Exact bond-ordered ground states and excited states of the generalized Hubbard chain

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We discuss the exact bond-ordered ground states of the one-dimensional half-filled generalized Hubbard model including three- and four-body terms, by decomposing the Hamiltonian into positive semidefinite parts. The obtained exact ground states are interpreted as Néel ordered states on the bond-located electrons. We determine parameter regions of the exact ground states. We also calculate elementary excitation energies as variational approach based on the matrix-product formalism.

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I. INTRODUCTION

The Hubbard model is one of the generic models to describe interacting electrons in narrow-band systems.[1] This model has played central roles to study magnetism and superconductivity. In spite of its simplicity, however, it is difficult to solve this model exactly except for one dimension. On the other hand, many extensions of the Hubbard model have been considered. The on-site repulsion of this model is due to the matrix elements of the Coulomb interaction corresponding to the on-site Wannier states, and the other matrix elements are neglected. Therefore, we consider effects of these neglected terms as site-off-diagonal interactions.[2,3] Furthermore we may also extend the Hubbard model including three- and four-body terms. Especially, the three-body part is justified as an effective interaction of the three-band mode.[4] For these generalized Hubbard models [see below (1)], exact results for ferromagnetism and superconducting states have been discussed.[5–12]

A few years ago Itoh *et al.* discussed a different type of exact ground state in a one-dimensional (1D) system, "bond Néel" (BN) state which is interpreted as a Néel ordered state of the bond-located electrons.[13] On the other hand, from the bosonization theory, it was suggested the existence of the fixed point of the "bond-spin-density-wave" state in 1D systems with the SU(2) symmetry, which is a spin-density-wave state of the bond-located spins.[14] The BN state is regarded as the anisotropic version of this BSDW state in the analogy of the relation between the spin-fluid state and the Néel state of the spin-1/2 *XXZ* chain. Therefore, the exact result has a role to clarify the physical picture of the predicted bond-ordered state. This situation is similar to the Majumder-Gohsh model[15] and the Affleck-Kennedy-Lieb-Tasaki model[16] in quantum spin systems.

The technique to construct the model for this exact ground state is to decompose the Hamiltonian into the sum of products of the projection operators for two sectors.[17] In this way, each of the terms becomes positive semidefinite operators, due to the staggered dimer structure of the BN state.

However, in the preceding works,[13,18] the model is limited in the two-body interactions ($X'=P=Q=0$). Although some extensions to the three-body terms have been done,[19] strategy to construct the general model (1) has not been established. It has also been insufficient to describe the ferromagnetic state and the phase-separated state that appear in the neighboring regions of the BN state. In this paper, therefore, we extend the projection operator method for the BN and other states to the general bond Hamiltonians. Moreover, we discuss the elementally excited states of the BN state.

This paper is organized as follows: In Sec. II, we discuss the method to construct the Hamiltonian for the exact BN ground state, and obtain the phase diagram including the ferromagnetic state and the phase-separated state. In Sec. III, we calculate correlation functions of the BN state based on the matrix-product method. Here we point out the importance of the anticommutation relation of the fermions in the finite-size systems which was not taken into account in the preceding work.[13] In Sec. IV, we calculate elementally the excitation spectrum of the BN state as a variational approach. Finally, we give a summary and a discussion of the results.

II. EXACT GROUND STATE

We consider the generalized Hubbard chain including three- and four-body terms at half-filling and zero-magnetic field, given by $\mathcal{H}=\Sigma_{i\sigma}h_{i,i+1,\sigma}$ with the local bond Hamiltonian,[12]

$$\begin{aligned} h_{ij\sigma} = & -t\,T_{ij\sigma} - \frac{\mu}{2}(n_{i\sigma}+n_{j\sigma}) + \frac{U}{4}(n_{i\sigma}n_{i\bar{\sigma}}+n_{j\sigma}n_{j\bar{\sigma}}) + V_{\parallel}n_{i\sigma}n_{j\sigma} \\ & + V_{\perp}n_{i\sigma}n_{j\bar{\sigma}} + XT_{ij\sigma}(n_{i\bar{\sigma}}+n_{j\bar{\sigma}}) + X'T_{ij\sigma}n_{i\bar{\sigma}}n_{j\bar{\sigma}} \\ & + \sum_{\sigma'}\left(\frac{W}{2}T_{ij\sigma}T_{ij\sigma'} + \frac{P}{2}(n_{i\sigma}n_{i\bar{\sigma}}n_{j\sigma'}+n_{i\sigma'}n_{j\sigma}n_{j\bar{\sigma}})\right) \\ & + \frac{Q}{2}n_{i\sigma}n_{i\bar{\sigma}}n_{j\sigma}n_{j\bar{\sigma}}, \end{aligned} \tag{1}$$

with the hopping and the density operators,

$$T_{ij\sigma} = c_{i\sigma}^{\dagger}c_{j\sigma} + \mathrm{H.c.}, \tag{2}$$

$$n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}, \tag{3}$$

where $c_{i,\sigma}^{\dagger}$ and $c_{i,\sigma}$ are electron creation and annihilation operators on a 1D lattice with periodic boundary conditions, i and σ label position and spin of the electrons on the chain. $\bar{\sigma}$ denotes the opposite spin of σ. The spin-SU(2) symmetry is broken for $V_{\parallel} \neq V_{\perp}$. Note that the bond-bond interaction (W) term can be rewritten as

$$-2W\left(\mathbf{S}_i \cdot \mathbf{S}_j + \boldsymbol{\eta}_i \cdot \boldsymbol{\eta}_j - \tfrac{1}{4}\right). \tag{4}$$

