

One-dimensional model for doubly degenerate electrons

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A Hubbard-like model with SU(4) symmetry for electrons with twofold orbital degeneracy is studied extensively. Exact solution in one dimension is derived by means of Bethe ansatz, where the sites are supposed to be occupied by at most two electrons. The features of ground state and excited states for repulsive coupling are shown. For finite N number of electrons, the configurations of quantum numbers are given explicitly and the spectra of excitations are obtained by solving Bethe-ansatz equation numerically. For infinite N , the ground state and various kinds of low-lying excitations are obtained on the basis of thermodynamics limit.

I. INTRODUCTION

There has been much interests in the studies on correlated electrons in the presence of orbital degree of freedom. The orbital degree of freedom is relevant to many transitional-metal oxides.¹⁻⁵ It may be also relevant to some C₆₀ materials⁶ and samples of artificial quantum dot arrays.⁷ For a theoretical understanding of the observed unusual properties, a SU(4) theory describing spin systems with orbital degeneracy was proposed.^{8,9} There were also numerical¹⁰ and perturbative¹¹ studies of one-dimensional models for these systems. The ground-state phase diagrams for the system with a symmetry breaking of SU(4)→SU(2)×SU(2) were discussed.^{11,12} The phase separation was recently¹³ observed in experiment. Along with the rapid developments in experiments where the metal ions has orbital degeneracy in addition to spin degeneracy, a theoretical study of such system by taking account of the kinetic terms caused by nearest neighbor hopping becomes important. In a recent letter¹⁴ the Hubbard model for electrons with orbital degeneracy was studied. It was shown that the model not only has an underlying SU(4) symmetry of spin-orbital double but also has a hidden charge SU(4) symmetry. An extended Lieb-Mattis transformation which maps those two SU(4) generators into each other is given. On the basis of elementary degenerate perturbative theory, it was shown that the effective Hamiltonian with strong repulsive coupling at half-filling is equivalent to the Hamiltonian of the SO(6) Heisenberg model, and that at quarter-filling is equivalent to the one of SU(4) Heisenberg model. Some features of the model in one dimension was also briefly described.

In present paper, we study the one-dimensional Hubbard-like model with SU(4) symmetry for electrons with twofold orbital degeneracy extensively. Its exact solution is formulated by means of the Bethe ansatz if sites are assumed to be occupied by at most two electrons. The features of the ground state and excited states for repulsive coupling are shown. For finite N number of electrons, the configurations of quantum numbers are given explicitly and the spectra of excitations are obtained by solving the Bethe-ansatz equation numerically. For infinite N , the ground state and various kinds of low-lying excitations are obtained on the basis of thermodynamics limit.

The paper is organized as follows. In next section we

propose the model Hamiltonian with some interpretative remarks. Employing standard method we carefully formulated the first quantized version of the Hamiltonian. We make an allowed modification so that the Bethe-Yang ansatz^{15,16} is applicable to this model. A detailed formulation from the Bethe-ansatz wave function to the Bethe-ansatz equation is given. In Sec. III, we explicitly show how the quantum numbers in the Bethe-ansatz equation should be taken for the nondegenerated ground state. We calculate the ground-state energy and Fermi momentum numerically for different numbers of electrons. We also compare them for different coupling constants. In Sec. IV, we study the excited states extensively by analyzing the possible variations in the sequence of quantum numbers. We indicate in each case how the quantum numbers change from integers to half-integers (or vice versa) with respect to that of the ground state. Numerical results of energy-momentum spectra for each excitation are given there. In Sec. V, two special cases, weak and strong coupling, are discussed. We are able to deduce several interesting properties from the Bethe-ansatz equation without solving it directly. In Sec. VI, we consider the thermodynamics limit. After giving some general formulas and expressions, we study the ground state and calculate the ground-state energy explicitly for strong coupling. In Sec. VII, we discuss low-lying excitations in the spin-orbital sector on the basis of thermodynamics limit. Both contributions of holes and two-strings¹⁷ are taken into account. The singlet excitation and several multiplet excitations are obtained. In Sec. VIII, we discuss low-lying excitations in charge sector by thermodynamics limit. The holon-antiholon and holon-holon excitations are obtained. Section IX is a summary of the main results of the paper and some conclusive discussions.

II. THE MODEL AND ITS EXACT SOLUTION

We consider a Hubbard-like model for electrons with twofold orbital degeneracy. The spin components are denoted by up (\uparrow) and down (\downarrow), the orbital components by top and bottom. The four possible states of electrons are

$$\begin{aligned} |1\rangle &= \begin{vmatrix} \uparrow \\ - \end{vmatrix}, & |2\rangle &= \begin{vmatrix} \downarrow \\ - \end{vmatrix}, \\ |3\rangle &= \begin{vmatrix} - \\ \uparrow \end{vmatrix}, & |4\rangle &= \begin{vmatrix} - \\ \downarrow \end{vmatrix}. \end{aligned} \quad (1)$$

We use 1, 2, 3, and 4 to label these states from now on. The model Hamiltonian then reads

$$H = -t \sum_{i,a} (C_{i,a}^\dagger C_{i+1,a} + C_{i+1,a}^\dagger C_{i,a}) + U \sum_{i,a < a'} n_{i,a} n_{i,a'}, \quad (2)$$

where $i = 1, 2, \dots, L$ identify the lattice site, $a, a' = 1, 2, 3, 4$ specify the spin and orbital as defined in the above. The C_{ia}^\dagger creates an electron with spin-orbital component a on site i , and $n_{ia} := C_{ia}^\dagger C_{ia}$ is the corresponding number operator on site i . Equation (2) is the Hamiltonian for four-component systems, and there were various discussions on the multicomponent Hubbard model in one dimension.^{18–22} However, the physics that Eq. (2) describes will be precise only when the representation space for the internal degree of freedom is specified.¹⁴ It is specified to the spin and orbital, and the site is assumed to be occupied by at most two electrons in our present model.

It is convenient to consider the states that span the Hilbert space of N particles:

$$|\psi\rangle = \sum_{\{a_j\}, \{x_j\}} \psi_{a_1, \dots, a_N}(x_1, \dots, x_N) C_{x_1 a_1}^\dagger \dots C_{x_N a_N}^\dagger |0\rangle.$$

where $x_j \in \{1, 2, \dots, L\}$, $a_j \in \{1, 2, 3, 4\}$, and $j = 1, 2, \dots, N$. The eigenvalue problem $H|\psi\rangle = E|\psi\rangle$ becomes an N -particle quantum-mechanical problem with the first quantized Schrödinger operator (Hamiltonian),

$$\mathcal{H} = -t \sum_{j=1}^N \Delta_j + \frac{U}{2} \sum_{i < j} (1 - \delta_{a_i, a_j}) \delta(x_i, x_j), \quad (3)$$

if site occupations of more than two electrons are excluded,²³ where $\Delta_j \psi := \psi(\dots, x_j + 1, \dots) + \psi(\dots, x_j - 1, \dots)$.

The wave function of Bethe ansatz form in the region $x \in \mathcal{C}(Q) := \{x | 1 \leq x_{Q1} < \dots < x_{QN} \leq L\}$ reads

$$\psi_a(x) = \sum_{P \in S_N} A_a(P, Q) e^{i(Pk|x)}, \quad (4)$$

where $x = (x_1, x_2, \dots, x_N)$, $a := (a_1, a_2, \dots, a_N)$, a_j stands for the spin-orbital component of the j th particle; Pk is the image of a given $k := (k_1, k_2, \dots, k_N)$ by a mapping $P \in S_N$; S_N denotes the permutation group of N objects; $(Pk|x) = \sum_{j=1}^N (Pk)_j(x)_j$. The coefficients $A(P, Q)$ are functionals on $S_N \otimes S_N$. We know that any permutations can always be expressed as the product of the neighboring interchanges $\Pi^j: (\dots, z_j, z_{j+1}, \dots) \mapsto (\dots, z_{j+1}, z_j, \dots)$. So the requirement of antisymmetry for fermionic permutation is $(\Pi^j \psi)_a(x) = -\psi_a(x)$, which gives

$$A(P, \Pi^j Q) = -\mathcal{P}^{Qj, Q(j+1)} A(\Pi^j P, Q), \quad (5)$$

where the spin-orbital labels are omitted and $\mathcal{P}^{Qj, Q(j+1)}$ is the SU(4) spinor representation of the permutation Π^j operator. An immediate consequence of Eq. (5) is $\delta_{a_i, a_j} \delta(x_j, x_i) \psi_a(x) = 0$, and hence we are allowed to consider, instead of Eq. (3), the following equivalent Schrödinger operator:

$$\mathcal{H} = -t \sum_{j=1}^N \Delta_j + U \sum_{i < j} \delta(x_i, x_j), \quad (6)$$

here the interaction terms are independent of the spin-orbital labels. Then the strategy of Refs. 15 and 24 can be used to solve the wave functions. The S matrix that relates the coefficients A 's between distinct regions in the configuration space of N electrons can be solved from the Schrödinger equation in the vicinity of hyperplane with $(Qx)_j = (Qx)_{j+1}$. Accordingly, we get

$$S^{Qj, Q(j+1)} = \frac{\sin(Pk)_{Qj} - \sin(Pk)_{Q(j+1)} + ic \mathcal{P}^{Qj, Q(j+1)}}{\sin(Pk)_{Qj} - \sin(Pk)_{Q(j+1)} + ic}, \quad (7)$$

where $2c = U/t$. As it satisfies Yang-Baxter equation,¹⁵ the Bethe-ansatz wave function is then consistently determined, i.e., the coefficients A 's in any region are determined up to an overall factor by the $\check{S}^{Qj, Q(j+1)} := -\mathcal{P}^{Qj, Q(j+1)} S^{Qj, Q(j+1)}$ and that in different regions are related by Eq. (5). If let $c \rightarrow \infty$ in Eq. (7), we know the wave function will be null if there are two k 's being the same value. So in the strong-coupling limit, the k 's must take distinct values though there can be four states corresponding to the same k_j in the absence of interaction.

