Magnetic properties of an SU(4) spin-orbital chain

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In this paper, we study the magnetic properties of the one-dimensional SU(4) spin-orbital model by solving its Bethe-ansatz solution numerically. It is found that the magnetic properties of the system for the case of $g_t=1.0$ differs from that for the case of $g_t=0.0$. The magnetization curve and susceptibility are obtained for a system of 200 sites. For $0<g_t<g_s$, the phase diagram depending on the magnetic field and ratio of Landé factors, g_t/g_s, is obtained. Four phases with distinct magnetic properties are found.

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Recently, much attention has been focused on strongly correlated electrons with orbital degrees of freedom[1–7] due to progress in experimental studies of transition-metal and rare-earth compounds such as $LaMnO_3$, CeB_6, and TmTe. Examples of spin-orbital systems in one dimension include quasi-one-dimensional tetrahis-dimethylamino-ethylene (TDAE)-C_{60},[8] artificial quantum dot arrays,[9] and degenerate chains in $Na_2Ti_2Sb_2O$ and $Na_2V_2O_5$ compounds.[10–12] In these systems, the low-lying electron states have orbital degeneracy in addition to spin degeneracy. This may result in various interesting properties associated with the orbital degrees of freedom in Mott insulating phases. For example, the magnetic ordering is influenced by the orbital structure which may change with pressure, or the magnetization is a nonlinear function of magnetic field even in the case of an isotropic exchange interaction of $S_i\cdot S_j$ type.[13]

The spin model with orbital degeneracy in a magnetic field was studied by means of effective field theories[5] recently. It has been shown that there exists critical behavior under a magnetic field. For a nonperturbative understanding of the magnetic properties of the model, the Bethe-ansatz solution of the SU(4) model is applicable when the exterior magnetic field is applied since the total z component of spin and orbital is a good quantum number. Although Ref. 6 studied the magnetic properties in terms of the Bethe-ansatz method, their result involves only a special case because the Landé factor was not taken into account. In the present paper, we study the model in the presence of an exterior field by solving the Bethe-ansatz equation numerically meanwhile taking account of the Landé g factor. We obtain a rich phase diagram in comparison to what was obtained in Ref. 6. Our results shed new light on the understanding of more realistic systems. The quantum phase transition (QPT) (Ref. 14) concluded from such a system is speculated to be found in experiments.

The one-dimensional quantum spin-1/2 system with two-fold orbital degeneracy is modeled by[15,16]

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

where the coupling constant is set to unity. The Hamiltonian (1) has not only $SU(2)\times SU(2)$ symmetry, but also an enlarged SU(4) symmetry.[16] It was solved by the Bethe-ansatz approach: the obtained secular equation reads[17,18]

$$2\pi I_a=N\theta_{-1/2}(\lambda_a)+\sum_{b=1}^{M}\theta_1(\lambda_a-\lambda_b)+\sum_{c=1}^{M'}\theta_{-1/2}(\lambda_a-\mu_c),$$

$$2\pi J_a=\sum_{b=1}^{M}\theta_{-1/2}(\mu_a-\lambda_b)+\sum_{c=1}^{M'}\theta_1(\mu_a-\mu_c)+\sum_{d=1}^{M''}\theta_{-1/2}(\mu_a-\nu_d),$$

$$2\pi K_a=\sum_{b=1}^{M'}\theta_{-1/2}(\nu_a-\mu_b)+\sum_{c=1}^{M''}\theta_1(\nu_a-\nu_c). \qquad (2)$$

where $\theta_\rho(x)=-2\tan^{-1}(x/\rho)$. The quantum numbers $\{I_a,J_a,K_a\}$ specify a state in which there are $N-M$ number of sites in the state $|\underline{\uparrow}\rangle$, $M-M'$ in $|\overline{\uparrow}\rangle$, $M'-M''$ in $|\underline{\downarrow}\rangle$, and M'' in $|\overline{\downarrow}\rangle$. The λ, μ, and ν are rapidities related to the three generators of the Cartan subalgebra of the SU(4) Lie algebra. The coupled transcendental equations (2) determine the energy spectrum of present model. To solve the Bethe-ansatz equation numerically, one needs to take into account of the following propositions.

(i) Given a N, $\mathrm{Max}(M)=3N/4$, $\mathrm{Max}(M')=N/2$, $\mathrm{Max}(M'')=N/4$, and $N-M\geqslant M-M'\geqslant M'-M''\geqslant M''$.

