Effect of one-ion $L$-$S$ coupling on magnetic properties of a correlated spin-orbit system

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By introducing a basis for a novel realization of the SU(4) Lie algebra, we exactly solve a spin-orbital chain with one-ion $L$-$S$ coupling (OILSC) via the Bethe ansatz (BA) approach. In the context of different Landé $g$ factors of the spin and orbital sectors, the OILSC results in rich and novel quantum phase transitions. Some accurate analytical expressions for the critical fields are obtained. Both spin ordering and orbital ordering are found in a gapped singlet phase. The system exhibits many interesting phenomena such as nonvanishing magnetization of the singlet phase, multi-entrance of the singlet in the ground state when the field varies, unsymmetric magnetization in two-component phase and magnetization crossover for different OILSC.

Strongly-correlated electron systems in the presence of orbital degeneracy have attracted much interest due to experimental advances in transition-metal compounds [1], and the orbital ordering as well as the orbital density wave has been observed in a family of manganites [2]. Among the experimental findings are materials related to spin-orbital systems in one dimension, such as tetrahals (dimethylamino) ethylene-C$_{60}$ [3], artificial quantum dot arrays [4], Na$_2$Ti$_2$Sb$_2$O and NaV$_2$O$_5$ degenerate chains [5], and so forth. A well-known spin-orbital model is the SU(4) model [6] which is exactly solvable in one dimension [7,8]. The competition of orbital degree of freedom with the spin results in three quantum phase transitions (QPT’s) in a magnetic field, according to both numerical [9] and analytic [10] analysis. Deviations from the SU(4) symmetry can be caused by variations of different-site interaction [3,5,11,12]. Another possibility for deviation was considered for an SU(2)$\otimes$SU(2) Ising-type same-site anisotropy in Ref. [13,10], which may occur when the external field turns the spin oriented in parallel to the orbital angular momentum frozen in some direction by a crystalline field. A more generally-existing same-site interaction is SU(3)$\otimes$U(1) one-ion $L$-$S$ coupling (OILSC), the strength of which varies substantially in a range of $0$\textasciitilde$10^4$cm$^{-1}$($1$cm$^{-1}$\textasciitilde$1$K\textasciitilde$10^{-4}$eV) for different elements [14]. As it is well understood now, $L$-$S$ coupling can cause magnetic anisotropy [15], as far as a single ion is concerned. An interesting problem is to investigate the influence of such an OILSC on the collective properties, especially the QPT’s of strongly-correlated spin-orbital systems in a magnetic field. It can be expected that the OILSC will bring about novel physics in the competition of spin and orbital degrees of freedom.

In the present paper we shall exactly solve a spin-orbital chain with such an OILSC via the Bethe ansatz (BA) approach. In the context of the different $g$ factors of spin and orbit sectors, the OILSC leads to a rich variety of novel QPT’s, with the analytic critical fields explicitly obtained. Both spin ordering and orbital ordering exist in a gapped singlet phase, accompanied by a nonvanishing magnetization. The energy of the singlet is no longer invariant in the field due to the different $g$ factors, which brings about five consecutive QPT’s. It also contributes to unsymmetric changes of the total magnetization within a same phase in weak and in strong fields.

We consider an $N$-site chain with the Hamiltonian

$$
\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{L-S}} + \mathcal{M}, \quad \mathcal{H}_0 = \sum_{i=1}^{N} P_{i,i+1}, \\
\mathcal{H}_{\text{L-S}} = \lambda \sum_{i} \vec{s}_i \cdot \vec{l}_i, \quad \mathcal{M} = -g_s H \sum_{i} (s^+_i s^-_i + g_l l^+_i l^-_i),
$$

