Phase diagram and symmetry breaking of an SU(4) spin-orbital chain in a generalized external field

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The ground-state phases of a one-dimensional SU(4) spin-orbital Hamiltonian in a generalized external field are studied on the basis of the Bethe-ansatz solution. Introducing three Landé g factors for spin, orbital, and their products in the SU(4) Zeeman term, we systematically discuss various symmetry breakings. The magnetization versus external field is evaluated by solving the Bethe-ansatz equations numerically. The phase diagrams corresponding to distinct residual symmetries are given by means of both numerical and analytical methods.

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I. INTRODUCTION

There has been much interest in the study of spin models with orbital degeneracy^{1–10} due to experimental progress related to many transition-metal and rare-earth compounds such as LaMnO₃ and CeB₆, and the perovskite lattice, as in KCuF₃. 5,6 Those systems involve an orbital degree of freedom in addition to that of spin. Almost three decades ago, Kugel and Khomskii¹¹ pointed out the possibility of orbital excitations in this system. As a model system, it exhibits some fascinating physical features that do not occur in the absence of the orbital degree of freedom. The isotropic case of a spin system with orbital degeneracy was shown to have an enlarged SU(4) symmetry, and the one-dimensional model is known to be exactly solvable.^{2,12} Materials related to spin-orbital systems in one dimension include quasi-onedimensional tetrahis-dimethylamino-ethylene C_{60} , $^{1\bar{3}}$ artificial quantum dot arrays, 14 and degenerate chains in Na₂Ti₂Sb₂O and Na₂V₂O₅ compounds. 15,16 It is therefore worthwhile to systematically study the features of the model. A theoretical study² found a strong interplay of the orbital and spin degrees of freedom in the excitation spectra. It has been noticed that the presence of the orbital degree of freedom may result in various interesting magnetic properties. Applying a conventional magnetic field, the spin-orbital chain with SU(4) symmetry is shown to reduce to a model with orbital SU(2) symmetry⁹ in the ground state. Recently, we showed that the magnetization process becomes more complicated if the contribution of the orbital sector is taken into account. 10 We explained that the competition between spin and orbital degrees of freedom leads to an orbital antipolarization phase. However, the external field we introduced in Ref. 10 is not the most general one for SU(4) systems. There is both anisotropy in spin-orbital superexchange and John-Teller distortion that break the degeneracy of the e_g orbital;⁵ this allows us to consider the most generalized external fields in the following.

In this paper, we study an SU(4) spin-orbital chain in the presence of a generalized external field on the basis of its

Bethe-ansatz solution. Our paper is organized as follows. In Sec. II, we introduce the Bethe-ansatz solution and the Zeeman-like term which is going to be added to the original SU(4) Hamiltonian. In Sec. III, we give some useful remarks about the quantum number configurations of the ground state in the presence of an external field that is characterized by three parameters. We also demonstrate the thermodynamic limit of the Bethe-ansatz equation and briefly present the dress-energy description of the ground state in the presence of an external field. In Sec. IV, we study the magnetization properties of a Hamiltonian in the regime with oneparameter symmetry breaking. In Sec. V, we study both the magnetization and the phase diagram in regimes with twoparameter symmetry breaking. Various phases and quantum phase transitions are investigated by both numerical calculation and analytical formulation. Concerning the various phases, we give a detailed explanation in terms of group theory. Section VI includes a summary.

II. THE MODEL AND ITS SOLUTION

We start from the following Hamiltonian:

$$\mathcal{H} = \sum_{j=1}^{N} \left[\left(2T_j \cdot T_{j+1} + \frac{1}{2} \right) \left(2S_j \cdot S_{j+1} + \frac{1}{2} \right) - 1 \right], \quad (1)$$

where S_j and T_j denote the spin and orbital operators at site j, respectively. Both of them are generators of the SU(2) group characterizing the spin and orbital degrees of freedom of outer shell electrons in some transition-metal oxides in the insulating regime. The coupling constant is set to unity for simplicity. It has been pointed out that the above Hamiltonian possesses an enlarged SU(4) symmetry¹ rather than SU(2)×SU(2) symmetry.

The four states that carry the fundamental representation of the SU(4) group are denoted by

$$|\uparrow\rangle = |1/2, 1/2\rangle, \quad |\bar{\uparrow}\rangle = |1/2, -1/2\rangle,$$
$$|\downarrow\rangle = |-1/2, 1/2\rangle, \quad |\bar{\downarrow}\rangle = |-1/2, -1/2\rangle. \tag{2}$$

TABLE I. The eigenvalues of S^z , T^z , U^z and the z component of O_1^z , O_2^z , O_3^z for the four basis states [Eq. (2)].