The periodic boundary condition is guaranteed provided that $A(P, \gamma Q) e^{i(Pk)_1 L} = A(P, Q)$ in which $\gamma = \Pi^{N-1} \Pi^{N-2} \dots \Pi^2 \Pi^1$. After applying the S matrices successively, one obtains an eigenvalue equation in the SU(4) spinor space:

$$S^{Q1, QN} S^{Q1, Q(N-1)} \dots S^{Q1, Q2} A(P, Q) = e^{-i(Pk)_1 L} A(P, Q). \quad (8)$$

The eigenvalue problem (8) can be diagonalized by means of quantum inverse scattering method²⁵ by defining the transfer matrix as $t(\alpha) = \text{tr } \mathcal{T}(\alpha)$ where

$$\mathcal{T}(\alpha) = T_{AN}(\alpha - \alpha_N) \dots T_{A2}(\alpha - \alpha_2) T_{A1}(\alpha - \alpha_1),$$

$$T_{Aj}(\alpha) := S^{Aj}(\alpha) \in \text{End}(V^A \otimes V^j).$$

End means endomorphism. It can also be diagonalized by similar procedure as in Ref. 16, where the general case of the continuous model with a δ -function interaction was solved. The Bethe-ansatz equations reads

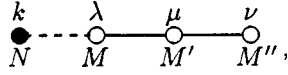
$$e^{ik_j L} = \prod_{\alpha=1}^M \Xi_{1/2}(\sin k_j - \lambda_\alpha),$$

$$1 = - \prod_{l=1}^N \Xi_{-1/2}(\lambda_\alpha - \sin k_l) \prod_{\alpha'=1}^M \Xi_1(\lambda_\alpha - \lambda_{\alpha'})$$

$$\times \prod_{\beta=1}^{M'} \Xi_{-1/2}(\lambda_\alpha - \mu_\beta),$$

$$\begin{aligned}
1 &= - \prod_{\alpha=1}^M \Xi_{-1/2}(\mu_{\beta} - \lambda_{\alpha}) \prod_{\beta'=1}^{M'} \Xi_1(\mu_{\beta} - \mu_{\beta'}) \\
&\times \prod_{\gamma=1}^{M''} \Xi_{-1/2}(\mu_{\beta} - \nu_{\gamma}), \\
1 &= - \prod_{\beta=1}^{M'} \Xi_{-1/2}(\nu_{\gamma} - \mu_{\beta}) \prod_{\gamma'=1}^{M''} \Xi_1(\nu_{\gamma} - \nu_{\gamma'}),
\end{aligned} \tag{9}$$

where $\Xi_n(x) := [x + inc]/[x - inc]$. Eq. (9) was given first in Ref. 19. Because a particular chemical potential was introduced in the Hamiltonian, the Bethe ansatz equation derived in Ref. 26 is the same as the SU(4) Heisenberg model.⁹ We write out the Bethe-ansatz equation in a form so that it is easy to be remembered by means of the ‘‘Dynkin diagram’’²⁷ of A_3 Lie algebra



where the dark dot is added to represent the charge rapidity k_j which also has an angle of 120° relative to the first simple root r_1 . The subscripts in Ξ in Eq. (9) are then related to the covariant components of the simple roots when the simple roots are chosen as nonorthogonal basis, accordingly, $r_1 = (-1/2, 1, -1/2, 0)$, $r_2 = (0, -1/2, 1, -1/2)$, $r_3 = (0, 0, -1/2, 1)$. The highest weight vector $\mathbf{w} = (w_1, w_2, w_3)$ labeling the representation of SU(4) carried out by the corresponding eigenstates is given by

$$\begin{aligned}
w_1 &= N - 2M + M', \\
w_2 &= M - 2M' + M'', \\
w_3 &= M' - 2M''.
\end{aligned} \tag{10}$$

A set of coupled transcendental equations are derived by taking the logarithm of Eq. (9),

$$\begin{aligned}
k_j + \frac{1}{L} \sum_{\alpha=1}^M \Theta_{-1/2}(\sin k_j - \lambda_{\alpha}) &= \frac{2\pi}{L} h_j, \\
\sum_{l=1}^N \Theta_{-1/2}(\lambda_{\alpha} - \sin k_l) + \sum_{\alpha'=1}^M \Theta_1(\lambda_{\alpha} - \lambda_{\alpha'}) \\
+ \sum_{\beta=1}^{M'} \Theta_{-1/2}(\lambda_{\alpha} - \mu_{\beta}) &= 2\pi I_{\alpha}, \\
\sum_{\alpha=1}^M \Theta_{-1/2}(\mu_{\beta} - \lambda_{\alpha}) + \sum_{\beta'=1}^{M'} \Theta_1(\mu_{\beta} - \mu_{\beta'}) \\
+ \sum_{\gamma=1}^{M''} \Theta_{-1/2}(\mu_{\beta} - \nu_{\gamma}) &= 2\pi J_{\beta}, \\
\sum_{\beta=1}^{M'} \Theta_{-1/2}(\nu_{\gamma} - \mu_{\beta}) + \sum_{\gamma'=1}^{M''} \Theta_1(\nu_{\gamma} - \nu_{\gamma'}) &= 2\pi K_{\gamma},
\end{aligned} \tag{11}$$

where $\Theta_n(x) := -2 \tan^{-1}(x/nc)$. The quantum number h_j for charge rapidity k_j takes integer or half-integer value depending on whether $M-1$ is odd or even. The quantum numbers I_{α} , J_{β} , or K_{γ} for flavor (we refer to the spin-orbital double) rapidities λ_{α} , μ_{β} , or ν_{γ} , take integer or half-integer values, respectively, depending on whether $N-M-M'$, $M-M'-M''$, or $M'-M''$ is odd or even. These properties arise from the logarithm function. Once the roots are solved from the above Eq. (11), the energy and momentum will be calculated by

$$\begin{aligned}
E &= -2t \sum_{j=1}^N \cos k_j, \\
P &= \frac{2\pi}{L} \left[\sum_{l=1}^N h_l + \sum_{\alpha=1}^M I_{\alpha} + \sum_{\beta=1}^{M'} J_{\beta} + \sum_{\gamma=1}^{M''} K_{\gamma} \right].
\end{aligned} \tag{12}$$

III. GROUND STATE

The ground state is nondegenerate only if $N=4n$ for n being odd numbers. This is easily seen by considering noninteracting case. The momentum eigenvalues (with periodic boundary condition) of noninteracting electrons are $k = m(2\pi/L)$, $m=0, \pm 1, \pm 2, \dots$. For example, $N=4n$ for $n=even$, the ground state has a 70-fold degeneracy. In the following we will restrict ourselves to the case of $N_0=4n$ for $n=odd$, and consider the nondegenerated ground state. The nondegenerated ground state is a SU(4) singlet, which is characterized by a four-row and n -column Young tableau. The quantum numbers in Eq. (11) for the ground state are

$$\begin{aligned}
\{h_j\} &= \{-(N_0-1)/2, \dots, (N_0-1)/2\}, \\
\{I_{\alpha}\} &= \{-(3N_0-4)/8, \dots, (3N_0-4)/8\}, \\
\{J_{\beta}\} &= \{-(N_0-2)/4, \dots, (N_0-2)/4\}, \\
\{K_{\gamma}\} &= \{-(N_0-4)/8, \dots, (N_0-4)/8\}.
\end{aligned} \tag{13}$$

Obviously, h 's and J 's are consecutive half-integers while I 's and K 's are consecutive integers. As a result of Eqs. (13) and (12), the momentum of the nondegenerate ground state is zero. We plot the ground-state energy with respect to the filling factor N/L for various coupling constant in Fig. 1. The relation between Fermi momentum and the filling factor for different coupling constant is also plotted there. These numerical results are calculated for $L=20$ and N from 4 to 40. For $N \rightarrow \infty$, we can take thermodynamics limit which will be discussed in Sec. VI. The ground state for $N=N_0+1$, $N=N_0+2$, etc., are degenerate about which we will discuss later.

IV. EXCITED STATES

A. Excitations above the nondegenerate ground state

The excited states are obtained by variation in the sequence of quantum numbers $\{h_j\}$, $\{I_{\alpha}\}$, $\{J_{\beta}\}$, or $\{K_{\gamma}\}$ from that for the ground state. The simplest case is to remove one of the h 's from the sequence of ground-state equation (13) and add a new h_0 outside of the original sequence, that is,

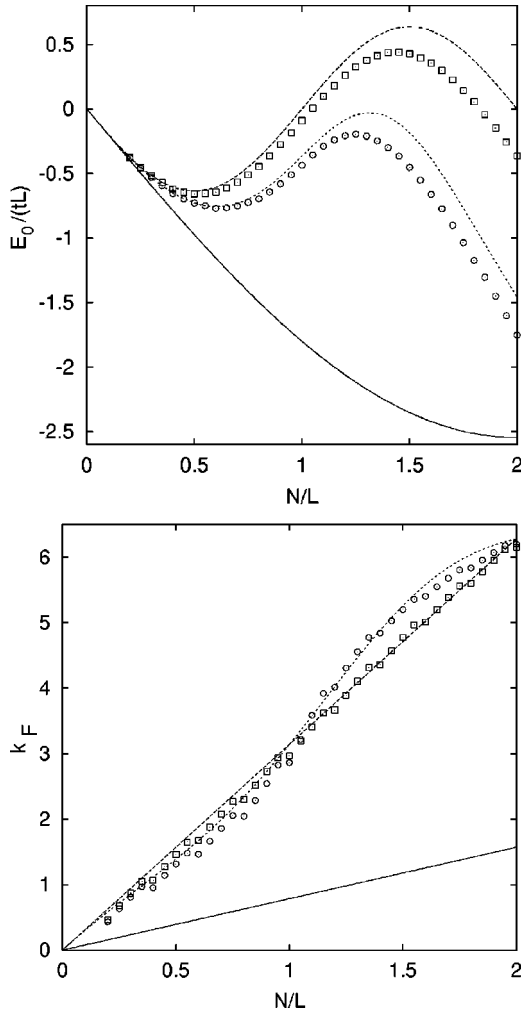


FIG. 1. The relations between filling factor N/L and ground-state energy E_0 (upper figure) or the Fermi momentum k_F (lower figure). The points are calculated with $U/t=10$ (\square) and $U/t=2$ (\circ) by taking N from 4 to 40 for $L=20$. Noninteracting case is plotted by solid lines. The other lines (dashed lines for $U/t=\infty$ and dotted lines for $U/t=10$) are plotted from the results of thermodynamics limit.

$$\{h_j\} = \left\{ -\frac{N_0-1}{2}, \dots, -\frac{N_0-1}{2} + n_0 - 1, -\frac{N_0-1}{2} + n_0 + 1, \dots, \frac{N_0-1}{2}, h_0 \right\}, \quad (14)$$

with $|h_0| > (N_0-1)/2$ and the other sequences in Eq. (13) keep unchanged. Clearly, the $(N_0-1)/2 + n_0$ is absent in the set (14). In Fig. 2, we plot the numerical results for energy-momentum spectrum, which is a two-parameter family of excitation. This kind of excitations are singlet states.

