Spin-orbital entanglement and quantum phase transitions in a spin-orbital chain with SU(2)×SU(2) symmetry

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Spin-orbital entanglement in quantum spin-orbital systems is quantified by a specifically reduced von Neumann entropy and is calculated for the ground state of a coupled spin-orbital chain with SU(2)×SU(2) symmetry. By analyzing the discontinuity and local extreme of the reduced entropy, we deduce a rich phase diagram describing quantum phase transitions in this system with complex correlations between multiple degrees of freedom.

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Exotic states associated with the orbital degrees of freedom in transition-metal oxides have attracted considerable interest recently. Examples of such systems with spin-orbital couplings include spin-gap materials $Na_2Ti_2Sb_2O$ and NaV_2O_5, manganites $La_{1-x}Sr_xMnO_3$, and V_2O_3.[1–5] There are many intriguing physical properties in these systems such as the emergence of orbital ordering and the appearance of complex coupled excitations involving both spin and orbital degrees of freedom. Starting from a multiband Hubbard model at strong coupling limit and at the integer electron fillings per unit cell, the charge degree of freedom may be integrated out so that one may derive an effective spin-orbital model.[6,7] One of the simplest such systems is the SU(2)×SU(2) model with SU(2) symmetries for spin-1/2 operator $\mathbf{S}_i$ as well as for pseudospin-1/2 operator $\mathbf{T}_i$ representing two degenerate orbitals. In particular, this coupled spin-orbital model can be derived from a two-band orbitally degenerate Hubbard model at quarter filling. There have recently been a lot of activities on the one-dimensional quantum spin-orbital coupled systems,[8,9] especially on its phase diagram.[10–14] Rich quantum phases include both conventional ferromagnetic and/or antiferromagnetic (FM/AFM) gapless phases and symmetry broken gapped states. In the strong-coupling regime, where the interplay between spin and orbital quantum fluctuations is crucial, the detailed phase diagram still remains controversial and a more comprehensive understanding is awaited.

Very recently, theoretical study of quantum entanglement[15] from the perspective of quantum information has provided much insight to better understand quantum phase transitions (QPTs) in quantum many-particle systems, including one-dimensional spin-1/2 systems[16–21] and interacting fermion and boson systems.[22,23] Various entanglement measures[24] have been quantified in terms of the spin-spin concurrence,[16] the contiguous block entanglement,[19] and the sublattice entanglement.[21,23] Some evidences for a close connection between a QPT point and a local extreme or singularity of an appropriately measured quantum entanglement have been reported.[21] In the coupled spin-orbital systems, the spin-orbital entanglement (SOE), a kind of entanglement measure between the different degrees of freedom, is expected to manifest itself particularly near QPT points. Recent theoretical study has also demonstrated that the SOE could lead to the violation of the Goodenough-Kanamori rules.[25]

It is well known that the conventional methods meet a great difficulty to crack the mystery of complicated phase diagrams of the strongly correlated system with multiple degrees of freedom. Here, we are motivated to introduce a quantitative measure of the SOE and to reveal and/or establish an interdisciplinary connection between the SOE and the rich quantum phases in complicated spin-orbital coupled systems. In the present paper, a specifically reduced von Neumann entropy is proposed to quantify the SOE, which measures the interplay between spin and orbital degrees of freedom in the quantum states. We use finite system exact numerical diagonalization method to calculate the reduced entropy of the ground state of the spin-orbital chain given by Hamiltonian [Eq. (1)] and study its relation with the QPTs of the system. Our results show that this measure of the entanglement entropy can reveal faithfully and systematically the phase boundaries of the complex phase diagram of the system from the perspective of quantum information theory, which is quite promising for the future exploration of complex strongly correlated systems with the multiple degrees of freedom.

