Exploring Quantum Phase Transitions with a Novel Sublattice Entanglement Scenario

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We introduce a new measure called reduced entropy of sublattice to quantify entanglement in spin, electron and boson systems. By analyzing this quantity, we reveal an intriguing connection between quantum entanglement and quantum phase transitions in various strongly correlated systems: the local extremes of reduced entropy and its first derivative as functions of the coupling constant coincide respectively with the first and second order transition points. Exact numerical studies merely for small lattices reproduce several well-known results, demonstrating that our scenario is quite promising for exploring quantum phase transitions.

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Quantum entanglement, a key concept in quantum information theory that has no classical counterpart\textsuperscript{[1]}, has been recognized to play also an important role in the study of quantum many-particle physics\textsuperscript{[2]}. However, how to quantify appropriately entanglement in many-body systems has been a challenging question for a long time. So far, a number of interesting theoretical attempts have been made on various notions of entanglement in several one-dimensional (1D) correlated systems as well as their possible links to quantum phase transitions (QPTs) that occur at absolute zero temperature\textsuperscript{[3, 4, 5, 6, 7, 8, 9]}. Among these various measures, it is remarkable as the reduced entropy of sublattice plays a crucial role in QPTs, similar to that of the thermal entropy in classical phase transitions: the local extremes of reduced entropy and its first derivative as functions of the coupling constant coincide respectively with the first and second order transition points. Exact numerical studies merely for small lattices reproduce several well-known results, demonstrating that our scenario is quite promising for exploring quantum phase transitions.

In this paper, by introducing a well-defined reduced entropy of sublattice as a measure of entanglement, which is an extensive quantity, we have found a distinct connection between quantum entanglement and QPTs in such an intriguing way: the local extremes of reduced entropy and its first derivative as functions of the coupling constant coincide respectively with the first and second order transition points of QPTs. This finding is remarkable as (i) it implies that the reduced entropy of sublattice plays a crucial role in QPTs, similar to that of the thermal entropy in classical phase transitions; and (ii) the analysis of reduced entropy enables us to identify and classify unambiguously QPT points for a wide class of systems.

While we have studied more than ten strongly correlated systems with the same conclusion, here we first analyze the best understood transverse-field quantum Ising chain as a benchmark, and then present our main results for three types of two-dimensional (2D) spin-$1/2$ systems and one type of electron system: a coupled dimer antiferromagnet (Fig.1a), a frustrated $J_1$-$J_2$ model (Fig.1b), a checkerboard antiferromagnet (Fig.1c), and a 1D half-filled extended Hubbard model (Fig.1d). The corresponding Hamiltonians read

\begin{equation}
H_\alpha = \sum_{i,j} J_{ij}^\alpha \mathbf{S}_i \mathbf{S}_j,
\end{equation}

\begin{equation}
H = -\sum_{\langle i,j \rangle} c_i^\dagger c_j + U \sum_i n_i\bar{n}_i + V \sum_i n_i n_j,
\end{equation}

where $\mathbf{S}_i$ is the spin operator and $\alpha$ is a model label. The coupling parameters in all models are explicitly shown in Fig.1. For the coupled dimer antiferromagnet model ($\alpha = a$), the anisotropy parameter is denoted by $\lambda$. $J_1$ and $J_2$ correspond to the nearest-neighbor and next-nearest-neighbor exchange couplings in the 2D frustrated

\begin{figure}[h]
\centering
\includegraphics[width=0.7\textwidth]{fig1}
\caption{Schematic configurations of the four studied strongly correlated systems. a) Coupled dimer antiferromagnet, b) 2D frustrated $J_1$-$J_2$ system, c) checkerboard antiferromagnet and d) 1D extended Hubbard model. Two subsystems are denoted as X (crosses) and • (solid symbols) in the figures.}
\end{figure}
Heisenberg Hamiltonian \((\alpha = b)\). In the checkerboard antiferromagnet spin system \((\alpha = c)\), the Hamiltonian contains nearest-neighbor couplings along the nearest-neighbor coupling \(J\) and the diagonal link \(J_x\). As for the 1D half-filled extended Hubbard model, \(c_{j\sigma}^\dagger\) and \(c_{j\sigma}\) are creation and annihilation operators of electron with spin \(\sigma\) at site \(j\), respectively, \(U\) and \(V\) represent the on-site repulsion/atraction and nearest-neighboring interaction.