There are several further possibilities. After moving one box from the fourth row in the Young tableau of the ground state to the first row, we get a Young tableau labeling a 15-dimensional irreducible representation of $SU(4)$ according to the knowledge of group theory. It requires $M = 3N_0/4 - 1$, $M' = N_0/2 - 1$, and $M'' = N_0/4 - 1$. This causes the h 's and J 's to take integer values instead of half-integer values that were taken for ground state. There are now M allowed values for the $M-1$ distinct I 's, and M'' allowed

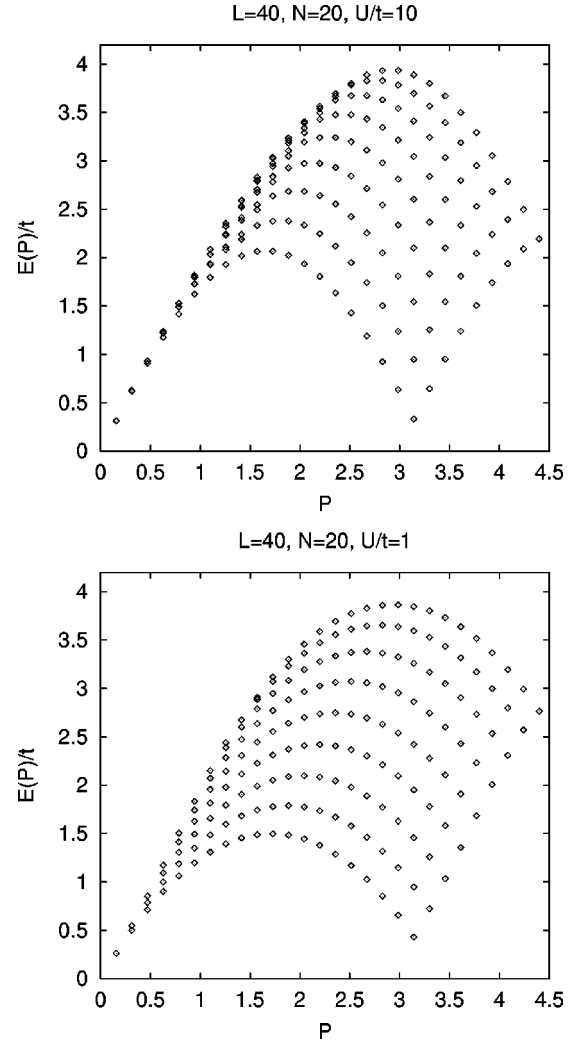


FIG. 2. "Particle"-hole excitation spectrum for the model of 40 sites with 20 electrons. The overall structure of the spectrum does not change much between the strong ($U/t=10$) and weak ($U/t=1$) correlation strengths.

values for the $M''-1$ distinct K 's. Consequently, holes in the I 's and K 's sequences indispensably occurred, and then the low-energy states are parametrized by,

$$\{h_j\} = \{-N_0/2 + 1, \dots, N_0/2 - 1, N_0/2\},$$

$$\{J_\beta\} = \{-N_0/4 + 1, \dots, N_0/4 - 1\},$$

$$I_1 = -\frac{3N_0-4}{8} + \delta_{1,\alpha_1}, \quad (15)$$

$$I_\alpha = I_{\alpha-1} + 1 + \delta_{\alpha,\alpha_1} \left(\alpha = 2, \dots, \frac{3N_0-1}{4} \right),$$

$$K_1 = -\frac{N_0-4}{8} + \delta_{1,\gamma_1},$$

$$K_\gamma = K_{\gamma-1} + 1 + \delta_{\gamma,\gamma_1} \left(\gamma = 2, \dots, \frac{N_0}{4} - 1 \right),$$

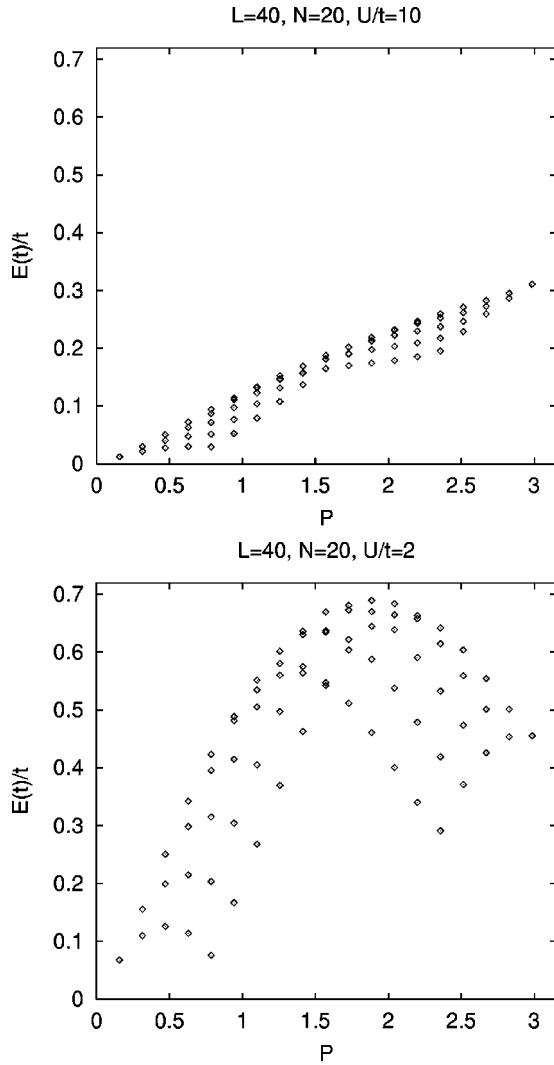


FIG. 3. 15-fold excitation spectrum for the model of 40 sites with 20 electrons. The overall structure of the spectrum changes much according to the correlation strengths. The lowest excitation energy and the whole pattern are raised when the correlation strength decreased.

where $1 \leq \alpha_1 \leq 3N_0/4, 1 \leq \gamma_1 \leq N_0/4$. Numerical results of the energy-momentum spectra for this type of excitation are plotted in Fig. 3, which is a two-parameter family of excitation. The states with negative momentum are just obtained by shifting the $\{h_j\}$ in Eq. (15) to the left by one unit.

Moving one box from the fourth and one from the third row of the Young tableau for the ground state to the first and second row, we get the 20-fold excitation with $M = 3N_0/4 - 1$, $M' = N_0/2 - 2$, and $M'' = N_0/4 - 1$. The I 's and K 's that took integer values in the ground state now take half-integer values: the h 's that took half-integer values now takes integer values, and the J 's still take half-integer values. As a result, two holes in $\{J_\beta\}$ are indispensably appeared,

$$\begin{aligned} \{h_j\} &= \{-N_0/2 + 1, \dots, N_0/2 - 1, N_0/2\}, \\ \{I_\alpha\} &= \{-3N_0/8 + 1, \dots, 3N_0/8 - 1\}, \\ \{K_\gamma\} &= \{-N_0/8 + 1, \dots, N_0/8 - 1\}, \end{aligned} \quad (16)$$

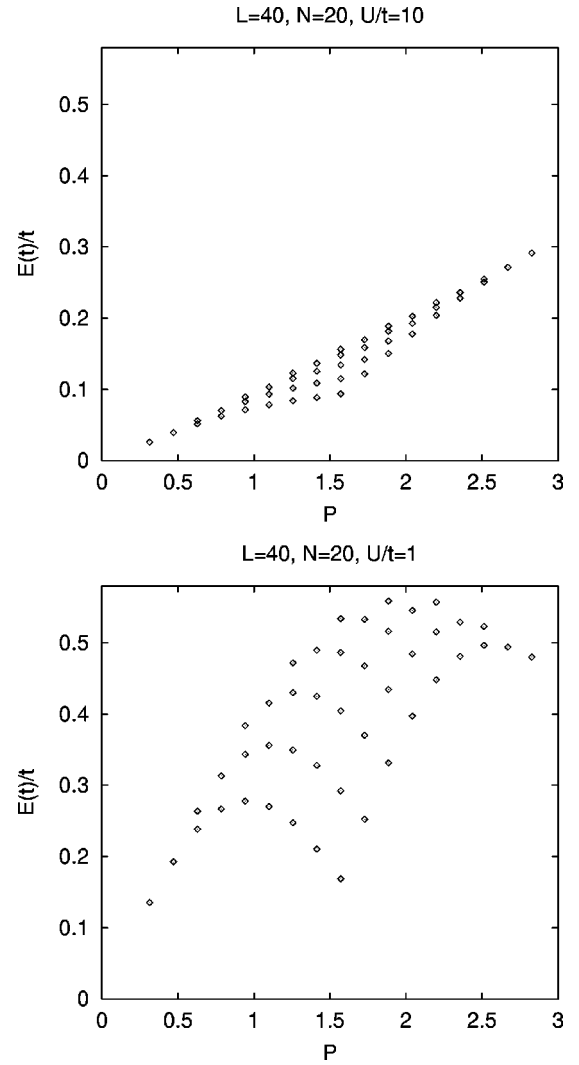


FIG. 4. 20-fold excitation spectrum for the model of 40 sites with 20 electrons. Some of points in the upper figure almost overlap. The overall structure of the spectra changes much with respect to the correlation strength. The lowest excitation energy as well as the pattern are raised when the correlation strength decreased.

$$J_1 = -\frac{N_0 - 2}{4} + \delta_{1,\beta_1},$$

$$J_\beta = J_{\beta-1} + 1 + \delta_{\beta,\beta_1} + \delta_{\beta,\beta_2},$$

where $\beta = 2, \dots, N_0/2 - 2$ and $1 \leq \beta_1 \leq \beta_2 \leq N_0/2$. Numerical results of the energy-momentum spectra for this type of excitation, a two-parameter family, are given in Fig. 4. Similarly, the states with negative momentum are just obtained by shifting the $\{h_j\}$ in Eq. (16) to the left by one unit.

