Excitonic Correlations, Spin-State Ordering, and Magnetic-Field Effects in One-Dimensional Two-Orbital Hubbard Model for Spin-Crossover Region

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The electronic properties of excitonic insulators have been examined precisely in recent years. Pictures of exciton condensation may be applied to the spin-state transition observed in perovskite cobalt oxides. We examine the crystal-field and magnetic-field dependences of spatial spin structures on the basis of the density matrix renormalization group method using an effective model for the one-dimensional two-orbital Hubbard model in strong-coupling limit. We find an excitonic insulating (EI) phase and a spin-state ordering (SSO) phase in the intermediate region between low-spin and high-spin phases. In the EI phase, spin-triplet excitons are spatially fluctuating due to quantum effects, and an incommensurate spin correlation realizes. The analyses of a spin gap and degeneracy of entanglement spectra suggest the realization of the Haldane-like edge state in the EI phase. In the SSO phase, 3-fold or incommensurate SSO structures realize depending on the crystal-field splitting. These structures are stabilized as a result of the competition of exchange interactions between spin states.

1. Introduction

The spin and orbital degrees of freedom provide a variety of physics in strongly correlated electron systems such as transition metal compounds,$^1$ Fe or Co ions in such compounds change their spin states in response to temperature and pressure. For these ions, the competition between the crystal-field splitting and the Hund coupling causes the spin-state transition in the 3d orbital. LaCoO$_3$ is a typical perovskite cobalt oxide that shows a spin-state transition. The magnetic susceptibility and electrical conductivity of LaCoO$_3$ increase rapidly as temperature increases below 100 K.$^2,3$ These temperature dependences are explained by three competing 3d electron configurations of the Co$^{3+}$ ion, which are a low-spin state with $s = 0$ for $(t_{2g})^6(e_g)^{10}$, an intermediate-spin state with $s = 1$ for $(t_{2g})^5(e_g)^1$, and a high-spin state with $s = 2$ for $(t_{2g})^4(e_g)^2$. The competition between these spin states also causes exotic phenomena such as giant magnetoresistance,$^5,6$ magnetic clustering,$^5,6$ and ferroelectricity.$^7$

Recently, the possibility of realizing excitonic insulators has been suggested in both experimental and theoretical studies.$^8–14$ In excitonic insulators, a macroscopic number of electron-hole pairs are spontaneously generated by Coulomb interaction, and the pairs move coherently. This is called exciton condensation. In the vicinity of the spin-state transition, the fluctuation between competing spin states results in the excitonic insulating (EI) state. Therefore, considering the EI phase is important around the spin-state transition.

In the perovskite cobalt oxide Pr$_{0.5}$Ca$_{0.5}$CoO$_3$, a first-order metal-insulator phase transition around 90K has attracted attention in regards to the excitonic insulator.$^9,15$ A first-order phase transition observed in high-magnetic-field experiments on LaCoO$_3$ has also been discussed in terms of its spin-state transition and exciton condensation.$^{16–19}$ Besides the EI phase, a spin-state ordering (SSO) phase is another candidate for the magnetically induced phase in LaCoO$_3$. In the SSO phase, the spin state is crystallized and shows a superlattice structure. Some spatial patterns have been suggested in numerical analyses.$^{11,16}$ The SSO phase has been observed in LaCoO$_3$ thin films on substrates [(LaAlO$_3$)$_{0.3}$(SrAl$_{0.5}$Ta$_{0.5}$O$_3$)$_{0.7}$], where various superlattice structures of spin states have been observed.$^{20–22}$ In such thin-film experiments, we can vary the spin state by controlling the crystal-field splitting, which is determined by the lattice constant of the substrate.

As described above, in the spin-state transition, the EI and SSO phases can be realized due to the spin and orbital degrees of freedom of 3d electrons. To understand the physics in the spin-state transition comprehensively, we need to develop a theory of multi-orbital strongly correlated electron systems that takes into account various types of spin structures and exciton condensation.

In this study, we examine the realization of the EI phase and various types of SSO on the basis of numerical analysis of the two-orbital Hubbard model.
(TOHM), which is the simplest strongly correlated model that describes spin-state transition. In previous theoretical studies, the realization of EI and SSO phases in the two-dimensional (2D) TOHM was confirmed under the framework of mean-field approximation and DMFT.\textsuperscript{11,12,23} However, in analyses using these methods, the order parameters or the spatial structures are assumed. In this study, the density matrix renormalization group method (DMRG)\textsuperscript{24,25} is performed on a low-energy effective model of the one-dimensional (1D) TOHM. With DMRG, we can perform an accurate analysis with a large system size without any assumptions on the various types of orderings or their spatial structures. Although the dimensionality is limited to 1D due to the limitation of the DMRG, an accurate picture of a 1D quantum system can be a probe to understand 2D or 3D ones. The main goal of this study is to make a ground-state phase diagram for the 1D TOHM in the vicinity of spin-state transition and to reveal the spatial structure in each phase.

In the analysis of the ground state of the low-energy effective model of TOHM, we find an EI phase and a SSO phase in the intermediate region between the low-spin (LS) phase and the high-spin (HS) phase. In the EI phase, an incommensurate spin correlation occurs, and its characteristic wavenumber changes continuously depending on the crystal field splitting. In the SSO phase, various types of SSO structures are found depending on the crystal-field splitting. As a particularly stable SSO structure, the 3-fold structure of LS/HS/HS is stabilized as a result of competing interactions between the near-orbital Coulomb interaction, orbital \( \lambda \), and spin \( \sigma = \uparrow, \downarrow \) as \( c_{i\lambda\sigma} \). The electron number operator is defined as \( n_{i\lambda\sigma} = c_{i\lambda\sigma}^\dagger c_{i\lambda\sigma} \). The first term in Eq. (1) describes the electron hopping between the same orbitals at the nearest sites \( \langle ij \rangle \) with its amplitude \( t_{\lambda} \). The second term describes the crystal-field splitting with its amplitude \( \Delta \). The remaining terms represent the onsite Coulomb interactions, where \( U \) is the intra-orbital Coulomb interaction, \( U' \) is the inter-orbital Coulomb interaction, \( J \) is the Hund coupling, and \( I \) is the pair hopping. We use the relational equations for the Coulomb interactions in an isolated ion: \( U = U' + 2J \) and \( I = J \). We focus on the case in which two electrons exist per site on average.