State	S^z	T^z	U^z	O_1^z	O_2^z	O_3^z
$ \uparrow\rangle$	1/2	1/2	1/2	1/2	0	0
$ \uparrow\rangle$	1/2	-1/2	-1/2	-1/2	1/2	0
11)	-1/2	1/2	-1/2	0	-1/2	1/2
$ \overline{\downarrow}\rangle$	-1/2	-1/2	1/2	0	0	-1/2

These bases are labeled by the eigenvalues of S^z and T^z , i.e., $|S^z,T^z\rangle$. As the su(4) Lie algebra is of rank 3, there exists a third generator $2S^zT^z$ which is simply the anisotropic hybridized spin-orbital interaction and possesses a simultaneous eigenvalue together with S^z and T^z . For convenience, we denote this new generator by U^z hereafter. In the terminology of group theory, however, the quadruplet can also be labeled by the weight vectors defined by eigenvalues of O_1^z , O_2^z , and O_3^z that constitute the Cartan subalgebra of the su(4) Lie algebra. Here we adopt the Chevalley basis because the physical quantities can be conveniently expressed in this basis.

The eigenvalues of S^z , T^z , U^z as well as that of O_1^z , O_2^z , O_3^z are given in Table I. The relation between these two bases reads²

$$S^{z} = O_{1}^{z} + 2O_{2}^{z} + O_{3}^{z},$$

$$T^{z} = O_{1}^{z} + O_{3}^{z},$$

$$U^{z} = O_{1}^{z} - O_{3}^{z}.$$
(3)

The present model (1) has been solved by Bethe-ansatz method.^{2,12} Its energy spectrum is given by

$$E_0(M, M', M'') = -\sum_{a=1}^{M} \frac{1}{1/4 + \lambda_a^2},$$
 (4)

where the λ 's are solutions of the following coupled transcendental equations:

$$2\pi I_{a} = N\theta_{-1/2}(\lambda_{a}) + \sum_{a'=1}^{M} \theta_{1}(\lambda_{a} - \lambda_{a'})$$

$$+ \sum_{b=1}^{M'} \theta_{-1/2}(\lambda_{a} - \mu_{b}),$$

$$2\pi J_{b} = \sum_{a=1}^{M} \theta_{-1/2}(\mu_{b} - \lambda_{a}) + \sum_{b'=1}^{M'} \theta_{1}(\mu_{b} - \mu_{b'})$$

$$+ \sum_{c=1}^{M''} \theta_{-1/2}(\mu_{b} - \nu_{c}),$$

$$2\pi K_{c} = \sum_{b=1}^{M'} \theta_{-1/2}(\nu_{c} - \mu_{b}) + \sum_{c'=1}^{M''} \theta_{1}(\nu_{c} - \nu_{c'}),$$

where $\theta_{\alpha}(x) = -2 \tan^{-1}(x/\alpha)$. λ , μ , and ν are rapidities related to the three generators of the Cartan subalgebra of the su(4) Lie algebra. The quantum numbers $\{I_a, J_b, K_c\}$ specify a state in which there are N-M sites in the state $|\uparrow\rangle$, M-M' in $|\bar{\uparrow}\rangle$, M'-M'' in $|\downarrow\rangle$, and M'' in $|\downarrow\rangle$. Hence the z components of total spin, orbital, and U^z are obtained as $S_{\text{tot}}^z = N/2 - M'$, $T_{\text{tot}}^z = N/2 - M + M' - M''$, and $U_{\text{tot}}^z = N/2 - M + M''$.

In the present SU(4) model, a three-parameter external field (h_1, h_2, h_3) can be introduced to express the most general Zeeman-like energy:

$$\mathcal{H}_{\text{Zee}} = \sum_{m}^{3} h_{m} O_{m}^{z}. \tag{6}$$

To make the physics clearer, we reselect the parameters to write the effective magnetization \mathcal{M}^z as

$$\mathcal{M}^z = g_s S_{\text{tot}}^z + g_t T_{\text{tot}}^z + g_u U_{\text{tot}}^z, \tag{7}$$

where g_s , g_t , and g_u are generalized Landé g factors for S^z , T^z , and U^z , respectively. Equation (7) can be expressed in terms of the number of rapidities,

$$\mathcal{M}^{z} = \frac{N}{2} (g_{s} + g_{t} + g_{u}) - M(g_{t} + g_{u}) - M'(g_{s} - g_{t})$$
$$-M''(g_{t} - g_{u}). \tag{8}$$

Because the Zeeman-like term commutes with the SU(4) Hamiltonian (1), the energy spectrum in the presence of an external field is simply related to the energy spectrum in the absence of the external field h:

$$E(h, M, M', M'') = E_0(M, M', M'') - h\mathcal{M}^z, \tag{9}$$

where $E_0(M, M', M'')$ is determined by Eqs. (5). Obviously, the application of an external field with a different magnitude just brings about various level crossings.

In terms of O_1 , O_2 , and O_3 , the magnetization (7) becomes

$$\mathcal{M}^{z} = (g_{s} + g_{t} + g_{u})O_{1}^{z} + 2g_{s}O_{2}^{z} + (g_{s} + g_{t} - g_{u})O_{3}^{z},$$
(10)

which breaks SU(4) symmetry down to various lower symmetries depending on the distinct regions in parameter space.

III. THE GROUND-STATE CONFIGURATION

Based on the Bethe-ansatz solution of the model, we first give the quantum number description of the ground state, which is useful for numerical calculation. We also give the dress-energy description for the ground state and propose the conditions that determine quantum phase transitions, which is useful for analytic study.