(ii) $\{I_a,J_a,K_a\}$ are consecutive integers (or half integers) arranged symmetrically around the zero, which are integers or half integers depending on whether $N-M-M'$, $M-M'-M''$, $M'-M''$ are odd or even, respectively.

The latter comes from the logarithm and the former is due to the property of the Young tableau. Once Eqs. (2) are solved, the energy in the absence of exterior field is evaluated by

$$E_0(M,M',M'')=-\sum_{a=1}^{M}\frac{1}{1/4+\lambda_a^2}. \qquad (3)$$

As the z component of total spin and that of total orbital are given by $S_z=N/2-M'$ and $T_z=N/2-M+M'-M''$, the magnetization $M_z=g_sS_z+g_tT_z$ reads

$$M_z=\frac{N}{2}(g_s+g_t)-Mg_t-M'(g_s-g_t)-M''g_t, \qquad (4)$$

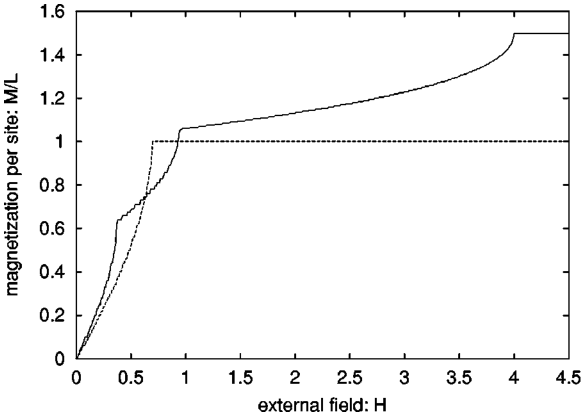


FIG. 1. Magnetization of SU(4) spin-orbital chain vs external field for a 200-site system. The solid line corresponds to $g_t = 1.0$ and the dashed line corresponds to $g_t = 0.0$.

where g_s and g_t are Landé g factors for spin and orbital, respectively. In the presence of the magnetic field H the energy becomes

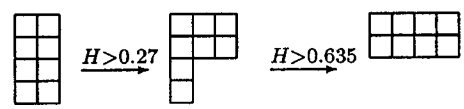
$$E(H,M,M',M'') = E_0 - HM_z. \tag{5}$$

In the absence of a magnetic field, the lowest-energy state is a SU(4) singlet where $M'' = N/4$, $M' = N/2$, and $M = 3N/2$. In the presence of a magnetic field, however, level crossing occurs and the state with $M'' = N/4$, $M' = N/2$, and $M = 3N/2$ is no longer the ground state. Therefore the values M, M', M'' for the lowest state depend on the magnitude of the applied magnetic field H. By analyzing the level crossing between the lowest-energy state and the others in terms of Eq. (5), we are able to calculate the magnetization by Eq. (4).

We set $g_s = 2.0$ and observe various situations for different values of g_t. The dependence of magnetization versus the magnetic field H is plotted in Fig. 1 for the cases of $g_t = 0.0$ and $g_t = 1.0$, respectively. Clearly, the magnetic properties of these two cases are quite different. We find that there exist three critical points in the magnetization process of which we will give interpretations on the basis of symmetry analysis and the evolution of the Young tableau as well as the physics picture by means of the mean-field analysis later on.

For an easier understanding, we first give an explanation by means of the Young tableau for an eight-site system. In Table I, we present the whole 15 different multiplets, their energy in the absence of a magnetic field, and the corresponding magnitudes of magnetization. Each multiplet corresponds to a distinct Young tableau.

The application of an exterior field will make each energy level corresponding to a multiplet that carries out an SU(4) irreducible representation split into Zeemann sublevels. If $g_t = 0.0$, the energy level of the SU(4) singlet labeled by the Young tableau $[2^4]$ will cross with the sublevel of the highest weight state labeled by the Young tableau [3311] when the applied exterior field reaches a value of 0.27. If the exterior field increases further, this state becomes the ground state. The magnitude of magnetization plays the role of slope of the energy curves determined by Eq. (5). When $H = 0.635$ its energy level will cross with that of the state labeled by the Young tableau [44]. For $H > 0.635$ the spins are totally polarized and the magnetization is saturated:



When $g_t = 1$, the level crossing occurs to the highest weight states labeled by the Young tableaux [3311], [332], [422], [44], [53], [62], [71], and [8] for the eight-site system.