Here $S_i^{\alpha} = \frac{1}{2} c_{i\sigma}^{\dagger} \tau_{\sigma\sigma'}^{\alpha} c_{i\sigma'}$ with τ^{α} being the Pauli matrices are the usual spin operators, and $\boldsymbol{\eta}_i$ denotes the η-pseudospin operator whose components are defined by

$$\eta_j^{+} = (-1)^j c_{j\uparrow}^{\dagger} c_{j\downarrow}^{\dagger}, \quad \eta_j^{-} = (-1)^j c_{j\downarrow} c_{j\uparrow}, \quad \eta_j^{z} = \tfrac{1}{2}(n_j - 1). \tag{5}$$

Now, we introduce the following bond operators:

$$A_{ij\sigma}^{\dagger} = \frac{1}{\sqrt{2}}(c_{i\sigma}^{\dagger} + c_{j\sigma}^{\dagger}), \quad B_{ij\sigma}^{\dagger} = \frac{1}{\sqrt{2}}(c_{i\sigma}^{\dagger} - c_{j\sigma}^{\dagger}). \tag{6}$$

These operators on the same bond satisfy the anticommutation relations

$$\{A_{ij\sigma}, A_{ij\sigma'}^{\dagger}\} = \{B_{ij\sigma}, B_{ij\sigma'}^{\dagger}\} = \delta_{\sigma\sigma'}, \quad \text{otherwise} = 0.$$

Using these operators, two electron states are described as

$$B_{ij\sigma}^{\dagger} A_{ij\sigma}^{\dagger} = c_{i\sigma}^{\dagger} c_{j\sigma}^{\dagger}. \tag{7}$$

Then the density operators for the bond operators and the original fermions are given by

$$n_{A\sigma} \equiv A_{ij\sigma}^{\dagger} A_{ij\sigma} = \tfrac{1}{2}(n_{i\sigma} + n_{j\sigma} + T_{ij\sigma}), \tag{8}$$

TABLE I. Projection operators used in this paper $\mathcal{Q}_{i\sigma}$. To project out the BN state, the minimum set of the operators are $\mathcal{Q}_{1\sigma}$, $\mathcal{Q}_{3\sigma}$, and $\mathcal{Q}_{4\sigma}$. $\mathcal{R}_{1\sigma}$ and $\mathcal{R}_{2\sigma}$ are projection operators used in Refs. 13 and 18. The number of free parameters become six in the former case, while three in the latter case.

		$\lvert 0\rangle$	$\lvert A_{\sigma}\rangle$	$\lvert B_{\sigma}\rangle$	$\lvert B_{\sigma}A_{\sigma}\rangle$
$\mathcal{Q}_{1\sigma}$	$(1-n_{A\sigma})(1-n_{B\sigma})$	1	0	0	0
$\mathcal{Q}_{2\sigma}$	$n_{A\sigma}(1-n_{B\sigma})$	0	1	0	0
$\mathcal{Q}_{3\sigma}$	$(1-n_{A\sigma})n_{B\sigma}$	0	0	1	0
$\mathcal{Q}_{4\sigma}$	$n_{A\sigma}n_{B\sigma}$	0	0	0	1
$\mathcal{R}_{1\sigma}$	$1-n_{A\sigma}$	1	0	1	0
$\mathcal{R}_{2\sigma}$	$n_{B\sigma}$	0	0	1	1

$$n_{B\sigma} \equiv B_{ij\sigma}^{\dagger} B_{ij\sigma} = \tfrac{1}{2}(n_{i\sigma} + n_{j\sigma} - T_{ij\sigma}), \tag{9}$$

$$n_{A\sigma} n_{B\sigma} = n_{i\sigma} n_{j\sigma}, \tag{10}$$

$$n_{i\sigma} = \tfrac{1}{2}(n_{A\sigma} + n_{B\sigma} + T_{AB\sigma}), \tag{11}$$

$$n_{j\sigma} = \tfrac{1}{2}(n_{A\sigma} + n_{B\sigma} - T_{AB\sigma}), \tag{12}$$

where $T_{AB\sigma} \equiv A_{ij\sigma}^{\dagger} B_{ij\sigma} + \text{H.c.}$ Since we restrict our attention only on the neighboring two sites i, j, we drop these indices from the operators defined above. Using these relations, the local Hamiltonian (1) is rewritten by the bond operators as follows:

$$\begin{aligned} h_{ij} = & -t\sum_{\sigma}(n_{A\sigma} - n_{B\sigma}) - \frac{\mu}{2}\sum_{\sigma}(n_{A\sigma} + n_{B\sigma}) + \frac{U}{4}(n_{A\uparrow}n_{A\downarrow} + n_{B\uparrow}n_{B\downarrow} + n_{A\uparrow}n_{B\downarrow} + n_{B\uparrow}n_{A\downarrow} + T_{AB\uparrow}T_{AB\downarrow}) + V_{\parallel}\sum_{\sigma} n_{A\sigma}n_{B\sigma} \\ & + \frac{V_{\perp}}{2}(n_{A\uparrow}n_{A\downarrow} + n_{B\uparrow}n_{B\downarrow} + n_{A\uparrow}n_{B\downarrow} + n_{B\uparrow}n_{A\downarrow} - T_{AB\uparrow}T_{AB\downarrow}) + W(n_{A\uparrow}n_{A\downarrow} + n_{B\uparrow}n_{B\downarrow} - n_{A\uparrow}n_{B\downarrow} - n_{B\uparrow}n_{A\downarrow}) \\ & + \frac{W}{2}\sum_{\sigma}(n_{A\sigma} + n_{B\sigma} - 2n_{A\sigma}n_{B\sigma}) + 2X(n_{A\uparrow}n_{A\downarrow} - n_{B\uparrow}n_{B\downarrow}) + X'\sum_{\sigma}(n_{A\sigma} - n_{B\sigma})n_{A\bar{\sigma}}n_{B\bar{\sigma}} \\ & + P\sum_{\sigma}(n_{A\sigma} + n_{B\sigma})n_{A\bar{\sigma}}n_{B\bar{\sigma}} + Qn_{A\uparrow}n_{B\uparrow}n_{A\downarrow}n_{B\downarrow}. \end{aligned} \tag{13}$$