We define the annihilating operator of an electron at site \( i \), orbital \( \lambda = (a, b) \), and spin \( \sigma = \uparrow, \downarrow \) as \( c_{i\lambda\sigma} \). The electron number operator is defined as \( n_{i\lambda\sigma} = c_{i\lambda\sigma}^\dagger c_{i\lambda\sigma} \). The first term in Eq. (1) describes the electron hopping between the same orbitals at the nearest sites \( \langle ij \rangle \) with its amplitude \( t_{\lambda} \). The second term describes the crystal-field splitting with its amplitude \( \Delta \). The remaining terms represent the onsite Coulomb interactions, where \( U \) is the intra-orbital Coulomb interaction, \( U' \) is the inter-orbital Coulomb interaction, \( J \) is the Hund coupling, and \( I \) is the pair hopping. We use the relational equations for the Coulomb interactions in an isolated ion: \( U = U' + 2J \) and \( I = J \). We focus on the case in which two electrons exist per site on average.

In the case of the spin-state transition, where \( t_{\lambda} \ll U, U', J, \Delta \), the low-energy effective Hamiltonian of Eq. (1) is derived by Kanamori et al.\textsuperscript{26} by treating the electron hopping terms as perturbations and truncating high-energy bases. The local bases of the effective Hamiltonian are

\[
|L\rangle = \left(f_{b\uparrow}^\dagger c_{b\uparrow}^\dagger - g_{a\uparrow}^\dagger c_{a\downarrow}^\dagger\right)|0\rangle, \quad (2)
\]

\[
|H_{+1}\rangle = c_{a\uparrow}^\dagger c_{b\downarrow}^\dagger |0\rangle, \quad (3)
\]

\[
|H_0\rangle = \frac{1}{\sqrt{2}} \left(c_{a\uparrow}^\dagger c_{b\downarrow}^\dagger + c_{a\downarrow}^\dagger c_{b\uparrow}^\dagger\right)|0\rangle, \quad (4)
\]

\[
|H_{-1}\rangle = c_{a\downarrow}^\dagger c_{b\uparrow}^\dagger |0\rangle, \quad (5)
\]

where \( |0\rangle \) is a vacuum. The factors in Eq. (2) are given as \( f = \frac{1}{\sqrt{1 + (\Delta' - \Delta)^2/T^2}} \) and \( g = \sqrt{1 - f^2} \), where \( \Delta' = \sqrt{\Delta^2 + T^2} \). \( |L\rangle \) is the LS state, where the amplitude of the one-site spin is \( s = 0 \). In the case of \( I = 0 \), then \( f = 1 \) and \( g = 0 \), and \( |L\rangle \) is the state in which two electrons occupy the low-energy orbital. If \( I \) becomes finite, then \( |L\rangle \) contains the state in which two electrons occupy the high-energy orbital as hybridization. \( |H_{s^z=0,\pm 1}\rangle \) are HS states, where the amplitude of the one-site spin is \( s = 1 \). In this paper, the terms "LS state" and "HS state" refer to the one-site bases and not refer to global ones.

We truncate the following high-energy bases which has two electrons in a site,

\[
|uL\rangle = \left(g_{b\downarrow}^\dagger c_{b\uparrow}^\dagger + f_{a\uparrow}^\dagger c_{a\downarrow}^\dagger\right)|0\rangle, \quad (6)
\]

\[
|iL\rangle = \frac{1}{\sqrt{2}} \left(c_{a\uparrow}^\dagger c_{b\downarrow}^\dagger - c_{a\downarrow}^\dagger c_{b\uparrow}^\dagger\right)|0\rangle, \quad (7)
\]

where \( |uL\rangle \) is the state in which two electrons mainly
occupies the high energy orbital, and \(|iL\rangle\) is the state in which one electron in the high-energy orbital and the other electron in the low-energy orbital form a singlet. This state is regarded as the singlet-exciton state while \(|H_{0,\pm 1}\rangle\) are regarded as the triplet-exciton states. If \(J > 0\), triplet-exciton states become more stable than the singlet one. This behaviour has been presented in previous study.\(^{27}\) In this study, we focus on the singlet-state transition, where \(\Delta\) and \(J\) are large. In this region, \(|uL\rangle\) and \(|iL\rangle\) are negligible.

The second order perturbation of \(t_a\) and \(t_b\) on the on-site basis \(\{|L\rangle, |H_{+1}\rangle, |H_0\rangle, |H_{-1}\rangle\}\) gives the following effective Hamiltonian,

\[
\mathcal{H}^{\text{eff}} = E_H \sum_i P_{Hi} + E_L \sum_i P_{Li} + \delta E_{LL} \sum_{(ij)} P_{Li}P_{Lj} + \delta E_{HL} \sum_{(ij)} (P_{Hi}P_{Lj} + P_{Li}P_{Hj}) + J_s \sum_{(ij)} (\vec{s}_i \cdot \vec{s}_j - 1) P_{Hi}P_{Hj} + J' \sum_{(ij)} \left[ P_i^- (\vec{s}_i \cdot \vec{s}_j + 1) P_j^+ + \text{H.c.} \right] + I' \sum_{(ij)} \left[ (\vec{s}_i \cdot \vec{s}_j - 1) P_i^+ P_j^+ + \text{H.c.} \right]. \tag{8}
\]

The operators in Eq. (8) are given as

\[
P_{Li} = \langle L_i | \langle L_i \rangle, \tag{9}
\]

\[
P_{Hi} = \sum_{s'=-1,0,1} |H_{s'}\rangle_i \langle H_{s'}|_i, \tag{10}
\]

\[
P_i^+ = |H_0\rangle_i \langle L_i \rangle, \tag{11}
\]

\[
P_i^- = |L_i\rangle_i \langle H_0|_i. \tag{12}
\]

