$ and $F_2 > 0$ which are independent of the system size such that

$$\frac{\|P_0 O_l \Psi(\zeta)\|^2}{\|O_l \Psi(\zeta)\|^2} < F_2 l^{d+1} (L^d + 1) R^{-2L^{d-1}} \quad \text{for } L > L_1. \tag{53}$$

Here, we describe some physical meanings of Theorem 4.1. We emphasize that the excited state in Theorem 4.1 is constructed by acting a local operator which consists of finite number of electron operators $c_{x,\sigma}^\dagger$ and $c_{x,\sigma}$. As discussed when we defined the ground state $\Psi(\zeta)$, one can confirm whether the system takes the ground state $\Psi(\zeta)$ or not by local observation. After one checks the ground state $\Psi(\zeta)$ once, one can obtain a locally deformed state, say $O_l \Psi(\zeta)$, by a local operation to the system. In this sense, Theorem 4.1 claims that one can change the state of the system from the ground state $\Psi(\zeta)$ by the local operation with energy as small as one wants. Particularly, the second result in

Theorem 4.1 guarantees that the deformed state $O_l\Psi(\zeta)$ has a non-zero orthogonal component to all ground states of the model. This fact implies that the local operation represented in O_l is really effective to deform the ground state $\Psi(\zeta)$ of the system. Therefore, we can claim that there exists a gapless excitation above the domain wall ground state $\Psi(\zeta)$.

Remark. Theorem 4.1 should imply the existence of a gapless excitation in the infinite-volume limit under the condition of the fixed electron number, if the corresponding ground state in the infinite system to $\Psi(\zeta)$ were shown to be pure and unique as in the XXZ model.⁽⁷⁾

We can prove the following property of the lowest excitation energy eigenvalue of H directly from Theorem 4.1.

Corollary 4.2. (Spectra of a finite system with open boundary condition). Suppose the d -dimensional Hubbard model defined by the Hamiltonian (15) with $d \geq 2$. Let E_1 be the lowest energy eigenvalue of excitation in the model with the system volume $|\Lambda_o| = L^d$ under the open boundary condition. There exist constants $L_2 > 0$ and $F_3 > 0$ which are independent of the system size such that

$$E_1 \leq F_3 U L^{-1} \quad \text{for } L \geq L_2. \quad (54)$$

4.2. Expansion in the Original Basis

Here we prepare for the proof of Theorem 4.1 and Corollary 4.2. To evaluate the inner product between two states, we represent them in terms of original electron operator $c_{x,\sigma}^\dagger$. This representation has good properties which help us to estimate expectation values of observables.

4.2.1. Space of Configurations

To introduce a representation of states in terms of original electron operators, we define the decoration of a site $x \in \Lambda$ by a set

$$\bar{x} := \bigcup_{j=1}^d \{x, x + e^{(j)}, x - e^{(j)}\} \cap \Lambda.$$

Note $\Lambda = \bigcup_{x \in \Lambda_o} \bar{x}$, which is not a disjoint union. Also we define the decoration \bar{X} of a subset $X \subset \Lambda_o$ by

$$\bar{X} := \bigcup_{x \in X} \bar{x}.$$

To expand the ground state $\Psi(\zeta)$ in terms of an orthogonal basis, we define the function $\xi_{x,\sigma}(\zeta)$ for $x \in \Lambda$ by

$$\xi_{x,\sigma}(\zeta) = \begin{cases} \lambda \eta_{x,\sigma} = \lambda \zeta^{-p(\sigma)/2} q^{-p(\sigma)[x]/2} & \text{for } x \in \Lambda_o, \\ -\eta_{x,\sigma} = -\zeta^{-p(\sigma)/2} q^{-p(\sigma)[x]/2} & \text{for } x \in \Lambda'. \end{cases} \quad (55)$$

Since the operator $\alpha_x^\dagger(\zeta)$ is written in terms of this function

$$\alpha_x^\dagger(\zeta) = \sum_{y \in \bar{x}} \sum_{\sigma = \uparrow, \downarrow} \xi_{y,\sigma}(\zeta) c_{y,\sigma}^\dagger,$$

the ground state is represented in

$$\Psi(\zeta) = \left(\prod_{x \in \Lambda_o} \sum_{y \in \bar{x}} \sum_{\sigma = \uparrow, \downarrow} \xi_{y,\sigma}(\zeta) c_{y,\sigma}^\dagger \right) \Phi_{\text{vac}}, \quad (56)$$

To represent the ground state in terms of the electron creation operators on sites, we define a set \mathcal{C}_R of all configurations for the ground state. We define a position configuration for the ground state by a one-to-one mapping $f: \Lambda_o \rightarrow \Lambda$ with a constraint $f(x) \in \bar{x}$ for each $x \in \Lambda_o$. This mapping f selects a site in each decoration \bar{x} . We denote a set of all position configurations for the ground state by \mathcal{P}_R . Also we define a spin configuration for the ground state by a mapping $g: \Lambda_o \rightarrow \{\uparrow, \downarrow\}$. We denote a set of all spin configurations for the ground state by \mathcal{S} . A position configuration $f \in \mathcal{P}_R$ and a spin configuration $g \in \mathcal{S}$ define a configuration in \mathcal{C}_R which is a mapping $\varphi: \Lambda_o \rightarrow \Lambda \times \{\uparrow, \downarrow\}$ such that $\varphi: x \mapsto \varphi(x) = (f(x), g(x))$ for $x \in \Lambda_o$. An arbitrary configuration is also a one-to-one mapping. Then the ground state (56) is represented as a summation over all configurations in orthogonal basis

$$\Psi(\zeta) = \sum_{\varphi \in \mathcal{C}_R} \left(\prod_{x \in \Lambda_o} \xi_{\varphi(x)}(\zeta) c_{\varphi(x)}^\dagger \right) \Phi_{\text{vac}}. \quad (57)$$

Several terms in this summation over all configurations are linearly dependent, and they cancel each other. Therefore the summation over all configurations in \mathcal{C}_R is reducible.

4.2.2. Simple Loop

To obtain an irreducible configuration space, we consider two different configurations φ and φ' in \mathcal{C}_R . Assume that two terms defined by φ and φ' are linearly dependent, namely, there exists a number C ,

$$\left(\prod_{x \in \Lambda_o} \xi_{\varphi(x)}(\zeta) c_{\varphi(x)}^\dagger \right) \Phi_{\text{vac}} = C \left(\prod_{x \in \Lambda_o} \xi_{\varphi'(x)}(\zeta) c_{\varphi'(x)}^\dagger \right) \Phi_{\text{vac}}. \quad (58)$$

We say that two configurations $\varphi, \varphi' \in \mathcal{C}_R$ are linearly dependent if the terms defined by φ and φ' are linearly dependent. This relation implies

$$\{\varphi(x) | x \in \Lambda_o\} = \{\varphi'(x) | x \in \Lambda_o\}, \quad (59)$$

otherwise one cannot obtain the relation (58) for any number C . Nonetheless, $\varphi \neq \varphi'$ implies $\varphi(x) \neq \varphi'(x)$ for some $x \in \Lambda_o$. Let us consider a set of sites for two linearly dependent $\varphi, \varphi' \in \mathcal{C}_R$

$$X(\varphi, \varphi') = \{x \in \Lambda_o | \varphi(x) \neq \varphi'(x)\}. \quad (60)$$

To study properties of this set, we define several terms. We say that a sequence

$$\{x_{m+1}, x_{m+2}, \dots, x_{m+n}\} \subset \Lambda_o$$

for arbitrary positive even integers m and n is a simple loop with a length n , if $\bar{x}_k \cap \bar{x}_{k+1} \neq \emptyset$ for $k = m+1, \dots, m+n-1$ and $\bar{x}_{m+n} \cap \bar{x}_{m+1} \neq \emptyset$. We say that a configuration $\varphi = (f, g) \in \mathcal{C}_R$ for the ground state has a simple loop $\{x_{m+1}, x_{m+2}, x_{m+3}, \dots, x_{m+n}\}$, if $f(x_k) \in \bar{x}_{k+1}$ for $k = m+1, m+2, \dots, m+n-1$ and $f(x_{m+n}) \in \bar{x}_{m+1}$.