In order to discuss exact ground states, the local Hamiltonian must be brought to the following form:

$$h_{ij} - (\varepsilon_0 - \mu) = \sum_{\alpha\beta} \lambda_{\alpha\beta} \mathcal{Q}_{\alpha\uparrow} \mathcal{Q}_{\beta\downarrow}, \tag{14}$$

where ε_0 is the ground state energy per site. $\mathcal{Q}_{\alpha\sigma}$ is a positive semidefinite projection operator, and the coefficients $\lambda_{\alpha\beta}$ are real and symmetric $\lambda_{\alpha\beta} = \lambda_{\beta\alpha}$ reflecting the spin-reversal symmetry. The left-hand side of Eq. (14) is also positive semidefinite when $\lambda_{\alpha\beta} > 0$. Since there exist four states in each bond for each spin sector, we introduce four projection operators as summarized in Table I, satisfying $\Sigma_{\alpha=1}^{4} \mathcal{Q}_{\alpha\sigma} = 1$. Therefore, the number of independent projection operators for the state $\lvert A_{\sigma}\rangle$ are three for each sector, so that there are six free parameters. On the other hand, in the preceding paper,[13,18] a Hamiltonian (1) with $X' = P = Q = 0$ has been

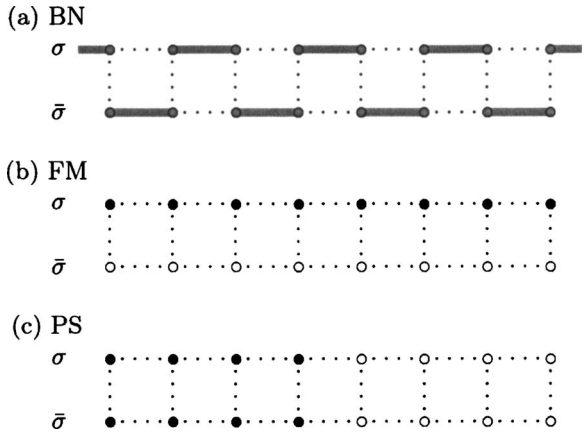

FIG. 1. Three states at half-filling described by the present projection operator method, (a) bond-Néel (BN), (b) ferromagnetic (FM), and (c) phase separated (PS) states.

constructed by two projection operators $1-n_{A\sigma}$ and $n_{B\sigma}$, however, this choice is not sufficient to treat arbitrary bond Hamiltonians, because the number of free parameters are three.

Here we mention relations between projection operators and some unitary transformations. It is well known that roles of the spin operators and the η operators (5) are interchanged by the following canonical transformation:

$$c_{j\uparrow} \to c_{j\uparrow}, \quad c_{j\downarrow} \to (-1)^j c_{j\downarrow}^\dagger. \tag{15}$$

This charge-spin transformation (15) gives $\mathcal{Q}_{1\downarrow} \leftrightarrow \mathcal{Q}_{4\downarrow}$, so that this transformation partly exchanges diagonal and off-diagonal elements of $\lambda_{\alpha\beta}$. Moreover the particle-hole transformation and the staggered phase transformation,

$$c_{j\sigma} \leftrightarrow (-1)^j c_{j\sigma}^\dagger, \tag{16}$$

$$c_{j\sigma} \leftrightarrow (-1)^j c_{j\sigma}, \tag{17}$$

give $\mathcal{Q}_{1\sigma} \leftrightarrow \mathcal{Q}_{4\sigma}$ and $\mathcal{Q}_{2\sigma} \leftrightarrow \mathcal{Q}_{3\sigma}$, respectively.

A. Bond Néel state

We consider the bond Néel wave function given by

$$|\mathrm{BN}_\sigma\rangle \equiv \prod_{m=1}^{L/2} A_{2m-1,2m,\sigma}^\dagger A_{2m,2m+1,\bar{\sigma}}^\dagger |0\rangle, \tag{18}$$

where $|0\rangle$ denotes a vacuum. In order to have the above state as the exact ground state, the Hamiltonian should be decomposed as in Eq. (14) with the parameters satisfying the following conditions:

$$\lambda_{11}, \lambda_{33}, \lambda_{44}, \lambda_{13}, \lambda_{14}, \lambda_{34} \geqslant 0, \quad \text{otherwise} = 0. \tag{19}$$

