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Ferromagnetic Domain Wall Ground States in a Deformed Flat Band Hubbard Model

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Abstract

We construct a set of exact ground states with a localized ferromagnetic domain wall in a deformed flat-band Hubbard model. We show the uniqueness of the ground state for the half filled lowest band in a fixed magnetization sub-space. The ground states with these structures are degenerated with the all spins up or all spins down states. We represent spin one point functions in terms of local electron number density, and find the domain wall structure in our model. We expect that the properties of the ground state and the excitations above the domain wall ground state are similar to those in the XXZ quantum spin model.

1 Introduction

Domain structures in a ferromagnetic system are interesting phenomena. If the system has a translational symmetry, this symmetry is broken spontaneously by the domains. In classical spin systems, universal natures of the domain wall have been studied extensively. For example in the Ising model on the cubic lattice, Dbrushin 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 Frölich proved that the horizontal domain wall on the d -dimensional hypercubic lattice is stable also 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 classical systems, since many local operators can deform the diagonal domain wall state to many other states without loss of energy. Nonetheless, the quantum perturbation is known to stabilize the diagonal domain wall structure. No local operator can deform the diagonal domain wall ground state to other ground states. 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]. Koma and Nachtergaele discussed the stability of the diagonal domain wall in the exact solution of the XXZ quantum spin systems [4]. Datta and Kennedy also discuss the stability of a domain wall in one-dimensional quantum spin models by a rigorous perturbation method [5]. The role of the quantum effects should be studied more in many other contexts.

In this report, we study a diagonal domain wall ground state in a deformed flat-band Hubbard model. The flat-band Hubbard model is proposed recently 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 with special properties, which are called flat-band Hubbard models [6, 7]. Tasaki proved also the stability of the saturated ferromagnetism against a perturbation which bends the electron band [8]. Tanaka and Ueda have shown the stability of the saturated ferromagnetism in a more complicated two-dimensional model in Mielke's

class [9]. Contrary to the Nagaoka ferromagnetism, this ferromagnetism is believed to be stable against a small perturbation or change the electron number density [10]. The flat-band Hubbard model can be a standard one in which we consider problems related to ferromagnetism in many-electron systems. 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 leads the electrons to a microscopic entangled state with respect to the site configuration. 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 $U(1)$ in our deformed model. This 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 see the profile of the ferromagnetic domain wall.

This report 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 state sub-space 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 describe some results obtained in a one-dimensional model. By the estimate of the correlation function, we observe the cluster property for the spin and the density of the electrons. Therefore, we expect stability of this ferromagnetic domain wall ground state. And we summarize in section 5.

2 Definition of the Model

The Hubbard model is a model which represents a many-electron system on an arbitrary lattice. An electron is described by a fermion operator. In this section, we define a d -dimensional model with illustrating it's physical meanings.

2.1 Lattice

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

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

Λ_o is d -dimensional integer lattice with linear size L , which 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' is obtained as a half site translation of Λ_o to j -th direction,

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

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

$$e^{(j)} := (0, \dots, 0, \underset{\substack{\uparrow \\ j\text{-th}}}{\frac{1}{2}}, 0, \dots, 0). \quad (5)$$

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

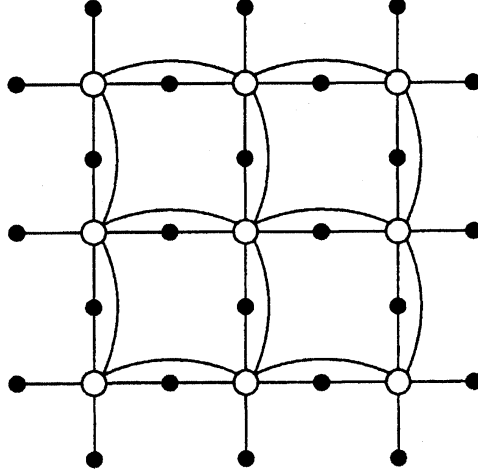


Figure 1: Two dimensional lattice (with $L = 3$). The white circles are sites in Λ_o and the black dots are sites in Λ' . Electrons at a site can hop to other site if the site is connected to the original site with a line or a curve.