The factors in Eq. (8) are given as

\[
E_H = \Delta + U' - J, \tag{13}
\]

\[
E_L = \Delta + U - \Delta', \tag{14}
\]

\[
\delta E_{LL} = \frac{4f^2 g^2 (t_a^2 + t_b^2)}{2U' - U - J + 2\Delta'}, \tag{15}
\]

\[
\delta E_{HL} = (t_a^2 + t_b^2) \left[ \frac{f^2}{-\Delta + U' + \Delta'} + \frac{g^2}{\Delta + U' + \Delta'} \right], \tag{16}
\]

\[
J_s = \frac{t_a^2 + t_b^2}{U + J}. \tag{17}
\]

\[
J' = 2t_a t_b \left[ \frac{f^2}{-\Delta + U' + \Delta'} + \frac{g^2}{\Delta + U' + \Delta'} \right], \tag{18}
\]

\[
I' = 2t_a t_b f g \left[ \frac{1}{U + J} + \frac{1}{2U' - U - J + 2\Delta'} \right]. \tag{19}
\]

We introduce a spin and pseudospin representation\(^{10}\) of Eq. (8) to clarify the anisotropy of the Hamiltonian. First, we introduce descending and ascending operators between the \(s = 0\) LS state and \(s = 1\) HS quadrupoles, which are defined as

\[
P_X^- = \frac{1}{\sqrt{2}} (|L\rangle \langle H_{-1}| - |L\rangle \langle H_{+1}|), \tag{20}
\]

\[
P_Y^- = \frac{1}{\sqrt{2}} (|L\rangle \langle H_{-1}| + |L\rangle \langle H_{+1}|), \tag{21}
\]

\[
P_Z^- = |L\rangle \langle H_0|, \tag{22}
\]

\[
P_i^\pm = (P_i^-)\dagger \quad (\Gamma = X, Y, Z). \tag{23}
\]

Second, the pseudospin operators \(\tau_i^\gamma\) for \(\Gamma = X, Y, Z\) are defined with the descending and ascending operators in Eqs. (20)-(23) as

\[
\tau_i^x = P_i^+ + P_i^-, \tag{24}
\]

\[
\tau_i^y = i(P_i^- - P_i^+), \tag{25}
\]

\[
\tau_i^z = P_i^+ P_i^- - P_L. \tag{26}
\]

Note that the representations of the pseudospin operators \(\tau_i^\gamma\) are twice as much as the ones of the spin 1/2 operator. Finally, the spin and pseudospin representation of the effective Hamiltonian in Eq. (8) is

\[
\mathcal{H}^{\text{eff}} = E_{0\tau} - h_{\tau z} \sum_i \tau_i^z + J_s \sum_i \vec{s}_i \cdot \vec{s}_j + J_z \sum_i \tau_i^z \tau_j^z + \frac{\tilde{\varphi}}{4} \sum_{\Gamma = X, Y, Z} \sum_{(ij)} \tau_i^\gamma \tau_j^\gamma, \tag{27}
\]

where \(\vec{s}\) is the spin operator whose amplitude is \(s = 1\), and \(\tau_i^\gamma = \tau_{X, i}^\gamma + \tau_{Y, i}^\gamma + \tau_{Z, i}^\gamma\). Note that the spin operator \(\vec{s}\) is generally not commutative with the pseudospin operator \(\tau_i^\gamma\). The factors in Eq. (27) are given as

\[
E_{0\tau} = NE_L - \frac{N_{ns} \delta E_{LL}}{2} + \frac{3N\tilde{\varphi}}{4} + \frac{9N_{ns} J_n}{32}, \tag{28}
\]

\[
h_{\tau z} = -\left( \frac{\tilde{\varphi}}{4} + \frac{3N_{ns} J_n}{16} \right), \tag{29}
\]

\[
J_z = \frac{J' + I'}{2}, \tag{30}
\]

\[
J_y = \frac{J' - I'}{2}, \tag{31}
\]

\[
J_z = \frac{J_0}{16}. \tag{32}
\]
where
\[ \Delta = E_H - E_L + n_z (\delta E_{LL} - \delta E_{HL}), \]
\[ J_{x} = 2\delta E_{HL} - \delta E_{LL} - J_s, \]
where \( n_z \) is the number of the nearest sites, and \( z = 2 \) in the 1D system. When \( J \) is nonzero in Eq. (1), then \( J_x > J_y \) in Eq. (27), and the number of excitons (HS states) does not conserve. Naively, the anisotropy of \( J_x > J_y \) in the pseudospin-pseudospin interaction seems to induce a long-range order for \( \langle \tau_{\Gamma}^x \rangle \). However, since there are spin-spin and the other pseudospin-pseudospin interactions in Eq. (27), the long-range order for \( \langle \tau_{\Gamma}^x \rangle \) can be suppressed as a result of the competition of the interactions. In fact, no symmetry breakings of \( \langle \tau_{\Gamma}^x \rangle \) are obtained in this study. In addition to Eq. (27), the Zeeman energy term is introduced as
\[ H_{\text{Zeeman}} = -H \sum_i s_i^z. \]

Before showing the results of the numerical analysis in Sect. 3, we show in Table I the typical configurations of pseudospins in the effective model in Eq. (27), where spin degrees of freedom and quantum fluctuations are not taken into consideration.

| Phase | \( \tau_{\Gamma} \) configurations | Parameter conditions |
|-------|----------------------------------|----------------------|
| LS    | \( \downarrow \downarrow \downarrow \downarrow \) | \( h_{xz} \ll 0 \) (\( \propto \Delta \gg U - U' + J \)) |
| HS    | \( \uparrow \uparrow \uparrow \uparrow \) | \( h_{y} > 0 \) (\( \propto \Delta \ll U - U' + J \)) |
| EI    | \( \leftrightarrow \leftrightarrow \leftrightarrow \leftrightarrow \) | \( h_{x} \gg 0 \), \( J_x > J_y > J_z \) |
| SSO   | \( \uparrow \downarrow \uparrow \downarrow \) | \( \Delta \sim U - U' + J, t_a/t_b \sim 1 \) |