It is known^{1,2} that the ground state of the Hamiltonian (1) is an SU(4) singlet for the case of N=4n. The configuration of the quantum number for the ground state $\{I_a, J_b, K_c\}$ (a=1,2,...,3n; b=1,2,...,2n; c=1,2,...,n) is consecutive integers (or half integers) arranged symmetrically around zero. In the presence of a magnetic field, however, the Zeeman

term brings about level crossings, and the state with M = 3n, M' = 2n, M'' = n is no longer the ground state. Therefore the numbers M, M', M'' for the lowest-energy state are related to the magnitude of the applied external field.

In order to solve the Bethe-ansatz equation numerically, we need to determine the possible configurations of quantum numbers for given values of M, M', and M''. The property of the Young tableau requires that Max(M) = 3N/4, Max(M') = N/2, Max(M'') = N/4, and $N - M \ge M - M'$ $\ge M' - M'' \ge M''$ for a given N. Then one is able to analyze the change of energy level for each state, which determines the true ground state for a given external field. One can also calculate the magnetization by Eq. (8).

In the thermodynamic limit, the energy (9) is expressed in terms of the densities of the rapidities,

$$E/N = -\frac{h}{2} (g_s + g_t + g_u) + \int_{-\lambda_0}^{\lambda_0} \sigma(\lambda) [-2\pi K_{1/2}(\lambda)] + (g_t + g_u)h d\lambda + (g_s - g_t)h \int_{-\mu_0}^{\mu_0} \omega(\mu)d\mu + (g_t - g_u)h \int_{-\nu_0}^{\nu_0} \tau(\nu)d\nu.$$
(11)

These densities satisfy the following coupled integral equations:

$$\sigma(\lambda) = K_{1/2}(\lambda) - \int_{-\lambda_0}^{\lambda_0} K_1(\lambda - \lambda') \sigma(\lambda') d\lambda'$$

$$+ \int_{-\mu_0}^{\mu_0} K_{1/2}(\lambda - \mu) \omega(\mu) d\mu,$$

$$\omega(\mu) = \int_{-\lambda_0}^{\lambda_0} K_{1/2}(\mu - \lambda) \sigma(\lambda) d\lambda - \int_{-\mu_0}^{\mu_0} K_1(\mu - \mu')$$

$$\times \omega(\mu') d\mu' + \int_{-\nu_0}^{\nu_0} K_{1/2}(\mu - \nu) \tau(\nu) d\nu,$$

$$\tau(\nu) = \int_{-\mu_0}^{\mu_0} K_{1/2}(\nu - \mu) \omega(\mu) d\mu - \int_{-\nu_0}^{\nu_0} K_1(\nu - \nu')$$

$$\times \tau(\nu') d\nu', \qquad (12)$$

where $K_n(x) = \pi^{-1} n/(n^2 + x^2)$ and λ_0 , μ_0 , and ν_0 are determined by

$$\int_{-\lambda_0}^{\lambda_0} \sigma(\lambda) = \frac{M}{N},$$

$$\int_{-\mu_0}^{\mu_0} \omega(\lambda) = \frac{M'}{N},$$

$$\int_{-\nu_0}^{\nu_0} \tau(\nu) = \frac{M''}{N}.$$
(13)

It is more convenient to introduce the dress energy. ¹⁷ The iteration of Eq. (12) gives rise to

$$\begin{split} \varepsilon(\lambda) &= -2 \pi K_{1/2}(\lambda) + (g_t + g_u)h - \int_{-\lambda_0}^{\lambda_0} K_1(\lambda - \lambda') \\ &\times \varepsilon(\lambda') d\lambda' + \int_{-\mu_0}^{\mu_0} K_{1/2}(\lambda - \mu) \zeta(\mu) d\mu, \\ \zeta(\mu) &= (g_s - g_t)h + \int_{-\lambda_0}^{\lambda_0} K_{1/2}(\mu - \lambda) \varepsilon(\lambda) d\lambda \\ &- \int_{-\mu_0}^{\mu_0} K_1(\mu - \mu') \zeta(\mu') d\mu' + \int_{-\nu_0}^{\nu_0} K_{1/2}(\mu - \nu) \\ &\times \xi(\nu) d\nu, \\ \xi(\nu) &= (g_t - g_u)h + \int_{-\mu_0}^{\mu_0} K_{1/2}(\nu - \mu) \zeta(\mu) d\mu \end{split}$$

$$\xi(\nu) = (g_t - g_u)h + \int_{-\mu_0}^{\mu_0} K_{1/2}(\nu - \mu)\zeta(\mu)d\mu$$
$$- \int_{-\nu_0}^{\nu_0} K_1(\nu - \nu')\xi(\nu')d\nu', \tag{14}$$

where ε , ζ , and ξ are the dress energies in the λ , μ , and ν sectors, respectively. It is worthwhile to point out that the dress energies are also the thermal potentials at zero temperature, i.e., $\exp(\varepsilon/T) = \rho^h/\rho$, $\exp(\zeta/T) = \sigma^h/\sigma$, and $\exp(\xi/T) = \omega^h/\omega$. The thermal Bethe-ansatz equation in the zero-temperature limit turns into Eq. (14). In terms of the dress energy, the energy (11) is simplified to

$$E/N = -\frac{h}{2}(g_s + g_t + g_u) + \int_{-\lambda_0}^{\lambda_0} K_{1/2}(\lambda)\varepsilon(\lambda)d\lambda. \quad (15)$$