Moving one box from the fourth and one from the third row of the Young tableau for the ground state to the first row, we get the 45-fold excitation with $M = 3N_0/4 - 2$, $M' = N_0/2 - 2$, and $M'' = N_0/4 - 1$. This makes it possible for the J 's to take integer values instead of half-integer ones and K 's to take half-integer values instead of integer ones. In this case, there exist two holes in $\{I_\alpha\}$ and one hole in $\{J_\beta\}$, namely,

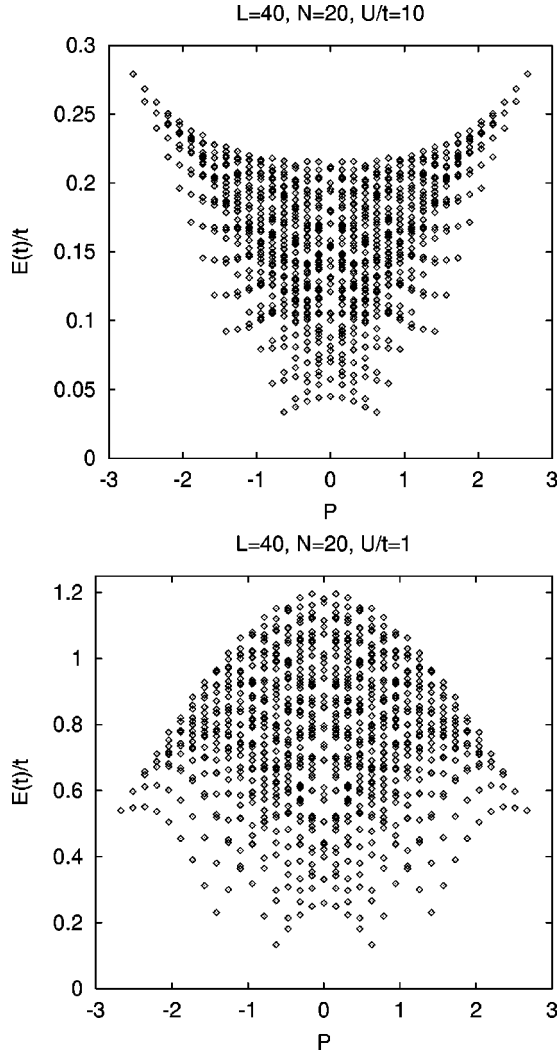


FIG. 5. 45-fold excitation spectrum for the model of 40 sites with 20 electrons.

$$\begin{aligned}
 \{h_j\} &= \{-N_0/2 + 1, \dots, N_0/2 - 1\}, \\
 \{K_\gamma\} &= \{-N_0/8 + 1, \dots, N_0/8 - 1\}, \\
 I_1 &= -\frac{3N_0 - 4}{8} + \delta_{1,\alpha_1}, \\
 I_\alpha &= I_{\alpha-1} + 1 + \delta_{\alpha,\alpha_1} + \delta_{\alpha,\alpha_2}, \\
 J_1 &= -\frac{N_0}{4} + 1 + \delta_{1,\beta_1}, \\
 J_\beta &= J_{\beta-1} + 1 + \delta_{\beta,\beta_1} \quad \left(\beta = 2, \dots, \frac{N_0}{2} - 2 \right),
 \end{aligned} \tag{17}$$

where $\alpha = 2, \dots, 3N_0/4 - 2$, $1 \leq \alpha_1 < \alpha_2 \leq 3N_0/4$, and $1 \leq \beta_1 \leq N_0/2 - 1$. Numerical results are plotted in Fig. 5. It is a three-parameter family of excitation.

Taking out one box respectively from the second, the third, and the fourth row and putting them together on the first row of the Young tableau, we have a 35-fold excitation. Due to $M = 3N_0/4 - 3$, $M' = N_0/2 - 2$, and $M'' = N_0/4 - 1$, we have four holes in $\{I_\alpha\}$, accordingly,

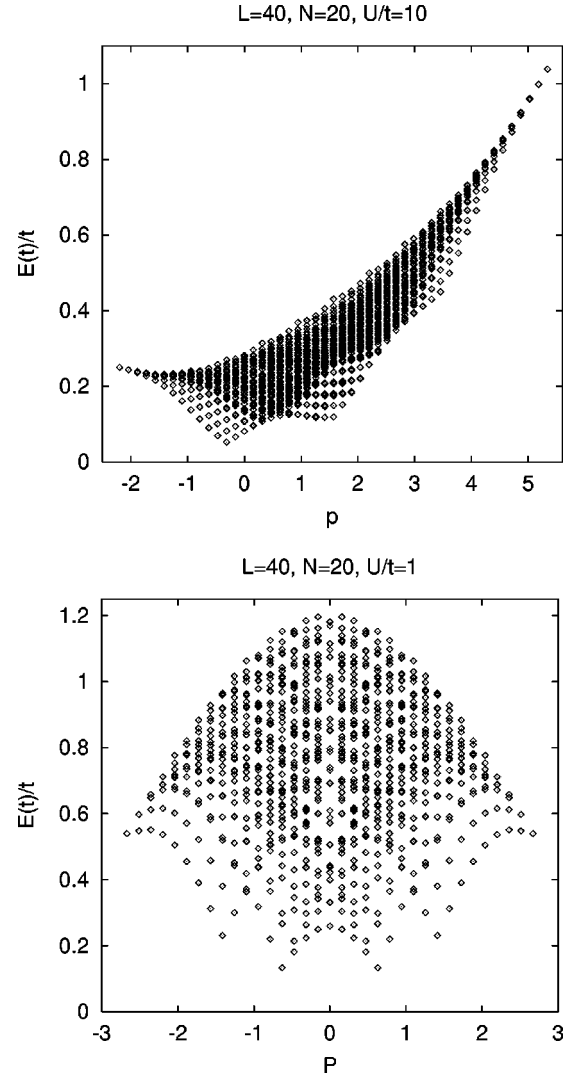


FIG. 6. 35-fold excitation spectrum for the model of 40 sites with 20 electrons. The complete spectra include another part that is just the mirror image of the above pattern and is not plotted.

$$\begin{aligned}
 \{h_j\} &= \{-N_0/2 + 1, \dots, N_0/2 - 1, N_0/2\}, \\
 \{J_\beta\} &= \{-(N_0 - 6)/4, \dots, (N_0 - 6)/4\}, \\
 \{K_\gamma\} &= \{-N_0/8 + 1, \dots, N_0/8 - 1\}, \\
 I_1 &= -\frac{3N_0}{4} + \delta_{1,\alpha_1}, \\
 I_\alpha &= I_{\alpha-1} + 1 + \sum_{i=1}^4 \delta_{\alpha,\alpha_i} \quad (\alpha = 2, \dots, 3N_0/4 - 3),
 \end{aligned} \tag{18}$$

where $1 \leq \beta_1 < \beta_2 < \beta_3 < \beta_4 \leq 3N_0/4 + 1$. The numerical results are plotted in Fig. 6, where we did not plot the pattern obtained by shifting $\{h_j\}$ in Eq. (18) to the left by one unit, which is just the mirror image of the plotted pattern. This is a four-parameter family of excitation.

B. Adding particles

If the number of electrons are $N_0 + 1$, $N_0 + 2$, or $N_0 + 3$, the corresponding states can be obtained by adding one, two

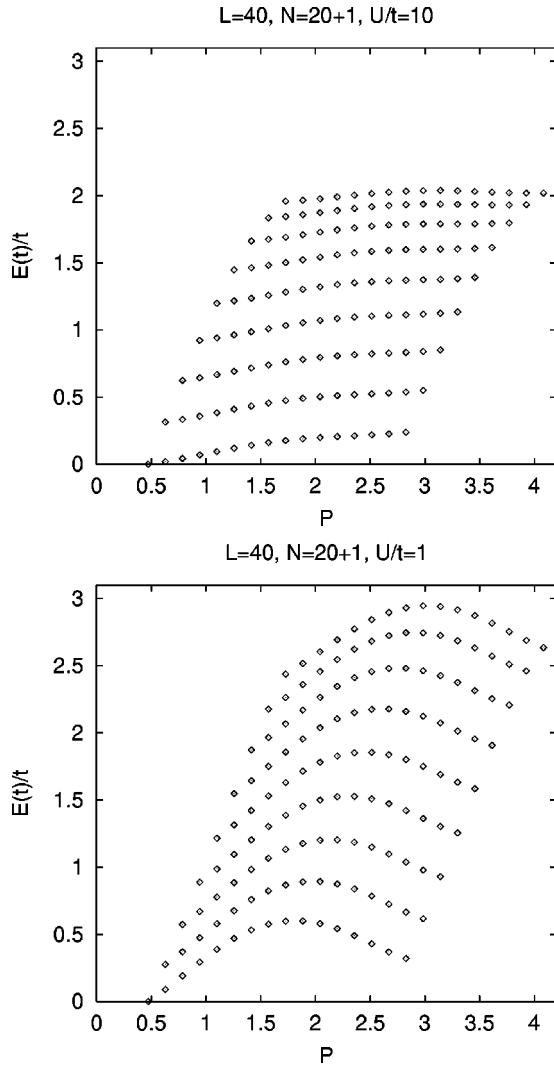


FIG. 7. Excitation spectrum for one particle added into the model of 40 sites with 20 electrons. The zero energy corresponds to the 21-electron ground state.

or three particles into the system of N_0 electrons. Adding one particle to the N_0 ground state and leaving M , M' , and M'' unchanged, the h 's, I 's, and J 's are half odd integers but K 's are integers. Comparing to that for the nondegenerate ground state of $N_0 = 4n$, there are now $3N_0/4 + 1$ allowed values for the $3N_0/4$ distinct I 's. So there is always a "hole" in the I 's sequence, namely,

$$\begin{aligned} \{h_j\} &= \{-(N_0 - 1)/2, \dots, (N_0 - 1)/2, h_0\}, \\ I_1 &= 3N_0/8 + \delta_{1,\alpha_1}, \\ I_\alpha &= I_{\alpha-1} + 1 + \delta_{\alpha,\alpha_1} \quad (\alpha = 2, \dots, 3N_0/4), \end{aligned} \quad (19)$$

where $1 \leq \alpha_1 \leq 3N_0/4 + 1$. The J and K sequences are the same as those in Eq. (13). The numerical results for $h_0 > 0$ are plotted in Fig. 7, where the zero energy corresponds to the ground state for $N = N_0 + 1$. The spectra with negative momentum are obtained by using $h_0 < 0$. It is easy to know by evaluating Eq. (10) that each point in the figure represents a quadruplet.

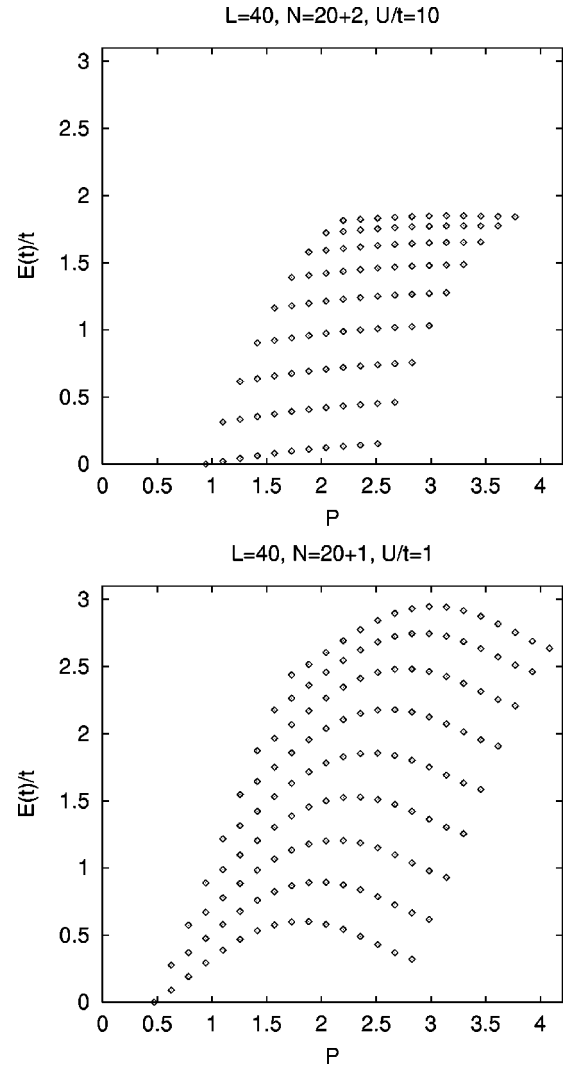


FIG. 8. Excitation spectrum for two particles added into the model of 40 sites with 20 electrons. The zero energy corresponds to the 22-electron ground state.