It is clear that the exterior field only breaks the spin SU(2) symmetry and the orbital SU(2) symmetry remains when $g_t = 0$. The magnetization process is similar to that of the traditional Heisenberg model but the intermediate states are those labeled by the Young tableau $[m_1, m_2, m_3, m_4]$ with $m_1 = m_2$ and $m_3 = m_4$, i.e., $M' = 2M''$, $N + M' = 2M$. This implies that the evolution of the Young tableau caused by the exterior field is realized by moving a couple of boxes lying in the third and fourth rows to the first and second rows. Unlike in the traditional Heisenberg model where an increasing exterior field flips the down spins to up spins one by one, it always flips a pair of parallel spins that constitute an orbital singlet. As a result, present spin-orbital model presents larger magnetic susceptibility; meanwhile, it undergoes two phases (i.e., phases I and III in Fig. 2) versus the exterior field.

Because the orbital SU(2) symmetry is also broken for nonvanishing g_t, the magnetization process becomes complicated when $0.0 < g_t < 2.0$. The whole process undergoes four regimes as long as $g_t < g_s$. The first regime consists of strong spin polarization and weak orbital polarization (SSP-WOP) processes, where the level crossing occurs to the

TABLE I. Ground-state energy E_0 in the vanished exterior field, the z component of the total spin S_z, that of the total orbital T_z, and magnetization M_z of all possible configuration of an eight-site system.

Multiplet	$[2^4]$	[3221]	[3311]	[332]	[4211]	[422]	[431]	[44]	$[51^3]$	[521]	[53]	[511]	[62]	[71]	[8]
E_0	−14.92	−13.73	−13.84	−13.41	−12.76	−12.85	−12.04	−11.30	−10.83	−9.95	−10.25	−7.41	−7.99	−4.00	0
T_z	0	1	0	1	1	2	1	0	2	2	1	3	2	3	4
S_z	0	1	2	2	2	2	3	4	2	3	4	3	4	4	4
$M_z(g_t=0)$	0	2	4	4	4	4	6	8	4	6	8	6	8	8	8
$M_z(g_t=1)$	0	3	4	5	5	6	7	8	6	8	9	9	10	11	12

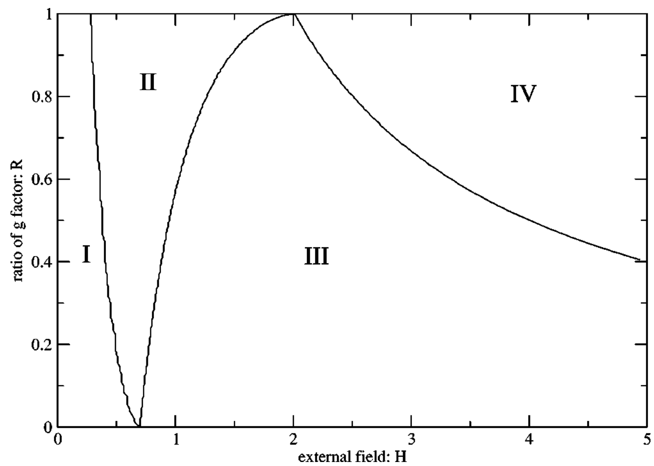


FIG. 2. Phase diagram of magnetic field H and the ratio of Landé g factors, $R=g_t/g_s$. There exist separated phases: (I) (SSP-WOP), (II) (SSP-OAP), (III) (SF-OP), and (IV) (SF-OF) in the region of $0<R<1$.

states labeled by four-row Young tableaux $[m_1,m_2,m_3,m_4]$. The contributions to M_z of both spin and orbital are positive in this regime. The second regime corresponds to the level crossing between the state labeled by three-row Young tableaux, i.e., $m_4=0$. Because the contribution of spin to M_z is positive, but that of orbital to M_z may be negative, we call it the regime of strong spin polarization and orbital antipolarization (SSP-OAP). The third regime is related to the level crossing occurring among the states labeled by two-row Young tableaux $(m_3=m_4=0)$ where spin degree of freedom is frozen and the orbital degree of freedom takes part in the polarization process only. We call it the regime of spin frozen and orbital polarization (SF-OP). Eventually, the magnetization reaches saturation and then both the spin and orbital become frozen (SF-OF) which is the phase IV indicated in Fig. 2. For $g_t=1.0$ the three critical values of the magnetic field are $H_1^c=0.31$, $H_2^c=0.93$, and $H_3^c=4.0$.