2.2 Electron Operators and the Fock Space

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

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

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

$$c_{x,\sigma} \Phi_{\text{vac}} = 0 \quad (7)$$

for all $x \in \Lambda$ and $\sigma = \uparrow, \downarrow$. We construct a set of basis of Fock space which is domain of the electron operators

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

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 electron at site x with spin σ . Note anticommutation relations $\{c_{x,\sigma}^\dagger, c_{x,\sigma}^\dagger\} = 0$ i.e. $c_{x,\sigma}^\dagger c_{x,\sigma}^\dagger = 0$. The latter implies the Pauli Principle. We take the open boundary condition which is realized by $c_{x,\sigma} = 0$ if $x_j > L/2$ for some $j = 1, 2, \dots, d$ with $x = (x_l)_{l=1}^d$.

2.3 Deformed Flat-Band Hubbard Model

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

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

and

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

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

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

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

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

and

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

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

$$\left\{ \left(\prod_{x \in A} a_{x,\uparrow}^\dagger \right) \left(\prod_{x \in B} a_{x,\downarrow}^\dagger \right) \Phi_{\text{vac}} \mid A, B \subset \Lambda \right\}. \quad (14)$$

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

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

with a parametrization $q = |q|e^{i\theta}$ by $0 \leq \theta < 2\pi$. Each term $t_{x,y}^{(\sigma)} c_{x,\sigma}^\dagger c_{y,\sigma}$ 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 a on-site repulsive interaction, we regard this Hamiltonian as a simplification of the Coulomb interaction between two electrons.

Note that this system conserve 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 as we want. In present report, we only consider that electron number is equal to $|\Lambda_o|$ i.e. we consider only the Hilbert space \mathcal{H} which is spanned by the following basis¹

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

or

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

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

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

¹Through out the present report, we denotes a complex conjugate of $\alpha \in \mathbb{C}$ by α^* and it's 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 a cardinality of a set A .

The Hamiltonian commutes with the third component of total spin operator

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

with

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

Note that this symmetry is enhanced to a $SU(2)$ symmetry in the case of $q = 1$ *i.e.* Hamiltonian commutes with any component of total spin operator. In this case, this model become original flat-band Hubbard model given by Tasaki [7, 8]. Another important symmetry is generated by a product of a parity and spin rotation defined by

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

where P is a parity operator defined by $Pc_{x,\sigma}P = c_{-x,\sigma}$ and $Pc_{x,\sigma}^\dagger P = c_{-x,\sigma}^\dagger$. 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.

3 Ground States

In this section, we obtain the ground state of the model with fixed electron number $N_e = |\Lambda_o|$. The representation of the hopping Hamiltonian in terms of $d_{x,\sigma}$,

$$H_{\text{hop}} = \sum_{\sigma=\uparrow,\downarrow} \sum_{x \in \Lambda'} d_{x,\sigma}^\dagger d_{x,\sigma}, \quad (28)$$

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

$$H = H_{\text{hop}} + H_{\text{int}} \geq 0. \quad (29)$$

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

$$\Phi_\uparrow = \left(\prod_{x \in \Lambda_o} a_{x,\uparrow}^\dagger \right) \Phi_{\text{vac}}. \quad (30)$$

We easily verify $H\Phi_\uparrow = 0$ from the anticommutation relations of $a_{x,\sigma}^\dagger$ and $d_{x,\sigma}$, and therefore Φ_\uparrow is a ground state of H . Next, we determine all other ground states.

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

$$d_{x,\sigma}\Phi = 0 \quad (31)$$

for all $x \in \Lambda'$ with $\sigma = \uparrow, \downarrow$ and

$$c_{y,\uparrow}c_{y,\downarrow}\Phi = 0 \quad (32)$$

for all $y \in \Lambda$.

