Entanglement and Quantum Phase Transition in Low Dimensional Spin Systems

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Introduction. Quantum entanglement has attracted a lot of attention for its potential applications in quantum information processing \cite{1, 2}. More recently, entanglement has also been recognized to play an important role in the study of quantum many particle physics, and experimental measurements have demonstrated that it can affect the macroscopic properties of solids \cite{3}. There have been a number of theoretical studies of the entanglement and quantum phase transitions in one dimensional spin systems and in interacting fermion and boson systems \cite{4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16}. These studies showed that the entanglement can exhibit a non-trivial behavior in condensed matter systems, such as the coincidence of the singularity in the entanglement and quantum phase transition point in certain systems \cite{13}. Most of the previous works were mainly focused on spin chains and the spin-spin concurrence \cite{1} was used to describe (two-particle) the entanglement. The scaling behavior of entanglement between a block of contiguous spins and the rest of the system in a spin chain has been studied both near and at the quantum critical point \cite{15}, and a connection with quantum phase transitions was elaborated.

In this paper, we adopt a preferable and distinct way to partition the system to study the ground state of three low dimensional spin systems: the XXZ spin chain, dimerized Heisenberg chain, and two-leg spin ladder. We find that the entanglement entropy is superior over concurrence in revealing quantum transition points. In the dimerized Heisenberg system, this entanglement entropy has maxima and minima which are in one-to-one correspondence with the transition points, while the concurrence fails to locate them. Even though the spin ladder system exhibits a complex phase structure, our entanglement entropy scenario is likely to enable us to identify the phase boundaries. It is expected that our approach is more efficient and powerful in exploring quantum phase transitions in various systems.

The models. We here study the entanglement in three types of spin-1/2 systems: XXZ chain, dimerized Heisenberg chain, and two-leg XXZ ladder, with the Hamiltonian given by

\begin{equation}
H_{XXZ} = \sum_{i=1}^{N} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z),
\end{equation}

\begin{equation}
H_D = \sum_{i=1}^{N/2} (J_1 S_{2i-1} \cdot S_{2i} + J_2 S_{2i} \cdot S_{2i+1}),
\end{equation}

\begin{equation}
H_L = \sum_{i=1}^{N} \sum_{j=1}^{2} \left( S_{i,j}^x S_{i,j+1}^x + S_{i,j}^y S_{i,j+1}^y + \Delta S_{i,j}^z S_{i,j+1}^z \right) + J' \sum_{j=1}^{N} \left( S_{1,j}^x S_{2,j}^x + S_{1,j}^y S_{2,j}^y + \Delta S_{1,j}^z S_{2,j}^z \right),
\end{equation}

where $S_i$ is the spin operator, $N$ is the linear dimension of the lattice (we adopt periodic boundary conditions). The anisotropy parameter is denoted by $\Delta$ in the XXZ model. $J_1$ and $J_2$ are two nearest-neighbor exchange couplings in the dimerized Heisenberg Hamiltonian. In the ladder system, the Hamiltonian contains inter-site interactions along the chains ($J$) and the rungs ($J'$).

To quantify the entanglement in these spin systems, we first adopt concurrence to describe two-spin entanglement \cite{1}. This quantity can be calculated from correlation functions $G^{\alpha\alpha} := \langle \sigma^\alpha \otimes \sigma^\alpha \rangle$, $(\alpha = x, y, z)$ \cite{4}:

\begin{equation}
C = \frac{1}{2} \max \left[ 0, 2 |G^{xx} + G^{yy} - G^{zz} - 1| \right],
\end{equation}

where the two site indexes are omitted. Since the correlation function decays rapidly, the concurrence is nonzero only between two closer sites. Therefore, the concurrence seems to provide limited information on the quantum phase transition. In a different approach, Vidal et al. \cite{15} studied the entanglement between a block of $L$ contiguous spins $B_L$ and the rest of the system $R_L$. The entropy of entanglement for the ground state $\Psi_g$ is given by,