In an earlier paper, Vidal \textit{et al.} \[7\] studied the ground state entanglement between a block of contiguous spins and the rest of the system. Their approach is, however, not applicable to the above four systems and many others. In the present work, it is in fact crucial to choose one size-\(N\) sublattice \(R_N\) reduced from the whole lattice in such a preferable way (i) the number of connecting bonds between the chosen sublattice and the rest \((B_N)\) of the system is maximized so that the correlation effect between the two parts can be best revealed; and (ii) the structure of sublattice \(R_N\) should be the same as (or, if impossible, most similar to) that of the original lattice, in the same spirit of the real-space renormalization idea. Under such choice, a new appropriate measure of entanglement for correlated systems, i.e., the reduced entropy of sublattice, is naturally given by

\[
S_N = N \log_2 \rho_N,
\]

where \(\rho_N\) is the reduced density matrix by the partial trace of the density matrix over \(B_N\). Being different from some conventional quantities (e.g., the spin susceptibility) which are only related to a two-body correlation function, this reduced entropy of sublattice contains all the contributions including two-body, three-body, and even \(N/2\)-body correlation functions. Since this reduced entropy can capture essentially the nonlocal nature of many-particle correlation, particularly around the transition points of QPTs, we naturally anticipate that it should have a close connection to QPTs, as we will elaborate later. In the numerical calculations (except for the first algorithm addressed below), we employed Lanczos algorithms with periodic boundary conditions to calculate exactly the ground state \(|\Psi_g\rangle\), from which we obtained

\[
\rho_N = \text{tr}_{B_N} |\Psi_g\rangle \langle \Psi_g|,
\]

and then \(S_N\), with the lattice size \(N\) and choice of the sublattice \(R_N\) (the lattice of \(X\)-points (crosses)) used in our calculation being illustrated in Fig.1.

As a benchmark illustration, we first analyze an exactly solvable model intensively studied before \[3, 7, 9\], i.e., the transverse-field quantum Ising chain with the Hamiltonian as

\[
H = -\sum_{i=1}^{L} (S_i^x S_{i+1}^x + \lambda S_i^z).
\]

It is well known that this system undergoes a second order phase transition between an ordered ferromagnetic state and a quantum paramagnetic state at \(\lambda_c = 1\). As depicted in Fig. 2 (with the even sites \(S_N\)), \(S_N\) monotonically decreases as \(\lambda\) changes from 0 to 2, while the first derivative of \(d(S_N/N)/d\lambda\) shows explicitly a local minimum at \(\lambda = \lambda_c\), indicating clearly that this local extreme corresponds to a critical point of the second-order QPT. This one-to-one correspondence between the reduced entropy and QPTs has also been tested and justified in the study of the Anderson localization model describing disorder-driven metal-insulator transition \[11\]. In fact, from our numerical results including those to be addressed later/elsewhere, we state more firmly that the extreme of the first derivative of reduced entropy in a finite system corresponds to the transition point of second-order QPTs. Moreover, as shown clearly in Fig. 2, as the lattice size increases from \(N = 10\) to 1280, the determined critical point is unchanged, and the curves of the renormalized first derivative (and reduced entropy) converge very rapidly (for \(N \geq 160\), all curves merge to one within the present resolution) \[12\]. Therefore, our reduced entropy of sublattice indeed captures essentially the nonlocal nature of many-particle correlation and reveals QPTs with negligible (or very weak) finite size effect, which is a remarkable advantage in exploring QPTs in other complicated systems.