4.2.3. Loop Decomposition of Linearly Dependent Configurations

Here, we show the following lemma.

Lemma 4.3. Let n be a number of elements of the set $X(\varphi, \varphi')$ given in (60) for two linearly dependent configurations $\varphi, \varphi' \in \mathcal{C}_R$. There exist a positive integer N and some positive even integers $0 = m_0 < m_1 <$

$\dots < m_N = n$ for $X(\varphi, \varphi')$, such that $X(\varphi, \varphi')$ can be written in a disjoint union of some simple loops

$$X(\varphi, \varphi') = \bigcup_{j=1}^N \{x_{m_{j-1}+1}, x_{m_{j-1}+2}, x_{m_{j-1}+3}, \dots, x_{m_j}\}$$

and $\varphi(x_{k-1}) = \varphi'(x_k)$ for $m_{j-1} + 1 < k \leq m_j$ and $\varphi(x_{m_j}) = \varphi'(x_{m_{j-1}+1})$. Therefore, both configurations φ and φ' have each simple loop.

Proof. We attach indices to all sites in $X(\varphi, \varphi')$ in the following inductive manner. Let x_1 be an arbitrary site in $X(\varphi, \varphi')$. From the relation (59), there exists a site $x_2 \in X(\varphi, \varphi')$ for the site x_1 such that $\varphi(x_1) = \varphi'(x_2)$. Note $x_1 \neq x_2$ and $\bar{x}_1 \cap \bar{x}_2 \neq \emptyset$. By the relation $\varphi(x_2) \neq \varphi'(x_2)$ there exists $x_3 \in X(\varphi, \varphi')$ for x_2 such that $\varphi(x_2) = \varphi'(x_3)$ and $x_3 \neq x_1, x_2$. There exists $x_4 \in X(\varphi, \varphi')$ for x_3 such that $\varphi(x_3) = \varphi'(x_4)$ and $x_4 \neq x_1, x_2, x_3$. If $\varphi(x_4) = \varphi'(x_1)$, then we obtain a simple loop $\{x_1, x_2, x_3, x_4\}$ with a length $m_1 = 4$ and both configurations φ and φ' have this simple loop. This is because $\bar{x}_4 \cap \bar{x}_1 \neq \emptyset$. If $\varphi(x_4) \neq \varphi'(x_1)$, we define $x_5 \in X(\varphi, \varphi')$ such that $\varphi(x_4) = \varphi'(x_5)$ and $x_5 \neq x_1, x_2, x_3, x_4$. We assume already defined $x_{k-1} \in X(\varphi, \varphi')$ for an arbitrary natural number $k \leq n$ with $x_{k-1} \neq x_i$ for any $i = 1, 2, \dots, k - 2$, such that $\varphi(x_j) = \varphi'(x_{j+1})$ for $j = 1, \dots, k - 2$. If $\varphi(x_{k-1}) = \varphi'(x_1)$, then we obtain a simple loop $\{x_1, x_2, x_3, \dots, x_{k-1}\}$ with a length $m_1 = k - 1$ and both configurations φ and φ' have this loop. If $\varphi(x_{k-1}) \neq \varphi'(x_1)$, we define $x_k \in X(\varphi, \varphi')$ such that $\varphi(x_{k-1}) = \varphi'(x_k)$ and $x_k \neq x_i$ for any $i = 1, \dots, k - 1$. This can be proved as follows. If $x_k = x_i$ for some $i = 2, 3, \dots, k - 1$, then $\varphi(x_{k-1}) = \varphi'(x_k) = \varphi'(x_i) = \varphi(x_{i-1})$. This equality and the definition of a one-to-one mapping imply $x_{k-1} = x_{i-1}$, which contradicts the assumption of the inductivity. Also the assumption $\varphi(x_{k-1}) \neq \varphi'(x_1)$ excludes $x_k = x_1$. Thus, x_k cannot be any element in $\{x_1, x_2, x_3, \dots, x_{k-1}\}$. Note $\bar{x}_{k-1} \cap \bar{x}_k \neq \emptyset$. There exists a number $m_1 \leq n$ such that $\varphi(x_{m_1}) = \varphi'(x_1)$ and $\bar{x}_{m_1} \cap \bar{x}_1 \neq \emptyset$. We obtain a simple loop $\{x_1, x_2, x_3, \dots, x_{m_1}\}$ with a length m_1 , and both configurations φ and φ' have this simple loop. If $X(\varphi, \varphi') \setminus \{x_1, x_2, x_3, \dots, x_{m_1}\} = \emptyset$, then $X(\varphi, \varphi') = \{x_1, x_2, x_3, \dots, x_{m_1}\}$ is a simple loop itself with a length $n = m_1$. If $X(\varphi, \varphi') \setminus \{x_1, x_2, x_3, \dots, x_{m_1}\} \neq \emptyset$, then $n - m_1 > 0$ and we continue to attach indices $m_1 + 1, \dots, n$ to the elements in $X(\varphi, \varphi') \setminus \{x_1, x_2, x_3, \dots, x_{m_1}\}$. By attaching the indices $m_1 + 1, \dots, n$, we can continue to identify a subset of $X(\varphi, \varphi') \setminus \{x_1, x_2, x_3, \dots, x_{m_1}\}$ to a simple loop that both configurations have. Finally, we can write the set $X(\varphi, \varphi')$ as a disjoint union of some simple loops by attaching the indices $1, 2, 3, \dots, n$ to all the elements in $X(\varphi, \varphi')$. Both configurations φ and φ' have each

simple loop $\{x_{m_{j-1}+1}, x_{m_{j-1}+2}, x_{m_{j-1}+3}, \dots, x_{m_j}\}$ with a length $m_j - m_{j-1}$, and for two sites in each loop we have $\varphi(x_{k-1}) = \varphi'(x_k)$ for $m_{j-1} + 1 < k \leq m_j$ and $\varphi(x_{m_j}) = \varphi'(x_{m_{j-1}+1})$. Thus, we have proved the lemma. ■

4.2.4. Irreducible Configuration Space

We define the irreducible set of all configurations for the ground state by

$$\mathcal{C} := \{\varphi \in \mathcal{C}_R \mid \varphi \text{ has no simple loop}\}.$$

Here, we obtain the following lemma by proving that the terms given by two configurations with a common simple loop are cancelled.