Due to the staggered dimer structure of the BN state as shown in Fig. 1(a), the positive semidefinite operator (14) gives 0. Therefore, Eq. (18) gives the exact ground state. Note that the projection operator for $|A_\sigma\rangle$ state $1-\mathcal{Q}_{2\sigma}$ is not needed, because it depends on the other three operators. Then one can find relations among the parameters of the model as

$$V_\perp = \frac{U}{2}, \quad V_\parallel = W - X' - P, \quad X = t - W,$$

$$\varepsilon_0 = \frac{U}{2}, \quad \mu = 2t + U - W, \tag{20}$$

and the coefficients are identified as

$$\lambda_{11} = 2t + \frac{U}{2} - W, \tag{21}$$

$$\lambda_{33} = 4W, \tag{22}$$

$$\lambda_{44} = -2t + \frac{U}{2} + 3W - 2X' + 2P + Q, \tag{23}$$

$$\lambda_{13} = 2t, \tag{24}$$

$$\lambda_{14} = -\frac{U}{2} + W - X' - P, \tag{25}$$

$$\lambda_{34} = -2t + 4W - 2X'. \tag{26}$$

Therefore, the parameter space of the exact BN ground state is given by the following six conditions:

$$t \geqslant 0, \quad W \geqslant 0, \quad W \geqslant \frac{t}{2} + \frac{X'}{2},$$

$$W \leqslant 2t + \frac{U}{2}, \quad W \geqslant \frac{U}{2} + X' + P,$$

$$W \geqslant \frac{2}{3}t - \frac{U}{6} + \frac{2}{3}X' - \frac{2}{3}P - \frac{1}{3}Q. \tag{27}$$

Thus we determine the BN regime in the U/t-W/t parameter space as is shown in Fig. 2. The lines surrounding the shaded regions do not necessarily mean the phase boundary. The three conditions of the BN state obtained in Refs. 13 and 18 for $X'=P=Q=0$ are identical with the last three conditions in Eqs. (27), while the first three conditions are implicit ones. However, these hidden conditions play essential roles to determine the regions of the ferromagnetic and the phase-separated states discussed below and the BN regions for finite X', P, Q. Especially at $X'/t=-1$ and $U=W=P=Q=0$ ($\lambda_{33}=\lambda_{34}=\lambda_{44}=0$), the local Hamiltonian becomes

$$-t\sum_\sigma T_{ij\sigma}(1-n_{i\bar{\sigma}})(1-n_{j\bar{\sigma}}), \tag{28}$$

which has the same eigenstates of the Hubbard model at $U=\infty$. Therefore, the BN ground state is highly degenerated.

We should also consider the possibility of the dual BN (DBN) ground state which is given by replacing $A_{ij\sigma}$ by $B_{ij\sigma}$ in the BN wave function,

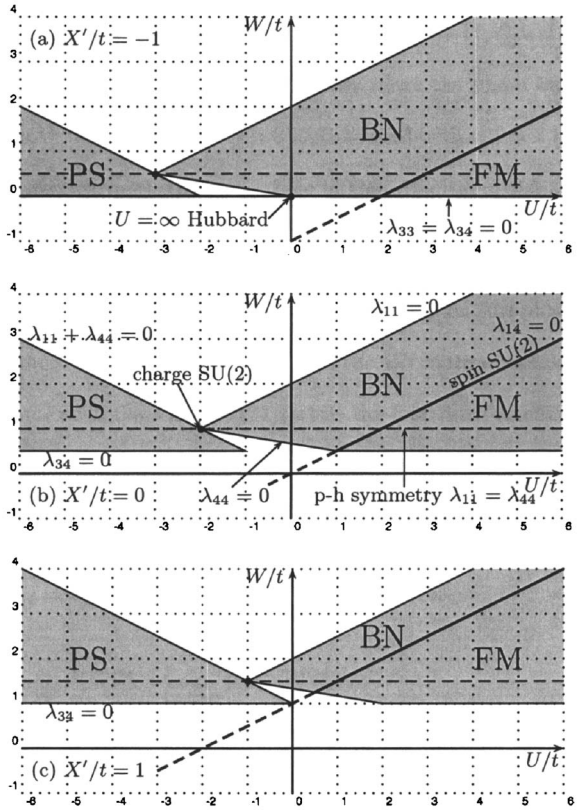

FIG. 2. Phase diagrams of the generalized Hubbard chain (1) with $P=Q=0$, in the U/t-W/t parameter space with $t>0$. The other parameters are set as $X=t-W$, $V_{\parallel}=W-X'-P$, and $V_{\perp}=U/2$. BN, FM, and PS denote bond-Néel, ferromagnetic, and phase-separated states, respectively. $\lambda_{14}=0$ corresponds to the spin SU(2) symmetry. Intersection of the particle-hole symmetric line ($\lambda_{11}=\lambda_{44}$, $\lambda_{13}=\lambda_{34}$) and the line for the PS state ($\lambda_{11}+\lambda_{44}=0$) gives the SU(2) symmetric point of the η-pseudospin. The three phases do not appear in the negative-W regions due to the condition $\lambda_{33}>0$.

$$|\mathrm{DBN}_{\sigma}\rangle \equiv \prod_{m=1}^{L/2} B^{\dagger}_{2m-1,2m,\sigma} B^{\dagger}_{2m,2m+1,\bar{\sigma}}|0\rangle. \tag{29}$$

The corresponding decomposed Hamiltonian of the DBN ground state is that of the BN state replacing the projection operators as $\mathcal{Q}_{2\sigma}\leftrightarrow\mathcal{Q}_{3\sigma}$. Then the condition of the DBN state is obtained by the phase transformation (17) which gives $A\leftrightarrow B$, $t\rightarrow -t$, $X\rightarrow -X$, $X'\rightarrow -X'$. Therefore, there is one-to-one correspondence between the BN state for $t>0$ and the DBN state for $t<0$, so that we only consider the parameter space with $t>0$. This situation is the same as that for the transformation of the exchange interactions in the Heisenberg model.