We now use the above scenario to look into a coupled Heisenberg dimer Hamiltonian with two spins per unit cell, a typical model for illustration of novel QPTs in the literature \[14\]. The transition may be tuned by varying a dimensionless parameter \(\lambda\) \((0 < \lambda < 1)\). As shown in Fig.1 (a), the bonds represented by the solid-line form the coupled dimers while the dashed-line represents the coupling between the neighboring dimers. In the case of \(\lambda \ll 1\), the ground state is a paramagnetic state consisting of a product of decoupled dimers, in each of which the spins pair into a valence bond singlet. At \(\lambda = 1\), the system corresponds to the square lattice antiferromagnet; its ground state has a long-range magnetic Neel order. Obviously, these two limits cannot be connected continuously and a transition point is expected between

![FIG. 2: The ground state renormalized reduced entropy \(S_N/N\) (a) and its first derivative versus the external parameter \(\lambda\) (b). The curves correspond to different lattice sizes \(N = 10, 40, 160, 1280\).](image-url)
them. Recently, a field theory study indicated that the transition between the two phases is of second-order \cite{13}, and the critical point was estimated around 0.5 from a Monte Carlo simulation \cite{14}. For the sublattice specified in Fig.1(a), the reduced entropy $S_N$ and its first derivative as functions of coupling $\lambda$ are shown in Fig. 3(a). $S_N$ monotonically decreases as $\lambda$ changes from 0 to 1, while the first derivative $d(S_N/N)/d\lambda$ shows a clear local minimum around $\lambda \sim 0.4$, which is now identified to be a critical point of the second-order QPT, in good agreement with the well-accepted result.

For the 2D frustrated $J_1$-$J_2$ Heisenberg model (Fig.1(b)), it is known that the ground state of the model possesses the conventional Neel long range order at $J_2/J_1 \ll 1$ and has a collinear antiferromagnetic quasi-long range order if $J_2/J_1 \sim 1$. The reduced entropy and its first derivative are illustrated as functions of $J_2/J_1$ in Fig.3 (b). By analyzing the first derivative $d(S_N/N)/d(J_2/J_1)$ as a function of $J_2/J_1$, we locate two local extreme points at $J_2/J_1 \sim 0.37$ and 0.62, respectively. According to the above criterion, we identify two critical points in the system. Besides, there is also a local maximum of $S_N$ at $J_2/J_1=0.5$, which is predicted to be another first-order QPT point according to our earlier study \cite{10} and many new results including those to be presented later. Interestingly, there is indeed a general consensus in previous studies that three distinct QPT points are present around $J_2/J_1 \sim 0.38$, 0.5 and 0.6 \cite{13, 14, 17, 18}. In view of the small $4 \times 4$ cluster used in our calculation, the good agreement of our results with the above consensus is very impressive.

Next we consider one of the most frustrated 2D antiferromagnets, the checkerboard antiferromagnet, which was investigated by some analytical and numerical approaches before \cite{19}. Its ground state has Neel long-range order at $J_x/J \ll 1$, whereas it corresponds decoupled Heisenberg chains when $J_x/J \gg 1$. At $J_x/J = 1$, it is a valence bond crystal in singlet plaquettes. These three phases are separated by two quantum critical points at $U/V = 0.80$ and 1.10, respectively. A recent field theory study reported a new candidate phase diagram with additional intermediate ordered phase \cite{20}. In Fig. 4(a), the calculated reduced entropy and its derivative are plotted as functions of $J_x/J$. As we can see, there exist a local maximum in $S_N$ and two local extremes in its first derivative located respectively at $J_x/J \sim 0.93$, $J_x/J \sim 0.82$, and 1.02. Based on our scenario, we predict that there exist eventually four different phases divided by three transition points. The same technique is also applied to study the hard-core bosons on the checkerboard lattice, revealing its possible superfluid to super-solid transition \cite{21}.