We consider a restricted Hilbert space \mathcal{H}_M spanned by the states with a magnetization M which is an eigenvalue of the operator $S_{\text{tot}}^{(3)}$. Since the magnetization is good quantum number by the commutation relation (25), we look for other ground states in each restricted sub-space \mathcal{H}_M . Let $\Phi(M)$ be a ground state with a magnetization M . We expand $\Phi(M)$ into the following series

$$\Phi(M) = \sum_{A,B} \psi(A, B) \left(\prod_{x \in A} a_{x,\uparrow}^\dagger \right) \left(\prod_{y \in B} a_{y,\downarrow}^\dagger \right) \Phi_{\text{vac}}, \quad (33)$$

where the sum is taken over all subsets $A, B \subset \Lambda$ with $|A| = (L + 2M)/2$ and $|B| = (L - 2M)/2$ and $\psi(A, B)$ is a coefficient. The first condition (31) implies that $\psi(A, B)$ does not vanish only for $A \cap \Lambda' = \emptyset$ and $B \cap \Lambda' = \emptyset$. The second condition (32) for $y \in \Lambda_o$ becomes

$$d_{y,\uparrow} d_{y,\downarrow} \Phi(M) = 0, \quad (34)$$

since the definition of $d_{y,\sigma}$ for $y \in \Lambda_o$. To satisfy this condition, $\psi(A, B)$ takes 0 for $A \cap B \neq \emptyset$. Thus the expansion (33) can be written in the form:

$$\Phi(M) = \sum_{\sigma \in \mathcal{S}_M} \phi(\sigma) \prod_{x \in \Lambda_o} a_{x,\sigma_x}^\dagger \Phi_{\text{vac}} \quad (35)$$

where \mathcal{S}_M is a set of all possible spin configurations $\sigma = (\sigma_x)_{x \in \Lambda_o}$ with a magnetization M :

$$\mathcal{S}_M = \left\{ \sigma = (\sigma_x)_{x \in \Lambda_o} \left| \frac{1}{2} \sum_{x \in \Lambda_o} (-1)^{\frac{1-p(\sigma_x)}{2}} = M, \sigma_x = \uparrow, \downarrow \right. \right\}. \quad (36)$$

In this representation, the second condition (32) for $y \in \Lambda_j$ is equivalent to

$$(d_{y-e(j),\uparrow} d_{y+e(j),\downarrow} - q d_{y-e(j),\downarrow} d_{y+e(j),\uparrow}) \Phi = 0. \quad (37)$$

We find that the coefficient satisfies

$$\phi(\sigma) = q^{\{p(\sigma_{y-e(j)}) - p(\sigma_{y+e(j)})\}/2} \phi(\sigma_{y-e(j), y+e(j)}) \quad (38)$$

for $y \in \Lambda_j$, 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 can be related by successive exchanges of two nearest neighbour spins. Therefore the degeneracy of those ground states is exactly the same as that in the SU(2) symmetric model, as in the domain wall ground states in the XXZ model [3].

We define S_q^- by

$$S_q^- = \sum_{x \in \Lambda} q^{[x]} a_{x,\downarrow}^\dagger d_{x,\uparrow}, \quad (39)$$

where $[x] = \sum_{j=1}^d x_j$. The ground state with a magnetization M is obtained by acting this operator certain times on the all spins up state

$$\Phi(M) = (S_q^-)^{|\Lambda_o| - 2M} \Phi_\uparrow. \quad (40)$$

3.1 Canonical States

To explore the nature of the ground state, we write it in a more explicit way as obtained by Gottstein and Werner in [11]. We define the canonical state $\Psi(\zeta)$ by

$$\Psi(\zeta) = \left(\prod_{x \in \Lambda_0} \alpha_x^\dagger(\zeta) \right) \Phi_{\text{vac}} = \sum_{n=0}^L \zeta^n (S_q^-)^n \Phi_\uparrow \quad (41)$$

where $\alpha_x^\dagger(\zeta) = a_{x,\uparrow}^\dagger + \zeta q^{[x]} a_{x,\downarrow}^\dagger$. Since the state which corresponds to this canonical state in the XXZ model is pure state in the infinite volume limit, we expect that this canonical state in our model is also pure state as well in the infinite volume limit. Note that the state $\Psi(\zeta)$ defined here in the Hubbard model is not a product state unlike in the XXZ model.