(1)

where $\vec{s}$ and $\vec{l}$ are spin-1/2 operators for spin and orbit and $g_s$ and $g_l$ are the corresponding Landé $g$ factors, $P_{i,i+1} = (2\vec{s}_i \cdot \vec{s}_{i+1} + \frac{1}{2}) (2\vec{l}_i \cdot \vec{l}_{i+1} + \frac{1}{2})$ exchanges the neighbor-site states. $H$ is the magnetic field and periodic boundary conditions are applied throughout. $\mathcal{H}_{\text{L-S}}$ is the OILSC from the $N$ sites and note that electrons have positive $\lambda$ whereas holes have negative $\lambda$ [15]. In the absence of the field, $\mathcal{H}_{\text{L-S}}$ breaks the system symmetry into SU(3)$\otimes$U(1) when the bulk part $\mathcal{H}_0$ is SU(4) invariant [6]. The basis consists of singlet and triplet of the SU(2) Lie algebra \{$s^+ l^+, s^- l^-, s^z l^z\}$, which is valid in the presence of the field only if $g_s = g_l$ as in the integrable spin ladder [16,17]. However, $\mathcal{H}_{\text{L-S}}$ and $\mathcal{M}$ do not commute due to the different $g$ factors of spin and orbit, the conventional singlet and triplet are no longer their common eigenstates and fail to be the solution in the spin-orbital system. Nevertheless, we can diagonalize $\mathcal{H}_{\text{L-S}} + \mathcal{M}$ as a whole, which requires a new basis for all sites

$$
\varphi_0 = \frac{\phi_1 - y^{-1} \phi_2}{\sqrt{1+y^{-2}}}, \quad \varphi_1 = \phi_3, \quad \varphi_2 = \frac{\phi_1 + y \phi_2}{\sqrt{1+y^2}}, \quad \varphi_3 = \phi_4,
$$

where $\phi_1 = |\uparrow\downarrow\rangle$, $\phi_2 = |\downarrow\uparrow\rangle$, $\phi_3 = |\uparrow\uparrow\rangle$, $\phi_4 = |\downarrow\downarrow\rangle$ denote site state $|s^z l^z\rangle$ and $y^{\pm1} = \pm g_s H/\lambda + \gamma(H/\lambda)$,
\[ \gamma(h) = (1 + g^2 \hbar^2)^{1/2}, \quad g_{\pm} = g_{\pm} \pm g_{\mp}. \] 

The new realization of the SU(4) Lie algebra takes \( S_{mn} \varphi_i = \delta_{mn} \varphi_i, \)

\[ S_{10} = p(y)r(y)[y^2(1/2 + s^2) - s^2(t^2 + 1/2)], \]

\[ S_{30} = p(y)r(y)[ys(1/2 - t^2) - t(1/2 - s^2)], \]

\[ S_{12} = r(y)[y^2(1/2 + s^2) + y^2(1/2 - t^2)], \]

\[ S_{32} = r(y)[ys(1/2 - t^2) + yt(1/2 - s^2)], \]

\[ S_{33} = s^4 t^4, \]

\[ S_{02} = p(y) r^2(y)(y^2 s^2 t^2 - s^2 t^2 + y(s^2 - t^2)), \]

where \( r(y) = 1/\sqrt{1+y^2}, \ p(y) = y/|y|, \) other operators are their conjugates \( S_{nm} = S_{nm}'. \) For a certain choice of the basis order, the three Cartan operators \( I_k \) \( (k = 1, 2, 3) \) can be generated by commutations, e.g., \( I_1 = [S_{23}, S_{32}], \ I_2 = [S_{12}, S_{21}] \) and \( I_3 = [S_{01}, S_{10}] \) for basis \( \varphi_0, \varphi_1, \varphi_2, \varphi_3 \) \( T \). 

The new basis \( \{ \varphi_0 \} \) and \( \{ \varphi_1, \varphi_2, \varphi_3 \} \) form the singlet and triplet of a new SU(2) Lie algebra \( A^+, A^-, A^2 \) where \( A^2 = s^2 + t^2 \)

\[ \varphi^\pm = \sqrt{2} r(y) [(y - 1)(s^2 t^2 - l^2 s^2) + \frac{y+1}{2}(s^2 + t^2)], \]

though the field breaks the symmetry into four U(1)'s.