Apparently, the ground state is a quasi-Dirac sea where the states of negative dress energy $\varepsilon(\lambda) < 0$, $\zeta(\mu) < 0$, $\xi(\nu) = 0$ are fully occupied. The Fermi points of the three rapidities are determined by

$$\varepsilon(\lambda_0) = 0, \quad \zeta(\mu_0) = 0, \quad \xi(\nu_0) = 0.$$
 (16)

The system will be magnetized if the applied field enhances the dress energy, because it makes the corresponding Fermi points decline. A quantum phase transition occurs when any of the Fermi points shrinks to zero. As a result, the critical values of the external field are solved using

$$\varepsilon(0)|_{h=h_c} = 0, \quad \zeta(0)|_{h=h_c'} = 0, \quad \xi(0)|_{h=h_c''} = 0. \quad (17)$$

These conditions together with Eq. (14) enable one to calculate these critical values.

IV. REGIMES WITH ONE-PARAMETER SYMMETRY BREAKING

The application of an external field makes the SU(4) symmetry break down to various regimes with different residual symmetries. In this section, we shall discuss the simplest case of a single parameter hierarchy. There are three special directions in the weight space of SU(4). If the external field is supplied along those directions, i.e., either h_1 , h_2 , or h_3 in Eq. (6) does not vanish, a partial breaking of a SU(2) to U(1) will take place. Let us consider the different cases.

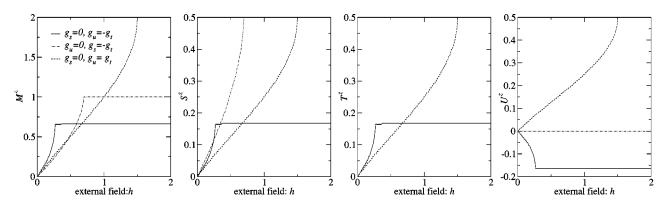


FIG. 1. The magnetization \mathcal{M}^z , S^z , T^z , U^z of the system with (1) $g_s = 0$, $g_t = -g_u$; (2) $g_u = 0$, $g_s = -g_t$; and (3) $g_s = 0$, $g_t = g_u$.

A. Residual $SU(3) \times U(1)$ symmetry

If $g_s = 0$, $g_t = -g_u > 0$, the Zeeman interaction (10) becomes

$$\mathcal{M}^z = 2g_t O_3^z = g_t M' - 2g_t M''. \tag{18}$$

The occurrence of the operator O_3^z makes the Hamiltonian noncommutable with O_3^\pm . Thus an SU(2) subgroup generated by O_3^z , O_3^+ , O_3^- is broken down to U(1). Analyzing the level crossing from Eq. (9), we shown the magnetization curve in Fig. 1.

Because the terms $g_t + g_u$ and $g_s - g_t$ in the first two equations of Eqs. (14) are nonpositive, the external field cannot enhance the two dress energies $\varepsilon(\lambda)$ and $\zeta(\mu)$; the Fermi points in both λ and μ sectors are fixed. On the contrary, the Zeeman term has a positive contribution to $\xi(\nu)$, and its two Fermi points will decline when the external field increases. Although it is an SU(4) singlet labeled by the Young tableau $[n^4]$ in the absence of an external field, the ground state possess a residual SU(3)×U(1) symmetry in the presence of the aforementioned one-parameter external field at small magnitude, which corresponds to phase IV labeled by the four-row Young tableau. In this regime there are still three types of rapidity that solve the Bethe-ansatz equation. The U(1) is generated by O_3^z , while the SU(3) is generated by the following eight operators:

$$O_{1}^{z} = \frac{1}{2} (T^{z} + U^{z}), \quad O_{2}^{z} = \frac{1}{2} (S^{z} - T^{z}),$$

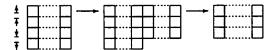
$$O_{1}^{+} = \left(\frac{1}{2} + S^{z}\right) T^{+}, \quad O_{2}^{+} = S^{+} T^{-},$$

$$O_{1}^{-} = \left(\frac{1}{2} + S^{z}\right) T^{-}, \quad O_{2}^{-} = S^{-} T^{+},$$

$$O_{1+2}^{+} = S^{+} \left(\frac{1}{2} + T^{z}\right), \quad O_{1+2}^{-} = S^{-} \left(\frac{1}{2} + T^{z}\right). \quad (19)$$

There exists a critical field when those two Fermi points shrink to zero; the rapidity ν disappears in the Bethe-ansatz equation. Thus a quantum phase transition occurs at the critical field which separates two phases; we call them phase IV and phase III.