In the case of \( \Delta \gg U - U' + J \), where the crystal-field splitting is sufficiently large, \( h_{xz} \ll 0 \) in the effective model in Eq. (27), and the ground state is in a low-spin (LS) phase with \( \langle \tau_{\Gamma} : \downarrow \downarrow \ldots \downarrow \rangle \). In the case of \( \Delta \ll U - U' + J \), the ground state is in a high-spin (HS) phase with \( \langle \tau_{\Gamma} : \uparrow \uparrow \ldots \uparrow \rangle \). In the case where \( \Delta \) and \( U - U' + J \) are comparable, the inter-pseudospin interaction \( J_x \) and the inter-spin interaction \( J_{y} \) are dominant. The inter-pseudospin interaction \( J_{x} \) is anisotropic for \( \gamma = x, y, z \). Since \( J_x \propto t_x^2 + t_y^2 \) and \( J_{y} \propto 2t_{a}t_{b} \), the behavior of the ground state depends on the parameter \( \eta = 2t_{a}t_{b}/(t_x^2 + t_y^2) \), which characterizes the anisotropy of the pseudospin-pseudospin interaction. The range of \( \eta \) is \( 0 \leq \eta \leq 1 \), where \( t_a/t_b = 0 \) for \( \eta = 0 \), and \( t_a/t_b = 1 \) for \( \eta = 1 \). In the case of \( \eta \ll 1 \), the anisotropy becomes \( J_z \gg J_x, J_y \), and the ground state tends to show a SSO with \( \langle \tau_{\Gamma} : \uparrow \downarrow \ldots \uparrow \downarrow \rangle \). If \( \eta \) is not small, the anisotropy can be \( J_x < J_y < J_z \), and pseudospins tend to form a state in which the pseudospin points in the \( x \)-axis, \( \langle \tau_{\Gamma} : \rightarrow \ldots \rightarrow \rangle \). In this configuration, the LS and HS states are hybridized. Since the HS state is regarded as a spin-triplet exciton, the configuration \( \langle \tau_{\Gamma} : \rightarrow \leftarrow \ldots \rightarrow \rangle \) represents the EI configuration, in which the excitons move coherently. In practice, the picture of the ground state of the effective model becomes more complicated due to the competition of multiple interactions in Eq. (27), which include the spin-spin interaction and three types of pseudospin-pseudospin interactions identified by \( \Gamma = X, Y, Z \).

We apply the DMRG method to the effective model. The system is 1D and has the open boundary condition unless otherwise specified. We set the truncation number in DMRG to \( \chi = 256 \) (and exceptionally \( \chi = 64 \) to determine some phase boundaries). Under this setting, the truncation error of the reduced density matrix is less than \( 10^{-5} \). We additionally use the periodic boundary condition for analyses of the SSO phase, where incommensurate spin structures are found.

### 3. Results

#### 3.1 Ground-state phase diagram

In this subsection, we present phase diagrams obtained by the numerical analysis with DMRG.

First, we fix the anisotropy factor for the pseudospin interaction at \( \eta = 1 \) \( \leftrightarrow \) \( t_a = t_b \) and make a phase diagram in the plane of the Hund coupling \( J \) and the crystal-field splitting \( \Delta \), where we set the parameters of the Coulomb interactions to \( U/\sqrt{t_a^2 + t_b^2} = 12 \), \( U' = U - 2J \), and \( J = I \) as a strongly correlated region. The \( \Delta - J \) phase diagram is shown in Fig. 1(a). In Fig. 1(a), as \( \Delta \) increases, the phase shifts as HS \( \rightarrow \) EI \( \rightarrow \) LS, where HS, EI, and LS stand for a low-spin phase, an excitonic insulating phase, and a high-spin phase, respectively. We obtain the phase boundaries by the rapid changes of the entanglement entropy, which is discussed in Subsect. 3.4.

In Fig. 1(b), we present the populations of the HS state \( \langle \rho_U \rangle \) and LS state \( \langle \rho_L \rangle \) along the dashed line in Fig. 1(a). In the EI phase, the LS state and the HS state coexist, and the population of the LS state increases as \( \Delta \) increases.

We can understand the property of the EI phase in the nearest correlation functions. We show the nearest correlation functions, \( \langle \tau_{\Gamma}^{-1} \tau_{\Gamma}^{-1} \rangle, \langle \tau_{\Gamma}^{1} \tau_{\Gamma}^{-1} \rangle, \langle \tau_{\Gamma}^{-1} \tau_{\Gamma}^{-1} \rangle \), and \( \langle s_1^x s_2^+ \rangle \) in Fig. 1(c). Note that the product of the nearest pseudospin, \( \langle \tau_{\Gamma}^{1} \rangle \), is not subtracted from \( \langle \tau_{\Gamma}^{-1} \tau_{\Gamma}^{-1} \rangle \) although \( \langle \tau_{\Gamma}^{1} \rangle \) is positive in the HS phase and negative in the LS phase. We compute the correlation function at the center of the system. The values of the pseudospin correlations are independent of the quadrupole basis \( \Gamma = X, Y, Z \) because of the rotational symmetry. The large value of \( \langle \tau_{\Gamma}^{1} \tau_{\Gamma}^{1} \rangle \) in the EI phase indicates that the EI phase is stabilized by the local kinetic energy of excitons. Compared with \( \langle \tau_{\Gamma}^{1} \tau_{\Gamma}^{1} \rangle, \langle \tau_{\Gamma}^{2} \tau_{\Gamma}^{2} \rangle \) does not show strong antiferromagnetism. This is because the antiferromagnetic inter-
actions between pseudospins satisfy $J_x > J_y$, $J_{ij} = \langle \tau^z_{i,j} \tau^z_{i+1,j+1} \rangle$ also does not show strong antiferromagnetism even near the center of the EI phase as a result of $J_x > J_z$. Near the HS(LS) phase, large value of $-h_{zz}$ makes $\langle \sigma^z_{i,j} \sigma^z_{i+1,j+1} \rangle$ ferromagnetic. In terms of long-range correlation functions, $\langle \tau^z_{i,j} \tau^z_{j,i} \rangle$ and $\langle \sigma^z_{i,j} \sigma^z_{j,i} \rangle$ become zero at $|i-j| \to \infty$. This means that there is no long-range order in the EI phase, that is $\langle \tau^x_{i,j} \rangle = \langle \tau^y_{i,j} \rangle = 0$ for $\Gamma = X, Y, Z$ and $i$ at any site. Since there are spin-spin interaction and three types of pseudospin-pseudospin interactions identified by $\Gamma$ in Eq. (27), the long-range order of EI can be suppressed as a result of the competition of the interactions.