3.2 Spin One Point Functions

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

$$\langle S_x^{(j)} \rangle_\zeta = \frac{1}{2} \sum_{\sigma, \tau = \uparrow, \downarrow} \mathcal{P}_{\sigma, \tau}^{(j)} \frac{(\Psi(\zeta), c_{x, \sigma}^\dagger c_{x, \tau} \Psi(\zeta))}{\|\Psi(\zeta)\|^2} = \frac{1}{2} \sum_{\sigma, \tau = \uparrow, \downarrow} \mathcal{P}_{\sigma, \tau}^{(j)} \frac{(c_{x, \sigma} \Psi(\zeta), c_{x, \tau} \Psi(\zeta))}{\|\Psi(\zeta)\|^2}. \quad (42)$$

The following anticommutation relations with $y \in \Lambda_\sigma$,

$$\{c_{x, \sigma}, \alpha_y^\dagger(\zeta)\} = \lambda \{d_{x, \uparrow}, a_{y, \uparrow}^\dagger + \zeta q^y a_{y, \downarrow}^\dagger\} = \lambda \eta_{x, \sigma} \delta_{x, y}, \quad (43)$$

for $x \in \Lambda_\sigma$, and

$$\{c_{x, \sigma}, \alpha_y^\dagger(\zeta)\} = -\eta_{x, \sigma} \left(q^{-\frac{1}{4}} \delta_{x-e^{(j)}, y} + q^{\frac{1}{4}} \delta_{x+e^{(j)}, y} \right), \quad (44)$$

for $x \in \Lambda_j$ are useful to calculate the expectation value, where $\eta_{x, \uparrow} = 1$ and $\eta_{x, \downarrow} = \zeta q^{[x]}$. These anticommutation relations (43) and (44) yield an equation

$$c_{x, \sigma} \Psi(\zeta) = \eta_{x, \sigma} \Psi_x(\zeta), \quad (45)$$

where $\Psi_x(\zeta)$ is defined by

$$\Psi_x(\zeta) = \begin{cases} \text{sgn}(x) \lambda \left(\prod_{y \neq x} \alpha_y^\dagger(\zeta) \right) \Phi_{\text{vac}} & \text{if } x \in \Lambda_\sigma \\ \left(\text{sgn}(x - e^{(j)}) q^{-\frac{1}{4}} \prod_{y \neq x - e^{(j)}} \alpha_y^\dagger(\zeta) + \text{sgn}(x + e^{(j)}) q^{\frac{1}{4}} \prod_{y \neq x + e^{(j)}} \alpha_y^\dagger(\zeta) \right) \Phi_{\text{vac}} & \text{if } x \in \Lambda_j \end{cases}, \quad (46)$$

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

$$\langle c_{x, \sigma}^\dagger c_{x, \tau} \rangle_\zeta = \eta_{x, \sigma}^* \eta_{x, \tau} \frac{\|\Psi_x(\zeta)\|^2}{\|\Psi(\zeta)\|^2}. \quad (47)$$

And also an expectation value of the electron number operator at site x can be written in

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

where $n_x = n_{x,\uparrow} + n_{x,\downarrow}$. Thus we obtain the representations of spin one-point function at site $x \in \Lambda$ in terms of a electron number density $\langle n_x \rangle_\zeta$,

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

$$\langle S_x^{(2)} \rangle_\zeta = \frac{\langle n_x \rangle_\zeta \zeta q^{[x]} - (\zeta q^{[x]})^*}{2i(1 + |\zeta q^{[x]}|^2)}, \quad (50)$$

$$\langle S_x^{(3)} \rangle_\zeta = \frac{\langle n_x \rangle_\zeta (1 - |\zeta q^{[x]}|^2)}{2(1 + |\zeta q^{[x]}|^2)}. \quad (51)$$

where $\epsilon = \lambda^2 + |q|^{\frac{1}{2}} + |q|^{-\frac{1}{2}}$. We can expect the electron number density in the canonical state takes almost constant on Λ_o or on Λ' respectively, from the definition of $\Psi(\zeta)$. Indeed, in one-dimensional model, we have confirmed that this conjecture by obtaining the exact bounds [12]. These results are shown in section 4.

As discussed the domain wall ground state in the XXZ models in [4, 13, 14], 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 the zeros of $\langle S_x^{(3)} \rangle_\zeta$ which is located at $x = -\log_{|q|} |\zeta|$. The function $\frac{1}{2} \langle n_x \rangle_\zeta - |\langle S_x^{(3)} \rangle_\zeta|$ decays exponentially as x leave 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 sub-lattice Λ_o or Λ' as we conjectured, the behaviors of the one point spin functions are not controlled by the number density mainly. In large λ limit for real $q > 1$, electrons are completely localized at integer sites, and the one point spin functions 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 $\theta \sum_{j=1}^d x_j$ around the third spin axis depending on the site $x = (x_j)_{j=1}^d$. 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.