We consider a one-dimensional spin-orbital Hamiltonian with SU(2)×SU(2) symmetry

$$H = \sum_i (\mathbf{S}_i \cdot \mathbf{S}_{i+1} + x)(\mathbf{T}_i \cdot \mathbf{T}_{i+1} + y), \quad (1)$$

where $\mathbf{S}_i$ are spin-1/2 operators while $\mathbf{T}_i$ denote the orbital pseudo-spin 1/2 operators. x and y are two tuning parameters. At $x=y$, the model has an interchange symmetry between spin and orbital. The model at $x=y=1/4$ is a special case, which possesses a higher SU(4) symmetry and has three gapless modes (spin, orbital, and spin-orbital) in the low-lying excitations.[26,27] It is also known that the model at $x=y=3/4$ has an exact ground state, in which the spin and orbital form dimerized singlets in a staggered pattern, and the doubly degenerate ground states can be expressed as a gapped matrix product state.[28]

There exists conceptual connection between quantum entanglement and QPTs. Both of them manifest themselves as intrinsic properties of quantum many particle system. In particular, quantum entanglement represents the nature of many-body wave function unable to be decomposed as direct products of single-particle wave functions. A general strategy or principle using the von Neumann entropy for a wide class of strongly correlated systems has been proposed in our earlier papers, Refs. 21 and 23. We introduced a measure of entanglement entropy between a selected sublattice and the rest of the lattice in spin, electron, and boson systems. In particular, direct connections between the occurrence of QPTs and the local extreme of this sublattice entanglement entropy were revealed. Exact numerical studies merely for small lattices reproduce many well-known results, demonstrating that this scenario is quite promising for exploring quantum phase transitions. In fact, we have examined more than 20 different strongly correlated models with consistent results.

In the spin-orbital model, the importance of the SOE has previously been recognized.[25,26,29] However, an appropriate quantitative measure for the entanglement is still awaited. We propose here to measure the SOE by a specifically reduced von Neumann entropy defined as

$$S^{so} := -\,\mathrm{tr}_s(\rho_s \log_2 \rho_s), \quad (2)$$

where $\rho_s \equiv \mathrm{tr}_o|\Psi\rangle\langle\Psi|$ is the reduced density matrix of the spin part in the state $|\Psi\rangle$ by integrating out all the orbital degrees of freedom. Obviously, Eq. (2) gives $S^{so}=0$ if spin $\mathbf{S}$ and orbital $\mathbf{T}$ are decoupled. The motivation for such a measure is to better reveal the correlation between two distinctive degrees of freedom. This measure is related to a recent proposal of the reduced entropy S_L of a sublattice in the study of the relations between entanglement and QPTs, where the sublattice entanglement S_L is defined by

$$S_L := -\,\mathrm{tr}(\rho_L \log_2 \rho_L), \quad (3)$$

where $\rho_L \equiv \mathrm{tr}_L|\Psi\rangle\langle\Psi|$ is the reduced density matrix for a sublattice B_L. The analogy of the SOE with the sublattice entanglement becomes more transparent if we map the model of Eq. (1) onto a two-leg "spin" ladder system with one chain described by spin $\mathbf{S}$ and the other chain by orbital $\mathbf{T}$ and the two sites on each leg are coupled by a four-operator interactions.[30]

Let us first examine the SOE defined in Eq. (2) for some simplest states. For a single-site system, the SOE has a one-to-one correspondence to a system of two spin-1/2 with one spin for $\mathbf{S}$ and the other for $\mathbf{T}$. We denote a state of single site by $|S_z,T_z\rangle$. It is obvious that the spin and orbital are highly entangled in the states $\frac{1}{\sqrt{2}}(|\frac{1}{2},-\frac{1}{2}\rangle \pm |-\frac{1}{2},\frac{1}{2}\rangle)$ or $\frac{1}{\sqrt{2}}(|\frac{1}{2},\frac{1}{2}\rangle \pm |-\frac{1}{2},-\frac{1}{2}\rangle)$. From Eq. (2), we have $S^{so}=1$ for these states, consistent with our intuition. For a two-site system, the spin (orbital) states can be either a singlet $|\Psi_S^s\rangle$ ($|\Psi_O^s\rangle$) or triplet $|\Psi_S^t\rangle$ ($|\Psi_O^t\rangle$). It is straightforward to find that $S^{so}=0$ in all the spin-orbital decoupled states, and $S^{so}=1$ in the states $1/\sqrt{2}(|\Psi_S^s\rangle|\Psi_O^{t(s)}\rangle \pm |\Psi_S^t\rangle|\Psi_O^{s(t)}\rangle)$. Next, we proceed to consider a four-site (labeled as 1,2,3,4) cluster, which is the smallest system size to form an SU(4) singlet state $|SGL\rangle$; to evaluate the above SOE, this state can be most conveniently written as