Defining $R=g_t/g_s$, we plot the phase diagram of H and R in Fig. 2. The critical lines that separate the aforementioned regimes are plotted in Fig. 2. Both the spin and orbital degrees of freedom are frozen in the phase IV. There is a simple relation for the boundary line between SF-OP and SF-OF regimes, $R=2/H$, which arises from competition between the state related to the Young tableau $[N-1,1]$ and $[N]$. The state in SSP-WP regime are quantum liquid of spin-orbital mixture while SF-OP is orbital quantum liquid. If $R=0.0$, the state in SSP-WOP has $SU(2)\otimes U(1)$ symmetry, while that in SF-OP has SU(2) symmetry.[6] When R approaches unity, however, the third phase SF-OP disappears. The phase SSP-OAP directly transits to phase SF-OF at point $H^c=2.0$, and then it undergoes only three distinct regimes which will be explained again in the following.

In the above we interpreted the phases with the help of the properties of the Young tableaux. It can also be understood on the basis of our mean-field analysis. In the presence of a magnetic field, at first, the Zeemann term in the Hamiltonian brings about three processes: orbital flipping up, spin flipping up, or both spin and orbital flipping up simultaneously, which is the phase I indicated in Fig. 2. When the magnetic field exceeds a certain value for $0<g_t<g_s$, the three flipping processes $|\overline{\downarrow}\rangle\to|\underline{\downarrow}\rangle$, $|\overline{\downarrow}\rangle\to|\overline{\uparrow}\rangle$, and $|\overline{\downarrow}\rangle\to|\underline{\uparrow}\rangle$ are stopped. In phase II, the following flipping processes take place: $|\underline{\downarrow}\rangle\to|\underline{\uparrow}\rangle$, $|\overline{\uparrow}\rangle\to|\underline{\uparrow}\rangle$, and $|\underline{\downarrow}\rangle\to|\overline{\uparrow}\rangle$. The last one is a process of spin flipping together with orbital antiflipping, which suppresses the susceptibility (slop of the magnetization curve) in phase II in comparison to that in phase I. As is known[18] that the ground state of the present model in the absence of exterior field is an SU(4) singlet whose physics picture can be considered as the simultaneous singlet of *spin* and *orbital* as well as the *product of spin and orbital*. Starting from the Neél state of the *product of spin and orbital*, the mean-field analysis tell us that a pair of parallel spins will favor their orbital to be antiparallel or vice versa. This makes it easy for us to understand the spin flipping but orbital antiflipping process in phase II. Increasing the magnetic field will make it cross to the edge of phase II where the spins are completely polarized. Thus, in phase III, the orbital starts to flip back $|\overline{\uparrow}\rangle\to|\underline{\uparrow}\rangle$. Once all orbitals become completely polarized, it goes into phase IV.

If $g_t=0$, the phase I transits to phase III directly. Because the orbital SU(2) is not broken, orbital up and down are equivalent and always half were in orbital up and half in orbital down among the spin flipping process in phase I. Increasing the magnetic field until all spins are completely polarized, the orbital liquid state still stay in a liquid state and it will not flip even if increasing the magnetic field further. So it will not go into phase IV. If $g_t=g_s$, the pure spin flipping and orbital flipping have the same probability in phase I. In phase II the spin flipping with orbital antiflipping does not occur and pure spin flipping and orbital flipping have still the same probability. Thus spin polarization itself will not happen unless spin and orbital are completely polarized simultaneously. Therefore it transits from phase II into phase IV directly.

In summary, we have investigated the magnetic properties of SU(4) spin-orbital chains by numerical solutions of their Bethe-ansatz equations. If the exterior field is decoupled to the orbital degree of freedom, i.e., $g_t=0$, we found that there exists a critical point of the quantum phase transition which separates it into two regimes. If the magnetic contribution of the orbital is not neglected, however, there will be three critical points and four regimes that demonstrate different magnetic properties. Though our calculation is made in one dimension, the analysis based on the symmetry and symmetry breaking has no restrictions in dimension. For high-dimensional systems (two or three dimensional), it is speculated to have similar features.

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