The nearest spin correlation $\langle s^z_i s^z_{i+1} \rangle$ in Fig. 1(c) is antiferromagnetic in the HS and EI phases. In the HS phase, $\langle P_H \rangle \sim 1$. In this region, the effective Hamiltonian reduces to the antiferromagnetic spin-1 Heisenberg model, and the nearest spin correlations becomes negative. In the EI phase, $\langle P_H \rangle$ is finite, and antiferromagnetic spin-spin interaction between the HS states make the nearest spin correlation negative.

Next, we present a phase diagram in the plane of the anisotropy for the pseudospin interaction $\eta$ and the crystal-field splitting $\Delta/\sqrt{t_x^2 + t_y^2}$ in Fig. 2, where we fix the parameters of Coulomb interactions to $U/\sqrt{t_x^2 + t_y^2} = 12$, $U'/\sqrt{t_x^2 + t_y^2} = 8$, and $J/\sqrt{t_x^2 + t_y^2} = I/\sqrt{t_x^2 + t_y^2} = 2$. In addition to the HS, EI, and LS phases, the SSO phase is found in Fig. 2. In the SSO phase, the spin states show superlattice structures, in which the population of HS states varies from site to site. The spatial structure of SSO changes depending on $\Delta$ and $\eta$. We focus on the spatial structures in the next subsection.

We characterize the SSO phase on the basis of the existence of a superstructure of spin states. The criterion is that a state is in the SSO phase when $\max(P_{Hi}) - \min(P_{Hi}) > 10^{-2}$ for $i$ in the central 20 sites in a 60-sites system with open boundaries.

The outlines in the phase diagrams in Fig. 1 and Fig. 2 can be understood as the typical configurations of pseudospins which is shown in Table I, and is consistent with

![Fig. 1](image1.png)

![Fig. 2](image2.png)
the previous studies with mean-field approximation\textsuperscript{10} and dynamical mean-field approximation.\textsuperscript{19} However, no spin or pseudospin orderings are observed in the HS and EI phases. This is interpreted as the result of the effect of strong quantum fluctuations in a 1D system, which is considered in the DMRG method. In addition, various types of spin-state structures were obtained by using large 1D clusters.

3.2 Spatial structures of spin states in the EI and SSO phases

In this subsection, we present the spatial structures of the spin states in the EI phase and the SSO phase through correlation functions. We set the system size as $L = 60$ and use the periodic boundary condition.

We consider a Fourier transformed correlation functions for spin states as

\begin{equation}
C_X(k) = \frac{1}{L} \sum_{ij} \langle X_i X_j \rangle \cos k(i - j),
\end{equation}

where $X_i$ is a one-site operator at a site $i$. Note that the product of one-site expected values are not subtracted in $C_X(k)$.

First, we fix the parameters as $U/\sqrt{t_a^2 + t_b^2} = 12$, $J/\sqrt{t_a^2 + t_b^2} = I/\sqrt{t_a^2 + t_b^2} = 2$, $U' = U - 2J$, $\eta = 0.5$. In this region, the phase transition is HS $\rightarrow$ EI $\rightarrow$ LS as $\Delta/\sqrt{t_a^2 + t_b^2}$ increases.

In Fig. 3(a), we present the correlation function for the HS state $C_{PH}(k)$ in the EI phase. Since $\langle P_{HI} \rangle$ is uniform in the EI phase, $k$-dependence of $C_{PH}(k)$ corresponds to the spatial quantum fluctuation in the population of HS states. $C_{PH}(k = 0)$ originates in the uniform populations of the HS state. $k$-dependence of $C_{PH}(k > 0)$ is small in the HS phase and the LS phase and becomes large in the EI phase. This behavior means that, in the EI phase, there is a strong quantum fluctuation, and the ground state is far from the direct product state such as $\langle \tau: \rightarrow \leftarrow \cdots \rightarrow \leftarrow \rangle$, in which $C_{PH}(k > 0)$ is constant. In Fig. 3(a), we also show the wave number at $2k = \min(2\pi \langle P_{HI} \rangle, 2\pi(1 - \langle P_{HI} \rangle))$ by broken lines, where $\langle P_{HI} \rangle$ is the spatial average of the populations of HS states. If excitons are regarded as free fermions, $\tilde{k}$ is interpreted as the Fermi wavenumber. In the EI phase, $C_{PH}(k > 0)$ tends to rise as $k$ increases in $k < \tilde{k}$ and becomes constant in $k > \tilde{k}$. This behavior is similar to the behavior of 1D spinless free fermions. As a difference from the case of fermions, $C_{PH}(k \rightarrow 0)$ is non-zero in the EI phase. This originates in the anisotropy of $J_x > J_y$ in Eq. (27), which means the number of excitons does not conserve.

In Fig. 3(b), we show the Fourier transformed spin correlation $C_{s+}(k)$ with the same parameters as those in Fig. 3(a). $C_{s+}(k)$ has a peak at $k = \pi \langle P_{HI} \rangle$ in the EI and HS phases. This is interpreted as the spin correlation in the EI phase representing a spin density wave whose wavenumber corresponds to the population of the HS state, although there is no spin ordering.

