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Theory of electrons with orbital degeneracy

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The Hubbard model for electrons with orbital degeneracy is shown to have an underlying $SU_d(4)$ symmetry of spin-orbital double. A hidden charge $SU_c(4)$ symmetry is exposed and an extended Lieb-Mattis transformation, which maps these two symmetries into each other, is given. On the basis of elementary degenerate perturbative theory, it is shown that the system with strong repulsive coupling is equivalent to a SO(6) Heisenberg magnet at half-filling and a SU(4) one at quarter-filling. The band is half-filled at all temperature for $\mu=3U/2$. The features of ground-state and low-lying excitations in one dimension are indicated according to exact solutions.

I. INTRODUCTION

There has been much interest in the study of correlated electrons in the presence of orbital degree of freedom[1] because the orbital degree of freedom plays an important role in understanding the phenomena, such as metal-insulator transitions, high-temperature superconductivity, and colossal magnetoresistance. The orbital degree of freedom is relevant to many transitional-metal oxides.[2–6] It may be also relevant to some C_{60} materials[7] and samples of artificial quantum dot arrays.[8] For a theoretical understanding of the observed unusual properties, a SU(4) theory describing spin systems with orbital degeneracy was proposed.[9] There were also numerical[10] and perturbative[11] studies of one-dimensional models for these systems. The ground-state phase diagrams for the system with a symmetry breaking of $SU(4)\rightarrow SU(2)\times SU(2)$ were discussed.[11,12] Experimentally, the phase separation[13] was observed. Due to the rapid developments in experiments where the metal ions have orbital degeneracy in addition to spin degeneracy, a theoretical study of such a system, by taking account of the kinetic terms caused by nearest-neighbor hopping, becomes indispensable.

In this paper we study a Hubbard-type model for electrons with orbital degeneracy. In Sec. II, we show that the model has an underlying SU(4) symmetry of spin-orbital double. The spin and orbital operators are related to the SU(4) generators, which will be helpful for further studies on the magnetization. A hidden charge SU(4) structure is exposed in Sec. III. An extended Lieb-Mattis transformation, which maps those two SU(4) symmetries into each other, is also presented. From a basic relation derived from particle-hole transformation, we show that the band is half-filled at all temperatures when the chemical potential equals $3U/2$. In Sec. IV, two kinds of ''partially negative U'' models are introduced and analyzed according to the strategy of Ref. 14. Three basic excitation modes are shown to exist in the spin-orbital sector. In Sec. V, with the help of the partially attractive models, we study the repulsive large U model on the basis of elementary degenerate perturbative theory. It is shown that the effective Hamiltonian with strong repulsive coupling at half-filling is equivalent to the Hamiltonian of a SO(6) Heisenberg model, and that at quarter-filling it is equivalent to the Hamiltonian of a SU(4) Heisenberg models. In Sec. VI, several possibilities of SU(4) symmetry breaking are given. In Sec. VII, we summerize the main results and discuss the agreement with exact solutions in one dimension by describing the features of ground state and low-lying excitations.

II. UNDERLYING SU(4) SYMMETRY

We consider electrons with doubly 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

$$|1\rangle=|\ \begin{matrix}\uparrow\\ -\end{matrix}\ \rangle,\quad |2\rangle=|\ \begin{matrix}\downarrow\\ -\end{matrix}\ \rangle,$$

$$|3\rangle=|\ \begin{matrix}-\\ \uparrow\end{matrix}\ \rangle,\quad |4\rangle=|\ \begin{matrix}-\\ \downarrow\end{matrix}\ \rangle. \tag{1}$$

We use 1, 2, 3, and 4 to label these states from now on. Let us consider the Hamiltonian of electrons with twofold orbital degeneracy on a lattice

$$H=-t\sum_{\substack{a\\ \langle x,x'\rangle}} C_a^\dagger(x)C_a(x')+\sum_{\substack{a<a'\\ x}} U_{aa'}n_a(x)n_{a'}(x), \tag{2}$$

where x's identify the lattice site, and $a,a'=1,2,3,4$ specify the spin and orbital as defined in the above. The $C_a^\dagger(x)$ creates a fermion of state $|a\rangle$ located at x site and $n_a(x)$ is the corresponding number operator. Equation (2) is the Hamiltonian for four-component systems, and there were various discussions on a multicomponent Hubbard model in one dimension.[15,16] We remark that the four-component Hamiltonian can also describe either a spin-3/2 system[17] or a toy model of proton and neutron system with on-site strong interaction. In the terminology of group theory, the former forms a high-dimensional (here it is four dimensional) representation of A_1 Lie algebra, while the later forms the fundamental representation of D_2 Lie algebra. The physics that Eq. (2) describes will be precise only when the representa-

tion space for the internal degree of freedom is specified. It refers to the spin and orbital in our present discussion.