Adding two particles to the N_0 particle ground state, we have $N = N_0 + 2$, $M = 3N_0/4 + 1$, $M' = N_0/2$, and $M'' = N_0/4$ for the low-energy states. This requires h 's, J 's, and K 's to take integer values but I 's to take half odd-integer values. Referring to Eq. (13) we know that there must be a "hole" in the J sequence, consequently,

$$\begin{aligned} \{h_j\} &= \{-N_0/2, \dots, N_0/2, h_0\}, \\ \{I_\alpha\} &= \{-3N_0/8, \dots, 3N_0/8\}, \\ J_1 &= -\frac{N_0}{4} + \delta_{1,\beta_1}, \\ J_\beta &= J_{\beta-1} + 1 + \delta_{\beta,\beta_1} \quad (\beta = 2, \dots, N_0/2), \end{aligned} \quad (20)$$

where $1 \leq \beta_1 \leq N_0/2 + 1$. The K sequence is the same as that in Eq. (13). The numerical results are plotted in Fig. 8.

Adding three particles to the N_0 ground state, we have $N = N_0 + 3$, $M = 3N_0/4 + 2$, $M' = N_0/2 + 1$, and $M'' = N_0/4$ for low-energy states. This requires h 's and K 's to be half odd integers but I 's and J 's to be integers, and then

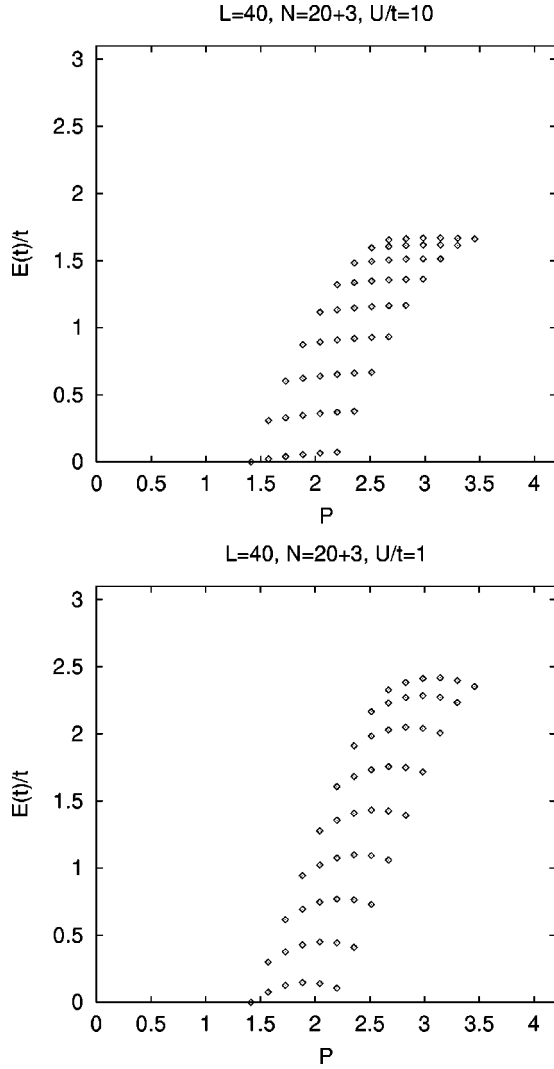


FIG. 9. Excitation spectrum for three particles added into the model of 40 sites with 20 electrons. The zero energy corresponds to the 23-electron ground state.

$$\begin{aligned}
 \{h_j\} &= \{-(N_0+1)/2, \dots, (N_0+1)/2, h_0\}, \\
 \{J_\alpha\} &= \{-(3N_0+4)/8, \dots, (3N_0+4)/8\}, \\
 \{J_\beta\} &= \{-N_0/8, \dots, N_0/4\}, \\
 K_1 &= -\frac{N_0}{8} + \delta_{1,\gamma_1}, \\
 K_\gamma &= K_{\gamma-1} + 1 + \delta_{\gamma,\gamma_1} \quad (\gamma=2, \dots, N_0/4),
 \end{aligned} \tag{21}$$

where $1 \leq \gamma_1 \leq N_0/4 + 1$. The numerical results are plotted in Fig. 9.

V. SPECIAL CASES

For some special limiting cases, one is able to obtain several interesting conclusions from the Bethe-ansatz equation without solving it directly.²⁸ In the following, we consider the weak coupling and strong coupling, respectively.

A. Weak coupling

Because $\Theta_1(x) = -\pi \operatorname{sgn}(x)$, $\Theta_{-1/2}(x) = \pi \operatorname{sgn}(x)$ for $c \rightarrow 0$, the Bethe-ansatz equation (11) becomes

$$\begin{aligned}
 k_j + \frac{\pi}{L} \sum_{\alpha=1}^M \operatorname{sgn}(\sin k_j - \lambda_\alpha) &= \frac{2\pi}{L} h_j, \\
 \sum_{l=1}^N \operatorname{sgn}(\lambda_\alpha - \sin k_l) - \sum_{\alpha'=1}^M \operatorname{sgn}(\lambda_\alpha - \lambda_{\alpha'}) \\
 + \sum_{\beta=1}^{M'} \operatorname{sgn}(\lambda_\alpha - \mu_\beta) &= 2I_\alpha, \\
 \sum_{\alpha=1}^M \operatorname{sgn}(\mu_\beta - \lambda_\alpha) - \sum_{\beta'=1}^{M'} \operatorname{sgn}(\mu_\beta - \mu_{\beta'}) \\
 + \sum_{\gamma=1}^{M''} \operatorname{sgn}(\mu_\beta - \nu_\gamma) &= 2J_\beta, \\
 \sum_{\beta=1}^{M'} \operatorname{sgn}(\nu_\gamma - \mu_\beta) - \sum_{\gamma'=1}^{M''} \operatorname{sgn}(\nu_\gamma - \nu_{\gamma'}) &= 2K_\gamma.
 \end{aligned} \tag{22}$$

Without loss of generality, the γ label can be so chosen that K_γ is arranged in an increasing order. Then the fourth equation in Eq. (22) becomes

$$\sum_{\mu=1}^{M'} \operatorname{sgn}(\nu_\gamma - \mu_\beta) = 2K_\gamma + 2\gamma - M'' - 1. \tag{23}$$

Because $|K_\gamma| \leq (M'' - 1)/2$ and $M'' \leq M'/2$ (restricted by the Young tableau), the minimum value of right-hand side of Eq. (23) is $-M' + 2$. This means that the smallest μ_β is smaller than the smallest ν_γ . From Eq. (23) we easily derive

$$\sum_{\beta=1}^{M'} [\operatorname{sgn}(\nu_{\gamma+1} - \mu_\beta) - \operatorname{sgn}(\nu_\gamma - \mu_\beta)] = 2(K_{\gamma+1} - K_\gamma + 1). \tag{24}$$

Obviously, if $K_{\gamma+1} - K_\gamma = m''$, there must exist exactly $m'' + 1$ solutions μ_β satisfying $\nu_\gamma < \mu_\beta < \nu_{\gamma+1}$.

Again from the third equation in Eq. (22), we have

$$\begin{aligned}
 \sum_{\alpha=1}^M [\operatorname{sgn}(\mu_{\beta+1} - \lambda_\alpha) - \operatorname{sgn}(\mu_\beta - \lambda_\alpha)] \\
 = 2J_{\beta+1} - 2J_\beta + 2 - \sum_{\gamma=1}^{M''} [\operatorname{sgn}(\mu_{\beta+1} - \nu_\gamma) \\
 - \operatorname{sgn}(\mu_\beta - \nu_\gamma)].
 \end{aligned} \tag{25}$$

Obviously, if there is a ν_γ such that $\mu_\beta < \nu_\gamma < \mu_{\beta+1}$ then the right-hand side of Eq. (25) equals $2(J_{\beta+1} - J_\beta)$, otherwise it equals $2(J_{\beta+1} - J_\beta + 1)$. Proceeding the same strategy to the second equation and the first equation in Eq. (22) successively, we obtain a sequence of relations that are summarized as follows.

(i) If $K_{\gamma+1} - K_\gamma = m''$, there exist exactly $m'' + 1$ solutions μ_β satisfying $\nu_\gamma < \mu_\beta < \nu_{\gamma+1}$.

(ii) For $J_{\beta+1} - J_{\beta} = m'$, if there exists a ν_{γ} satisfying $\mu_{\beta} < \nu_{\gamma} < \mu_{\beta+1}$, there will be m' λ 's such that $\mu_{\beta} < \lambda_{\alpha} < \mu_{\beta+1}$; otherwise if there is no ν_{γ} satisfying that, then there will be $m' + 1$ λ 's such that $\mu_{\beta} < \lambda_{\alpha} < \mu_{\beta+1}$.

(iii) For $I_{\alpha+1} - J_{\alpha} = m$, if there is a μ_{β} satisfying $\lambda_{\alpha} < \mu_{\beta} < \lambda_{\alpha+1}$, there will exist m $\sin k_l$'s such that $\lambda_{\alpha} < \sin k_l < \lambda_{\alpha+1}$; otherwise there will be $m + 1$ $\sin k_l$'s such that $\lambda_{\alpha} < \sin k_l < \lambda_{\alpha+1}$.

(iv) For $h_{j+1} - h_j = n'$, if there exists such a λ_{α} that $\sin k_j < \lambda_{\alpha} < \sin k_{j+1}$, then we will have $k_{j+1} - k_j = 2\pi(n' - 1)/L$; otherwise we will have $k_{j+1} - k_j = 2\pi n'/L$.

