Topological Estimator of Block Entanglement for Heisenberg Antiferromagnets

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We introduce a computable estimator of block entanglement entropy for many-body spin systems admitting total singlet ground states. Building on a simple geometrical interpretation of entanglement entropy of the so-called valence bond states, this estimator is defined as the average number of common singlets to two subsystems of spins. We show that our estimator possesses the characteristic scaling properties of the block entanglement entropy in critical and noncritical one-dimensional Heisenberg systems. We invoke this new measure to examine entanglement scaling in the two-dimensional Heisenberg model on a square lattice revealing an ''area law'' for the gapped phase and a logarithmic correction to this law in the gapless phase.

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The study of ground state entanglement properties of strongly interacting quantum many-body systems has recently been the subject of intense research [1,2]. This has allowed a new perspective on quantum phase transitions [3], especially in low-dimensional systems [4]. Additionally, the obtained results have helped in the development of improved simulation techniques for quantum many-body systems [5,6].

A central question in this field regards the scaling characteristics of the entanglement (or geometric) entropy—which fully quantifies the degree of entanglement (in a pure state) between a distinguished subsystem of a many-body system and the rest, in critical and noncritical systems. This problem actually was considered earlier [7] in the context of black hole physics. Specifically, in the case of one-dimensional spin systems, it has been shown that the entanglement of a contiguous block of spins saturates with block size L (related to the finite correlation length) for noncritical systems, while it logarithmically diverges ($S(L) \sim \log L$) in critical systems [4]. This logarithmic divergence depends on the universality class of the studied quantum phase transition and is governed by the central charge of the corresponding conformal field theory [8,9]. In $d > 1$ spatial dimensions, it is believed that the entanglement entropy originates only from the boundary separating two regions of noncritical systems ($S(L) \sim L^{d-1}$), while a logarithmic deviation from this ''area law'' might characterize critical systems, i.e., $S(L) \sim L^{d-1} \log L$. This is supported by results for some fermionic systems [10,11], where the violation of the area law accompanies algebraically decaying correlation functions and absence of energy gap; however, it seems that the area law is not necessarily violated in harmonic lattice systems [12]. In two dimensions for a topologically ordered gapped system, the area law is modified by an additive universal constant related to the total quantum dimension of the system [13]. Topological corrections to the entanglement scaling law have also appeared in the context of quantum gravity models [14].

In spite of the progress listed in the previous paragraph, the scaling of entanglement entropy in ($d > 1$)-dimensional spin systems has seldom been examined (however, see Ref. [15] for an ''infinite''-dimensional lattice). Such studies seem especially warranted in two dimensions where the competition between quantum fluctuations and different lattice topologies lead to interesting quantum phase transitions resulting in novel spin phases. The following reasons have contributed to the lack of results for these systems: (1) The explicit characterization of the ground state of these systems is generically hard, (2) The exact evaluation of the scaling of entanglement entropy with the size of the distinguished subsystem requires, in general, the diagonalization of exponentially growing matrices.

A different solution, which we propose in this Letter, amounts to the identification of estimators (specifically chosen for the examined system or class of systems) yielding the relevant entanglement scaling information that can be evaluated using quantum many-body techniques. This approach has the added advantage of encompassing a physical interpretation of the problem and its solutions.

We consider the isotropic antiferromagnetic Heisenberg spin-1/2 model

$$H = \sum_{i,j} J_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j. \qquad (1)$$

A crucial property of the exact ground state of this Hamiltonian, with an even number of sites, is that it is believed to be a total spin singlet state [16,17]. Therefore every such ground state can be represented in the so-called valence bond basis. We show below how this feature can be used to introduce an intuitive and remarkably simple estimator of the entanglement entropy of a contiguous block of spins.

The singlet ground state of the model [Eq. (1)] in general takes the form of a resonating valence bond state [18], i.e., a superposition of various possible valence bond states $|c_i\rangle$ (or elementary two-spin singlet coverings; see Fig. 1) on the considered lattice

$$|\Psi_{\mathrm{gs}}\rangle = \sum_i w_i |c_i\rangle. \tag{2}$$

These valence bond states can each be conveniently chosen as a collection of ''bipartite'' singlets connecting, e.g., spins residing on even- and odd-numbered sites. These states form an over-complete basis of the singlet sector of the underlying space, which we hereafter refer to as the valence bond basis.