We can verify that the Hamiltonian (2) with $U_{aa'}=U$ commutes with following 15 operators,

$$O_m=\frac{1}{2}\sum_x [C_m^\dagger(x)C_m(x)-C_{m+1}^\dagger(x)C_{m+1}(x)],$$

$$E_{\alpha_m}=\sum_x C_m^\dagger(x)C_{m+1}(x),$$

$$E_{-\alpha_m}=(E_{\alpha_m})^\dagger, \quad m=1,2,3, \tag{3}$$

and additionally, $E_{\alpha_1+\alpha_2}=[E_{\alpha_1},E_{\alpha_2}]$, $E_{\alpha_2+\alpha_3}=[E_{\alpha_2},E_{\alpha_3}]$, $E_{\alpha_1+\alpha_2+\alpha_3}=[E_{\alpha_1+\alpha_2},E_{\alpha_3}]$, $E_{-\alpha_1-\alpha_2}=(E_{\alpha_1+\alpha_2})^\dagger$, $E_{-\alpha_2-\alpha_3}=(E_{\alpha_2+\alpha_3})^\dagger$, and $E_{-\alpha_1-\alpha_2-\alpha_3}=(E_{\alpha_1+\alpha_2+\alpha_3})^\dagger$, here α_m's stand for the simple roots of A_3 Lie algebra. These operators precisely obey the commutation relations of A_3 Lie algebra.[18] The Hamiltonian (2) with $U_{aa'}=U$ is invariant under any global SU(4) rotation. We denote this underlying symmetry of spin-orbital double by $\mathrm{SU}_d(4)$. There are several equivalent ways to write out the generators of the Lie algebra. We adopt the Chevalley basis because physical quantities can be conveniently evaluated in this basis. Because the A_3 Lie algebra is of rank three, i.e., three generators in its Cartan subalgebra, there are three conserved quantum numbers that label the eigenstates. In terms of these O_m's that commute to each other, the z components of both total spin S^z_{tot} and total orbital T^z_{tot} are given by

$$S^z_{\mathrm{tot}}=O_1+O_3,$$

$$T^z_{\mathrm{tot}}=O_1+2O_2+O_3. \tag{4}$$

They are useful for evaluating magnetizations once the ground state in the presence of magnetic field is solved.

III. HIDDEN CHARGE SU(4) SYMMETRY

In addition to the above symmetry, one may easily think of the U(1) charge invariance.[19] Moreover, there exists a larger hidden symmetry in the present model on a bipartite lattice, we call charge $\mathrm{SU}_c(4)$ symmetry. Their Chevalley bases are given by

$$Q_m=\frac{1}{2}\sum_x [C_m^\dagger(x)C_m(x)+C_{m+1}^\dagger(x)C_{m+1}(x)-1],$$

$$F_{\alpha_1}=\sum_x e^{i\boldsymbol{\pi}\cdot\mathbf{x}}C_1^\dagger(x)C_2^\dagger(x),$$

$$F_{\alpha_2}=\sum_x e^{i\boldsymbol{\pi}\cdot\mathbf{x}}C_2(x)C_3(x),$$

$$F_{\alpha_3}=\sum_x e^{i\boldsymbol{\pi}\cdot\mathbf{x}}C_3^\dagger(x)C_4^\dagger(x), \quad m=1,2,3, \tag{5}$$

where $\boldsymbol{\pi}=(\pi,\pi,\ldots)$, and the Q_m's are generators of Cartan subalgebra of the A_3 Lie algebra. The other generators are given by standard relations that we demonstrated previously when observing the underlying $\mathrm{SU}_d(4)$ symmetry. The charge $\mathrm{SU}_c(4)$ symmetry is not only valid for the Hamiltonian (2) at high-energy scale $t\gg U$ but also valid for a kind of on-site coupling that we are going to show. Considering $U_{13}=U_{24}=-U$, while $U_{ab}=U$ for the other subscripts, and taking account of the chemical potential term in the Hamiltonian, we obtain

$$[H',F_{\alpha_m}]=(-1)^m(2\mu-U)F_{\alpha_m},$$

$$H'=H-\mu\sum_{x,a} n_a(x). \tag{6}$$

The commutators between H' and Q_m's always vanish. Apparently, the model has a charge $\mathrm{SU}_c(4)$ symmetry when $\mu=U/2$. The mentioned requirement for the sign of the on-site coupling constants is unnecessary for the traditional Hubbard model, which has a hidden charge SU(2) symmetry[20] because there is only one constant for coupling of spin up and spin down.