B. Ferromagnetism

We consider the fully polarized ferromagnetic (FM) ground state,

$$|\mathrm{FM}_{\sigma}\rangle \equiv \prod_{j=1}^{L} c^{\dagger}_{j\sigma}|0\rangle = \prod_{m=1}^{L/2} B^{\dagger}_{2m-1,2m,\sigma} A^{\dagger}_{2m-1,2m,\sigma}|0\rangle$$
$$= \prod_{m=1}^{L/2} B^{\dagger}_{2m,2m+1,\sigma} A^{\dagger}_{2m,2m+1,\sigma}|0\rangle. \tag{30}$$

The corresponding decomposed Hamiltonian is given by the same as that of the BN state (14) with (19), but the one condition is changed as

$$\lambda_{14}\geqslant 0 \rightarrow \lambda_{14}\leqslant 0. \tag{31}$$

Due to the structure of the FM state as shown in Fig. 1(b), the operator (14) takes the lowest eigenvalue for (30). Therefore, a first-order transition between the BN state and the FM state takes place at $\lambda_{14}=0$.

When $\lambda_{14}=0$, the spin degrees of freedom recover the SU(2) symmetry, $V_{\parallel}=V_{\perp}$. Then the total spin operators, $S^{\alpha}_{\mathrm{tot}}=\Sigma_i S^{\alpha}_i$ ($\alpha=+,-,z$), commute with the Hamiltonian. In this case, the BN state, and the states given by $(S^{\pm}_{\mathrm{tot}})^n|\mathrm{BN}_{\sigma}\rangle$ ($0\leqslant n\leqslant L/2$) and their linear combinations are degenerate. Therefore, this is a multicritical line where the ground state is highly degenerate.

C. Phase separation

We also consider the phase-separated (PS) state which has large degeneracy with order L,

$$|\mathrm{PS}\rangle \equiv \frac{1}{\sqrt{L}}\sum_{j=1}^{L} |\mathrm{PS}\rangle_j,$$

$$|\mathrm{PS}\rangle_j \equiv \prod_{m=j/2}^{j/2+L/4-1} \prod_{\sigma=\uparrow,\downarrow} B^{\dagger}_{2m,2m+1,\sigma} A^{\dagger}_{2m,2m+1,\sigma}|0\rangle. \tag{32}$$

In 1D systems, the surface energy for PS states is considered sufficiently small, so that we neglect the surface energy. Then the corresponding decomposed Hamiltonian is given by the same as that of the BN state (14) with (19), except for the following two conditions:

$$\lambda_{11},\lambda_{44}\geqslant 0 \rightarrow \lambda_{11}+\lambda_{44}\leqslant 0. \tag{33}$$

Then due to the structure of the PS state as shown in Fig. 1(c), the operator (14) takes the lowest eigenvalue for (32).

The line of $\lambda_{11}+\lambda_{44}=0$ is related to the BN-FM boundary by the charge-spin transformation (15), which interchanges the projection operators as $\mathcal{Q}_{1\downarrow}\leftrightarrow\mathcal{Q}_{4\downarrow}$. On the other hand, it follows from Eq. (16) that the conditions

$$\lambda_{11}=\lambda_{44}, \quad \lambda_{13}=\lambda_{34}, \tag{34}$$

which give $W=X'/2+t$ with $2P+Q=0$ denote the particle-hole symmetry. The crossing point of the particle-hole symmetric line and the line of $\lambda_{11}+\lambda_{44}=0$ corresponds to the SU(2) symmetry of the η-pseudospin operators. At this point, the η-pairing operator $\eta^{\alpha}_{\mathrm{tot}}\equiv\Sigma_i\eta^{\alpha}_i$ commutes with the Hamiltonian. Therefore, similar to the $\lambda_{14}=0$ line, the states $(\eta^{\pm}_{\mathrm{tot}})^n|\mathrm{BN}_{\sigma}\rangle$ ($0\leqslant n\leqslant L/2$) which includes the η-pairing state, and their linear combinations are degenerate with the

ground states. Therefore, the intersection of these two lines is a multicritical point where the ground state is highly degenerate.

As shown in Fig. 2, the FM and the PS states appear in the U/t-W/t parameter space with $W/t>0$ almost symmetrically in the positive- and in the negative-U regions, respectively. This is consistent with the fact that the W term is the ferromagnetic exchange interactions of the spins and the pseudospins (4), and the PS state is regarded as the FM state of the pseudospin space.

III. CORRELATION FUNCTIONS

We calculate the correlation functions in the bond-Néel state using the matrix product method.[20,21] This method has been applied to spin ladder systems[22,23] and electron systems.[24–26] The present bond-Néel state is described as

$$|\mathrm{BN}_\sigma\rangle = 2^{-L/2}\,\mathrm{Tr}(\tau^z g_{1,\sigma} g_{2,\bar{\sigma}} \cdots g_{L-1,\sigma} g_{L,\bar{\sigma}}), \tag{35}$$

where

$$g_{i\sigma} \equiv \begin{pmatrix} c^\dagger_{i,\sigma} & c^\dagger_{i,\sigma} c^\dagger_{i,\bar{\sigma}} \\ 1 & c^\dagger_{i,\bar{\sigma}} \end{pmatrix} |0\rangle_i. \tag{36}$$

Since the matrix product $g_{i,\sigma} g_{j,\bar{\sigma}}$ creates the bond $A^\dagger_{ij\sigma}$ between ith and jth sites, $[h_{i,j}-(\varepsilon_0-\mu)]g_{i,\sigma}g_{j,\bar{\sigma}}=0$ is satisfied. Note that the Pauli matrix τ^z in (35) plays a role to cancel an additional negative sign reflecting the anticommutation relation of the fermions.[27] We also introduce 4×4 transfer matrices $G_{\sigma\sigma'} \equiv g^\dagger_{i\sigma} \otimes g_{i\sigma'}$. Here the tensor product $\otimes$ relates the matrix elements as $(G_{\sigma\sigma'})_{l_1 l_2} = ((g_{i\sigma})_{n_1 n_2})^\dagger (g_{i\sigma'})_{m_1 m_2}$, where $l_k=(n_k,m_k)$ and the indices correspond as $l_k = 1,2,3,4 \leftrightarrow (n_k,m_k)=(1,1),\ (1,\ 2),\ (2,\ 1),\ (2,\ 2)$, respectively.