Next, we fix $\eta = 0.3$. In this region, the phase transitions are HS $\rightarrow$ EI $\rightarrow$ SSO $\rightarrow$ EI $\rightarrow$ LS as $\Delta/\sqrt{t_a^2 + t_b^2}$ increases. Figure 4(a) shows $C_{PH}(k)$ in the SSO phase. We also show the peak wavenumbers against the crystal-field splitting in Fig. 4(b). The sharp peaks in Fig. 4(a) represent the structure of the SSO. There is a strong peak for $k = 2\pi/3$ in $\Delta/\sqrt{t_a^2 + t_b^2} = 5.75$. This peak represents the LS/HS/HS structure shown in Fig. 4(d).

As shown in Fig. 4(b), the spin-state structure in the SSO phase changes against the crystal-field splitting $\Delta/\sqrt{t_a^2 + t_b^2}$. The plateau at $k = 2\pi/3$ in Fig. 4(b) indicates the LS/HS/HS structure is stable. According to the Hamiltonian in Eq. (27), the nearest LS-HS pair is stabilized by the $J_z$ term, and the nearest HS-HS pair is stabilized by the $J_x$ term. The LS/HS/HS structure is realized as a result of the competition between these interactions. In the other region in the SSO phase, two peaks branch from the peak at $k = 2\pi/3$. The two peaks have generally incommensurate wavenumbers, and one of them follows the population of the HS
The expected values of $\Delta/\sqrt{t_a^2 + t_b^2}$ against the crystal-field splitting $\Delta$ seems to originate from the finite system size $L$. In this subsection, we present the magnetic-field effects in the effective model. Figures 5(a) and 5(b) are phase diagrams in the plane of the crystal-field splitting $\Delta/\sqrt{t_a^2 + t_b^2}$ and a magnetic field $H/\sqrt{t_a^2 + t_b^2}$, where we fix the parameters, $U/\sqrt{t_a^2 + t_b^2} = 12$, $J/\sqrt{t_a^2 + t_b^2} = 1/\sqrt{t_a^2 + t_b^2} = 2$, $U' = U - 2J$ and $\eta = 1$ ($\leftrightarrow t_a = t_b$). In these parameters, the EI phase exists in the intermediate region between the HS and LS phases. In Figs.5(a) and 5(b), in addition to the HS, EI, and LS phases, there appears a type-1 magnetized excitonic insulating phase (MEI-1), a type-2 magnetized excitonic insulating phase (MEI-2), a magnetized high-spin phase (MHS), and a fully polarized phase (Full Polar). We determine the phase boundary on the basis of the discontinuity of the first derivative of the magnetization curve. Basically, we set the system size as $L = 60$ and set the truncation number in DMRG as $\chi = 64$.

The value of a magnetic field at the phase boundaries for HS-MHS, EI-MEI-2, and LS-MEI-1 corresponds to the spin gaps in HS, EI, and LS phases, respectively. As shown in Figs.5(a) and 5(b), spin gaps are obtained in the HS, EI, and LS phases, and the spin gaps appear to be closed at the EI-LS phase boundary. To determine the spin gaps in the HS and EI phases, system-size extrapolations are performed. The extrapolation is performed with the function

$$\Delta_s(L) = \Delta_s(\infty) + a/L + b/L^2,$$  \hspace{1cm} (37)

where $\Delta_s(\infty)$, $a$, and $b$ are the fitting parameters. $\Delta_s(L)$ is a spin gap in the system whose size is $L$. $\Delta_s(L)$ is computed by $\Delta_s(L) = E^{(m=3)}(L) - E^{(m=0)}(L)$, where $E^{(m)}(L)$ is the energy of the ground state at $\langle \sum_i s_i^2 \rangle = m$. We avoid $E^{(m=1)}(L) - E^{(m=0)}(L)$ because it corresponds to the spin excitation at the edges, and this magnetization is ignored in an infinite system. We use $L = 128, 192, 256$ under the open boundary condition and set the truncation number in DMRG to $\chi = 256$. Some examples for the $L$ dependence of the $\Delta_s(L)$ are shown in Fig. 6. Figure 6(a) and (b) show that there is a finite spin gap in the HS and EI phases. In the EI phase near the LS phase of $5.90 < \Delta/\sqrt{t_a^2 + t_b^2} < 6.15$, the spin gap becomes small and its existence is not obtained with state $\langle P_H \rangle$. The discretization of the $k_{\text{peak}}$ in Fig. 4(b) seems to originate from the finite system size $L = 60$ and should become continuous in $L \to \infty$. Some snapshots of the spin-state structures in the SSO phase are shown in Fig. 4(c1)-(c3). Figure 4(c1) shows the LS/HS/HS structure shown in Fig. 4(d). Figure 4(c2) shows the structure at $\Delta/\sqrt{t_a^2 + t_b^2} = 5.77$, which is near the parameter at which LS/HS/HS structure realizes. Here some kinks are inserted into the basic LS/HS/HS structure. Figure 4(c3) shows the structure at $\Delta/\sqrt{t_a^2 + t_b^2} = 5.79$, which is far from the parameter of LS/HS/HS structure. Here a complex spin state is found. In the region where $\langle P_H \rangle < 0.5$, the SSO phase is not found. This result indicates that the spin-spin interaction between the HS states contributes to the stabilization of the SSO with the LS/HS/HS structure.
The spin gap in the HS phase is the Haldane-gap because in $\Delta \ll U - U' + J$, the low-energy effective Hamiltonian in Eq. (27) reduces to the spin-1 Heisenberg model. In fact, the value of the spin gap in the HS phase in Fig. 5(b) is in good agreement with $\Delta_{\text{Haldane}} J_s = 0.0293$, where $J_s = (t_{a}^2 + t_{b}^2)/(U + J) = 0.0714$ is the amplitude of spin-spin interaction in Eq. (27), and $\Delta_{\text{Haldane}} = 0.4105$ is the value of Haldane gap of the spin-1 Heisenberg model obtained in the previous study.\(^{25}\)

The spin gap in the EI phase is similar to the one of the spin-1 Heisenberg model as follows. First, the value of spin gap in the EI phase connects to the one in the HS phase. Second, the ground state energies in the EI phase degenerate for $m = 0, \pm 1$ under the open boundary condition, and the degeneracy lifts under the periodic boundary condition. This result suggests the existence of free 1/2 spins at edges similar to the case of the AKLT model. We discuss the edge state in detail in Subsect. 3.5 through the observation of entanglement spectra.