Equation (6) implies that the raising operators F_{α_m} of the charge $\mathrm{SU}_c(4)$ create some pair of electrons to a given state. Precisely, F_{α_1} or F_{α_3} creates a double occupancy of spin singlet, however, $F_{-\alpha_2}$ creates a double occupancy of spin triplet. These operators provide mappings between states in distinct sectors of different electron numbers.

There exists an extended Lieb-Mattis transformation:

$$C_i(x)\mapsto e^{i\boldsymbol{\pi}\cdot\mathbf{x}}C_i^\dagger(x), \quad i=2,4,$$

$$C_j(x)\mapsto C_j(x), \quad j=1,3, \tag{7}$$

which maps $\mathrm{SU}_c(4)$ into $\mathrm{SU}_d(4)$ and vice versa. The application of particle-hole transformation gives rise to a basic relation[16] for bipartite lattice:

$$E(N_a,U)=E(L-N_a,U)+3(N-2L)U, \tag{8}$$

where L is the total number of lattice sites and N the total number of electrons. Using this relation we can derive a relation for the thermal average:

$$\langle\hat{N}\rangle_{\mu,T}=4L-\langle\hat{N}\rangle_{3U-\mu,T}, \tag{9}$$

where $\hat{N}=\Sigma_{x,a}n_a(x)$. As a result, the band is half-filled at all temperature when $\mu=3U/2$.

IV. PARTIALLY ATTRACTIVE MODELS

The magnitude and sign of the on-site coupling may vary from system to system. For isotropic pure attractive coupling $U_{ab}=U<0$, the unperturbed ground state has $N/4$ of the sites occupied by ''quaternarys.'' The ground state is degenerate when $N/4<L$ because the energy $3NU/2$ is independent of which sites are occupied. As a generalization of a Cooper pair, the quaternary might have abundant physical meanings. It can form a SU(4) singlet for $U_{ab}=U$. It can also form either two pairs being spin singlet but orbital triplet or that being spin triplet but orbital singlet, or form a ''resonance'' state being alternations of them depending on the symmetries remaining in a general U_{ab}. For example, a

triplet-pairing supper conductivity model was discussed[21] by a particular choice of U_{ab}.

We have particular interests in two kinds of partially attractive on-site couplings: (i) $U_{13}=U_{24}=-U$, while $U_{ab}=U$ for the others and (ii) $U_{12}=U_{23}=U_{13}=-U$, while $U_{14}=U_{24}=U_{34}=U$. Here $U<0$ for both cases. Let us consider these two cases, respectively.

In case (i), the local favorite states in energy are a quaternary and four types of pairs. The quaternary is an instantaneous state that may separate into two pairs randomly because there is no difference in energy between them. The hoping terms in the Hamiltonian split the degeneracy to form a band of charge-density wave states where the quaternary and pairs move from site to site. As is known in the absence of orbital degree of freedom[14] that the spin-density excitation turns over a spin to break a pair at a cost $|U|$ in energy. The spin-orbital-density excitation, however, turns over either a spin or a orbital, which results in three basic processes. In addition to the process of breaking a pair at the cost $|U|$ in energy, one process transmits a favorite pair into an unfavorite pair at the cost $2|U|$ in energy. The process of breaking a quaternary into a trinity and a single costs $|U|$. Breaking a quaternary into two unfavorite pairs will cost $4|U|$, which is not a basic process because it can be represented by two processes of the second type. All the other complicated processes can always be represented as a composition of those three basic processes. Thus we believe that there are three elementary quasiparticles involved in the excitations in the spin-orbital sector.

For the case (ii), the favorite states in energy are two types of trinitys and three types of pairs. The charge-density wave states arising from the hopping terms are of the movement of the trinitys and pairs from site to site. The spin-orbital-density excitation that turns over either a spin or an orbital involves three basic processes that cost $|U|$, $2|U|$, and zero in energy. Therefore, there are three elementary quasiparticles, in which a gapless mode is expected to exist.