First, we calculate the overlap integral of the wave functions $\langle \mathrm{BN}_\sigma | \mathrm{BN}_{\sigma'} \rangle$. For $\sigma=\sigma'$, the transfer matrix $G \equiv G_{\sigma\sigma}$ is calculated as

$$G = \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}, \tag{37}$$

and $(\tau^z g_{1\sigma})^\dagger \otimes (\tau^z g_{1\sigma}) = G$. Since $G^L = 2^{L-1} G$, the norm of the BN wave function becomes 1,

$$\langle \mathrm{BN}_\sigma | \mathrm{BN}_\sigma \rangle = 2^{-L}\,\mathrm{Tr}\, G^L = 1. \tag{38}$$

On the other hand, for $\sigma'=\bar{\sigma}$, we need the following transfer matrices:

$$G_{\uparrow\downarrow} = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \tag{39}$$

and $(\tau^z g_\uparrow)^\dagger \otimes (\tau^z g_\downarrow) = -(G_{\uparrow\downarrow})^3$, $(G_{\uparrow\downarrow})^4 = I$, where I is the identity matrix. We should note that a negative sign of $(G_{\uparrow\downarrow})_{14}$ stems from the anticommutation relation of the fermions. Due to this negative sign, the overlap integral in finite-size systems shows different properties for $L=4n$ and for $L=4n+2$ with n being an integer,

$$\langle \mathrm{BN}_\sigma | \mathrm{BN}_{\bar{\sigma}} \rangle = \begin{cases} -2^{-L}\,\mathrm{Tr}(G_{\uparrow\downarrow})^2 = 0 & (L=4n), \\ -2^{-L}\,\mathrm{Tr}\, I = -2^{2-L} & (L=4n+2). \end{cases} \tag{40}$$

In the thermodynamic limit, however, these two states are always orthogonal. This means that the BN ground state has twofold degeneracy due to the spontaneous breaking of the translational symmetry.

Next, we calculate the correlation functions as follows:[28]

$$\langle O_i O_j \rangle = 2^{-L}\,\mathrm{Tr}(g^\dagger_{i\alpha} \otimes O_i g_{i\alpha}) G^{j-i-1} (g^\dagger_{j\beta} \otimes O_j g_{j\beta}) G^{L-j+i-1}. \tag{41}$$

The charge-charge correlation function $O_i = n_i \equiv n_{i\uparrow} + n_{i\downarrow}$ is obtained as

$$\langle n_i n_{i+1} \rangle = \tfrac{3}{4}. \tag{42}$$

For $|i-j| \geqslant 2$, $\langle n_i n_j \rangle = 1$ and $\langle n_i \rangle = 1$, so that we obtain

$$\langle n_i n_j \rangle - \langle n_i \rangle \langle n_j \rangle = 0. \tag{43}$$

The spin-spin correlation functions are

$$\langle S^z_i S^z_{i+1} \rangle = -\tfrac{1}{16}, \tag{44}$$

$$\langle S^\pm_i S^\mp_{i+1} \rangle = 0. \tag{45}$$

For $|i-j| \geqslant 2$, we obtain

$$\langle S^z_i S^z_j \rangle = 0. \tag{46}$$

These results indicate that there is a finite energy gap between the ground state and the excited states with respect to site-located charges and spins.

The bond-bond correlation function is given by

$$\begin{aligned} &\langle T_{i,i+1,\sigma} T_{j,j+1,\sigma'} \rangle \\ &\quad = 2^{-L}\,\mathrm{Tr}[(g_{i,\alpha} g_{i+1,\bar{\alpha}})^\dagger \otimes T_{i,i+1,\sigma} g_{i,\alpha} g_{i+1,\bar{\alpha}}] G^{j-i-2} \\ &\qquad \times [(g_{j,\beta} g_{j+1,\bar{\beta}})^\dagger \otimes T_{j,j+1,\sigma'} g_{j,\beta} g_{j+1,\bar{\beta}}] \\ &\qquad \times G^{L-j+i-2} = \frac{1 \pm (-1)^{|j-i|}}{2}, \end{aligned}$$

where the upper and the lower signs denote the cases for $\sigma'=\sigma$ and $\sigma'=-\sigma$, respectively. The order parameter of the bond-spin-density wave (BSDW) is defined by

$$O^\alpha_i \equiv \frac{1}{2}(-1)^i \sum_{\sigma,\sigma'} (c^\dagger_{i,\sigma} \tau^\alpha_{\sigma,\sigma'} c_{i+1,\sigma'} + c^\dagger_{i+1,\sigma} \tau^\alpha_{\sigma,\sigma'} c_{i,\sigma'}). \tag{47}$$