The spin gap in the LS phase is due to the energy difference between the LS state and the HS state. From here, we present the magnetization processes in the phases along the dashed lines (c)-(h) in Fig. 5(a).

The magnetization process in a wide range of the HS phase is HS → MHS → Full Polar (the dashed line at (c) and (d) in Fig. 5(a)). In the MHS phase, the population of the LS state is almost zero, and $\langle r_{i,j}^x r_{i,j+1}^x \rangle$ is almost zero. Therefore, the magnetization process in the MHS phase is the process in which $s = 1$ spins are aligned by a magnetic field.
The magnetization process in the EI phase is EI \rightarrow MEI-2 \rightarrow MEI-1 \rightarrow Full Polar (the dashed line at (e) and (f) in Fig. 5(a)), where we call the MEI phase in a low magnetic field MEI-2 and the phase in a high magnetic field MEI-1. As shown in Fig. 5(e), in the MEI-2 phase, the population of the HS state is finite for all bases of \( s^z = \pm 1 \), whereas in the MEI-1 phase, the populations of \( s^z = \pm 1 \) is finite, and that of \( s^z = 0 \) is almost zero. Therefore, the phase transition of MEI-2 \rightarrow MEI-1 occurs when the \( s = 1 \) spins are fixed to \( s^z = +1 \) by a magnetic field. Because of the antiferromagnetic spin-spin interaction, MEI-2 phase survives even in a finite magnetic field. Because of the antiferromagnetic spin-spin interaction, MEI-2 phase survives even in a finite magnetic field.

The magnetization process in the LS phase is LS \rightarrow MEI-1 \rightarrow Full Polar (the dashed line at (g) and (h) in Fig. 5(a)). The MEI-1 phase is the same phase as in the magnetization process in the EI phase. As shown in Figs. 5(g) and 5(h), the properties of the populations and the nearest correlations are consistent with the MEI-1 phase in the magnetization process in the EI phase.

In Fig. 5(a), we presented the magnetic-field effects around the EI phase, where \( \eta = 1 \) (\( \Leftrightarrow t_a = t_b \)). The magnetic field effects for smaller \( \eta \) are left for future work, where the magnetized SSO phase may be found because the LS/HS phase was obtained under a magnetic field with a mean-field analysis.\(^{11}\)

### 3.4 Entanglement entropy

![Fig. 6](image6.png)

**Fig. 6.** (Color online) Samples of Spin gap extrapolations with Eq. (37). \( \Delta \sqrt{t_a^2 + t_r^2} = 5.40,5.50 \) are in the HS phase, and the others are in the EI phase. \( \Delta \sqrt{t_a^2 + t_r^2} = 5.90,6.00,6.10 \) are near the LS phase.

![Fig. 7](image7.png)

**Fig. 7.** (Color online) Entanglement entropy in the HS, EI, and LS phases, where the system whose size is \( L = 60 \) is divided into the left and right one whose size is \( l = 30 \). The base of logarithm is \( e \). The model parameters are \( \eta = 1.0 \) (\( \Leftrightarrow t_a = t_b \)), \( U/\sqrt{t_a^2 + t_r^2} = 12, U' = U - 2J \) and \( J = I \).

In this subsection, we present the properties of entanglement entropy in the HS, EI, and LS phases. Generally, entanglement entropy is sensitive to phase transitions, and is useful to determine the phase boundaries.\(^{28-30}\)

Figure 7 shows the entanglement entropy as a function of crystal-field splitting. The entanglement entropy is defined for the density matrix of a 30 site subsystem in a 60 site system. The system has the periodic boundary condition. The truncation number in DMRG is set to \( \chi = 256 \) for Fig. 7. We set \( \eta = 1.0 \) (\( \Leftrightarrow t_a = t_b \)), \( U/\sqrt{t_a^2 + t_r^2} = 12, U' = U - 2J \) and \( J = I \), which are the same as the parameters in the dashed line in Fig. 1(a).

The value of entanglement entropy in the HS phase is consistent with the one of the spin-1 Heisenberg model.\(^{31}\) The entanglement entropy in the HS phase is not far from \( 2 \log 2 \sim 1.39 \). The value of \( 2 \log 2 \) is derived from the valencebond in the AKLT model. The picture of valence bond solid (VBS) in the AKLT model is applied to the picture in the HS phase. In this picture, the value of \( 2 \log 2 \) originates in the two valence bonds in the edges of the subsystem, and the additional value comes from the modulation from the AKLT model. In the EI phase, the entropy is larger than the one in the HS and LS phases. The rapid changes in the entanglement entropy are found in the HS-EI and EI-LS boundaries. Based on these changes, we determined the phase boundaries in Fig. 1 and Fig. 2. In the LS phase, the entropy is quite small. This is because the electrons in the LS phase cannot move due to the Pauli exclusion principle.
Fig. 8. (Color online) Entanglement spectra. The vertical axis $-\log(\Lambda_{L/2})$ means the entanglement spectra, where the divided systems have the same number of sites. The base of the logarithm is Napier’s constant. For each parameter of $\Delta/\sqrt{t_a^2 + t_b^2}$, we show 16 entanglement spectra whose singular values are the largest ones. At panels (a), (b), and (c), the boundary conditions are open ones, and $m = \langle \sum_i s_i^z \rangle = 1$. The system sizes are (a) $L = 16$, (b) $L = 32$, and (c) $L = 64$. At panels (d), (e), and (f), the boundary conditions are periodic ones, and $\langle \sum_i s_i^z \rangle = 0$. The system sizes are (d) $L = 12$, (e) $L = 24$, and (f) $L = 60$.