3.3 Spin Correlation Functions

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

$$\langle S_x^{(j)} S_y^{(l)} \rangle_\zeta = \sum_{\sigma, \tau, \sigma', \tau'} \frac{\eta_{x, \sigma}^* \frac{1}{2} \mathcal{P}_{\sigma, \tau}^{(j)} \eta_{x, \tau}}{1 + |\zeta q^x|^2} \frac{\eta_{y, \sigma'}^* \frac{1}{2} \mathcal{P}_{\sigma', \tau'}^{(l)} \eta_{y, \tau'}}{1 + |\zeta q^y|^2} \langle n_x n_y \rangle_\zeta. \quad (52)$$

We can rewrite

$$\langle S_x^{(j)} S_y^{(l)} \rangle_\zeta = \langle S_x^{(j)} \rangle_\zeta \langle S_y^{(l)} \rangle_\zeta \frac{\langle n_x n_y \rangle_\zeta}{\langle n_x \rangle_\zeta \langle n_y \rangle_\zeta}. \quad (53)$$

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. In the following section, actually we show that this can be done for the one-dimensional model.

4 Results in the One-Dimensional Model

In one-dimensional case, we can evaluate the following normalization function

$$A(x, y; \zeta) := \left\| \left(\prod_{w=x}^y \alpha_w^\dagger(\zeta) \right) \Phi_{\text{vac}} \right\|^2, \quad (54)$$

for $y, x \in \Lambda_o$ with $y > x$. Note $A(-\frac{L-1}{2}, \frac{L-1}{2}; \zeta) = \|\Psi(\zeta)\|^2$. This normalization function obeys a recursion relation

$$A(x, y; \zeta) = \epsilon(1 + |\zeta q^{y/2}|^2) A(x, y-1; \zeta) - (1 + |\zeta q^{y-\frac{1}{2}}|^2)^2 A(x, y-2; \zeta) \quad (55)$$

where $\epsilon = \lambda^2 + |q|^{\frac{1}{2}} + |q|^{-\frac{1}{2}}$. We can extract the main x dependent part out of $A(x, y, \zeta)$ as follows

$$A(x, y, \zeta) = B(x, y, \zeta) r^{y-x+1} \prod_{w=x}^y (1 + |\zeta q^w|^2), \quad (56)$$

where $r = (\epsilon + \sqrt{\epsilon^2 - 4})/2$. The quotient $B(x, y, \zeta)$ satisfies a useful recursion relation

$$B(x, y, \zeta) = \left(1 + \frac{1}{r^2}\right) B(x, y-1, \zeta) - \frac{1 - f(y + \log_{|q|} |\zeta|)}{r^2} B(x, y-2, \zeta), \quad (57)$$

where the function $f(x)$ is defined by

$$f(x) = \frac{(|q|^{\frac{1}{2}} - |q|^{-\frac{1}{2}})^2}{(|q|^{x-1} + |q|^{-x+1})(|q|^x + |q|^{-x})}. \quad (58)$$

The solution of this recursion relation is determined by the formally defined boundary condition $B(-L, -L-2, \zeta) = 0$ and $B(-L, -L-1, \zeta) = 1$. The one point function is represented in terms of the normalization function

$$\langle n_x \rangle_\zeta = \frac{\lambda^2 B(-L, x-1, \zeta) B(x+1, L, \zeta)}{r B(-L, L, \zeta)}, \quad (59)$$

for $x \in \Lambda_o$. The expression for $x \in \Lambda'$ is easily obtained also as a closed form but complicated. The recursion relation (57) enables us to estimate bounds for expectation values of several local operators in the domain wall ground states [12]. We find the following bounds for number density

$$\begin{aligned} 0 &< \frac{\lambda^2}{\sqrt{\epsilon^2 - 4}} - \langle n_x \rangle_\zeta < F(x, L, \zeta) && \text{if } x \in \Lambda_o \\ -F^-(x, L, \zeta) &< 1 - \frac{\lambda^2}{\sqrt{\epsilon^2 - 4}} - \langle n_x \rangle_\zeta < F^+(x, L, \zeta) && \text{if } x \in \Lambda' \end{aligned} \quad (60)$$