We calculate the correlation function of the z component of the BSDW operator as

$$\langle O^z_i O^z_j \rangle = \tfrac{1}{64}. \tag{48}$$

The z component of the BSDW order parameter is obtained as

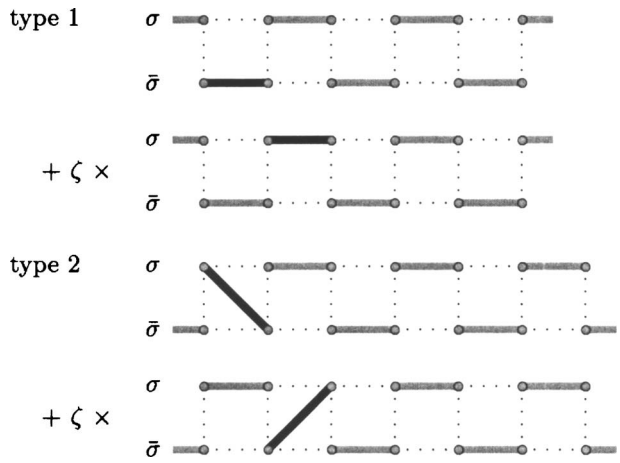

FIG. 3. Variational states for the elementary excited states in even and odd site systems.

$$\langle O_i^z \rangle = \pm \tfrac{1}{2}, \tag{49}$$

so that the system shows the BN long range order. The BSDW-z order corresponds to the Néel order of the bond-located spins.

IV. ELEMENTARY EXCITATIONS

In this section, we consider elementary excited states as variational wave functions with a soliton pair in the bond-Néel state following the approach for spin ladder systems by Kolezhuk and Mikeska.[23] We consider the variational states as the matrix product state where defects are inserted. To describe these excitations, we introduce a variational parameter ζ and momentum p ($\in[0,\pi]$). Now we consider the following two cases as shown in Fig. 3.

Type 1: The BN state with even number of sites $2N$ where a defect is inserted in one spin sector,

$$|\Psi_{1,\alpha}\rangle \equiv \sum_{n=2}^{N-1} \mathrm{e}^{\mathrm{i}p(2n+1)}|n\rangle,$$

$$|n\rangle = \left(\prod_{i=1}^{n-1} g_{2i-1}^{\sigma} g_{2i}^{\bar{\sigma}}\right)(\tau^{\alpha} g_{2n-1}^{\sigma} g_{2n}^{\bar{\sigma}} + \zeta g_{2n-1}^{\sigma} \tau^{\alpha} g_{2n}^{\bar{\sigma}}) \times \left(\prod_{i=n+1}^{N} g_{2i-1}^{\sigma} g_{2i}^{\bar{\sigma}}\right), \tag{50}$$

where $\tau^{\alpha}=\tau^{z}$, τ^{+}, τ^{-} corresponding to insertion of defects, $(1/\sqrt{2})(c_{i\sigma}^{\dagger}-c_{j\sigma}^{\dagger})$, $c_{i\sigma}^{\dagger}c_{j\sigma}^{\dagger}$, and 1, respectively.

Type 2: The BN state with odd number of sites $2N+1$ where a defect connecting different spin sectors is inserted,

$$|\Psi_{2,\alpha}\rangle \equiv \sum_{n=1}^{N-1} \mathrm{e}^{\mathrm{i}p(2n+1)}|n\rangle,$$

$$|n\rangle = \left(\prod_{i=1}^{n} g_{2i-1}^{\sigma} g_{2i}^{\bar{\sigma}}\right)(\tau^{\alpha} g_{2n+1}^{\bar{\sigma}} + \zeta g_{2n+1}^{\sigma} \tau^{\alpha})\left(\prod_{i=n+1}^{N} g_{2i}^{\sigma} g_{2i+1}^{\bar{\sigma}}\right), \tag{51}$$

where $\tau^{\alpha}=\tau^{0}$, τ^{z}, τ^{+}, τ^{-} corresponding to insertion of defects, $(c_{i\sigma}^{\dagger}+c_{j\bar{\sigma}}^{\dagger})/\sqrt{2}$, $(c_{i\sigma}^{\dagger}-c_{j\bar{\sigma}}^{\dagger})/\sqrt{2}$, $c_{i\sigma}^{\dagger}c_{j\bar{\sigma}}^{\dagger}$, and 1, respectively. τ^{0} is the 2×2 identity matrix.

Since the bond-Néel ground state has two-site periodicity due to the spontaneous breaking of the translational symmetry, we need a linear combination of two terms with a variational parameter $\zeta=\pm 1$. Note that we only consider one of the two degenerate states due to the orthogonality in the thermodynamic limit (40). We should also note that, for the type 2, we need two solitons to satisfy the consistency with the periodic boundary conditions.

The excitation energy $\varepsilon_{\nu,\alpha}(p)$ is expressed as

$$\varepsilon_{\nu,\alpha}(p) = \frac{\langle \Psi_{\nu,\alpha}| \sum (h_{i,i+1} - \varepsilon_0 + \mu)|\Psi_{\nu,\alpha}\rangle}{\langle \Psi_{\nu,\alpha}|\Psi_{\nu,\alpha}\rangle}. \tag{52}$$

We consider the case $X'=P=Q=0$ for simplicity. After long but straightforward calculations, we obtain the following results:

$$\varepsilon_{1,z}(p) = 2W, \tag{53}$$

$$\varepsilon_{1,\pm}(p) = \tfrac{1}{2}[3W - t \mp (t-W)], \tag{54}$$

$$\varepsilon_{2,0}(p) = \frac{8W-U}{120}(8\cos 2p + 17) - \zeta(t-W)\frac{7-2\cos 2p}{30}, \tag{55}$$

$$\varepsilon_{2,z}(p) = \frac{8W-U}{120}(8\cos 2p + 17) + \zeta(t-W)\frac{\cos 2p + 1}{3}, \tag{56}$$

$$\varepsilon_{2,\pm}(p) = \frac{\{U + 8W + \zeta[W \pm (W-t)]\}(17 - 8\cos 2p) \mp 2(t-W)(4+5\zeta)(4\cos 2p - 1)}{24[5 + 2\zeta(1+\cos 2p)]}, \tag{57}$$