Lemma 4.4. The ground state is represented in the summation over irreducible set of all configurations

$$\Psi(\zeta) = \sum_{\varphi \in \mathcal{C}} \left(\prod_{x \in \Lambda_o} \xi_{\varphi(x)}(\zeta) c_{\varphi(x)}^\dagger \right) \Phi_{\text{vac}}. \quad (61)$$

Proof. From Lemma 4.3, we consider a configuration $\varphi \in \mathcal{C}_R$ which has a simple loop $\{x_1, \dots, x_n\}$ with the length $n = 2m$. We show that this configuration φ has a counter contribution which cancels the contribution from φ . For the configuration φ , there exists a unique configuration φ' with the same simple loop such that $X(\varphi, \varphi') = \{x_1, \dots, x_n\}$. In this case, $\varphi(x_k) = \varphi'(x_{k+1})$ for any natural number $k \leq n - 1$ and $\varphi(x_n) = \varphi'(x_1)$. Then, the fermion statistics of the electron operators gives the following relation:

$$\prod_{k=1}^{2m} c_{\varphi(x_k)}^\dagger = \prod_{k=1}^{2m} c_{\varphi'(x_{k+1})}^\dagger = - \prod_{k=1}^{2m} c_{\varphi'(x_k)}^\dagger,$$

where we define $x_{2m+1} = x_1$. This relation implies $C = -1$ in the relation (58), therefore the contributions of φ and φ' in (57) cancel each other. Now, we rewrite the representation (57) of the ground state into summation over independent terms. As discussed above, all configurations which give linearly dependent terms in the representation (57) have at least one simple loop and all terms are cancelled. Therefore, the representation (57) of ground state can be rewritten into a summation over all configurations with no simple loop, which consists of only linearly independent terms. ■

The set \mathcal{C} of all configurations can be decomposed into a set \mathcal{P} of all position configurations and a set \mathcal{S} of all spin configurations, where the set of all position configurations is defined by

$$\mathcal{P} := \{f \in \mathcal{P}_R \mid f \text{ has no simple loop}\},$$

as well as \mathcal{C} . On the other hand, all spin configurations have no constraint. Therefore, after summing over all the spin configurations, the ground state is represented in the summation over irreducible set of all position configurations

$$\Psi(\zeta) = \sum_{f \in \mathcal{P}} \left[\prod_{x \in \Lambda_o} (\xi_{f(x), \uparrow}(\zeta) c_{f(x), \uparrow}^\dagger + \xi_{f(x), \downarrow}(\zeta) c_{f(x), \downarrow}^\dagger) \right] \Phi_{\text{vac}}. \quad (62)$$

4.3. Proof of Theorem 4.1

We define the following hyper cube on the lattice with a positive number l

$$Y_l := \left(\left\{ (x_1, x_2, \dots, x_d) \in \mathbb{R}^d \mid \|[x]\| \leq \frac{l-1}{2}, |x_j| < \frac{l-1}{2} \right. \right. \\ \left. \left. \text{for all } j=1, 2, \dots, d \right\} + \frac{z}{d}(1, 1, \dots, 1) \right) \cap \Lambda_o, \quad (63)$$

where we define $z \in \mathbb{R}$ by $|\zeta| = q^{-z}$. Note that the sublattice Y_l has a linear size l . We define a local operator

$$\tilde{S}_{Y_l}^{(3)} = \frac{1}{2} \sum_{x \in Y_l} \sum_{\sigma, \tau = \uparrow, \downarrow} \tilde{a}_{x, \sigma}^\dagger \mathcal{P}_{\sigma, \tau}^{(3)} d_{x, \tau}, \quad (64)$$

and its deviation from the ground state expectation value

$$\delta \tilde{S}_{Y_l}^{(3)} = \tilde{S}_{Y_l}^{(3)} - \frac{(\Psi(\zeta), \tilde{S}_{Y_l}^{(3)} \Psi(\zeta))}{\|\Psi(\zeta)\|^2}. \quad (65)$$

We define a normalized state $\tilde{\Psi}(\zeta)$ by

$$\tilde{\Psi}_l(\zeta) := \frac{\delta \tilde{S}_{Y_l}^{(3)} \Psi(\zeta)}{\|\delta \tilde{S}_{Y_l}^{(3)} \Psi(\zeta)\|}, \quad (66)$$

which is obviously orthogonal to the ground state $\Psi(\zeta)$.

First, we evaluate the norm of $\delta\tilde{S}_{Y_l}^{(3)}\Psi(\zeta)$.

$$\|\delta\tilde{S}_{Y_l}^{(3)}\Psi(\zeta)\|^2 = \|(\tilde{S}_{Y_l}^{(3)} - \langle\tilde{S}_{Y_l}^{(3)}\rangle_\zeta)\Psi(\zeta)\|^2. \quad (67)$$

Lemma 4.4 allows us to represent the state in a summation over the configurations. If we define an indicator function χ by $\chi[\text{true}] = 1$ and $\chi[\text{false}] = 0$, the state can be represented in

$$\begin{aligned} \tilde{S}_{Y_l}^{(3)}\Psi(\zeta) &= \sum_{y \in Y_l} \sum_{f \in \mathcal{P}} \chi[f(y) = y] \operatorname{sgn}(y) \sum_{w \in \bar{y}} (\xi_{w,\uparrow}(\zeta)c_{w,\uparrow}^\dagger - \xi_{w,\downarrow}(\zeta)c_{w,\downarrow}^\dagger) \\ &\quad \times \left[\prod_{x \in \Lambda_o \setminus \{y\}} (\xi_{f(x),\uparrow}(\zeta)c_{f(x),\uparrow}^\dagger + \xi_{f(x),\downarrow}(\zeta)c_{f(x),\downarrow}^\dagger) \right] \Phi_{\text{vac}}, \end{aligned} \quad (68)$$

where $\operatorname{sgn}(y) = \pm 1$ is a sign factor coming from the fermion statistics. Note that for an arbitrary $f \in \mathcal{P}$ with $f(y) \neq y$, there exists $g \in \mathcal{P}$ such that $g(y) = y$ and $f|_{\Lambda_o \setminus \{y\}} = g|_{\Lambda_o \setminus \{y\}}$. Thus we can represent $\tilde{S}_{Y_l}^{(3)}\Psi(\zeta)$ by

$$\begin{aligned} \tilde{S}_{Y_l}^{(3)}\Psi(\zeta) &= \sum_{y \in Y_l} \sum_{f \in \mathcal{P}} \left[\prod_{x \in \Lambda_o} (\xi_{f(x),\uparrow}(\zeta)c_{f(x),\uparrow}^\dagger \right. \\ &\quad \left. + (-1)^{\chi[x=y]} \xi_{f(x),\downarrow}(\zeta)c_{f(x),\downarrow}^\dagger \right] \Phi_{\text{vac}} + \Phi_\perp. \end{aligned} \quad (69)$$