\begin{equation}
S_L := -\text{tr} (\rho_L \log_2 \rho_L),
\end{equation}
way that bi-partitions the system into two sublattices to few one dimensional models. Here we adopt a distinct way away from the critical point; while this idea is applicable with the size of the boundary between them \[19, 20\]. The motivation of such partition is the antiferromagnetic isotropic point, \(\Delta = 1\) for different number of sites \(L\). Because the concurrence here is expressed in terms of the two-site correlation function of the nearest-neighbor sites, its value converges quickly as \(L\) increases. As we can see, the concurrence at one phase transition point \(\Delta = 1\) reaches the maximum while the concurrence emerges at another transition point \(\Delta = -1\) as \(L\) approaches infinity. These two quantum phase transition points can be identified from the analysis of concurrence in this case. We now address the entanglement entropy of the sublattice \(B_L = \{\text{odd sites}\}\) with \(L = N/2\) \[23\]. Fig. 1(b) displays the numerical results of the entanglement entropy \(S_L/L\) as a function of \(\Delta\). We obtain the reduced subsystem of crosses by tracing out the spin degree of freedom on circle points. As the system is in the vicinity of the quantum phase transition point, we may expect \(S_L/L\) to reach its extreme value. We find that the transition points \(\Delta = 1\) and \(\Delta = -1\) correspond to the maximum and minimum of the sublattice entanglement entropy. As for the latter case, a simple analysis of the scaling behavior around the minimum point shows that the location of the transition point approaches to \(\Delta = -1\) and \(S_L/L = 0\) as the size of the subsystem increases. Thus at \(L \to \infty\), \(S_L/L \to 0\) for \(\Delta < -1\). Therefore, the two transition points can be clearly specified and a distinct connection between quantum phase transition and the entanglement entropy has been established.

**Dimerized Heisenberg chain.** We now consider the dimerized Heisenberg chain \[24\]; this model is characterized by an alternation of strong and weak bonds between two nearest neighboring spins. In the case of \(0 < J_2/J_1 < 1\), the ground state is just an ensemble of \(N/2\) uncoupled dimers around the strong bonds. Consequently, there is an energy gap of order of \(J_1\) to separate the singlet ground state \((S_z = 0)\) from the first excited state with \(S_z = 1\). All the spins are locked into singlet states. At \(J_2/J_1 = 1\), the system is reduced to the isotropic antiferromagnetic Heisenberg chain that is quasi-long-range ordered, and belongs to a different universality class from the dimerized system. In the case of \(J_2/J_1 < 0\), the ground state is a product of spin singlet pairs coupled by ferromagnetic bonds. We can define two concurrences \(C_1\) and \(C_2\), which correspond to two nearest-neighboring spins coupled by bonds \(J_1\) and \(J_2\), respectively. The pairwise concurrence as a function of \(J_2/J_1\) for different lattice size \(L\) is shown in Fig. 2(a). It can be easily seen that the value of concurrence is independent of the lattice size. In the limit of strong dimerization, \(J_2/J_1 = 0\) (or equivalently \(J_2/J_1 \to \infty\)), the concurrence \(C_1\) (\(C_2\)) reaches a maximum value. However, the concurrence analysis does not enable us to identify the transition point \(J_2/J_1 = 1\) unambiguously. Below, all the above three Hamiltonians have a rotational symmetry around the z-axes. The calculations presented below are carried out in an invariant subspace with \(S_z = 0\). Lanczos algorithms are employed to calculate the ground state \(|\Psi_g\rangle\), from which we construct the density matrix for the whole system. We then obtain the reduced density matrix \(\rho_L\) by tracing out \(R_L\), and compute its Von Neumann entropy in Eq.(5).

**XXZ-chain.** Let us first consider the one-dimensional XXZ model. As a simple toy model, a great deal of work has been devoted to analyze its entanglement and quantum phase transition \[22\]. It is well known that \(\Delta = 1\) is the antiferromagnetic isotropic point, \(\Delta = -1\) is the ferromagnetic isotropic point, and \(\Delta = 0\) is the pure XY point. This allows us to describe the various domains as a function of \(\Delta\). The system is in an Ising ferromagnetic phase at \(\Delta < -1\), Ising antiferromagnetic phase at \(\Delta > 1\), and XY phase at \(-1 < \Delta < 1\). In Fig. 1(a), we show two concurrences as a function of anisotropy \(\Delta\) for different number of sites \(L\). Because the concurrence here is expressed in terms of the two-site correlation function of the nearest-neighbor sites, its value converges quickly as \(L\) increases. As we can see, the concurrence at one phase transition point \(\Delta = 1\) reaches the maximum while the concurrence emerges at another transition point \(\Delta = -1\) as \(L\) approaches infinity. These two quantum phase transition points can be identified from the analysis of concurrence in this case. We now address the entanglement entropy of the sublattice \(B_L = \{\text{odd sites}\}\) with \(L = N/2\) \[23\]. Fig. 1(b) displays the numerical results of the entanglement entropy \(S_L/L\) as a function of \(\Delta\). We obtain the reduced subsystem of crosses by tracing out the spin degree of freedom on circle points. As the system is in the vicinity of the quantum phase transition point, we may expect \(S_L/L\) to reach its extreme value. We find that the transition points \(\Delta = 1\) and \(\Delta = -1\) correspond to the maximum and minimum of the sublattice entanglement entropy. As for the latter case, a simple analysis of the scaling behavior around the minimum point shows that the location of the transition point approaches to \(\Delta = -1\) and \(S_L/L = 0\) as the size of the subsystem increases. Thus at \(L \to \infty\), \(S_L/L \to 0\) for \(\Delta < -1\). Therefore, the two transition points can be clearly specified and a distinct connection between quantum phase transition and the entanglement entropy has been established.