We notice that a time-dependent single L-S coupled particle was solved by an SU(2) gauge transformation \([18]\), but here we consider a many-body system with \( N \) correlated ions. Note that \( P_{i,j} \) is still the permutation operator in the new basis, and \( H_{L,S} + M \) commutes with the SU(4) bulk part \( H_0 \). Based on the above new SU(4) realization we can exactly solve the model via the BA approach \([8]\) with the BA equations and the eigenenergy

\[ E = -\sum_{i=1}^{N_{I}} 2\pi a_{1}(\mu^{(1)}_{i}) + \sum_{i=1}^{N_{I}} E_{i} N_{i}, \]

where \( \Xi_{x}^{(k,l)}_{(m,n)} = (\mu^{(k)} - \mu^{(l)} - x)/\mu^{(k)} - \mu^{(l)} + x), \)

\[ \mu^{(i)}_{0} = 0, \ M^{(0)} = N, \ M^{(i)} = 0, \ 1 \leq k \leq 3; \ a_{1}(\mu) = \frac{1}{2\pi} \mu_{1}^{2} + \frac{1}{2\pi} \mu_{2}^{2} + \frac{1}{2\pi} \mu_{3}^{2} + \frac{1}{2\pi} \mu_{4}^{2}, \]

\[ E_{0} = -\frac{1}{2} - \frac{\gamma}{2}(H/\lambda), \ E_{1} = \frac{1}{2} - \frac{1}{2}(g_{t} + H), \]

\[ E_{3} = \frac{1}{2} + \frac{1}{2}(g_{t} + H) \]

\[ N_{i} \] is the total site number in state \( \varphi_{i}. \) The basis order is chosen as \( (\varphi_{1}, \varphi_{2}, \varphi_{3}, \varphi_{4})^{T} \), where \( P_{i} \in \{1, 2, 3, 4\} \) and \( P_{i} \) is energetically the most favorable while \( P_{4} \) is the least favorable. The relation \( N_{P_{i}} = M^{(i-1)} - M^{(i)} \) gives another form of energy \( E = \sum_{j=1}^{M^{(i)}} g^{(j)}(\mu_{j}) + g^{(3)}(M^{(3)}) \)

\[ M^{(3)} \]

\[ M^{(3)} \] the field shifts the order from \( (\varphi_{0}, \varphi_{1}, \varphi_{2}, \varphi_{3})^{T} \) to \( (\varphi_{0}, \varphi_{2}, \varphi_{3})^{T} \) for \( \lambda > 0 \), and \( (\varphi_{1}, \varphi_{2}, \varphi_{3})^{T} \) to \( (\varphi_{1}, \varphi_{2}, \varphi_{3})^{T} \) for \( \lambda < 0 \), at point \( H_{F} = g_{t} \). Following Ref. \([19]\) and Ref. \([20]\) one can obtain the ground state (GS) equations for three dressed energy \( c^{(i)} \):

\[ c^{(i)} = g^{(i)} - a_{2} * c^{(i)} - a_{1} * (c^{(i-1)} + c^{(i+1)}), \]

where \( c^{(0)} = c^{(4)} = 0 \) and the symbol * denotes the convolution. Fermis seas filled by negative \( c^{(i)} \) form the GS.

In the absence of the field, the GS is composed of all the four basis components when \( \lambda_{-} < \lambda < \lambda_{+} \) where \( \lambda_{+} = 4, \lambda_{-} = -2a_{0}/3 \) and \( a_{0} = (\sqrt{3} \pi - 3 \ln 3)/2 \). But a strong positive OILSC \( \lambda > \lambda_{+} \) keeps the triplet gapful, the GS only consists of singlet and the system exhibits spin and orbital ordering, as shown later on. The first QPT will occur when the field brings down the triplet \( \varphi_{1} \) and closes the gap \( \Delta = g^{(1)}(0) \) at a critical field

\[ H_{c0} = \frac{\lambda - 8 + \sqrt{\lambda^{2} - \Delta_{g}^{2} 16(\lambda - 4)}}{g_{t} + (1 - \Delta_{g}^{2})}, \]