The residual state Φ_\perp is orthogonal to the first term in the right hand side as well as any ground state $\Psi(\zeta)$, since Φ_\perp has no term written in a basis of irreducible configurations \mathcal{C} . The ground state expectation value is represented as

$$\begin{aligned} \langle\tilde{S}_{Y_l}^{(3)}\rangle_\zeta &= \frac{1}{2\|\Psi(\zeta)\|^2} \sum_{f \in \mathcal{P}} \sum_{x_1 \in Y_l} \frac{|\xi_{f(x_1),\uparrow}|^2 - |\xi_{f(x_1),\downarrow}|^2}{|\xi_{f(x_1),\uparrow}|^2 + |\xi_{f(x_1),\downarrow}|^2} \\ &\quad \times \prod_{x \in \Lambda_o} (|\xi_{f(x),\uparrow}|^2 + |\xi_{f(x),\downarrow}|^2), \end{aligned} \quad (70)$$

where \mathcal{P} denotes the irreducible set of all the position configurations of the ground state. Another important part in the norm of $\delta\tilde{S}_{Y_l}^{(3)}\Psi(\zeta)$ is

$$\begin{aligned}
 & \|\tilde{S}_{Y_l}^{(3)}\Psi(\zeta)\|^2 \\
 &= \sum_{f \in \mathcal{P}} \frac{1}{4} \left\{ \sum_{x_1=x_2 \in Y_l} 1 + \sum_{x_1 \neq x_2 \in Y_l} \frac{|\xi_{f(x_1), \uparrow}|^2 - |\xi_{f(x_1), \downarrow}|^2}{|\xi_{f(x_1), \uparrow}|^2 + |\xi_{f(x_1), \downarrow}|^2} \frac{|\xi_{f(x_2), \uparrow}|^2 - |\xi_{f(x_2), \downarrow}|^2}{|\xi_{f(x_2), \uparrow}|^2 + |\xi_{f(x_2), \downarrow}|^2} \right\} \\
 &\quad \times \prod_{x \in \Lambda_o} (|\xi_{f(x), \uparrow}|^2 + |\xi_{f(x), \downarrow}|^2) + \|\Phi_{\perp}\|^2 \\
 &\geq \sum_{f \in \mathcal{P}} \frac{1}{4} \left\{ \sum_{x_1 \in Y_l} \left[1 - \left(\frac{|\xi_{f(x_1), \uparrow}|^2 - |\xi_{f(x_1), \downarrow}|^2}{|\xi_{f(x_1), \uparrow}|^2 + |\xi_{f(x_1), \downarrow}|^2} \right)^2 \right] \right. \\
 &\quad \left. + \left(\sum_{x_1 \in Y_l} \frac{|\xi_{f(x_1), \uparrow}|^2 - |\xi_{f(x_1), \downarrow}|^2}{|\xi_{f(x_1), \uparrow}|^2 + |\xi_{f(x_1), \downarrow}|^2} \right)^2 \right\} \prod_{x \in \Lambda_o} (|\xi_{f(x), \uparrow}|^2 + |\xi_{f(x), \downarrow}|^2).
 \end{aligned}$$

Thus, the norm of $\delta\tilde{S}_{Y_l}^{(3)}\Psi(\zeta)$ has the following lower bound

$$\begin{aligned}
 \|\delta\tilde{S}_{Y_l}^{(3)}\Psi(\zeta)\|^2 &\geq \sum_{f \in \mathcal{P}} \left\{ \sum_{x_1 \in Y_l} \frac{1}{4} \left[1 - \left(\frac{|\xi_{f(x_1), \uparrow}|^2 - |\xi_{f(x_1), \downarrow}|^2}{|\xi_{f(x_1), \uparrow}|^2 + |\xi_{f(x_1), \downarrow}|^2} \right)^2 \right] \right. \\
 &\quad \left. + \frac{1}{4} \left[\sum_{x_1 \in Y_l} \frac{|\xi_{f(x_1), \uparrow}|^2 - |\xi_{f(x_1), \downarrow}|^2}{|\xi_{f(x_1), \uparrow}|^2 + |\xi_{f(x_1), \downarrow}|^2} - 2\langle S_{Y_l}^{(3)} \rangle_{\zeta} \right]^2 \right\} \\
 &\quad \times \prod_{x \in \Lambda_o} (|\xi_{f(x), \uparrow}|^2 + |\xi_{f(x), \downarrow}|^2) \\
 &\geq \sum_{f \in \mathcal{P}} \sum_{x_1 \in Y_l} \frac{1}{4} \left[1 - \left(\frac{|\xi_{f(x_1), \uparrow}|^2 - |\xi_{f(x_1), \downarrow}|^2}{|\xi_{f(x_1), \uparrow}|^2 + |\xi_{f(x_1), \downarrow}|^2} \right)^2 \right] \prod_{x \in \Lambda_o} (|\xi_{f(x), \uparrow}|^2 + |\xi_{f(x), \downarrow}|^2) \\
 &\geq \sum_{x_1 \in Y_l} \frac{1}{4} \left[1 - \left(\frac{|q|^{|[x_1]-z|+1/2} - |q|^{-|[x_1]-z|-1/2}}{|q|^{|[x_1]-z|+1/2} + |q|^{-|[x_1]-z|-1/2}} \right)^2 \right] \\
 &\quad \times \sum_{f \in \mathcal{P}} \prod_{x \in \Lambda_o} (|\xi_{f(x), \uparrow}|^2 + |\xi_{f(x), \downarrow}|^2). \tag{71}
 \end{aligned}$$

If we define $G_1 = (|q|^{\frac{1}{2}} + |q|^{-\frac{1}{2}})^{-2}$, we obtain

$$\|\delta\tilde{S}_{Y_l}^{(3)}\Psi(\zeta)\|^2 \geq G_1 l^{d-1} \|\Psi(\zeta)\|^2. \tag{72}$$

Next, we estimate $(\delta\tilde{S}_{Y_l}^{(3)}\Psi(\zeta), H\delta\tilde{S}_{Y_l}^{(3)}\Psi(\zeta))$. The hopping energy of $\delta\tilde{S}_{Y_l}^{(3)}\Psi(\zeta)$ vanishes

$$(\delta\tilde{S}_{Y_l}^{(3)}\Psi(\zeta), H_{\text{hop}}\delta\tilde{S}_{Y_l}^{(3)}\Psi(\zeta))=0, \quad (73)$$

since $\delta\tilde{S}_{Y_l}^{(3)}\Psi(\zeta)$ consists of only operators $a_{x,\sigma}^\dagger$ with $x \in \Lambda_o$ acting on Φ_{vac} . The interaction term

$$\begin{aligned} (\delta\tilde{S}_{Y_l}^{(3)}\Psi(\zeta), H_{\text{int}}\delta\tilde{S}_{Y_l}^{(3)}\Psi(\zeta)) &= (\tilde{S}_{Y_l}^{(3)}\Psi(\zeta), H_{\text{int}}\tilde{S}_{Y_l}^{(3)}\Psi(\zeta)) \\ &= U \sum_{y \in \partial Y_l} \|c_{y,\uparrow}c_{y,\downarrow}\tilde{S}_{Y_l}^{(3)}\Psi(\zeta)\|^2, \end{aligned} \quad (74)$$

where we define $\partial Y_l = \bar{Y}_l \cap \overline{\bar{Y}_l^c} \subset \Lambda'$. Note that for any $y \in \partial Y_l$, there exist $x_1 \in \Lambda_o \setminus Y_l$ and $x_2 \in Y_l$ such that $\bar{x}_1 \cap \bar{x}_2 = y$. Thus, we find a bound