$$|SGL\rangle = \sqrt{2/3}[(12)_S(34)_S(14)_O(23)_O - (14)_S(23)_S(12)_O(34)_O],$$

where $(12)_{S(O)}$ denotes the spin (orbital) singlet state of the sites 1 and 2. This $|SGL\rangle$ state contains 24 terms in terms of the single-site spin-orbital state and is rotationally invariant under the 15 SU(4) generators.[26,31] After tracing over the orbital degrees of freedom, we find $S^{so}=1$ in this high-symmetry state. The ground state of Hamiltonian [Eq. (1)] for $(x=y=3/4)$ is a dimerized state and can be written as a matrix product state in both spin and orbital parts.[28] For the four-site system, we find that $S^{so}\approx 0.40$.

In what follows, we will calculate the SOE of the ground state of Hamiltonian [Eq. (1)] in a larger but finite system. We will demonstrate a close connection between the SOE and QPTs in the model. Since the Hamiltonian is invariant under the rotations around the z axes in both $\mathbf{S}$ and $\mathbf{T}$ spaces, the exact diagonalization calculation for the ground state $|\Psi_G\rangle$ is carried out in the Hilbert subspace of $S_z=0$ and $T_z=0$. We then construct the density matrix of the system and obtain the reduced density matrix ρ_s of the spin part by tracing out the orbital degree of freedom, and compute the reduced entropy given by Eq. (2). In our calculation, the length of the chain ranges from 8 to 12 sites.

The spatial profiles of the SOE as a function of x and y are displayed in Fig. 1. A salient feature shows the existence of a region with zero entanglement, where the spin and orbital degrees of freedom are decoupled. The boundary lines to separate this region from the region with finite entanglement are sharp, and S^{so} changes discontinuously across the boundaries. This suggests a first-order phase transition at the boundaries for the jump in S^{so}. In the zero entanglement region, the spins and/or orbitals are completely ferromagnetic, so that the orbitals and/or spins are ferromagnetic or antiferromagnetic depending on effective coupling. On the other hand, if both $\mathbf{S}$ and $\mathbf{T}$ are coupled antiferromagnetically, the four-operator term may frustrate the system and possibly lead to the emergence of various nontrivial ground states with finite values of S^{so}. Note that the ground states of the boundary lines are highly degenerate; thus, S^{so} on the boundary depends on the explicit form of the state. The values of S^{so} on the boundary lines we show in the figure are the

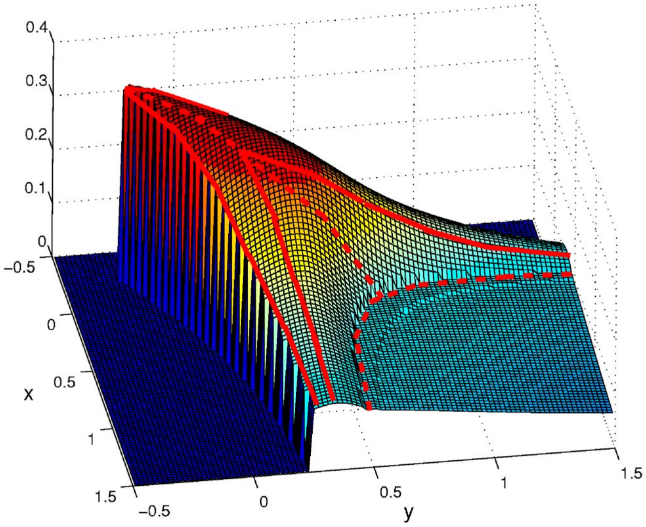

FIG. 1. (Color online) The spin-orbital entanglement per site S^{so}/L for the ground state of Hamiltonian [Eq. (1)] in $L=8$ site system as a function of x and y. The phase boundaries (solid and dashed lines) are drawn to guide the eyes.