where \( \Delta_{g} = g_{-}/g_{+} \). Further increase of the field will exhaust all the singlet and so fully polarize the GS at

\[ H_{c} = \frac{\lambda + 8 + \sqrt{\lambda^{2} + \Delta_{g}^{2} 16(\lambda + 4)}}{g_{t} + (1 - \Delta_{g}^{2})}, \]

which is valid for all values of \( \lambda \). For a weak OILSC \( 0 < \lambda < \lambda_{-} \), the field brings out the components \( \varphi_{3}, \varphi_{2}, \varphi_{0} \) in turn at three different critical points.

For \( \lambda < 0 \), the single-ion energy \( E_{0} \) of the singlet \( \varphi_{0} \) rises when the field becomes stronger. The triplet component \( \varphi_{3} \) has lower energy in zero field but will be raised by the field in a quicker way than \( \varphi_{0} \). The energy competition of \( \varphi_{3} \) and \( \varphi_{0} \) results in new kinds of QPT’s. In the four-component GS a weak negative OILSC does not expel the singlet far away from the triplet. In an increasing field \( \varphi_{3} \) rises in energy more quickly and soon goes beyond \( \varphi_{0} \), so \( \varphi_{3} \) gets out of the GS before \( \varphi_{0} \). There are three critical fields consecutively exhausting \( \varphi_{3}, \varphi_{0}, \varphi_{2} \) from the GS. However, a stronger negative OILSC leaves a longer distance between the triplet and singlet. Before \( \varphi_{3} \) covers this distance to \( \varphi_{0} \), the singlet \( \varphi_{0} \) has already risen completely out of the GS, which happens in the first critical point. But \( \varphi_{3} \) soon draws very near to \( \varphi_{0} \) such that \( \varphi_{0} \) becomes close enough to the GS, in which \( \varphi_{3} \) still lies, and is drawn back into the GS. This brings about the second QPT. Afterwards, the field overwhelms the influence of OILSC and pump out \( \varphi_{3}, \varphi_{0} \) and \( \varphi_{2} \) one by one, which gives other three QPT’s. Therefore the system undergoes five consecutive QPT’s (5-QPT) in this case, the variations of the components in the GS are: \( 1230 \rightarrow 1230 \) (and \( 1203 \rightarrow 1203 \) and \( 1212 \rightarrow 1212 \)).
λQ will expel the singlet too far away from the GS composed of the triplet. The triplet component ϕ3 itself will get out of the GS before it becomes adhesive and draw the singlet into the GS. We then have only the two QPT’s.

We present a detailed phase diagram in Fig.1, the inset illustrates the 5- and 4-QPT. 5-QPT exist if C−QPT exist if C\_Q tends to rise up at C\_Q, with requirement on the g factors \( G_{12} \leq (1 + \Delta_{\phi}) g_1 / (1 + \Delta_{\phi}) = 0.516 g_1 \), where \( \Delta_{\phi} = 3(1 + w) \omega_0^{1/2} / (4 \pi) \) and \( w = 2/3 \), satisfied for most typical spin-orbital systems. When the triplet ϕ3 attracts the singlet ϕ2 into the GS, some density of ϕ2 themselves are attracted upwards a bit by ϕ0, which causes a quicker increase in magnetization. This attraction-and-counter-attraction is more sensitive near the point Q where ϕ3 has small proportion in the GS. A 4-QPT magnetization ϕ\_4\_M\_Q tends to rise up at C\_Q−C\_M. After C\_Q−C\_M it tends to rise up at C\_−C\_M\_Q. For C\_Q above analytic results are compared with the numerical results of infinity Fermi points (FP), the other terms come into the GS. Curve d in Fig.2A shows a quicker climbing than the regions thereafter, which happens in a same phase with only two components ϕ0 and ϕ1 in the GS. Curve d only involves these two components from the beginning and provides a full view of this unsymmetry. Besides the slowdown of d⟨M\_z⟩/dH\_0, another contribution to the unsymmetry comes from the variation in the energy-difference increasing rate. The energy difference |E\_0 − E\_1| between the GS components ϕ\_1 and ϕ\_0 varies in a slower rate d|E\_0 − E\_1|/dH when the field reaches higher.