Fig. 9. (Color online) Schematic VBS pictures in the AKLT model. Panel (a) shows the picture for $m = 1$ under the open boundary condition, where $m = (\sum_i s_i^z)$. Panel (b) shows the picture for $m = 0$ under the periodic boundary condition. The hollow circles represent sites that have $s = 1$ spins. The filled circles represent 1/2 spins, which form a singlets represented by the solid lines. The arrows at edges represent 1/2 spins. The red dashed lines divide the system into two sides.

3.5 Entanglement spectra

In this section, we discuss the quantum state in the EI phase through the observation of entanglement spectra. As described in SubSect. 3.3, spin gaps are obtained in the HS and EI phases, which suggests the relationship with the Haldane gap.

In the case of the spin-1 Heisenberg model, it is known that the entanglement spectra with the largest singular values are degenerate. This degeneracy comes from the fact that the ground state is understood by the VBS picture in the AKLT model. In the VBS picture, singlet composed by virtual 1/2 spins results in the degeneracy of $\uparrow\downarrow$ and $\downarrow\uparrow$.

In Fig. 8, we show the entanglement spectra for the HS, EI, and LS phases in our model. The parameters are set to $U/\sqrt{t_a^2 + t_b^2} = 12$, $J/\sqrt{t_a^2 + t_b^2} = 2$, $I/\sqrt{t_a^2 + t_b^2} = 2$, $U' = U - 2J$ and $t_a = t_b$, which are the parameters at the $H = 0$ line in Fig. 5(a). As (boundary condition, $m = (\sum_i s_i^z)$), we show the cases of (open, $m = 1$) and (periodic, $m = 0$). The reasons for adopting these settings are described later in this sub-section. For the system sizes, we adopt $L = 16, 32, 64$ for the open boundary condition, and $L = 12, 24, 60$ for the periodic one.

In the HS phase, the entanglement spectra for the maximum singular values degenerate to 2-fold under the open boundary condition as the system size increases as (a)→(b)→(c), and degenerate to 4-fold under the periodic boundary condition as (d)→(e)→(f). These degeneracies are explained by VBS pictures in Figs. 9(a) and 9(b). When the system is divided, the degeneracy in the entanglement spectra appears due to the singlet composed of 1/2 spins on the cross sections of both sides. Under the open boundary condition, one set of singlet is divided, and under the periodic one, two sets of singlets are divided. Therefore, there appears 2-folded degeneracy under the open boundary condition and 4-folded degeneracy under the periodic boundary condition. The reason why we adopt the condition of $m = 1$ under the open
boundary condition is to align the almost free 1/2 spins at both edges in the same direction. These results for the entanglement spectra in the HS phase are consistent with previous studies in the spin-1 Heisenberg model.\(^{33, 34}\)

In the EI phase, as the system size increases, the spectra for the maximum singular values degenerate to 4-fold under the open boundary condition and degenerate to 8-fold under the periodic boundary condition. These degeneracies are explained as follows. First, as in the case of the HS phase, singlets at edges form entanglement of 2-folded degeneracy in the open boundary condition and 4-folded degeneracy in the periodic one. Second, in the EI phase, there are contributions to entanglements due to motions of excitons and fluctuations in the number of excitons. In our model in Eq. (8), we can obtain the following commutation relation \(\left[ P^{(2)}_H, \mathcal{H}^{(2)} \right] = 0 \) where \(P^{(2)}_H\) is a projection operator to the space where the total number of excitons is odd. \(P^{(2)}_H\) is represented by \(P^{(2)}_H = \sum_\Lambda \left( \prod_{\lambda \in \Lambda} P^{(2)}_\lambda \right)\), where \(\Lambda\) denotes any set of site indexes with an odd number of elements. We introduce \(N^{(2)}_{\Lambda} = 0, 1\) as a eigenvalues of \(P^{(2)}_\Lambda\). The eigenstate of \(N^{(2)}_{\Lambda} = 0\) indicates the superposition of the states where the number of excitons is even, and the other indicates the odd one. We consider the case when whole system is divided into two parts where \(N^{(2)}_{\Lambda}\) of the whole system is fixed to 0. This condition is used in obtaining Fig. 8. In this case, the possible combinations of \(N^{(2)}_{\Lambda}\) of sub-systems are \((N^{(2)}_{\Lambda}) = (0, 0)\) or \((1, 1)\). If the sizes of the both subsystems and the number of excitons are large enough, the two entanglement spectra originating from \((0, 0)\) and \((1, 1)\) are degenerate. The degree of degeneracy of this entanglement spectrum is not affected by boundary conditions since \(N^{(2)}_{\Lambda}\) is a property of bulk.

From the above, the combination of singlets in the valence bonds and fluctuations of the excitations explains the 4(8)-folded degeneracy of the entanglement spectra under the open(periodic) boundary condition in Fig. 8. These results suggest that the spin gap obtained in the EI phase is given by the same mechanism as that of Haldane gap.

4. Summary

We made a ground-state phase diagram of the low-energy effective model of the one-dimensional two-orbital Hubbard model for the spin-crossover region on the basis of the density matrix renormalization group method. We found an excitonic insulating (EI) phase and spin-state ordering (SSO) phase in the intermediate region between a low-spin (LS) phase and a high-spin (HS) phase. The EI phase is realized in the region where \(t_a/t_b \sim 1\), and the SSO phase is realized in the region where \(t_a/t_b \ll 1\), where \(t_a/t_b\) is the ratio of electron transfers.

The spin correlation function in the EI phase has a peak wavenumber at \(k = \pi (P_H)\), resulting in an incommensurate spin correlation. The spin-state structure in the SSO phase shows the LS/HS/HS structure and various types of incommensurate structures depending on the crystal-field splitting.

We also made a phase diagram in a magnetic field. We found a spin gap not only in the LS and HS phases but also in the EI phase. The magnetization process in the EI phase has two stages, where the magnetization curve has different gradients corresponding to the phase transition, where the directions of \(s = \pm 1\) spins are fixed by a magnetic field.

In the entanglement spectra in the EI phase, the degeneracy in the largest singular values was found. The degree of degeneracy depended on the boundary conditions, which suggested the existence of the edge state similar to the valence bond solid state in the AKLT model.

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