$$\begin{aligned} &\|c_{y,\uparrow}c_{y,\downarrow}\tilde{S}_{Y_l}^{(3)}\Psi(\zeta)\|^2 \\ &= \sum_{f \in \mathcal{P}} \frac{\chi[f(x_1)=y] \chi[f(x_2)=x_2]}{(|\xi_{f(x_1),\uparrow}|^2 + |\xi_{f(x_1),\downarrow}|^2)(|\xi_{f(x_2),\uparrow}|^2 + |\xi_{f(x_2),\downarrow}|^2)} \\ &\quad \times \prod_{x \in \Lambda_o} (|\xi_{f(x),\uparrow}|^2 + |\xi_{f(x),\downarrow}|^2) \\ &\leq \sum_{f \in \mathcal{P}} \frac{1}{(|\xi_{f(x_1),\uparrow}|^2 + |\xi_{f(x_1),\downarrow}|^2)(|\xi_{f(x_2),\uparrow}|^2 + |\xi_{f(x_2),\downarrow}|^2)} \\ &\quad \times \prod_{x \in \Lambda_o} (|\xi_{f(x),\uparrow}|^2 + |\xi_{f(x),\downarrow}|^2) \\ &\leq \frac{\|\Psi(\zeta)\|^2}{(|q|^{|y|-1-z} + |q|^{-|y|+1+z})^2}, \end{aligned} \quad (75)$$

where we have used the indicator function again. For sufficiently large l , there exists $G_2 > 0$ such that

$$\sum_{y \in \partial Y_l} \frac{1}{(|q|^{|y|-1-z} + |q|^{-|y|+1+z})^2} \leq G_2 l^{d-2}.$$

Therefore, we have the following inequality:

$$(\delta\tilde{S}_{Y_l}^{(3)}\Psi(\zeta), H\delta\tilde{S}_{Y_l}^{(3)}\Psi(\zeta)) \leq G_2 U l^{d-2} \|\Psi(\zeta)\|^2. \quad (76)$$

From (72) and (76), we obtain

$$(\tilde{\Psi}_l(\zeta), H\tilde{\Psi}_l(\zeta)) < \frac{G_2}{G_1} U l^{-1}. \quad (77)$$

If we define $F_1 = G_2/G_1$, we find (52).

Here, we evaluate norm of $P_0\tilde{\Psi}_l(\zeta)$. First we consider inner product between two different ground states

$$\frac{|(\Psi(\zeta'), \Psi(\zeta))|}{\|\Psi(\zeta')\| \|\Psi(\zeta)\|}. \quad (78)$$

From Lemma 4.4, we can represent the inner product in the following

$$\frac{(\Psi(\zeta'), \Psi(\zeta))}{\|\Psi(\zeta')\| \|\Psi(\zeta)\|} = \frac{\sum_{\varphi \in \mathcal{C}} \prod_{x \in \Lambda_\sigma} \xi_{\varphi(x)}(\zeta')^* \xi_{\varphi(x)}(\zeta)}{\sqrt{\sum_{\varphi_1, \varphi_2 \in \mathcal{C}} \prod_{x \in \Lambda_\sigma} |\xi_{\varphi_1(x)}(\zeta')|^2 |\xi_{\varphi_2(x)}(\zeta)|^2}}. \quad (79)$$

The Schwarz inequality ensures the convergence of the inner product of the normalized ground state

$$\frac{|(\Psi(\zeta'), \Psi(\zeta))|}{\|\Psi(\zeta')\| \|\Psi(\zeta)\|} \leq 1.$$

We estimate this inner product with considering the constraints on the configurations. We evaluate the product of the norms

$$\begin{aligned} & \|\Psi(\zeta')\|^2 \|\Psi(\zeta)\|^2 \\ &= \sum_{f_1, f_2 \in \mathcal{P}} \prod_{x \in \Lambda_\sigma} (|\xi'_{f_1(x), \uparrow}|^2 + |\xi'_{f_1(x), \downarrow}|^2) (|\xi_{f_2(x), \uparrow}|^2 + |\xi_{f_2(x), \downarrow}|^2). \end{aligned} \quad (80)$$

Here, we abbreviate ζ and ζ' by

$$\xi_{f(x), \sigma} = \xi_{f(x), \sigma}(\zeta), \quad \xi'_{f(x), \sigma} = \xi_{f(x), \sigma}(\zeta').$$

We evaluate each term in this summation. A term with arbitrary $f_1, f_2 \in \mathcal{P}$ has a lower bound

$$\begin{aligned}
& \sum_{f_1, f_2 \in \mathcal{P}} \frac{1}{2} \left[\prod_{x \in \Lambda_o} (|\xi'_{f_1(x), \uparrow}|^2 + |\xi'_{f_1(x), \downarrow}|^2)(|\xi_{f_2(x), \uparrow}|^2 + |\xi_{f_2(x), \downarrow}|^2) + (f_1 \leftrightarrow f_2) \right] \\
& \geq \sum_{f_1, f_2 \in \mathcal{P}} \sqrt{\prod_{x \in \Lambda_o} (|\xi'_{f_1(x), \uparrow}|^2 + |\xi'_{f_1(x), \downarrow}|^2)(|\xi_{f_2(x), \uparrow}|^2 + |\xi_{f_2(x), \downarrow}|^2) \times (f_1 \leftrightarrow f_2)} \\
& = \sum_{f_1, f_2 \in \mathcal{P}} \prod_{x \in \Lambda_o} R(f_1(x), f_2(x))^2 |\xi'_{f_1(x), \uparrow} \xi_{f_1(x), \uparrow}^* + \xi'_{f_1(x), \downarrow} \xi_{f_1(x), \downarrow}^*| \\
& \quad \times |\xi'_{f_2(x), \uparrow} \xi_{f_2(x), \uparrow}^* + \xi'_{f_2(x), \downarrow} \xi_{f_2(x), \downarrow}^*|,
\end{aligned}$$

where a function $R(y_1, y_2)$ is defined for arbitrary $y_1, y_2 \in \Lambda$ by

$$R(y_1, y_2)^2 = \frac{\sqrt{(|\xi'_{y_1, \uparrow}|^2 + |\xi'_{y_1, \downarrow}|^2)(|\xi_{y_1, \uparrow}|^2 + |\xi_{y_1, \downarrow}|^2) \times (y_1 \leftrightarrow y_2)}}{|\xi'_{y_1, \uparrow} \xi_{y_1, \uparrow}^* + \xi'_{y_1, \downarrow} \xi_{y_1, \downarrow}^*| |\xi'_{y_2, \uparrow} \xi_{y_2, \uparrow}^* + \xi'_{y_2, \downarrow} \xi_{y_2, \downarrow}^*|}. \quad (81)$$

In the practical calculation, we can check $R(y_1, y_2) > 1$ for arbitrary $y_1, y_2 \in \Lambda$. Also the Schwarz inequality for the linearly independent two vectors $(\xi_{y, \uparrow}, \xi_{y, \downarrow})$ and $(\xi'_{y, \uparrow}, \xi'_{y, \downarrow})$ ensures this relation. We define a function

$$R(x) \equiv \min_{f_1, f_2 \in \mathcal{P}} R(f_1(x), f_2(x)),$$

which is also larger than 1. Therefore, we have an upper bound of the inner product between the normalized ground states

$$\frac{|(\Psi(\zeta'), \Psi(\zeta))|}{\|\Psi(\zeta')\| \|\Psi(\zeta)\|} \leq \prod_{x \in \Lambda_o} R(x)^{-1}. \quad (82)$$

Each factor $R(x)^{-1}$ with a fixed $[x]$ is a constant less than 1, since the both functions $\xi_{f(x), \sigma}(\zeta)$ and $\xi_{f(x), \sigma}(\zeta')$ depend on x only through $[x] = \sum_{k=1}^d x_k$ for any $f \in \mathcal{P}$. We define $R = \max_{x \in \Lambda_o} R(x)$, then we find

$$|(\Psi(\zeta'), \Psi(\zeta))| \leq R^{-L^{d-1}} \|\Psi(\zeta')\| \|\Psi(\zeta)\|. \quad (83)$$