The magnetization process can be clearly illustrated by the evolution of the Young tableau,



which shows the evolution from an SU(4) singlet to SU(3) \times U(1) states and then to an SU(3) singlet. Physically, we have $\mathcal{M}^z/N=0$ at zero external field because one-quarter of the total sites are each of the states $|\uparrow\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, and $|\downarrow\rangle$. Turning on the external field leads to the spin-orbital flippings $|\overline{\downarrow}\rangle \rightarrow |\uparrow\rangle$, $|\overline{\downarrow}\rangle \rightarrow |\uparrow\rangle$, and $|\overline{\downarrow}\rangle \rightarrow |\downarrow\rangle$, which result in nonvanishing magnetization. The $SU(3) \times U(1)$ symmetry causes the above three flipping processes to occur simultaneously. When the external field exceeds a critical value, the material goes into phase III where all the states $|\downarrow\rangle$ have been flipped over. In this phase the z components of the total spin and total orbital stay positive constant $S^z/N = T^z/N$ = 1/6, while that of U^z stays a negative constant $U^z/N=$ -1/6. Consequently, the magnetization reaches a saturation value $\mathcal{M}^z/N = 2/3$, and the ground state becomes the SU(3) singlet regardless of the magnitude of the external field in phase III.

B. Residual $SU(2) \times SU(2)$ symmetry

Applying the external field along the direction of the second simple root of su(4) Lie algebra, we will have a symmetry breaking from SU(4) to SU(2)×U(1)×SU(2) for the ground state. This is realized by the choice of Landé g factors $g_u = 0$, $g_s = -g_t$, which makes the magnetization

$$\mathcal{M}^z = 2g_s O_2^z = g_s M - 2g_s M' + g_s M''$$
 (20)

These two SU(2) are generated, respectively, by

$$\left\{ \frac{1}{2} \left(T^z + U^z \right), \left(\frac{1}{2} + S^z \right) T^{\pm} \right\},$$

$$\left\{ \frac{1}{2} \left(T^z - U^z \right), \left(\frac{1}{2} - S^z \right) T^{\pm} \right\}. \tag{21}$$

As $g_s - g_t$ in the second equation of Eq. (14) is positive but both $g_t + g_u$ and $g_t - g_u$ in the first and the third equations are

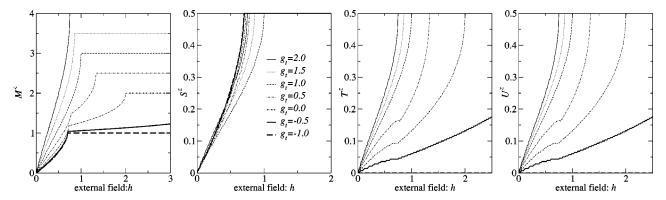
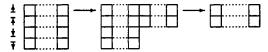


FIG. 2. The magnetization \mathcal{M}^z , S^z , T^z , U^z of the system with $g_s = 2$, $g_u = g_s + g_t$, and $g_t = 2.0, 1.5, 1.0, 0.5, 0.0, -0.5, -1.0$.

negative, the external field makes the Fermi points in the μ sector shrink. The critical value of the external field when the quantum phase transition occurs is determined by $\zeta(0)|_{h_c}=0$. This critical point separates two different phases; we call them phase IV and phase II.

The magnetization curve is shown in Fig. 1. It can also be illustrated by the evolution of the Young tableau



The spin-orbital flipping process caused by the applied external field has several characteristics. During the flipping process, $|\downarrow\rangle$ and $|\downarrow\rangle$ flip simultaneously into $|\uparrow\rangle$ and $|\uparrow\rangle$ pairs, which reduces the four-row Young tableau to a two-row Young tableau when across the critical field. Apparently, the eigenvalues of both T^z and U^z do not change during the magnetization process. Only S^z contributes to the magnetization \mathcal{M}^z . The total spin is completely polarized (i.e., \mathcal{M}^z is saturated) once phase IV transits to phase II. The phase that Yamashita $et\ al.^9$ discussed is in this special case.

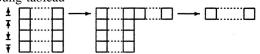
C. Residual $U(1) \times SU(3)$ symmetry

If $g_s = 0$ and $g_t = g_u$, the magnetization becomes

$$\mathcal{M}^z = 2g_t O_1^z = g_t (N - 2M + M'),$$
 (22)

which implies that the external field was applied along the first simple root of su(4) Lie algebra. This gives rise to a symmetry breaking down to U(1)×SU(3) for the ground state. For the sake of saving space, we omitt the operators that generate these symmetries. Because this parameter choice implies that $g_t + g_u$ in the λ sector is positive but the g factor terms in both μ and ν sectors are nonpositive, the quantum phase transition is related only to the λ sector. The critical value is determined by $\varepsilon(0)|_{h_c} = 0$. This critical point separates the system into two phases, phase IV and phase I. The magnetization process is shown in Fig. 1.