A valence bond state appears as the ground state, e.g., of the isotropic Heisenberg frustrated chain at the Majumdar-Ghosh point [19]. The entanglement entropy of a set of adjacent spins A is the number of singlets $\mathcal{N}_{A|\mathrm{rest}}$ crossing the boundary separating it from the rest of the system (Fig. 1). This identification allows the study of entanglement entropy in the random singlet phase of the Heisenberg antiferromagnet [20].

Consider now the general ground state in Eq. (2). It is intuitively clear that the entanglement between a block of spins and the rest of the system should be related to the ''average'' number of singlets crossing the boundary of the distinguished subsystem. We consider the case of bipartite lattices—by setting the order of spin pairs in the singlets globally in the valence bond basis, the w_i characterizing the ground state can be chosen to be non-negative [16,21]. We define the average number of singlets cutting the boundary constraining a contiguous block of spins as

$$\bar{N}_{A|\mathrm{rest}} = \frac{1}{\sum_i w_i} \sum_i w_i N^i_{A|\mathrm{rest}}, \tag{3}$$

where $\mathcal{N}^i_{A|\mathrm{rest}}$ is the contribution due to the basis state $|c_i\rangle$ that occurs with weight $w_i/\sum_i w_i$. This choice of definition is motivated by the concept of singlet bond length probability [18] in a resonating valence bond state that can be used to define, e.g., the average bond length characterizing a ground state. It is well-defined in the (over-complete) valence bond basis, as can be directly verified by comparison with results for small systems in the exact so-called resonating valence bond basis. The quantity $\bar{\mathcal{N}}_{A|\mathrm{rest}}$, as shown shortly, shares the same scaling properties with the entanglement entropy under certain conditions, and as such can then be considered an appropriate estimator of the latter. Interestingly, it depends only on the topological distribution of singlets in the ground state and, unlike the entanglement entropy, is easily computable given $|\Psi_{\mathrm{gs}}\rangle$ [Eq. (2)].

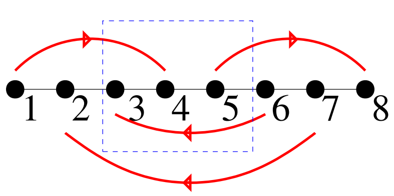

FIG. 1 (color online). A collection of singlets (a valence bond state) covering an exemplary lattice. The entanglement of the distinguished subsystem with its complement is the number of singlets crossing the boundary.

It is worth noting that $\bar{\mathcal{N}}_{A|\mathrm{rest}}$ correctly detects the lack of entanglement between unentangled regions and is also symmetrical with respect to the considered regions $\bar{\mathcal{N}}_{A|\mathrm{rest}} = \bar{\mathcal{N}}_{\mathrm{rest}|A}$. Furthermore, it takes on the value of 1 across a boundary containing any single spin signalling maximal entanglement of a spin with the rest of the system [22]. Finally, the average number of singlets crossing a boundary is manifestly subadditive, i.e., $\bar{\mathcal{N}}_{AB|\mathrm{rest}} \leq \bar{\mathcal{N}}_{A|\mathrm{rest}} + \bar{\mathcal{N}}_{B|\mathrm{rest}}$.

Nevertheless, $\bar{\mathcal{N}}_{A|\mathrm{rest}}$ is not generally equal to the corresponding entanglement entropy. In fact, the choice of the type of subsystem that is examined dictates the effectivity of describing its entanglement properties using $\bar{\mathcal{N}}_{A|\mathrm{rest}}$. For example, choosing the subsystem A from spins belonging only to one sublattice, $\bar{\mathcal{N}}_{A|\mathrm{rest}}$ is easily seen to be equal to the number of constituent spins independently of the actual entanglement [23]. Therefore, the possibility of estimating the entanglement entropy exists, in general for blocks of contiguous spins.