Applying these items to the ground state $n' = m = m'' = 1$, we conclude that the sequence $\{k_j\}$ is divided into groups with four successive values in each group. Between each pair (k_{4j-3}, k_{4j-2}) , (k_{4j-2}, k_{4j-1}) or (k_{4j-1}, k_{4j}) in the same group there is one λ , so totally there are three λ 's in each group. Furthermore, there are two μ 's, each lying between the adjacent λ 's. And between these two μ 's there is always a ν .

B. Strong coupling

For the strong-coupling limit case, $c \rightarrow \infty$ (i.e., large U limit), the ration $\sin k_j/c$ in the Bethe-ansatz equation is neglectable. The first equation in Eq. (9) then becomes

$$k_j = \frac{2\pi}{L} n_j - \frac{1}{L} P_H, \quad (26)$$

$$P_H = \sum_{\alpha=1}^M [\pi - 2 \tan^{-1}(2\lambda_{\alpha}/c)],$$

where n_j are integers. Obviously, the P_H is just the momentum of spin-orbital excitations in the SU(4) Heisenberg chain.^{9,29} The other three Bethe-ansatz equations turn to be those known for the SU(4) Heisenberg chain for the scaled rapidities, λ_{α}/c , μ_{β}/c , and ν_{γ}/c . Equation (26) indicates that the allowed quasimomenta k 's in the strong-coupling limit are quantized in units of $2\pi/L$, just like "spinless" noninteracting fermions. This is because the double occupancy is forbidden by the strong repulsive on-site coupling. The allowed quasimomenta due to periodic boundary condition are determined by spin-orbital momentum P_H . Particularly, for $N = 4n$ with $n = \text{odd}$, the ground-state spin-orbital momentum P_H is an odd multiple of π ⁹ so that the allowed k 's are half odd integers multiplied by $2\pi/L$. Therefore, the ground state for $N = 4n$ ($n = \text{odd}$) is uniquely determined, i.e., it is nondegenerate. This is different from the noninteraction case in which the allowed k 's are always integers multiplied by $2\pi/L$ for any N and for each k there are four states because of the spin-orbital degree of freedom.

VI. THERMODYNAMICS LIMIT

Replacing k_j , λ_{α} , μ_{β} , and ν_{γ} in Eq. (11) by continuous variables k , λ , μ , and ν but keeping the summation still over the solution set of these roots, we can consider the quantum numbers h_j , I_{α} , J_{β} , and K_{γ} as functions $h(k)$, $I(\lambda)$, $J(\mu)$, and $K(\nu)$ given by Eq. (11). Take $I(\lambda)$ as an example, when $I(\lambda)$ passes through one of the quantum numbers I_j , the corresponding λ is equal to one of the roots λ_j , similarly for

$J(\mu)$, $K(\nu)$, or $h(k)$. However, there may exist some integers or half-integers for which the corresponding λ (μ , ν , or k) is not in the set of roots. Such a situation is conventionally referred as a "hole." In the thermodynamics limit, $N \rightarrow \infty$, $L \rightarrow \infty$ but N/L kept finite, we may introduce the density of real roots and the density of holes (indicated by a subscript h),

$$\rho(k) + \rho_h(k) = (1/L) dh(k)/dk,$$

$$\sigma(\lambda) + \sigma_h(\lambda) = (1/L) dI(\lambda)/d\lambda.$$

$$\omega(\mu) + \omega_h(\mu) = (1/L) dJ(\mu)/d\mu,$$

$$\tau(\nu) + \tau_h(\nu) = (1/L) dK(\nu)/d\nu.$$

By replacing the summations by integrals, for example,

$$\lim_{L \rightarrow \infty} \frac{1}{L} \sum_{l=1}^N f(k_l) = \int_{-Q}^Q dk \rho(k) f(k), \quad (27)$$

$$\lim_{L \rightarrow \infty} \frac{1}{L} \sum_{\alpha=1}^M g(\lambda_{\alpha}) = \int_{-B}^B d\lambda \sigma(\lambda) g(\lambda),$$

and so forth, Eq. (11) gives rise to the following coupled integral equations,

$$\rho(k) + \rho^{(0)}(k) = \frac{1}{2\pi} - \cos k \int_{-B}^B K_{-1/2}(\sin k - \lambda) \sigma(\lambda) d\lambda,$$

$$\sigma(\lambda) + \sigma^{(0)}(\lambda) = - \int_{-Q}^Q K_{-1/2}(\lambda - \sin k) \rho(k) dk$$

$$- \int_{-B}^B K_1(\lambda - \lambda') \sigma(\lambda') d\lambda'$$

$$- \int_{-B'}^{B'} K_{-1/2}(\lambda - \mu) \omega(\mu) d\mu, \quad (28)$$

$$\omega(\mu) + \omega^{(0)}(\mu) = - \int_{-B}^B K_{-1/2}(\mu - \lambda) \sigma(\lambda) d\lambda$$

$$- \int_{-B'}^{B'} K_1(\mu - \mu') \omega(\mu') d\mu'$$

$$- \int_{-B''}^{B''} K_{-1/2}(\mu - \nu) \tau(\nu) d\nu,$$

$$\tau(\nu) + \tau^{(0)}(\nu) = - \int_{-B'}^{B'} K_{-1/2}(\nu - \mu) \omega(\mu) d\mu$$

$$- \int_{-B''}^{B''} K_1(\nu - \nu') \tau(\nu') d\nu',$$

where $K_n(x) := \pi^{-1} n c / (n^2 c^2 + x^2)$, and Q , B , B' , and B'' in the definite integrals should be determined self-consistently by

$$\frac{N}{L} = \int_{-Q}^Q \rho(k) dk,$$

$$\begin{aligned}\frac{M}{L} &= \int_{-B}^B \sigma(\lambda) d\lambda, \\ \frac{M'}{L} &= \int_{-B'}^{B'} \omega(\mu) d\mu, \\ \frac{M''}{L} &= \int_{-B''}^{B''} \tau(\nu) d\nu.\end{aligned}\quad (29)$$

They hold for the case in the absence of the complex roots. In the presence of complex roots, however, it has variants. In Eq. (28) we denoted the inhomogeneous terms by $\rho^{(0)}$, $\sigma^{(0)}$, $\omega^{(0)}$, and $\tau^{(0)}$, which not only stand for the densities of holes ρ_h , σ_h , etc., but also the contributions from complex roots, two-strings.

Once the density $\rho(k)$ is solved from Eq. (28), we have the z components of the total spin and the total orbital

$$\begin{aligned}\frac{S_{\text{tot}}^z}{L} &= \frac{1}{2} \int_{-Q}^Q \rho(k) dk + \int_{-B'}^{B'} \omega(\mu) d\mu - \int_{-B}^B \sigma(\lambda) d\lambda \\ &\quad - \int_{-B''}^{B''} \tau(\nu) d\nu, \\ \frac{T_{\text{tot}}^z}{L} &= \frac{1}{2} \int_{-Q}^Q \rho(k) dk - \int_{-B'}^{B'} \omega(\mu) d\mu.\end{aligned}\quad (30)$$

This is useful for a correct calculation of magnetizations. The energy is given by

$$\frac{E}{L} = -2t \int_{-Q}^Q \cos k \rho(k) dk. \quad (31)$$

The highest weight vector that characterizes the corresponding representation is given by

$$\begin{aligned}w_1 &= L \int_{-Q}^Q \rho(k) dk - 2L \int_{-B}^B \sigma(\lambda) d\lambda + L \int_{-B'}^{B'} \omega(\mu) d\mu, \\ w_2 &= L \int_{-B}^B \sigma(\lambda) d\lambda - 2L \int_{-B'}^{B'} \omega(\mu) d\mu + L \int_{-B''}^{B''} \tau(\nu) d\nu, \\ w_3 &= L \int_{-B'}^{B'} \omega(\mu) d\mu - 2L \int_{-B''}^{B''} \tau(\nu) d\nu.\end{aligned}\quad (32)$$

A. Ground-state properties

The ground state of the present model is a Fermi sea described by $\rho_0(k)$, which is the distribution function of charge with respect to momentum k . The $\tau_0(\nu)$ describes the distribution of states with spin down and orbital bottom in the ν -rapidity space. The $\omega_0(\mu)$ represents the distribution of either the state with spin up while orbital bottom or that with spin down while orbital bottom in the μ -rapidity space. The $\sigma_0(\lambda)$, however, stands for the distribution of either state $|2\rangle$, $|3\rangle$, or $|4\rangle$ in the λ -rapidity space. These distribution functions satisfy Eq. (28) with $B=B'=B''=\infty$ and no holes, i.e., $\rho^{(0)}=0$, $\sigma^{(0)}=0$, $\omega^{(0)}=0$, $\tau^{(0)}=0$. By making a Fourier transform of the second through fourth equation of Eq. (28), we have

$$\begin{aligned}\bar{\sigma}(q) &= \frac{1}{\sqrt{2\pi}} \int_{k_F}^{k_F} e^{-c|q|/2+iq \sin k} \rho(k) dk - \bar{\sigma}(q) e^{-c|q|} \\ &\quad + \bar{\omega}(q) e^{-c|q|/2}, \\ \bar{\omega}(q) &= \bar{\sigma}(q) e^{-c|q|/2} - \bar{\omega}(q) e^{-c|q|} + \bar{\tau}(q) e^{-c|q|/2}, \\ \bar{\tau}(q) &= \bar{\omega}(q) e^{-c|q|/2} - \bar{\tau}(q) e^{-c|q|}.\end{aligned}\quad (33)$$

It is not difficult to obtain a single integral equation that determines the $\rho_0(k)$

$$\rho_0(k) = \frac{1}{2\pi} + \frac{\cos k}{c} \int_{-k_F}^{k_F} R_{3/2} \left(\frac{\sin k - \sin k'}{c} \right) \rho_0(k') dk', \quad (34)$$

where k_F is the Fermi momentum and

$$R_n(x) = \int_{-\infty}^{\infty} \frac{dq}{2\pi} \frac{\sinh(nq)}{\sinh(2q)} e^{iqx - |q|/2}.$$

Once $\rho_0(k)$ is solved, the energy will be evaluated by the integral

$$E_0/L = -2t \int_{-k_F}^{k_F} \cos k \rho_0(k) dk.$$

Though an explicit expression cannot be obtained from Eq. (34) in the general case, it becomes easier for a numerical calculation.

It is immediate from Eq. (33) that the highest weight vector (32) of the ground state is a null vector. Therefore the ground state is a $SU(4)$ singlet; accordingly, both spin and orbital are antiferromagnetic.