With the help of the above discussions we are now in the position to employ elementary degenerate perturbation theory for more quantitative formulations. It is sufficient for calculating the low-temperature properties to consider the lowest band only. For those two types of partially attractive on-site couplings that were discussed previously, all electrons remain in either the favorite pairs, trinitys, or quaternary in the lowest band. Because it breaks pairs, trinitys, or quaternary, the perturbation part (the hopping term) has vanishing first-order matrix elements. Thus it must be calculated to second order by considering the virtual transitions into the next band. After some algebra one gets,

$$(\varepsilon-\varepsilon_0)a_g=\sum_{g'}\langle g|H_t^2|g'\rangle a_{g'},$$

$$a_g=\frac{\langle g|H_t|\psi\rangle}{\varepsilon-\varepsilon_0}, \tag{10}$$

where $|g\rangle$ denotes various degenerate states of the unperturbed ground states, i.e., $H_U|g\rangle=\varepsilon_0|g\rangle$. H_t stands for the hopping term and H_U for the interaction term of Eq. (2). After the similar calculation as in Ref. 14, we obtain the effective Hamiltonians that will be helpful for studying the repulsive model.

V. EFFECTIVE MODELS OF STRONG REPULSIVE COUPLING

We now study the repulsive model $U_{ab}=U>0$. First we consider the half-filled band ($N=2L$). For the ground state in this case, every site is doubly occupied by electrons. The excitation of charge-density waves brings about inevitably a triple occupancy of site at a cost of $|U|$ in energy at least. By making a particle-hole canonical transformation:

$$C_i(x)\mapsto C_i^\dagger(x),\quad i=2,4,$$

$$C_j(x)\mapsto C_j(x),\quad j=1,3,$$

the Hamiltonian becomes

$$\tilde{H}=t\sum_{\langle x,x'\rangle}^{a}(-1)^a C_a^\dagger(x)C_a(x')+U\sum_{\substack{a<a'\\ x}}(-1)^{a+a'}n_a(x)n_{a'}(x)+\sum_{x,a}V_a[n_a(x)+\tfrac{1}{2}], \tag{11}$$

where $V_a=[1-3(-1)^a]U/2$. Clearly, the repulsive on-site coupling becomes the partially attractive case (i), which we already discussed. In the unperturbed states, the sites originally occupied by

$$|\ \downarrow\ —\ \rangle$$
$$|\ —\ \downarrow\ \rangle$$

become empty, whereas those occupied by

$$|\ \uparrow\ —\ \rangle$$
$$|\ —\ \uparrow\ \rangle$$

are replaced by

$$|\ \uparrow\ \downarrow\ —\ —\ \rangle$$
$$|\ —\ —\ \uparrow\ \downarrow\ \rangle\ .$$

The other four kinds of double occupancies exchanged their positions. The degenerate perturbation theory can now be used in the same way as was done in the partially attractive models that we considered before. After reversing the canonical transformation, we obtain the effective Hamiltonian as follows

$$H_{\rm eff}=\frac{t^2}{|U|}\sum_{\langle x,x'\rangle}[h(x,x')-\tfrac{3}{4}],$$

$$h(x,x')=\sum_{mn}g^{mn}O_m(x)O_n(x')+\sum_{\alpha\in\Delta}E_\alpha(x)E_{-\alpha}(x'), \tag{12}$$

where Δ denotes the set of roots of the A_3 Lie algebra, $E_\alpha(x)$ and $O_m(x)$ are generators of the Lie algebra given by $E_{\alpha_m}(x)=C_m^\dagger(x)C_{m+1}(x)$, and $O_m(x)=C_m^\dagger(x)C_m(x)$

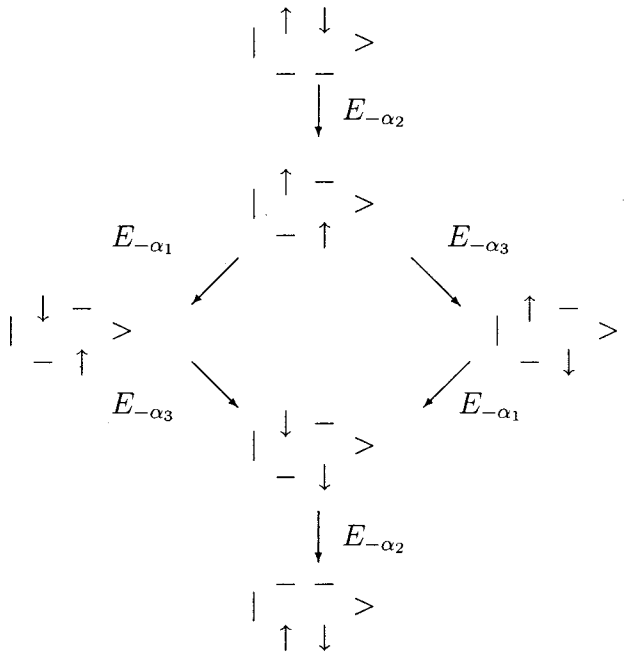

FIG. 1. The weight diagram of the representation of SO (6).