where $F(x, L, \zeta)$ and $F^\pm(x, L, \zeta)$ are strictly positive, and they consist of terms which decay exponentially as L or $|x + \log_{|q|} |\zeta| |$ become large. Then, the number density approaches to the asymptotic values $\lambda^2/\sqrt{\epsilon^2 - 4}$ for Λ_o or $1 - \lambda^2/\sqrt{\epsilon^2 - 4}$ for Λ' exponentially as x moves away from the site $-\log_{|q|} |\zeta|$. This fact ensures our conjecture that the number density is almost constant for Λ_o or Λ' respectively. We also find bounds

$$-F_1^-(x, y, L, \zeta) < \langle n_x n_y \rangle_\zeta - \langle n_x \rangle_\zeta \langle n_y \rangle_\zeta < F_1^+(x, y, L, \zeta) \quad (61)$$

where $F_1^\pm(x, y, L, \zeta)$ are positive and consist of terms which decay exponentially as L , $|x - y|$, $|x + \log_{|q|} |\zeta| |$ or $|y + \log_{|q|} |\zeta| |$ becomes large. This fact shows that electrons are localized, in other words $\Psi(\zeta)$ is a almost product state. The spin correlation functions are almost a product of two spin-one-point functions, and they satisfy the cluster property. Then, we expect that the ground state is a pure state in the infinite volume limit. In large λ limit, the spin correlation function is reduced to just a product of two one-point spin function. This property is the same as the domain wall ground state in XXZ model. We consider that our model is closely related to XXZ model if $q \in \mathbb{R}$.

To see the actual shape of the spin one point function, a numerical solution of the recursion relation (57) is useful in the one-dimensional model. We obtain the electron number density from this solution, then we calculate the spin one point function represented in the number density (51). We show the profile of the domain wall at $x = 0$ in Figure 2.

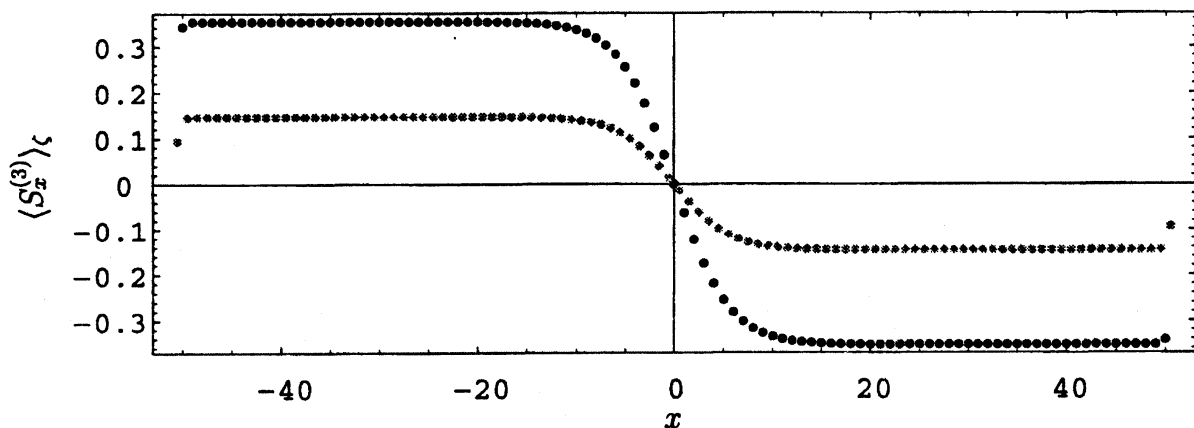


Figure 2: Spin one point function in the one-dimensional model calculated from the numerical solution of the recursion relation (57) for $L = 101$, $q = 1.2$, $\zeta = 1 (= q^0)$ and $\lambda = 2$. The black dots plot the spins on $x \in \Lambda_o$ and the gray dots plot the spins on $x \in \Lambda'$.

5 Summary

In this report, 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. We discuss similarity and difference of the domain wall solutions in our lattice electron model and quantum XXZ model. We proved these states satisfy the cluster property in a one-dimensional model. We expect that cluster property is satisfied in any dimensions, and therefore this curious structure should be stable in the infinite volume limit.

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