B. Ground-state energy for strong coupling

The ground-state energy can be calculated explicitly at strong on-site coupling, $c \gg 1$ (i.e., $U \gg t$). Because of $(\sin k - \sin k')/c \ll 1$ in this case and $4\pi R_{3/2}(0) = 3 \ln 2 + \pi/2$, Eq. (34) is written up to the order $O(1/c)$,

$$\rho_0^{\text{stro}} = \frac{1}{2\pi} + \left(3 \ln 2 + \frac{\pi}{2} \right) \frac{\cos k}{4\pi c} \frac{N}{L}.$$

The Fermi momentum determined from $N/L = \int_{-k_F}^{k_F} \rho_0(k) dk$ is

$$k_F = \frac{N}{L} \left[\pi - \left(3 \ln 2 + \frac{\pi}{2} \right) \frac{\sin(\pi N/L)}{2c} \right],$$

and then the energy is calculated

$$\begin{aligned}\frac{E_0}{L} &= -\frac{t \sin(\pi N/L)}{\pi/2} - \frac{t^2}{U} \left(\frac{N}{L} \right)^2 \left(3 \ln 2 + \frac{\pi}{2} \right) \\ &\quad \times \left[1 - \frac{\sin(2\pi N/L)}{2\pi N/L} \right],\end{aligned}\quad (35)$$

where N/L is the filling factor. It becomes $E_0^{(1/2)} = -Nt^2(6 \ln 2 + \pi)/U$ at half-filling $N=2L$. At quarter filling $L=N$ we have

$$\frac{E_0^{(1/4)}}{N} = -2 \frac{t^2}{U} \left(\frac{3}{2} \ln 2 + \frac{\pi}{4} \right),$$

which agrees with the result of the SU(4) Heisenberg model^{9,29} for $J=2t^2/U$. Because the model is solved under the assumption of excluding site occupations of more than two, the results here are not valid for above half-filling $N > 2L$ in which there must exist sites occupied by three electrons and the Bethe-ansatz wave-function failures at that point in configuration space. However, the energy is expected to be evaluate by a particle-hole transformation,¹⁴

$$E(N/L, U)/L = E(4 - N/L, U)/L + 3(N/L - 2)U. \quad (36)$$

In the next section and thereafter we will study low-lying excitations on the basis of the thermodynamics limit.

VII. SPIN-ORBITAL EXCITATIONS

It is convenient to study the excitations by introducing $\rho(k) = \rho_0(k) + \rho_1(k)/L$, $\sigma(\lambda) = \sigma_0(\lambda) + \sigma_1(\lambda)/L$, $\omega(\mu) = \omega_0(\mu) + \omega_1(\mu)/L$, and $\tau(\nu) = \tau_0(\nu) + \tau_1(\nu)/L$, where $\rho_0(k)$, $\sigma_0(\lambda)$, $\omega_0(\mu)$, and $\tau_0(\nu)$ satisfy the same set of integral equations as the ground state did. The excitation energy up to the order $O(1/L)$ is

$$\Delta E = - \int_{-Q}^Q dk (2t \cos k + \Lambda) \rho_1(k), \quad (37)$$

where Λ stands for the chemical potential.³⁰ Q can be replaced by k_F for a large system. Equation (37) is valid for both the spin-orbital excitation and the charge excitation. The excitation energy is related to $\rho_1(k)$, which, moreover, should be solved from the following coupled integral equations:

$$\begin{aligned} \rho_1(k) + \rho_1^{(0)}(k) &= -\cos k \int_{-\infty}^{\infty} K_{-1/2}(\sin k - \lambda) \sigma_1(\lambda) d\lambda, \\ \sigma_1(\lambda) + \sigma_1^{(0)}(\lambda) &= - \int_{-k_F}^{k_F} K_{-1/2}(\lambda - \sin k) \rho_1(k) dk \\ &\quad - \int_{-\infty}^{\infty} K_1(\lambda - \lambda') \sigma_1(\lambda') d\lambda' \\ &\quad - \int_{-\infty}^{\infty} K_{-1/2}(\lambda - \mu) \omega_1(\mu) d\mu, \end{aligned} \quad (38)$$

$$\begin{aligned} \omega_1(\mu) + \omega_1^{(0)}(\mu) &= - \int_{-\infty}^{\infty} K_{-1/2}(\mu - \lambda) \sigma_1(\lambda) d\lambda \\ &\quad - \int_{-\infty}^{\infty} K_1(\mu - \mu') \omega_1(\mu') d\mu' \\ &\quad - \int_{-\infty}^{\infty} K_{-1/2}(\mu - \nu) \tau_1(\nu) d\nu, \end{aligned}$$

$$\begin{aligned} \tau_1(\nu) + \tau_1^{(0)}(\nu) &= \int_{-\infty}^{\infty} K_{-1/2}(\nu - \mu) \omega_1(\mu) d\mu \\ &\quad + \int_{-\infty}^{\infty} K_1(\nu - \nu') \tau_1(\nu') d\nu'. \end{aligned}$$

The limits for the definite integrals are the same as that for ground state, which are valid for the low-lying excitations. Beyond low-lying excitations, however, the integration limits Q , B , B' , and B'' should be determined consistently. Here we only consider low-lying excitations.

In order to consider the excitations above the singlet ground state, we must analyze the decomposition of the direct product of the SU(4) fundamental representation for $N = 4n$. Using the Young tableau, we can obtain that the decomposition gives rise to a direct sum of a series of irreducible representations, i.e., (0, 0, 0), (1, 0, 1), (0, 2, 0), (2, 1, 0), (4, 0, 0), etc. So the excitation states in spin-orbital sector include both the singlet (0, 0, 0) and the multiplets of 15-fold (1, 0, 1), of 20-fold (0, 2, 0), and of 45-fold (2, 1, 0) or of 35-fold (4, 0, 0), etc. After evaluating the contributions of roots and two-strings to the highest weight vectors that characterize the irreducible representations of SU(4), we can get the correct compositions of holes and two-strings that create the possible excitations allowed by group theory.

A. The multiplets

One λ hole and one ν hole together create a 15-fold multiplet. Let $\sigma_1^{(0)}(\lambda) = \sigma^h(\lambda) = \delta(\lambda - \bar{\lambda})$, $\tau_1^{(0)}(\nu) = \tau^h(\nu) = \delta(\nu - \bar{\nu})$, and the other inhomogeneous terms in Eq. (38) be null. Equation (38) is reduced to a closed form by Fourier transform. The excitation energy is composed of two terms

$$\Delta E_{(15)} = \varepsilon_{\sigma}(\bar{\lambda}) + \varepsilon_{\tau}(\bar{\nu}),$$

and each of them can be identified as one of the SU(4) modes with energy

$$\varepsilon_f(\bar{x}) = - \int_{-k_F}^{k_F} dk (2t \cos k + \Lambda) \rho_1^f(k, \bar{x}), \quad (39)$$

where $f = \sigma, \tau$, or ω . The $\rho_1^{\sigma}(k, \bar{\lambda})$ is solved as

$$\begin{aligned} \rho_1^{\sigma}(k, \bar{\lambda}) &+ \frac{\cos k/(4c)}{\sqrt{2} \cosh \left[\frac{\pi}{2c} (\sin k - \bar{\lambda}) \right] - 1} \\ &= \frac{\cos k}{c} \int_{-k_F}^{k_F} R_{3/2} \left(\frac{\sin k - \sin k'}{c} \right) \rho_1^{\sigma}(k', \bar{\lambda}) dk', \end{aligned} \quad (40)$$

and the $\rho_1^{\tau}(k, \bar{\nu})$ satisfies the following integral equation:

$$\begin{aligned} \rho_1^{\tau}(k, \bar{\nu}) &+ \frac{\cos k/(4c)}{\sqrt{2} \cosh \left[\frac{\pi}{2c} (\sin k - \bar{\nu}) \right] + 1} \\ &= \frac{\cos k}{c} \int_{-k_F}^{k_F} R_{3/2} \left(\frac{\sin k - \sin k'}{c} \right) \rho_1^{\tau}(k', \bar{\nu}) dk'. \end{aligned} \quad (41)$$

Two μ holes, $\omega^{(0)}(\mu) = \delta(\mu - \bar{\mu}_1) + \delta(\mu - \bar{\mu}_1)$, create a 20-fold multiplet with excitation energy

$$\Delta E_{(20)} = \varepsilon_\omega(\bar{\mu}_1) + \varepsilon_\omega(\bar{\mu}_2),$$

where $\varepsilon_\omega(x)$ is evaluated by the same integral (39), but $\rho_1^\omega(k, \bar{\mu})$ should solve

$$\begin{aligned} \rho_1^\omega(k, \bar{\mu}) + \frac{\cos k/(4c)}{\cosh\left[\frac{\pi}{2c}(\sin k - \bar{\mu})\right]} \\ = \frac{\cos k}{c} \int_{-k_F}^{k_F} R_{3/2}\left(\frac{\sin k - \sin k'}{c}\right) \rho_1^\omega(k', \bar{\mu}) dk'. \end{aligned} \quad (42)$$

The 45-fold multiplet is a three-hole state created by two λ holes and one μ hole, i.e., $\sigma_1^{(0)}(\lambda) = \delta(\lambda - \bar{\lambda}_1) + \delta(\lambda - \bar{\lambda}_2)$ and $\omega_1^{(0)}(\mu) = \delta(\mu - \bar{\mu})$ for which the excitation energy is

$$\Delta E_{(45)} = \varepsilon_\sigma(\bar{\lambda}_1) + \varepsilon_\sigma(\bar{\lambda}_2) + \varepsilon_\omega(\bar{\mu}).$$

Four λ holes create a 35-fold multiplet with excitation energy

$$\Delta E_{(35)} = \sum_{j=1}^4 \varepsilon_\sigma(\bar{\lambda}_j).$$

In the above we have seen that there are three types of elementary excitation modes in the spin-orbital sector [let us call the SU(4) flavor degree of freedom]. It is easy to know the contributions of the holes to the highest weight vectors, and to the spin and orbital. Consequently, the quadruplets (1, 0, 0) or (0, 0, 1) are SU(4) modes carrying both spin $\frac{1}{2}$ and orbital $\frac{1}{2}$ with energies ε_σ or ε_τ , whereas the hexaplet (0, 1, 0) is one of the SU(4) modes carrying either spin 1 or orbital 1 with energy ε_ω . Clearly, spins and orbitals are mixed up in present isotropic on-site coupling. The spin orbital separation is expected to occur for the anisotropic cases that can be caused by Hund's rule. From Eqs. (40)–(42) we find that the asymptotic behavior of all the three densities of roots vanishes as the rapidities go to infinity. Thus these elementary excitations are gapless, i.e., $\varepsilon_f(\pm\infty) = 0$.