It is helpful to illustrated this process by the evolution of the Young tableau



From Fig. 1, we see that the spin, orbital, and U^z are polarized simultaneously versus external field. The above Young tableau indicates that the states $|\uparrow\rangle$, $|\downarrow\rangle$, $|\downarrow\rangle$, $|\downarrow\rangle$ change to the state $|\uparrow\rangle$ simultaneously because they carry out a SU(3) representation and the system possesses SU(3) symmetry. After the system is fully polarized, the magnetization reaches the maximum value $\mathcal{M}^z/N=1/2$. Then the residual symmetry of the ground state is only U(1).

V. REGIMES WITH TWO-PARAMETER SYMMETRY BREAKING

In the previous section, we discussed the simplest case where merely one SU(2) subgroup symmetry is broken. In the following, we will consider regimes with two-parameter symmetry broken, which involves more SU(2) subgroups.

A. Residual $U(1) \times U(1) \times SU(2)$ symmetry

Under the restriction $g_u = g_s + g_t$, the magnetization (8) becomes

$$\mathcal{M}^z = 2(g_s + g_t)O_1^z + 2g_sO_2^z,$$
 (23)

which indicates that the residual symmetry of the ground state is U(1)×U(1)×SU(2), in which the SU(2) is generated by $O_3^z = (T^z - U^z)/2$ and $O_3^{\pm} = T^{\pm}(1/2 - S^z)$.

The magnetization curves for different g_t are plotted in Fig. 2, and the phase diagram in terms of g_t/g_s versus h is given in Fig. 3. On the one hand, because the eigenvalue of T^z equals that of U^z for both states $|\uparrow\rangle$ and $|\bar{\uparrow}\rangle$, the flipping process occurring in phase II contributes to the magnetization of both T^z and U^z equivalently. On the other hand, the flipping from $|\downarrow\rangle$ and $|\bar{\downarrow}\rangle$ occurs simultaneously in phase IV due to the SU($\bar{2}$) symmetry. As a result, the magnetizations of T^z and U^z are expected to be the same in the whole process, which can be seen from our numerical calculation in Fig. 2.

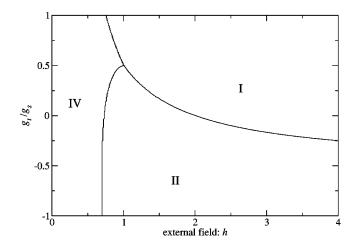


FIG. 3. The phase diagram of g_t/g_s versus h with $g_u = g_s + g_t$ and residual symmetry $U(1) \times U(1) \times SU(2)$.

For $g_t/g_s < 0.5$, there exist three distinct phases, denoted by IV, II, and I, respectively according to the number of rows of the Young tableau. The SU(2) symmetry makes the states $|\downarrow\rangle$ and $|\downarrow\rangle$ flip simultaneously when the external field increases. This makes the four-row Young tableau turn into a two-row Young tableau directly; hence the phase III labeled by a three-row Young tableau will not occur. The boundary between phase IV and phase II is determined from $\zeta(0)=0$ and $\xi(0)=0$ together,

$$g_t/g_s = \frac{1}{2} + \frac{1}{2h} K_{1/2}(0) * \varepsilon(0),$$
 (24)

where * denotes a convolution, and ε can be computed from Eqs. (14) numerically. For a sufficiently large external field, all S, T, and U are frozen in the z direction, which leads to phase I. The boundary between phase I and phase II is determined by $\varepsilon(0) = 0$, i.e.,

$$g_t/g_s = \frac{1}{h} - \frac{1}{2}. (25)$$

This can also be derived from the competition between the states related to the Young tableau [N-1,1] and [N].

The asymptotic behavior at large h is $g_t/g_s = -1/2$, which implies that the phase I will never occur as long as g_t/g_s

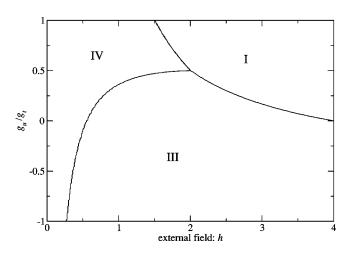
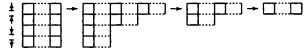


FIG. 5. The phase diagram of g_u/g_t versus h with $g_s=0$ and residual symmetry $U(1)\times SU(2)\times U(1)$.

<-1/2. The magnetization process in the region -1/2 < g_t/g_s <1/2 can be illustrated by the following evolution of the Young tableau:



The boundary between phase IV and phase I is determined by $\varepsilon(0) = 0$, $\zeta(0) = 0$, and $\xi(0)$ together,

$$g_t/g_s = \frac{3}{2h} - 1. (26)$$

The common solution of Eqs. (24)–(26) gives h=1 and $g_t/g_s=1/2$, which is a three-phase coexistence point.