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FIG. 2: For various lattice sizes \( N \) in a dimerized Heisenberg chain, (a) the ground state concurrences \( C_1 \) (solid line) and \( C_2 \) (dotted line) versus \( \Delta \), and (b) \( S_L/L \) as a function of the sublattice size \( L \). The inset in (b) shows the divergence of the \( d^2(S_L/L)/d(J_2/J_1)^2 \) at the block entanglement minimum point as the system size increases.

we examine the entanglement entropy of the chosen odd-site sublattice (or the even-site sublattice). In this case, the two transition points are found to correspond to a local maximum and a local minimum in the entanglement entropy [see Fig. 2(b)]. Here it is interesting to notice that the second derivative of \( S_L/L \) with respect to \( J_2/J_1 \) seems to exhibit singularity at the minimum point \( J_2/J_1 = 1 \) (see Fig. 2(b) inset), which corresponds to the only gapless point. Due to the limitation of our computational resources, a detailed scaling analysis is not available. In addition, it is seen that \( S_L/L \) is weakly size dependent and converges quickly to a fixed value at the transition point with increasing lattice size.

**Spin ladders.** Spin ladders have been attracting great interest in the field of low dimensional spin systems in recent several years [25]. The physics of Heisenberg ladders can be understood in some special limits. For large and negative \( J' \), the 2-leg ladder is equivalent to an \( S = 1 \) spin chain, and the system is gapful [26]. For large and positive \( J' \), the two spins along the rung are locked into a singlet state. The ground state is a collection of spin singlets on each rung and is gapful. The phase diagram of two coupled XXZ chains was previously determined by utilizing Hamiltonian mappings and Abelian bosonization [27]. Previous studies presumably indicated five distinct phases in this complicated phase diagram as a function of \( \Delta \) and \( J'/J \). We first examine the dependence on the coupling constant of two nearest-neighbor spin concurrence: this analysis failed to describe the rich structure of the phase diagram. Below we report our study on the entanglement entropy of the chosen subsystem and its relevance to quantum phase transition point. The spatial profiles and contour plots of \( S_L/L \) as a function of \( J'/J \) and \( \Delta \) are displayed in Fig. 3. From our analysis from above-mentioned two models, we know that both the ridges and valleys may correspond to possible phase boundaries. For example, one can distinguish the boundary \( J'/J = 0 \) (ridge or valley), \( \Delta = 1 \) for \( J'/J < 0 \) (ridge), \( \Delta = -1 \) for \( J' < 0 \) (ridge). Derived from the numerical results, Fig. 4 shows the schematic phase boundaries of a coupled 2-leg XXZ spin ladder system (the dashed line denotes the ridge of its derivative). Most phase boundaries are in agreement with those in Ref. 26. Our results suggest the existence of a new quantum phase in the region \( \Delta < -1.5 \) and \( J'/J > 0.5 \), which has not been reported in previous studies [27, 28, 29].

Finally, it is important to emphasize that, in comparison with the previous investigations [18], we do not have to deal with a large system i.e., a large \( L \), to capture its scaling behavior. This indicates that the finite size effects are not important in our approach; numerical results for a quite small system may disclose relevant information about the quantum phase transition points. In this sense, the present approach is broadly applicable to many other systems including spin and electron systems in higher dimension [19], not limited merely to the spin-chains.

**Summary.** We have investigated the ground-state entanglement in three one-dimensional spin systems by using both two-spin concurrence and entanglement entropy of the preferably chosen sublattice. Concurrence may provide some partial insights about certain quantum phase transition points. However, our entanglement entropy scenario allows us to establish a distinct connection between its local maxima/minima and transition points.

FIG. 3: \( S_L/L \) \((L = 8)\) as a function of the \( J'/J \) and \( \Delta \) in a coupled 2-leg XXZ spin ladder system. The results for \( L = 6 \) are essentially same.
FIG. 4: Schematic phase boundaries of a coupled 2-leg XXZ spin ladder system.

points, which is promising for shedding a new light on the understanding of quantum phase transition and quantum entanglement.

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