B. The singlet

By observing the contributions of two-strings to the highest weight vectors, we find that the SU(4) modes can compound to form a singlet. In addition to placing in the λ rapidity a hole at $\bar{\lambda}$ and in the ν rapidity a hole at $\bar{\nu}$, we take into account three two-strings in those three rapidities, $\lambda^\pm = \lambda_0 \pm ic/2$, $\mu^\pm = \mu_0 \pm ic/2$, and $\nu^\pm = \nu_0 \pm ic/2$. In this case,

$$M/L = \int_{-\infty}^{\infty} \sigma(\lambda) d\lambda + 2,$$

$$M'/L = \int_{-\infty}^{\infty} \omega(\mu) d\mu + 2,$$

$$M''/L = \int_{-\infty}^{\infty} \tau(\nu) d\nu + 2,$$

and the inhomogeneous terms of Eq. (38) read

$$\rho_1^{(0)}(k) = -\cos k K_1(\sin k - \lambda_0),$$

$$\begin{aligned} \sigma_1^{(0)}(\lambda) = \delta(\lambda - \bar{\lambda}) + K_{3/2}(\lambda - \lambda_0) + K_{1/2}(\lambda - \lambda_0) \\ - K_1(\lambda - \lambda_0), \end{aligned} \quad (43)$$

$$\begin{aligned} \omega_1^{(0)}(\mu) = K_{3/2}(\mu - \mu_0) + K_{1/2}(\mu - \mu_0) - K_1(\mu - \lambda_0) \\ - K_1(\mu - \nu_0), \end{aligned}$$

$$\begin{aligned} \tau_1^{(0)}(\nu) = \delta(\nu - \nu_0) + K_{3/2}(\nu - \nu_0) + K_{1/2}(\nu - \nu_0) \\ - K_1(\nu - \mu_0). \end{aligned}$$

Substituting them into Eq. (38) and taking Fourier transform, we find that the term containing ν_0 in the fourth equation cancels with the term containing ν_0 in the third equation. After substituting the result into the second equation, again the terms containing μ_0 cancel each other. The substituting of the obtained expression of $\sigma_1(\lambda)$ into the first equation brings about an exact cancellation of the terms containing λ_0 . As a result, the excitation energy is obtained:

$$\Delta E_{(1)} = \varepsilon_\sigma(\bar{\lambda}) + \varepsilon_\tau(\bar{\nu}),$$

where ε_σ and ε_τ are evaluated by Eq. (39) in which the ρ_1^σ and ρ_1^τ satisfy the Eq. (40) and Eq. (41), respectively. Clearly, the excitations of 15-fold multiplet and the singlet are degenerate in energy.

VIII. CHARGE EXCITATIONS

A. The holon-antiholon excitation

Let us consider the case of less than quarter-filling ($N < L$). We are allowed to add one ‘‘particle’’ outside the charge Fermi sea, $k_p \notin [-k_F, k_F]$ but leaving a hole inside the charge Fermi sea $\bar{k} \in [-k_F, k_F]$. The calculation of the energy is required to start from

$$E = -2t \cos k_p - 2tL \int_{-k_F}^{k_F} \cos k \rho(k) dk,$$

where the integration limit k_F is required to fulfill $\int_{-k_F}^{k_F} \rho(k) dk = (N-1)/L$.

By introducing $\rho(k) = \rho_0(k) + \rho_1(k)/L$, etc., the excitation energy $\Delta E = E - E_0$ is composed of two terms

$$\Delta E(\bar{k}, k_p) = \varepsilon_h(\bar{k}) + \bar{\varepsilon}_h(k_p). \quad (44)$$

Here we introduced the holon energy

$$\varepsilon_h(x) = 2t \cos x - \int_{-k_F}^{k_F} (2t \cos k + \Lambda) \rho_1^c(k, x) dk, \quad (45)$$

and antiholon (‘‘particle’’ state) energy $\bar{\varepsilon}_h(x) = -\varepsilon_h(x)$. In Eq. (45), the $\rho_1^c(k, x)$ should be solved from the following equation:

$$\begin{aligned} \rho_1^c(k, x) + \frac{\cos k}{c} R_{3/2} \left(\frac{\sin k - \sin x}{c} \right) \\ = \frac{\cos k}{c} \int_{-k_F}^{k_F} R_{3/2} \left(\frac{\sin k - \sin k'}{c} \right) \rho_1^c(k', x) dk'. \end{aligned} \quad (46)$$

This equation is derived from Eq. (38) by taking

$$\rho_1^{(0)}(k) = \delta(k - \bar{k}),$$

$$\sigma_1^{(0)}(\lambda) = -K_{1/2}(\lambda - \sin k_p),$$

$$\omega_1^{(0)}(\mu) = \tau_1^{(0)}(\nu) = 0,$$

which comes from the ‘‘particle’’ and the hole. Now we find that this kind of excitation consists of a holon carrying energy $\varepsilon(\bar{k})$ and an antiholon carrying energy $\bar{\varepsilon}_h(k_p)$. Obviously, Eq. (44) vanishes when $\bar{k} \rightarrow k_F$ and $k_p \rightarrow k_F$, and the holon-antiholon excitation is gapless.

B. The holon-holon excitation

In order to discuss states with double occupancy, we need to consider solutions containing complex k pairs. Suppose a configuration $\{h_j\}$ results in a complex pairs (two-strings), $k^\pm = \kappa \mp i\chi$, and two holes inside the Fermi sea, $\bar{k}_1, \bar{k}_2 \in [-k_F, k_F]$. After a careful analyses of the Bethe ansatz equation, one finds the string position is restricted to lie around a particular λ solution that we denote by λ_0 , i.e., it must satisfy

$$\sin(\kappa \pm i\chi) = \lambda_0 \mp ic/2 + O(e^{-\eta L}).$$

An exact deletion holds in the second equation in Eq. (9) for $\lambda_0 = (\sin \bar{k}_1 + \sin \bar{k}_2)/2$. After rewriting the Bethe-ansatz equation by separating the factors of the complex k pairs, we take the thermodynamics limit as before. In order to get the excitation energy we need to solve Eq. (38) with

$$\rho_1^{(0)}(k) = \delta(k - \bar{k}_1) + \delta(k - \bar{k}_2) + \cos k K_{-1/2}(\sin k - \lambda_0),$$

$$\sigma_1^{(0)}(\lambda) = \tau_1^{(0)}(\nu) = 0,$$

$$\omega_1^{(0)}(\mu) = K_{-1/2}(\mu - \lambda_0).$$

After careful calculation, we obtain the excitation energy

$$\Delta E(\bar{k}_1, \bar{k}_2) = \varepsilon_h(\bar{k}_1) + \varepsilon_h(\bar{k}_2) + \Delta(U, k_F),$$

where ε_h is the holon energy given by the same equation (45), and $\Delta(U, k_F)$ is given by

$$\begin{aligned} \Delta(U, k_F) = U + 2t \int_{-\pi}^{\pi} \cos^2 k K_1(\sin k - \lambda_0) dk \\ - \int_{-k_F}^{k_F} (2t \cos k + \Lambda) \rho_1^{\text{stri}}(k, \lambda_0) dk, \end{aligned}$$

with

$$\begin{aligned} \rho_1^{\text{stri}}(k, \lambda_0) = \frac{\cos k}{c} R_1 \left(\frac{\sin k - \lambda_0}{c} \right) \\ + \frac{\cos k}{c} \int_{-k_F}^{k_F} R_{3/2} \left(\frac{\sin k - \sin k'}{c} \right) \rho_1^{\text{stri}}(k', \lambda_0) dk' \\ + \frac{\cos k}{c} K_{1/2}(\sin k - \lambda_0). \end{aligned} \quad (47)$$

Clearly the holon-holon excitation always has a gap $\Delta_g = 2\varepsilon_h(k_F) + \Delta(U, k_F)$, which exists at any filling. However, the gapless modes of holon-antiholon are available to carry charges for away from quarter-filling. It is easy to shown by calculating Eq. (32) that both holon-antiholon and holon-holon excitations are SU(4) singlet; consequently, they carry neither spins nor orbitals.

IX. DISCUSSIONS

In the above we have presented an extensive discussion on one-dimensional Hubbard-like model with SU(4) symmetry, where the sites are restricted to be occupied by at most two electrons. The model was proposed to describe electrons with twofold orbital degeneracy. The symmetries and some general features were given previously.¹⁴ We focused on the one-dimensional case in this paper and studied the ground state and excitations by means of an exact solution. The excitation energies of the excited states are just sums of some particular terms related to quasiparticles. It provides an explicitly interpretation of the separation of charge excitations and spin-orbital excitations. Among the charge excitations, there are gapless holon-antiholon excitations and holon-holon excitations with gaps. Both excitations carry neither spins nor orbitals. They are completely decoupled from the spin-orbital degree of freedom. The holons and antiholons move throughout the crystal at less than quarter-filling. Various excitations in spin-orbital sector consist of three basic modes which are created by the holes in the three rapidities for the spin-orbital double. That means there are three kinds of quasiparticles that carry spins and orbitals, i.e., two quadruplets transforming according to the fundamental or conjugate representation, and one hexaplet forming the six-dimensional representation. These elementary excitations in spin-orbital sector are gapless.

As the on-site coupling in our model is isotropic for spin-orbital labels, there is no separation between spin and orbital. A complete separation between the spin waves and orbital waves is expected to occur after taking account of the contributions of Hund’s rule. This needs to introduce anisotropic on-site coupling in the spin and orbital configuration.

For finite N and L we plotted the excitation spectra by solving the Bethe-ansatz equation numerically. The variation of the quantum number for excited states from that for the ground state, and their changes from integer to half-integers (or vice versa) were shown in each cases. It provides a concrete interpretation about the collective excitations for the orbital degenerate electronic systems. The overall structure of the spectra for spin-orbital excitations changed greatly with respect to the changes of the correlation strength. The lowest excitation energy and the whole pattern are increased when the correlation strength decreased. However, the

“particle”-hole excitation spectrum does not change much from the strong to the weak correlation strengths.

In the quarter-filled band for strong repulsive on-site coupling, there will be no double occupied sites. In this case the total wave function will be separated into a product of Slater determinant of N “spinless” fermions and part of $SU(4)$ Heisenberg magnets. The direct results from the Bethe-ansatz equation by taking strong-coupling limit agree with it exactly.

It is worthwhile to mention that the model studied here is not a direct $SU(4)$ generalization of the Hubbard model, since a projection onto the subspace of states having at most two electrons at each site was made to render it solvable through the Bethe ansatz. The two models are therefore not expected to share the same physical features. Considering the

self-conjugate representation on a bipartite lattice in the strong repulsive coupling limit, Ref. 31 clarified the system is dimerized with doubly degenerate singlet ground state and indicated the excitations are massive symmetry and antisymmetric kinks. In our present model, however, the local states on each site carry out the fundamental representation of $SU(4)$.

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