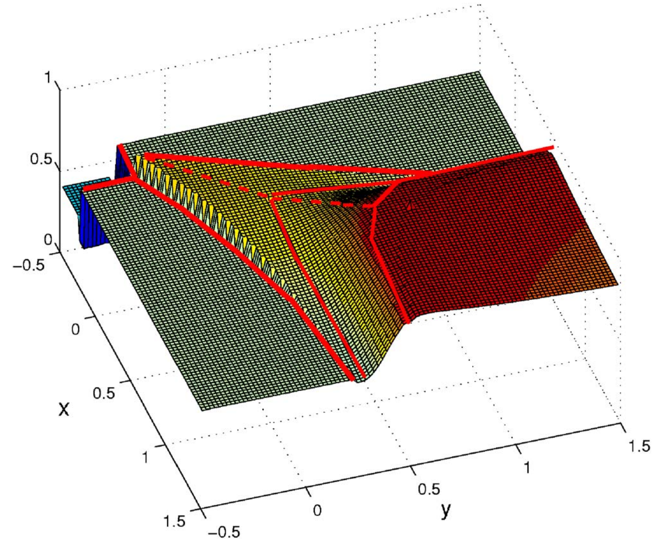

FIG. 2. (Color online) The rescaled sublattice entanglement $S_{L/2}/L$ ($L=8$) as a function of the x and y. The phase boundaries (solid and dashed lines) are essentially the same as that of Fig. 1.

values continuously evolved from the region with finite entropy.

In the region with finite S^{so}, there are two special points, as shown in the figure. One is the antiferromagnetic SU(4) symmetric point ($x=1/4$, $y=1/4$). This corresponds to a local maximum in S^{so}, consistent with the intuition that this high-symmetry point possesses a strong spin-orbital correlation. The other is a dimerized state point $(3/4,3/4)$, corresponding to a local minimum in S^{so} for the entanglement of the spin **S** and orbital **T** is suppressed in that state. Let us examine S^{so} along the symmetric line $x=y$. The line connecting the point $(-1/4,-1/4)$ and the SU(4) point is a ridge line (thin red solid line), where S^{so} are local maxima, while the line connecting the SU(4) point and (0.66, 0.66) is a valley line (thin red dashed line), where S^{so} are local minima. Besides, two more ridge lines connecting at the SU(4) point locate roughly along the $x(y)$ axes. Around the dimerized state point, one may observe the existence of a curved boundary line dividing the regions where the discontinuity of first derivative of entanglement as a function of parameters occurs.

For the large x and y regions, mean-field studies always suggest an antiferromagnetic ground state with respect to both **S** and **T**. In that case, we would expect that its corresponding SOE may approach zero. However, the SOE in this parameter region shows a plateau-like behavior with finite value, which contradicts the conclusion of mean-field results. Since the well-known dimerized state point is located within the large x and y regions, we conclude that this phase regime belongs to the gapped dimerized state rather than the gapless antiferromagnetic phase. It is worth noting that the strength of SOE may be regarded as an indicator to discern how good the mean-field approximation will be. In the strongly coupled regime, the interplay between spin and orbital quantum fluctuations becomes important and leads to some highly nontrivial quantum phases. Therefore, it is necessary to consider the effects of quantum entanglement more seriously beyond the mean-field theory. Certainly, we also find the vanishing of SOE in the large limits of x and y.

To study the additional entanglement between the intercalated sublattices of composite degrees of freedom and to best reveal all possible quantum phase boundaries, we also look into the standard sublattice entanglement,[21,23] which is obtained by tracing out both spin and orbital degrees of freedom at even (or odd) sites in the present chain. In Fig. 2, we plot the sublattice entanglement versus the coupling parameters. It is interesting to note that there is roughly one-to-one correspondence of local extreme and discontinuity between these two measures of entanglement. In contrast to that of SOE, the SU(4) point reaches a local minimum of sublattice entanglement while the dimerized state point corresponds to a local maximum. Since the SOE mainly captures the correlation between the spin and orbital degrees of freedom while the sublattice entanglement focuses on the correlation between the intercalated sublattices of composite degrees of freedom, these two measures may provide certain complementary information. In the case of conventional ferromagnetic and/or antiferromagnetic phases, the SOE vanishes while the sublattice entanglement remains nonzero. Thus, the measure of SOE is unlikely to distinguish these conventional phases. Instead, in Fig. 2, the corresponding phase boundaries could be identified. In addition, the enhancement of sublattice entanglement for the gapped dimerized state is clearly observed.