A typical electron example is the 1D extended Hubbard model at half filling (Fig.1(d)). It is well known that there are two classical phases: charge-density-wave (CDW) ($U/V \ll 1$) and spin-density-wave (SDW) ($U/V \gg 1$) for positive $U$. The classical first-order phase boundary lies at $U/V=2$ \cite{22}. By employing our approach, we can identify accurately this classical first-order boundary from the local maxima of the reduced entropy. On the other hand, a recent theoretical study presumably indicated the presence of a new quantum phase bond-order-wave (BOW) at the verge of the line $U/V=2$, with the QPTs between SDW/BOW and CDW/BOW appearing to be the second-order \cite{23}. By analyzing the local extreme of the first derivative $d(S_N/N)/dV$ at fixed

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**FIG. 3:** The ground state renormalized reduced entropy $S_N/N$ and its first derivative versus the external parameter $\lambda$. (a) Coupled Dimer Antiferromagnet, (b) 2D frustrated system.

**FIG. 4:** (a) The ground state renormalized reduced entropy $S_N/N$ (solid line) and its first derivative (dotted line) versus the external parameter $J_x/J$ for the 2D checkerboard antiferromagnet model. (b) The phase boundaries for the 1D extended repulsive Hubbard model.
two critical points close to the line $U/V=2$ show up. Thus we incline to predict that two new quantum phases emerge around the classical phase boundary where the residual CDW and SDW correlations may still survive in the presence of quantum fluctuations, with the two new phase boundaries being the second-order (Fig.4(b)). By increasing the lattice size (from $N=6$ to $10$), the shifts of local extreme lines of $d(S_N/N)/dV$ towards the line $U/V=2$ can be clearly observed (not shown here). Thus the phase region for BOW becomes narrower, which is consistent with a previous investigation [24]. It is notable that the well-known second-order superconducting phase transition is also revealed with the same analysis for a negative $U$.

For the above numerical finding of the relationship between the reduced entropy of sublattice and the transition points, particularly from the first example, we may heuristically understand its origin: as $N \rightarrow \infty$, the shape of the peaks or dips around the transition points (in Figs. 3 and 4) would become sharper [24], namely $d^2(S_N/N)/d\lambda$ (or $d(S_N/N)/d\lambda$) would be discontinuous at the second (first) order transition points, resembling to the cases in thermodynamic phase transitions.

Many QPTs are yet to be clearly understood due to the competing nature of highly degenerate quantum states. In the sense that the reduced entropy for a small system may capture essentially the nonlocal feature of entanglement in a real system, this appropriate measure of entanglement enables us to establish its clear connection to transition points of QPTs. Therefore, comparing with the conventional wisdoms, it is not compulsory for us to deal with a large system to make the scaling analysis. In our scenario, exact numerical results for a quite small correlated system are able to disclose relevant information about QPTs. This is indeed a unique and superior advantage of our approach, making it be quite promising for the future exploration of QPTs in various physical systems, particularly if they fail to be characterized by the conventional approach.

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11. Let us consider the three dimensional Anderson localization model, with $H = -\sum_{(ij)} c^\dagger_{i\sigma} c_{j\sigma} + \sum_{i\sigma} \epsilon_i c^\dagger_{i\sigma} c_{i\sigma}$. The disorder is incorporated into the diagonal parameter $\epsilon_i$, which changes randomly with a uniform distribution $[-W/2, W/2]$ where $W$ characterizes the strength of the disorder. We here examine the reduced entanglement and found clearly its monotonic decrease with respect to $W$, while its first derivative has a local minimum at $W_c \sim 16$ ($W_c$ is the critical disorder strength) which corresponds to a second-order metal-insulator transition, in excellent agreement the well-known result.
12. This feature implies that the reduced entropy of sublattice introduced by us is an extensive quantity just like the thermal entropy, which is distinctly from other entanglement measures proposed before and is a reason why it can play a similar role in QPTs as that played by the thermal entropy in thermodynamic phase transitions.

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[22] The hopping intergral $t$, nearest-neighbor repulsion $V$ and the boson creation operator $b^\dagger$. We use the same technique to analyze the reduced entropy and found a local maxima at $J_2/J_0 \sim 10$ which may correspond to a possible first-order superfluid to supersolid transition. It is clear that in the large $J_z(V)$ limit, a novel supersolid phase may show up due to the
remarkable geometrical frustration.

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