B. Residual $U(1) \times SU(2) \times U(1)$ symmetry

If the external field along the direction of the second simple root is quenched but those along the other directions are kept, we will have symmetry breaking down to $U(1) \times SU(2) \times U(1)$. This kind of symmetry breaking is caused by the Zeeman term of the following magnetization:

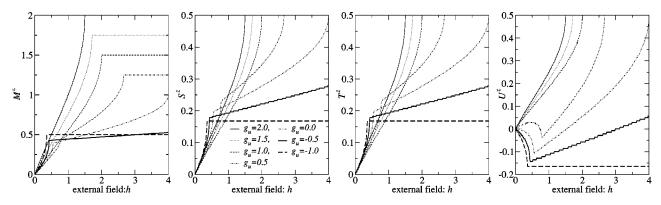


FIG. 4. The magnetization \mathcal{M}^z , S^z , T^z , U^z of the system with $g_s = 0$, $g_t = 2$, and $g_u = 2.0, 1.5, 1.0, 0.5, 0.0, -0.5, -1.0$.

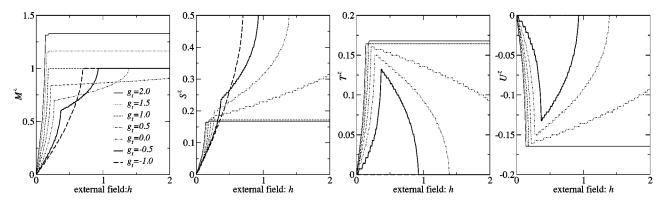


FIG. 6. The magnetization \mathcal{M}^z , S^z , T^z , U^z of the system with $g_s = 2$, $g_u = -g_s - g_t$, and $g_t = 2.0, 1.5, 1.0, 0.5, 0.0, -0.5, -1.0$.

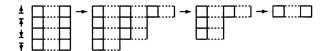
$$\mathcal{M}^{z} = (g_{t} + g_{u})O_{1}^{z} + (g_{t} - g_{u})O_{3}^{z}$$
 (27)

The magnetization curves with different g_u are plotted in Fig. 4, and the phase diagram in terms of g_u/g_t versus h is given in Fig. 5. For $g_u/g_t < 1/2$, there exist three phases denoted by IV, III, and I, respectively.

The boundary between phases IV and III is determined from $\xi=0$, which can be solved numerically. For a sufficiently large external field, the magnetization is saturated while reaching phase I. This phase transition occurs at

$$g_u/g_t = \frac{2}{h} - \frac{1}{2}. (28)$$

Thus if $g_u/g_t < -1/2$, phase I will never occur regardless of the magnitude of the external field. So in the region $-1/2 < g_u/g_t < 1/2$, the magnetization process can be illustrated by the Young tableau



In phase III, the length of the second row and that of the third row in the corresponding Young tableau are always equal due to the SU(2) symmetry. Thus the probability of pure spin flipping $|\overline{\downarrow}\rangle \rightarrow |\overline{\uparrow}\rangle$ and pure orbital flipping $|\overline{\downarrow}\rangle \rightarrow |\underline{\downarrow}\rangle$ is the same. Additionally, the process $|\overline{\downarrow}\rangle \rightarrow |\uparrow\rangle$ contributes the same for the magnetization of S^z and T^z . These properties result in the same magnetization curves of S^z and T^z shown in Fig. 4. Flipping over the state $|\overline{\downarrow}\rangle$ which has positive eigenvalue of U^z brings about a negative magnetization of U^z in phase IV.

Phase I will never occur for $g_u/g_t < -1/2$, is similar to the case of SU(3)×U(1). Actually, it recovers the case of residual SU(3)×U(1) symmetry at $g_u/g_t = -1$,

If $g_u/g_t > 1/2$, we can see from Fig. 5 that phase IV transits into phase I directly along with an increase of the external field. The boundary which separates these two phases is determined by

$$g_u/g_t = \frac{3}{h} - 1. (29)$$

Obviously, the point at $g_u/g_t=0.5$ and h=2 is a three-phase coexistence point. The magnetization properties in the region $g_u/g_t>1/2$ are similar to the case of U(1)×SU(3); in particular, a larger U(1)×SU(3) symmetry remains for $g_u/g_t=1$.

C. Residual $SU(2) \times U(1) \times U(1)$ symmetry

The third case of two-parameter symmetry breaking is produced by the Zeeman term with restriction to the Landé g factor $g_u = -g_s - g_t$. The magnetization now reads

$$\mathcal{M}^z = 2g_s O_2^z + 2(g_s + g_t) O_3^z, \tag{30}$$

which breaks the SU(4) symmetry down to SU(2) \times U(1) \times U(1).

The magnetization curves for different g_t/g_s are plotted in Fig. 6, and the phase diagram in terms of g_t/g_s versus h is given in Fig. 7. In the region of $g_t/g_s > -1/2$, there exist three phases denoted by IV, III, and II, respectively. The final state is characterized by a two-row Young tableau at sufficient large external field due to the SU(2) symmetry. The boundary separating phases III and II is determined by $\zeta(0) = 0$, which reads

$$g_t/g_s = \frac{1}{2} - \frac{\ln 2}{h}. (31)$$

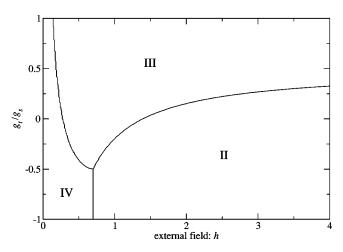


FIG. 7. The phase diagram of g_t/g_s versus h with $g_u = -g_s - g_t$. and residual symmetry $SU(2) \times U(1) \times U(1)$.