Next, we evaluate an inner product between $\delta \tilde{S}_{Y_l}^{(3)} \Psi(\zeta)$ and another ground state. First, we evaluate

$$\begin{aligned}
(\Psi(\zeta'), \tilde{S}_{Y_l}^{(3)}\Psi(\zeta)) &= \frac{1}{2} \sum_{f \in \mathcal{P}} \sum_{x_1 \in Y_l} \frac{\xi'_{f(x_1), \uparrow} \xi_{f(x_1), \uparrow}^* - \xi'_{f(x_1), \downarrow} \xi_{f(x_1), \downarrow}^*}{\xi'_{f(x_1), \uparrow} \xi_{f(x_1), \uparrow}^* + \xi'_{f(x_1), \downarrow} \xi_{f(x_1), \downarrow}^*} \\
&\quad \times \prod_{x \in \Lambda_o} (\xi'_{f(x), \uparrow} \xi_{f(x), \uparrow}^* + \xi'_{f(x), \downarrow} \xi_{f(x), \downarrow}^*). \tag{84}
\end{aligned}$$

Then, we have

$$\begin{aligned}
|(\Psi(\zeta'), \tilde{S}_{Y_l}^{(3)}\Psi(\zeta))| &\leq \frac{1}{2} \sum_{x_1 \in Y_l} \left| \sum_{f \in \mathcal{P}} \prod_{x \in \Lambda_o} (\xi'_{f(x), \uparrow} \xi_{f(x), \uparrow}^* + \xi'_{f(x), \downarrow} \xi_{f(x), \downarrow}^*) \right| \\
&= \frac{1}{2} G_3 l^d |(\Psi(\zeta'), \Psi(\zeta))|, \tag{85}
\end{aligned}$$

where we define G_3 by $\sum_{x_1 \in Y_l} 1 = G_3 l^d$. Also we obtain another upper bound

$$(\Psi(\zeta), \tilde{S}_{Y_l}^{(3)}\Psi(\zeta)) \leq \frac{1}{2} G_3 l^d \|\Psi(\zeta)\|^2. \tag{86}$$

Therefore, the inner product between $\delta \tilde{S}_{Y_l}^{(3)}\Psi(\zeta)$ and the ground state is estimated as

$$|(\Psi(\zeta'), \delta \tilde{S}_{Y_l}^{(3)}\Psi(\zeta))| \leq G_3 l^d R^{-L^{d-1}} \|\Psi(\zeta')\| \|\Psi(\zeta)\|. \tag{87}$$

Now we estimate $\|P_0 \tilde{\Psi}_l(\zeta)\|$. Since $\{\Psi(\zeta_j)\}_{j=0}^{L^d}$ is a complete basis of the ground states, we can represent $P_0 \tilde{\Psi}_l(\zeta)$ by

$$P_0 \tilde{\Psi}_l(\zeta) = \sum_{j=0}^{L^d} \frac{C_j}{\|\Psi(\zeta_j)\|} \Psi(\zeta_j), \tag{88}$$

where C_j is a complex coefficient. Thus, we have

$$\begin{aligned}
\|P_0 \tilde{\Psi}_l(\zeta)\|^2 &= \sum_{j=0}^{L^d} \frac{C_j}{\|\Psi(\zeta_j)\|} (\tilde{\Psi}_l(\zeta), \Psi(\zeta_j)) = \sum_{j=0}^{L^d} C_j \frac{(\delta \tilde{S}_{Y_l}^{(3)}\Psi(\zeta), \Psi(\zeta_j))}{\|\delta \tilde{S}_{Y_l}^{(3)}\Psi(\zeta)\| \|\Psi(\zeta_j)\|} \\
&< \frac{G_3}{\sqrt{G_1}} l^{(d+1)/2} R^{-L^{d-1}} \sum_{j=0}^{L^d} |C_j|, \tag{89}
\end{aligned}$$

where we have used (83) and (87). To evaluate $\sum_j |C_j|$, we consider

$$\begin{aligned} \frac{(\Psi(\zeta_j), P_0 \tilde{\Psi}_l(\zeta))}{\|\Psi(\zeta_j)\|} &= \sum_{k=0}^{L^d} C_k \frac{(\Psi(\zeta_j), \Psi(\zeta_k))}{\|\Psi(\zeta_j)\| \|\Psi(\zeta_k)\|} \\ &= C_j + \sum_{k \neq j} C_k \frac{(\Psi(\zeta_j), \Psi(\zeta_k))}{\|\Psi(\zeta_j)\| \|\Psi(\zeta_k)\|}. \end{aligned} \tag{90}$$

Then, we have

$$\begin{aligned} |C_j| &< \frac{|(\Psi(\zeta_j), P_0 \tilde{\Psi}_l(\zeta))|}{\|\Psi(\zeta_j)\|} + \sum_{k \neq j} |C_k| \frac{|(\Psi(\zeta_j), \Psi(\zeta_k))|}{\|\Psi(\zeta_j)\| \|\Psi(\zeta_k)\|} \\ &< \frac{G_3}{\sqrt{G_1}} l^{(d+1)/2} R^{-L^{d-1}} + R^{-L^{d-1}} \sum_{k \neq j} |C_k|, \end{aligned} \tag{91}$$

where we have used (83) and (87). If we define $|C_m| = \max\{|C_k|\}_{k=0}^{L^d}$, then we obtain

$$|C_k| \leq |C_m| < \frac{G_3}{\sqrt{G_1}} \frac{l^{(d+1)/2} R^{-L^{d-1}}}{1 - L^d R^{-L^{d-1}}}, \tag{92}$$

for any $k=0, 1, \dots, L^d$. Thus, we obtain

$$\|P_0 \tilde{\Psi}_l(\zeta)\|^2 < \frac{G_3^2 (L^d + 1) l^{d+1} R^{-2L^{d-1}}}{G_1 (1 - L^d R^{-L^{d-1}})}. \tag{93}$$

from (89) and (92). If we define L_1 by $1 - L_1^d R^{-L_1^{d-1}} = 1/2$ and F_2 by $F_2 = 2G_3^2/G_1$, then we obtain

$$\|P_0 \tilde{\Psi}_l(\zeta)\|^2 < F_2 (L^d + 1) l^{d+1} R^{-2L^{d-1}}. \tag{94}$$

By definition of the normalized state (66), this inequality completes the proof of Theorem 4.1. ■

4.4. Proof of Corollary 4.2

Here, we prove Corollary 4.2. We define a normalized state $\tilde{\Psi}_\perp$ by

$$\tilde{\Psi}_\perp := \frac{(1 - P_0) \tilde{\Psi}_L(1)}{\|(1 - P_0) \tilde{\Psi}_L(1)\|}. \tag{95}$$