$-C^{\dagger}_{m+1}(x)C_{m+1}(x)$, with $m=1,2,3$. These operators generate the whole states from the highest weight state

$$|\ \begin{matrix}\uparrow & \downarrow\\ - & -\end{matrix}\ \rangle$$

as shown in Fig. 1, where the x in $E_{\alpha}(x)$ is omitted. Those states form the vector representation of A_3 (isomorphic to D_3) Lie algebra. Whence it is a $SO(6)$ Heisenberg model.

As to the case of quarter-filling ($N=L$) with repulsive on-site coupling, the ground state has one electron on each site. The excitation of charge-density waves brings about double occupancy of sites indispensably and costs energy of $|U|$ at least. It is again interesting to make a canonical transformation

$$C_4(x)\mapsto C^{\dagger}_4(x),\quad C_l(x)\mapsto C_l(x),\quad l=1,2,3.$$

Consequently, the sites at first occupied by

$$|\ \begin{matrix}- & \\ \downarrow & \end{matrix}\ \rangle$$

are now empty whereas the other sites are doubly occupied, i.e., by either

$$|\ \begin{matrix}\uparrow & - \\ - & \downarrow\end{matrix}\ \rangle,\quad |\ \begin{matrix}\downarrow & - \\ - & \downarrow\end{matrix}\ \rangle,$$

or

$$|\ \begin{matrix}- & - \\ \uparrow & \downarrow\end{matrix}\ \rangle .$$

The repulsive on-site coupling becomes the partially attractive case (ii) which we discussed previously. Again, the degenerate perturbation theory can be applied as before. The effective Hamiltonian is obtained as a SU(4) Heisenberg model. The local states form the spinor representation of A_3 Lie algebra, and their relations in the weight diagram were given[9] by

$$|\ \begin{matrix}\uparrow & \\ - & \end{matrix}\ \rangle \xrightarrow{E_{-\alpha_1}} |\ \begin{matrix}\downarrow & \\ - & \end{matrix}\ \rangle \xrightarrow{E_{-\alpha_2}} |\ \begin{matrix}- & \\ \uparrow & \end{matrix}\ \rangle \xrightarrow{E_{-\alpha_3}} |\ \begin{matrix}- & \\ \downarrow & \end{matrix}\ \rangle .$$

The evaluation of correlation function in the strong-coupling limit will be considerably simple by means of the corresponding effective Hamiltonians.

VI. SYMMETRY BREAKING

The underlying $SU_d(4)$ symmetry is fulfilled for the isotropic on-side coupling $U_{aa'}=U$. There is no phase separation between spin wave and orbital wave at the SU(4) point. A complete separation is expected to occur after the anisotropic on-side couplings in the spin-orbital configuration are introduced. Since the ''diagonal'' coupling U_{aa} has no physical contribution due to fermionic wave function vanishing when two electrons at the same site have the same SU(4) state (i.e., $a=a'$), we can introduce six parameters $v_{ab}(a<b)$ to break down the SU(4) symmetry, i.e., $U_{aa'}=U+v_{aa'}$.

It is not difficult to find the possible symmetry breakings by calculating the commutation relations between the Hamiltonian and the SU(4) generators. There are two ways to break the SU(4) down to the SU(3)$\times U(1)$. For $v_{12}=v_{13}=v_{23},v_{14}=v_{24}=v_{34}$ (or $v_{12}=v_{13}=v_{14},v_{23}=v_{24}=v_{34}$), the residue symmetry SU(3)$\times U(1)$ is generated by $\{O_1,O_2,E_{\pm\alpha_1},E_{\pm(\alpha_1+\alpha_2)},E_{\pm\alpha_2},O_3\}$ (or by $\{O_1,O_2,O_3,E_{\pm\alpha_2},E_{\pm(\alpha_2+\alpha_3)}E_{\pm\alpha_3}\}$). This is a two-parameter hierarchy. For a three-parameter hierarchy, $v_{13}=v_{23}=v_{14}=v_{24}$, the residue symmetry is SU(2)$\times$SU(2)$\times U(1)$ generated by $\{O_1,E_{\pm\alpha_1},O_3,E_{\pm\alpha_3},O_2\}$. When $v_{12}=v_{13}$ and $v_{24}=v_{34}$, the residue symmetry becomes SU(2)$\times U(1)\times U(1)$ with $\{O_2,E_{\pm\alpha_2},O_1,O_3\}$ as its generators. This is obviously a four-parameter hierarchy. Furthermore, if either $v_{12}\neq v_{13}$ or $v_{24}\neq v_{34}$ the previous SU(2)$\times U(1)\times U(1)$ will be broken to the $U(1)\times U(1)\times U(1)$ generated by $\{O_1,O_2,O_3\}$.