Quantum phase diagram could be distilled from the analysis of the spatial profiles of entanglement as a function of parameters following the existing wisdom: both the ridges and valleys in the three-dimensional plot may correspond to possible phase boundaries.[21,23] Derived from the numerical results presented in Figs. 1 and 2, we plot the phase boundaries of a coupled spin-orbital chain for $L=8$ in Fig. 3. The results for $L=12$ are essentially the same. There are totally seven distinct quantum phases. Phases I, II, and III are con-

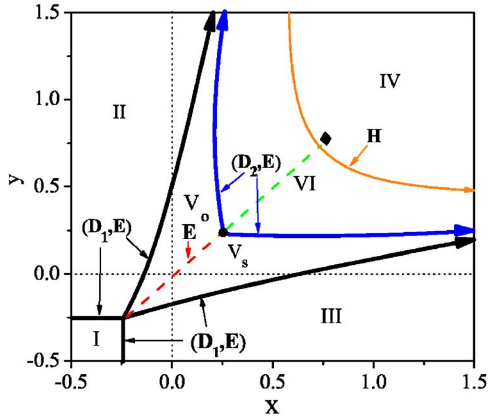

FIG. 3. (Color online) Ground-state phase diagram of a coupled spin-orbital chain. The dotted point is at $(1/4,1/4)$ while the diamond point is located at $(3/4,3/4)$. Quantum phases are identified according to the analysis of entanglements. Phase boundaries can be abstracted from previous theoretical studies. The symbols D_1 (Ref. 10) and D_2 (Ref. 13) represent the density-matrix renormalization-group (DMRG) calculations. Labels E (Ref. 12) and H (Ref. 14) correspond to the exact diagonalization method and high-temperature series expansion, respectively.

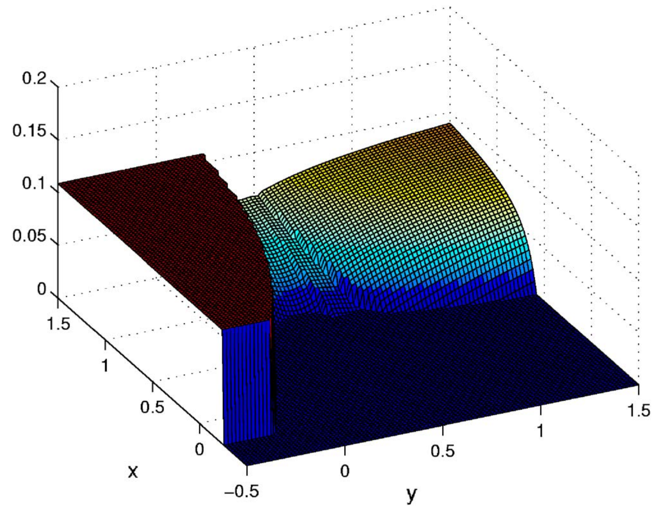

FIG. 4. (Color online) The spin pairwise concurrence for the ground state $L=8$ site system as a function of x and y.

ventional spin and orbital ferromagnetic and/or antiferromagnetic states. Phases V_o and V_s belong to gapless states which are consistent with that of the exact diagonalization analysis by Yamashita *et al.*[12] According to the previous DMRG study,[13] dimerized gapped phase exists in the parameter region for both positive x and y. The high-temperature series-expansion approach suggests the existence of two distinct gapped phases in such parameter region.[14] One phase corresponds to deconfined $S=1/2$ excitations while the other one belongs to confined $S=1$ triplet excitations. Our calculation supports the existence of two distinct gapped phases. In view of the fact that the exact ground state at the point $(3/4,3/4)$ belongs to staggered dimerized singlet and this dimerized state point is located within phase IV, we conclude that phase IV is a staggered dimerized singlet state. It is also expected that the gapped phase VI may be separated into two different phases (spin and orbital valence bond states) by the critical symmetric line (green dashed line), which is likely supported by a recent Schwinger boson mean-field analysis.[32] For comparison, each of the phase boundary line abstracted from previous studies is labeled by their theoretical methods in Fig. 3. Most of our phase boundaries are in good agreement with previous studies. It is remarkable that the most comprehensive phase diagram is now efficiently and straightforwardly obtained by using our entanglement approach.