An upper bound of $(\tilde{\Psi}_\perp, H\tilde{\Psi}_\perp)$ gives an upper bound on the lowest excitation energy in a finite system, since $\tilde{\Psi}_\perp(\zeta)$ is orthogonal to all of the ground state. Since $H\tilde{\Psi}_L(1) = H(1 - P_0)\tilde{\Psi}_L(1)$, the only remaining task is to estimate $\|(1 - P_0)\tilde{\Psi}_L(1)\|$. From (93), we obtain

$$\begin{aligned} \|(1 - P_0)\tilde{\Psi}_L(1)\|^2 &= \|\tilde{\Psi}_L(1)\|^2 - \|P_0\tilde{\Psi}_L(1)\|^2 \\ &< 1 - \frac{G_3^2 (L^d + 1)L^{d+1}R^{-2L^{d-1}}}{G_1 (1 - L^d R^{-L^{d-1}})}. \end{aligned} \tag{96}$$

If we define L_2 by

$$\frac{G_3^2 (L_2^d + 1)L_2^{d+1}R^{-2L_2^{d-1}}}{G_1 (1 - L_2^d R^{-L_2^{d-1}})} = \frac{1}{2}, \tag{97}$$

and set $F_3 = 2F_1$, then we obtain an upper bound

$$(\tilde{\Psi}_\perp, H\tilde{\Psi}_\perp) < F_3 U L^{-1}. \tag{98}$$

This gives an upper bound on the lowest excitation energy in a finite system, and so completes the proof of Corollary 4.2. ■

5. EXISTENCE OF THE SPIN-WAVE GAP

In this section, we consider our model under the periodic boundary condition. The properties of ground states and low energy excitations are very different from a system with the open boundary. We find only two ground states: the all-spin-up state and the all-spin-down state. We show that a one-magnon spin-wave excitation has an energy gap as in the XXZ model. The proof is based on Tasaki’s argument for the SU(2) invariant model.⁽¹⁸⁾ He proved that the one-magnon spin-wave excitation in the Tasaki model has the same dispersion relation as that in the ferromagnetic Heisenberg model. These spin-wave excitations in both models have no energy gap, since they are the Goldstone mode above the ground states which spontaneously break the SU(2) spin rotation symmetry. On the contrary, an energy gap is generated by the anisotropy in our model as in the XXZ model. Here, we show only a brief sketch of the proof.

5.1. Ground States and Spin-Wave Excitation

First we obtain ground states. We have already found the representation of a ground state (35) with the condition (36) in Section 3. The

periodic boundary condition allows no configuration which satisfies the condition (36) except in the two cases: $\sigma_x = \uparrow$ for all $x \in \Lambda_o$ or $\sigma_x = \downarrow$ for all $x \in \Lambda_o$. Thus, we conclude that all ground states in the periodic system are only two fully polarized states Φ_\uparrow and Φ_\downarrow .

Next we consider the one-magnon spin-wave excitation. For the spin-wave in our electron model, we consider properties of the spin-wave state in quantum spin models. The one-magnon spin-wave state with a wave-number $k \in \mathcal{K}$: $\Phi_{\text{SW}}(k)$ satisfies

$$T_x \Phi_{\text{SW}}(k) = e^{-ik \cdot x} \Phi_{\text{SW}}(k) \quad (99)$$

and

$$S_{\text{tot}}^{(3)} \Phi_{\text{SW}} = (S_{\text{max}} - 1) \Phi_{\text{SW}}, \quad (100)$$

where $x \in \Lambda_o$. The translation operator T_x is defined by

$$T_x c_{y,\sigma} T_x^{-1} = c_{x+y,\sigma} \quad \text{and} \quad T_x c_{y,\sigma}^\dagger T_x^{-1} = c_{x+y,\sigma}^\dagger. \quad (101)$$

\mathcal{K} is the space of wave-number vectors

$$\mathcal{K} := \left\{ \frac{2\pi n}{L} \mid n \in \mathbb{Z}^d \cap \left[-\frac{L-1}{2}, \frac{L-1}{2} \right]^d \right\}. \quad (102)$$

Then, the one-magnon spin-wave state is in the following Hilbert space \mathcal{H}_k

$$\mathcal{H}_k := \left\{ \Psi \in \mathcal{H} \mid T_x \Psi = e^{-ik \cdot x} \Psi \quad \text{and} \quad S_{\text{tot}}^{(3)} \Psi = \frac{1}{2} (|\Lambda_o| - 1) \Psi \right\}. \quad (103)$$

We define the one-magnon spin-wave state with wave-number k by the lowest energy state in \mathcal{H}_k . Let $E_{\text{SW}}(k)$ be the energy of one-magnon spin-wave state with wave-number k . We can prove the following theorem.

Theorem 5.1. (Spin-Wave Gap). Suppose the d -dimensional Hubbard model defined by the Hamiltonian (15). There exist positive constants $t_0, U_0, \lambda_0, C < \infty$ which are independent of system volume such that

$$\min_{k \in \mathcal{K}} E_{\text{SW}}(k) \geq \frac{2U}{\lambda^4} \left[\frac{d(|q| + |q|^{-1} - 2)}{2} - \frac{C}{\lambda} \right], \quad (104)$$

for $t \geq t_0, U \geq U_0$ and $\lambda \geq \lambda_0$.

This theorem shows that one-magnon spin-wave excitation has a finite gap for sufficiently large λ in a periodic system.

5.2. Sketch of Proof

Theorem 5.1 is proved by the same approach given in ref. 18. Here, we show only a sketch of the proof.

First we introduce a localized electron operator $a_{x,\sigma}^\dagger$ defined by

$$a_{x,\sigma}^\dagger := \sum_{y \in \Lambda} \psi_{y,\sigma}^{(x)} c_{y,\sigma}^\dagger, \quad (105)$$

where $\psi_{y,\sigma}^{(x)}$ is defined by

$$\psi_{y,\sigma}^{(x)} := \begin{cases} \delta_{x,y} - \sum_{j=1}^d \left(\frac{q^{p(\sigma)/4}}{\lambda} \delta_{x-e^{(j)},y} + \frac{q^{-p(\sigma)/4}}{\lambda} \delta_{x+e^{(j)},y} \right) & \text{if } x \in \Lambda_o, \\ \delta_{x,y} + \frac{(q^{-p(\sigma)/4})^*}{\lambda} \delta_{x-e^{(j)},y} + \frac{(q^{p(\sigma)/4})^*}{\lambda} \delta_{x+e^{(j)},y} & \text{if } x \in \Lambda_j. \end{cases} \quad (106)$$

The set $\{a_{x,\sigma}^\dagger \Phi_{\text{vac}}\}_{x \in \Lambda}$ is a basis in the space of single electron states. We define the dual operator $b_{x,\sigma}$ which satisfies

$$\{b_{x,\sigma}, a_{y,\tau}^\dagger\} = \delta_{x,y} \delta_{\sigma,\tau} \quad \text{and} \quad \{b_{x,\sigma}, b_{y,\tau}\} = 0 = \{a_{x,\sigma}^\dagger, a_{y,\tau}^\dagger\}. \quad (107)$$

We represent $b_{x,\sigma}$ in terms of the original electron operator by

$$b_{x,\sigma} = \sum_{y \in \Lambda} (\tilde{\psi}_{y,\sigma}^{(x)})^* c_{y,\sigma}. \quad (108)$$

Eqs. (105), (107) and (108) mean

$$\sum_{w \in \Lambda} (\tilde{\psi}_{w,\sigma}^{(x)})^* \psi_{w,\sigma}^{(y)} = \delta_{x,y} \quad \text{and} \quad \sum_{w \in \Lambda} (\tilde{\psi}_{x,\sigma}^{(w)})^* \psi_{y,\sigma}^{(w)} = \delta_{x,y}. \quad (109)$$

The original electron operators can be written in terms of $a_{x,\sigma}^\dagger$ and $b_{x,\sigma}$,

$$c_{x,\sigma}^\dagger = \sum_{y \in \Lambda} (\tilde{\psi}_{x,\sigma}^{(y)})^* a_{y,\sigma}^\dagger \quad \text{and} \quad c_{x,\sigma} = \sum_{y \in \Lambda} \psi_{x,\sigma}^{(y)} b_{y,\sigma}. \quad (110)$$

The Hilbert space with $|\Lambda_o|$ electrons is also spanned by the basis

$$\left\{ \left(\prod_{x \in A} a_{x,\uparrow}^\dagger \right) \left(\prod_{x \in B} a_{x,\downarrow}^\dagger \right) \Phi_{\text{vac}} \mid A, B \subset \Lambda \text{ with } |A| + |B| = |\Lambda_o| \right\} \quad (111)$$

because $c_{x,\sigma}^\dagger$ can be written in terms of $a_{x,\sigma}^\dagger$.