As the SU(4) Lie algebra is of rank 3 (there are three generators in its Cartan subalgebra) the Zeemann-like interactions with external fields reads

$$H_Z=\sum_{x,m} h_m O_m(x),$$

where $m=1,2,3$. In general, it breaks the symmetry down to the minimum residue symmetry $U(1)\times U(1)\times U(1)$. However, if $h_2=h_3=0$, it regains a SU(2)$\times U(1)\times U(1)$ generated by $\{O_1,O_2,O_3,E_{\pm\alpha_3}\}$. Similarly another SU(2)$\times U(1)\times U(1)$ generated by $\{O_1,E_{\pm\alpha_1}O_2,O_3\}$ regains for $h_1=h_2=0$.

Since it is the SU(4) singlet, the ground state is invariant under any SU(4) rotations. Except for the singlet-excitation

and the pure charge-excitation states, which are still invariant under SU(4) rotation, the other multiplet-excitation states vary. For the system with $N=4n$, there is always an axis in flavor space along which the multiplet-excitation states are invariant under a rotation of 2π.

VII. DISCUSSIONS

We have shown both the underlying and hidden symmetries of a Hubbard model with orbital degeneracy. We derived the effective Hamiltonian in strong repulsive coupling for both half-filled and quarter-filled band. The band is half-filled at all temperature if the chemical potential is $3U/2$. It is shown that there are three elementary modes involved in the excitations in the spin-orbital sector.

We did not specify the dimensions in the above discussions on the symmetries of the system and its low-temperature effective Hamiltonians. It is interesting to consider a one-dimensional case[22] because the exact solution in one dimension always provides nonperturbative features. The exact solution can be obtained by means of Bethe-Yang ansatz similar to Ref. 23 if states with site occupation of more than two are excluded.[24] Although the multicomponent generalizations of Hubbard model in one dimension were explored by several authors[15,16] in various aspects, the relationship between the enlarged internal degree of freedom and concrete physics was not clearly exhibited. It is convenient to take a thermodynamics limit to the Bethe ansatz equation by introducing density distributions of the quasimomentum k and that of three rapidities for the spin-orbital double [we call SU(4) flavor]. The ground state being of real roots and no holes is a SU(4) singlet, accordingly, both spin and orbital are in ''antiferromagnetic'' states. The features of low-lying excitations are studied by considering the contributions of holes and complex 2 strings. An important consequence is that the excitations in charge sector and flavor sector are separated. In charge sector the elementary modes are holon and antiholon (particle), and the real excitations are gapless particle-holon and gapful holon-holon excitations etc. There are three types (in agreement with the above general analyses in any dimension) of flavorons as the elementary excitation modes in flavor sector, namely, two quadruplets carrying spin-1/2 and orbital-1/2 that form, respectively, the fundamental representation and the conjugate representation of SU(4); a hexaplet carrying either spin-1 or orbital-1 that forms a six-dimensional representation moreover. These flavorons compound to constitute real excitations. The details of one-dimensional model are given in another paper.[22]

We also analyzed the possible symmetry breakings caused either by extending the model to anisotropic on-side coupling or by introducing an external field. Our analyses based on the Hamiltonian structure will be helpful for further discussions on the phase diagram by means of numerical density-matrix renormalization group.

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$$S^z=\sum_x \sum_{n=1}^{4} (n-5/2)C_n^\dagger(x)C_n(x),$$

$$S^+=\sum_x \sum_{m=-1}^{1} \sqrt{4-|m|}\,C_{3+m}^\dagger(x)C_{2+m}(x),$$

$$S^-=(S^+)^\dagger,$$

they obey $[S^+,S^-]=2S^z$.

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