We also present two typical magnetization for negative OILSC, shown by curves a and b in Fig.2A. The corresponding QPT’s are: (a) 123−12→12; (b) 1230 (and 1203)→120−12→1. One can notice the crossover of the two curves in plane 12 before full polarization, where only two components ϕ\_1 and ϕ\_2 are left in the GS. Curve b lies in four-component phase 1230 in the absence of the field, while a stronger OILSC expels the singlet off the GS and curve a starts from triplet phase 123. The negative λ makes ϕ\_0 rising in energy level while ϕ\_2 sinks when the field is applied. But the lowest state ϕ\_1 sinks fast and so all the other components are moving out of the GS. Thus there is one more component ϕ\_0 getting out of the GS for case b than case a. Therefore, the proportion of the most energetically favorable component ϕ\_1, with a positive magnetization \( g_1/2 \), increases more quickly in case b than in case a, which gives a quicker rise of magnetization in curve b before the first QPT. The component \( \phi_3\) in case b has smaller proportion in the beginning of a four-component phase 1230, while it has larger proportion in case a starting from a three-component phase 123. Consequently, \( \phi_3\) gets out of the GS earlier in case b and the first QPT occurs ahead of case a. But the rise of curve b soon slows down after its earlier first QPT, since the \( \phi_0\) has weaker negative magnetization than \( \phi_3\) in case a. After \( \phi_3\) gets out in case a, curve b soon rises
beyond curve a again as it has two components $\varphi_2$ and $\varphi_0$ moving out while only one component $\varphi_2$ in case a.

As a result, case b has higher magnetization than case a when they both come to phase 12. But in this phase, $\varphi_2$ rises away from the lower state $\varphi_1$ always more quickly in case a with a stronger $\lambda$, as shown by $d|E_2 - E_1|/dH$ in Fig.2B. Therefore, $\varphi_2$ gets out faster in case a, and its lower magnetization rises in advance of case b and reaches the saturation point first. This results in the crossover. Finally we stress only in the context of the different $g$ factors of spin and orbit that the OILSC leads to these properties. If $g_s = g_t$ [17], the novel phenomena including the five consecutive QPT’s, the spin and orbital ordering, nonzero magnetization of the singlet, the unsymmetric magnetization and the magnetization crossover, will all disappear.

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FIG. 1. Phase diagram of quantum phase transitions (QPT’s) in magnetic field, $g_s = 2.0, g_t = 1.0$. The number i labels the state $\varphi_i$, e.g., the state components in phase 0123 are $\varphi_0\varphi_1\varphi_2\varphi_3$ in which the singlet $\varphi_0$ is energetically the most favorable whereas the triplet component $\varphi_3$ is the least favorable. The discrepancy between the analytic and numerical critical fields is not visible for most region of $C_1$NQD and $C_1$MQ. The boundary of singlet phase and the full-polarized point are exact. INSET: the five consecutive QPT’s (dark dots) and four QPT’s (dark boxes), their full-polarized points are relatively far away.
FIG. 2. (A) Typical magnetization behaviors in different QPT’s, $g_s = 2.0$, $g_t = 1.0$. The dashed lines are gapped singlet phase with a nonzero magnetization $M^z$, both spin and orbital ordering can be observed in this phase. Curve d provides a full view of unsymmetric growth of $M^z$, the dotted-line region (phase 01) in weak field climbs faster than the solid-line region (phase 10) in strong field. Also note the crossover between curve a and b before full polarization. (B) Magnetization of four consecutive QPT’s, $\lambda = -0.76$, $H_{c4} = 3.65$, the numbers denote the phases as in Fig.1. (C) Comparison on increasing speed of energy difference $E_2 - E_1$ in the field for $\lambda = -1.5$ and $\lambda = -0.5$, the former always has a larger speed.