We represent the interaction Hamiltonian in terms of this basis

$$H_{\text{int}} = \sum_{x_1, x_2, x_3, x_4 \in \Lambda} \left(U \sum_{w \in \Lambda} (\tilde{\psi}_{w, \uparrow}^{(x_1)} \tilde{\psi}_{w, \downarrow}^{(x_2)})^* \psi_{w, \downarrow}^{(x_3)} \psi_{w, \uparrow}^{(x_4)} \right) a_{x_1, \uparrow}^\dagger a_{x_2, \downarrow}^\dagger b_{x_3, \downarrow} b_{x_4, \uparrow}. \quad (112)$$

It is convenient to introduce a new hopping Hamiltonian \tilde{H}_{hop} defined by

$$\tilde{H}_{\text{hop}} := t\lambda^2 \sum_{\sigma = \uparrow, \downarrow} \sum_{x \in \Lambda'} a_{x, \sigma}^\dagger b_{x, \sigma} \quad (113)$$

for the estimation of a lower bound of spin-wave excitation. \tilde{H}_{hop} satisfies

$$\tilde{H}_{\text{hop}} a_{x, \sigma}^\dagger \Phi_{\text{vac}} = \begin{cases} 0 & \text{if } x \in \Lambda_o, \\ t\lambda^2 & \text{if } x \in \Lambda'. \end{cases} \quad (114)$$

Since $H_{\text{hop}} a_{x, \sigma}^\dagger \Phi_{\text{vac}} = 0$ for $x \in \Lambda_o$ and $t\lambda^2$ is lowest energy eigenvalue of a single electron state which is orthogonal to the zero energy states, then we have $\tilde{H}_{\text{hop}} \leq H_{\text{hop}}$.

First, we define a basis of \mathcal{H}_k . To define a convenient basis of \mathcal{H}_k , we define a state $\Psi_{\mu, A}(k)$ for $\mu = 0, 1, \dots, d$ and for a set $A \subset \Lambda$ with $|A| = |\Lambda_o| - 1$ by

$$\Psi_{\mu, A}(k) := \sum_{w \in \Lambda_o} e^{ik \cdot w} T_w a_{e^{(\mu)}, \downarrow}^\dagger \left(\prod_{v \in A} a_{v, \uparrow}^\dagger \right) \Phi_{\text{vac}}, \quad (115)$$

where $e^{(\mu)} = o = (0, 0, \dots, 0)$ for $\mu = 0$ and $e^{(\mu)} = e^{(j)}$ for $\mu = j$ ($j = 1, 2, \dots, d$). This state satisfies both properties (99) and (100). We define another state $\Omega(k)$ by

$$\Omega(k) = \frac{1}{\alpha(k)} \sum_{w \in \Lambda_o} e^{ik \cdot w} T_w a_{o, \downarrow}^\dagger b_{o, \uparrow} \Phi_{\uparrow} \propto \Psi_{0, \Lambda_o \setminus \{o\}}, \quad (116)$$

which is an approximation of the spin-wave state. We will choose a constant $\alpha(k)$ in the proof. We define the following basis of \mathcal{H}_k by

$$\mathcal{B}_k := \{\Omega(k)\} \cup \{\Psi_{\mu, A} \mid \mu = 0, 1, \dots, d, \quad A \subset \Lambda \\ \text{with } |A| = |\Lambda_o| - 1 \text{ and } (\mu, A) \neq (0, \Lambda_o \setminus \{o\})\}. \quad (117)$$

We define \tilde{H} by $\tilde{H}_{\text{hop}} + H_{\text{int}}$ and matrix elements $h[\Phi, \Psi]$ between $\Phi, \Psi \in \mathcal{B}_k$ by the unique expansion

$$\tilde{H}\Phi = \sum_{\Psi \in \mathcal{B}_k} h[\Psi, \Phi]\Psi. \tag{118}$$

And we define $D[\Phi]$ by

$$D[\Phi] := \Re[h[\Phi, \Phi]] - \sum_{\Psi \in \mathcal{B}_k \setminus \{\Phi\}} |h[\Phi, \Psi]|. \tag{119}$$

Now, we can prove the following lemmas.

Lemma 5.2. Let $E_0(k)$ be the lowest energy eigenvalue of \tilde{H} in the Hilbert space \mathcal{H}_k . Then, we have

$$E_0(k) \geq \min_{\Phi \in \mathcal{B}_k} D[\Phi]. \tag{120}$$

Lemma 5.3. There exist positive constants $t_0, U_0, \lambda_0, C < \infty$ independent of system volume such that

$$\begin{aligned} \min_{\Phi \in \mathcal{B}_k} D[\Phi] &= D[\Omega(k)] \\ &\geq \frac{2U}{\lambda^4} \left[\frac{d(|q| + |q|^{-1})}{2} - \sum_{j=1}^d \cos(2k \cdot e^{(j)} + \theta) - \frac{C}{\lambda} \right] \end{aligned} \tag{121}$$

for $t \geq t_0, \lambda \geq \lambda_0$ and $U \geq U_0$.

We find the proof of Lemma 5.2 in subsection 6.1 of ref. 18. Lemma 5.3 is obtained by a direct evaluation.

Now, we can prove Theorem 5.1. Since $\tilde{H} \leq H$, then we have $E_0(k) \leq E_{\text{SW}}(k)$. Thus we find

$$\begin{aligned} \Delta E &\geq \min_{k \in \mathcal{K}} E_0(k) \\ &\geq \min_{k \in \mathcal{K}} \frac{2U}{\lambda^4} \left[\frac{d(|q| + |q|^{-1})}{2} - \sum_{j=1}^d \cos(2k \cdot e^{(j)} + \theta) - \frac{C}{\lambda} \right] \end{aligned} \tag{122}$$

from Lemmas 5.2 and 5.3. This concludes Theorem 5.1. ■

6. SUMMARY

In this paper, we construct a set of exact ground state with a ferromagnetic domain wall structure and a spiral structure in a deformed flat-band Hubbard model under an open boundary condition. We have studied excited states above the domain wall ground state. There exists a gapless excitation above the domain wall ground state in dimensions higher than one. This excited state is constructed by acting a local operator near the domain wall on the ground state. We study this model also under the periodic boundary condition. In this case a ground state becomes the all-spin-up or -down state. We have shown the energy gap of the spin-wave excitation above the all-spin-up ground state. These properties of the excitations above the ground states are similar to those in the XXZ model.

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