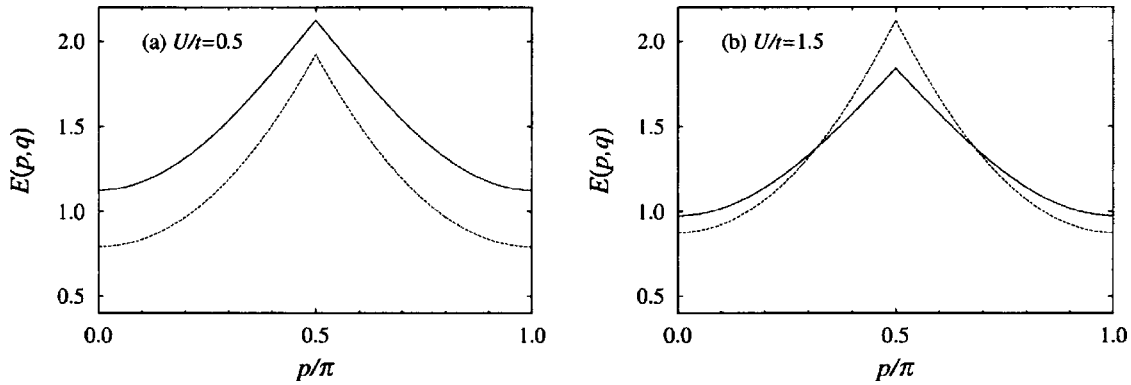

FIG. 4. Dispersion curves which give the upper bound of the bottom of the continuum (lower one of these two lines at each p) at $W=t$ for (a) $U/t=0.5$, (b) $U/t=1.5$. The solid and dashed lines are Eq. (58) for $(\alpha,\alpha')=(\pm,\mp)$, and for (0,0), respectively.

where the parameter ζ is determined according to the variational principle. We should choose $\zeta=\mathrm{sign}(t-W)$ for Eq. (55), and $\zeta=-\mathrm{sign}(t-W)$ for Eq. (56). The excitation spectra of type 1 turn out to be dispersionless. For simplicity, we consider the particle-hole symmetric case $W=t$. Then $\varepsilon_{2,0}(p)$ and $\varepsilon_{2,z}(p)$ are degenerate, and other two independent dispersion relations are $\varepsilon_{2,\pm}(p)/t$ with $\zeta=+1$ and $\varepsilon_{2,\pm}(p)/t$ with $\zeta=-1$.

Furthermore, we consider two-soliton excited states assuming that two defects do not interact,

$$E(p,q)=\varepsilon_{2,\alpha}((p+q)/2)+\varepsilon_{2,\alpha'}((p-q)/2). \tag{58}$$

Here, $p(\in[0,\pi])$ and $q(\in[0,\pi])$ are the total and the relative momenta, respectively. Due to the conservation of the electron number, we consider states $\varepsilon_{\nu,+}$ and $\varepsilon_{\nu,-}$ as a set. When $W=t$, the flat dispersion relations $\varepsilon_{1,z}$ and $\varepsilon_{1,+}+\varepsilon_{1,-}$ are degenerate, and they are not the lowest ones. We show the numerical data of excitations (58) for $(\alpha,\alpha')=(\pm,\mp)$ and for (0,0) at $U/t=0.5$ and at 1.5 in Fig. 4. The lower one of these dispersion relations gives the upper bound of the bottom of the continuum. In this region, we do not consider $\varepsilon_{2,\pm}(p)/t$ with $\zeta=-1$, because this gives always higher energies than that with $\zeta=+1$. The two dispersions cross depending on U/t. As is discussed in Sec. II, there are many degenerated states with the BN ground state near the BN-FM phase boundary or the charge SU(2) point. Therefore, we should also consider other excited states in these regions.

V. SUMMARY AND DISCUSSION

We have discussed an exact bond-ordered ground state of the generalized Hubbard chain including the site-off-diagonal interactions using the projection operator method. This state is regarded as a Néel ordering of bond-located spins, so that we call this bond Néel state. By changing the choice of the projection operators, we have extended the argument in Refs. 13 and 18, and constructed the models including three- and four-body terms. These ground states have twofold degeneracy, but the uniqueness has not been proven yet. This approach enables us to determine not only the BN region but also the ferromagnetic and the phase-separated regions. It is also useful to clarify the symmetry properties of the system. Moreover, we have calculated the excitation spectra as a variational approach based on the matrix product formalism.

The present BN state in the generalized Hubbard model corresponds to the staggered dimer state in the spin-$\frac{1}{2}$ two-leg ladder model with four spin exchanges.[23] In Refs. 23 and 26, the Hamiltonian is constructed based on more general argument. Comparing with the way to decompose the Hamiltonian to the projection operators in this approach, the present argument is quite simple. This is because the present BN state is given by direct product of bond operator for different spin sectors, and the model does not include hopping terms between different spin sectors.

This simplicity of the method is useful when we construct the Hamiltonian in higher dimensional systems. As is pointed out and demonstrated in the preceding works,[13,18] we can extend the present discussion to the Kagomé and the Checkerbord lattices in two dimensions and the Pyrochlore lattice in three dimensions, if we replace the bonds of this argument by plaquettes. These states are regarded as Néel ordered states on the dual lattices.

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[27] In Ref. 13, effect of the anticommutation relation of fermions is not taken into account. This gives a difference in the result of the finite-size systems such as Eq. (40).
[28] Result in Ref. 13 corresponding to Eqs. (42), (44), (48), and (49) should be corrected.