As depicted in Figs. 1 and 2, the phase boundaries between the conventional AFM/FM states and the many-body states are rather clear while the phase boundaries among many-body states become less remarkable. There appear three types of singularities of entanglement in our calculations. (i) The discontinuity of entanglement occurs at the boundary lines between I (II, III) and IV. (ii) The discontinuity of the first derivative of entanglement shows up at the boundary between IV and VI. (iii) The local extreme of the entanglement appears at the boundary, which separates phases V and VI. According to the renormalization-group (RG) analysis, the phase transition between phases V and VI belongs to a generalized Kosterlitz-Thouless universality class.[13,33] It is well known that a typical thermodynamic quantity may exhibit certain singularity at the phase boundary but it may become too weak to be observed in Kosterlitz-Thouless-type transition. Our entanglement approach shows the presence of local entanglement extreme at the boundary instead of the occurrence of entanglement divergence and/or discontinuity. This result is consistent with RG analysis. Furthermore, our present results indicate the existence of a gapped phase IV in the large x and y regions of the phase diagram, missed in previous exact diagonalization studies.[12] This phase agrees qualitatively with the perturbative series-expansion study.

Since the coupled spin-orbital chain can be regarded equivalently to a two-leg spin ladder with four-spin interactions, we may also employ a measure of concurrence to quantify the bipartite entanglement in terms of spin-spin, orbital-orbital as well as spin-orbital concurrences. A three-dimensional plot of spin pairwise concurrence is illustrated in Fig. 4. Our results show that the concurrence can merely reveal a few features of the phase diagram such as the ordinary phases I, II, and III, but, unfortunately, it fails to identify the detailed phase diagram in the strong-coupling regime. Another scenario is to analyze a so-called single-site entanglement. In this case, we obtain the reduced density matrix by tracing out all degrees of freedom except for a single site and then get its reduced entropy. However, one is still unable to identify many phase boundaries. In our opinion, the failure of these two measures highlights the importance of the nonlocal many-body correlation effect in characterizing some nontrivial quantum phases.

Exotic physical phenomena such as high-temperature superconductivity and colossal magnetoresistance effect in transition-metal oxides associated with the interplay of multiple degrees of freedom have attracted great interest. For a strongly correlated system with multiple degrees of freedom, it is natural and crucial to examine the entanglement between distinct degrees of freedom. In the present coupled spin-orbital model, we propose the measure of SOE to characterize straightforwardly the complicated quantum correlation between the spin and orbital degrees of freedom. As shown in the present study, this measure can be used to characterize the quantum phase transitions more explicitly. Moreover, one can easily generalize this scenario to study other more complicated systems. As an example, for a system with holon and spinon degrees of freedom, e.g., *t*-*J* model, we may firstly get the ground-state wave function of the finite-size system by exact diagonalization. Then, we compute the reduced density matrix of the holon part by integrating out all the spinon degrees of freedom. Finally, we obtain its corresponding von Neumann entropy as the quantification of holon-spinon entanglement. The study along this direction is in progress.

In conclusion, we present an approach to study the phase diagram of the coupled spin-orbital chain by coherently examining the entanglement related to two distinctive degrees of freedom. The analysis of the SOE supplemented by the sublattice entanglement scenario enables us to establish a one-to-one link between its local extreme and/or discontinuity and QPT points. A most comprehensive phase diagram has been systematically deduced for the first time from the perspective of quantum information theory based on exact numerical results for a finite lattice system. In contrast to the conventional methods employed in previous studies, our investigation presents not only an alternative approach but also a superior and efficient way to identify quantum phase boundaries in a coupled spin-orbital system. Our study demonstrates a distinct merit of evaluating entanglement measure to extract valuable information of quantum phase transitions for strongly correlated systems with multiple degrees of freedom. The present scenario may shed a light on the understanding of the complicated interplay among different degrees of freedom in terms of this entanglement measure.

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