Obviously, if $g_t/g_s > 1/2$, phase II will never occur regardless of the magnitude of the external field, and the magnetization process is similar to the case of SU(3)×U(1).

In the region $-1/2 < g_t/g_s < 1/2$, the magnetization process can be illustrated by the following Young tableau,

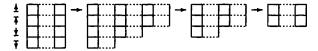


Figure 6 shows that the magnetization processes of S^z , T^z , and U^z are quite different. In phase IV, the flipping from $|\downarrow\rangle$ to three other states gives a positive contribution to S^z and T^z , but a negative contribution to U^z . In phase III, S^z undergoes polarization continually, while U^z undergoes polarization but T^z undergoes antipolarization. Since in the final phase both eigenvalues are zero and the spin magnetization is saturated, this phase will not change for any further increase of the external field.

The point $g_t/g_s = 0.5$, $h = \ln 2$ is a three-phase coexistence point. It can be seen that there exist two phases merely for $g_u/g_t < -1/2$, and phase IV transits into phase II directly. Actually, the residual symmetry of $SU(2) \times U(1) \times SU(2)$ is restored when $g_t/g_s = -1$.

VI. SUMMARY

In the above, we studied the magnetization properties of an SU(4) spin-orbital chain in the presence of a generalized external field that has three parameters because the Cartan subalgebra of Su(4) Lie algebra has three generators. These three parameters are reset so as to relate them to the spin Sv(4) orbital Tv(4), and their product Tv(4). We called them three Landé Tv(4)

factors, which makes it possible to investigate the problem in terms of a unified external field. Then all possible symmetry breakings and the corresponding magnetization processes induced by that external field are studied. The ground-state phase diagram caused by the competition of quantum fluctuation and the Zeeman-like effect is studied by solving the Bethe-ansatz equations numerically. The phase transition boundaries are derived by studying the dress-energy equations analytically. The features of various phases and transitions between them are explained in detailed by group theory analysis. Although the "magnetization" curves are calculated from the Bethe-ansatz solution of a one-dimensional model, the analysis of the symmetry broken is not restricted to one dimension.

Our results showed that a spin system with orbital degeneracy possesses a rich phase diagram in comparison to the spin-only Heisenberg model. These features in the phase diagram are expected to provide some clues toward detecting the competition and interplay between spin and orbital degrees of freedoms. Since the orbital state can be controlled by a magnetic, electric, or stress field, the quantification of the magnetization versus these generalized external fields in our discussion presented a possibly measurable description of the response with respect to those generalized external fields. They are actually relevant to the anisotropy in spin-orbital superexchange and John-Teller distortion.

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¹Y. Q. Li, M. Ma, D. N. Shi, and F. C. Zhang, Phys. Rev. Lett. **81**, 3527 (1998).

²Y. Q. Li, M. Ma, D. N. Shi, and F. C. Zhang, Phys. Rev. B **60**, 12781 (1999).

³T. Itakura and N. Kawakami, J. Phys. Soc. Jpn. **64**, 2321 (1995).

⁴ A. Joshi, M. Ma, F. Mila, D. N. Shi, and F. C. Zhang, Phys. Rev. B **60**, 6584 (1999).

⁵Y. Tokura and N. Nagaosa, Science **288**, 462 (2000).

⁶A. M. Oleś, L. F. Feiner, and J. Zaanen, Phys. Rev. B **61**, 6257 (2000).

⁷C. Itoi, S. Qin, and I. Affleck, Phys. Rev. B **61**, 6747 (2000).

⁸Y. L. Lee and Y. W. Lee, Phys. Rev. B **61**, 6765 (2000).

⁹Y. Yamashita, N. Shibata, and K. Ueda, Phys. Rev. B **61**, 4012

^{(2000).}

¹⁰S. J. Gu and Y. Q. Li, Phys. Rev. B **66**, 092404 (2002).

¹¹ K. I. Kugel and D. I. Khomskii, Zh. Eksp. Theor. Fiz. **64**, 1429 (1973) [Sov. Phys. JETP **37**, 725 (1973)].

 ¹²B. Sutherland, Phys. Rev. B **12**, 3795 (1975); Phys. Rev. Lett. **20**, 98 (1968).

¹³D. P. Arovas and A. Auerbach, Phys. Rev. B **52**, 10114 (1995).

¹⁴ A. Onufriev and J. B. Marston, Phys. Rev. B **59**, 12573 (1999).

¹⁵E. Axtell, T. Ozawa, S. Kauzlarich, and R. R. P. Singh, J. Solid State Chem. **134**, 423 (1997).

¹⁶S. K. Pati, R. R. P. Singh, and D. I. Khomskii, Phys. Rev. Lett. 81, 5406 (1998).

¹⁷H. Frahm and V. E. Korepin, Phys. Rev. B **42**, 10553 (1990).