The evaluation of Eq. (3) is facilitated by a recently proposed ground state projection scheme in the valence bond basis implemented via quantum Monte Carlo simulations [21]. The ground state is projected out from a trial state (which we choose as a valence bond basis state) through the action H^n of a high power of the considered Hamiltonian. In effect, the states $|c_i\rangle$ are output with the appropriate weights $\sim w_i$ and a subsequent counting of singlets yields $\bar{\mathcal{N}}_{A|\mathrm{rest}}$.

We now turn to the scaling properties of our estimator in one-dimensional systems. Consider first the critical Heisenberg chain consisting of equal nearest neighbor interactions $J = J' = 1$ [see Fig. 2(a)]. Taking into account the finite size N of the system, the entanglement entropy of a block of size L scales as [8]:

$$S(L, N) = \frac{c_0}{3} + \frac{c}{3} \log\left[\frac{N}{\pi} \sin\left(\frac{\pi}{N} L\right)\right], \tag{4}$$

where $c = 1$ is the relevant central charge [4]. The quantity

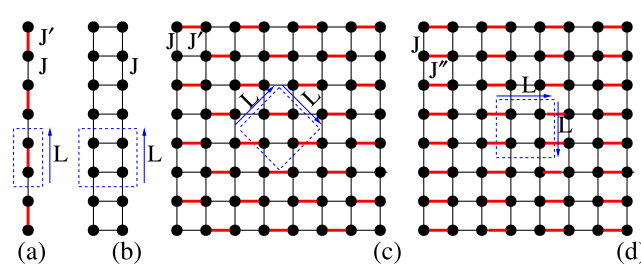

FIG. 2 (color online). Types of lattices considered below: (a) the $J - J'$ one-dimensional chain, (b) the ladder, (c) the $J - J'$ staggered square lattice, (d) the $J - J''$ columnar square lattice. All interactions are assumed to be antiferromagnetic J, $J' > 0$. Periodic boundary conditions are assumed throughout.

$\bar{\mathcal{N}}_L$ [Fig. 3(a)] also follows the same functional dependence on the block size, i.e., $\bar{\mathcal{N}}_L = \tilde{c}_0/3 + (\tilde{c}/3)\log x(L)$, where the effective length $x(L)$ is the argument of the logarithm in Eq. (4). The result shows that the entanglement entropy and estimator for identical blocks are linearly related. This leading order relation is evident also for small system sizes via exact diagonalization [inset in Fig. 3(a)]. The "charge" governing the logarithmic divergence of $\bar{\mathcal{N}}_L$ is close to the central charge for the Heisenberg model $\tilde{c} = 0.92 < c$.

The linear chain can be tuned away from criticality by setting $J'/J \neq 1$. In particular, for $J' = 0$ the ground state becomes a single valence bond state. The estimator $\bar{\mathcal{N}}_L$ trivially fulfills an area law. More generally, the noncritical chain is characterized by saturation of the estimator [Fig. 3(b)].

A different noncritical system is the Heisenberg antiferromagnet on a ladder [Fig. 2(b)], whose properties are intermediate between one- and two-dimensional systems [24]. The ground state is a spin liquid with a Haldane-type energy gap. The estimator of entanglement saturates with block size in this case as well [Fig. 3(b)—triangles].

The entanglement estimator and true entanglement are related through the properties of correlations, which are completely determined by the distribution of singlets in a resonating valence bond state, independently of the system dimension. Heuristically, long (short) range entanglement is connected with long (short) range singlets, which in turn, likewise determines the entanglement estimator. This is proved by the results presented so far and strongly indicates the utility of the introduced estimator in characterizing the properties of block entanglement in general.

We therefore examine the Heisenberg antiferromagnet on a square lattice with staggered and columnar dimerization [25] [Fig. 2(c) and 2(d)]. The two models undergo quantum phase transitions between Néel ordered and disordered valence bond states at $J'/J \approx 2.46$ [26] and $J''/J \approx 1.91$ [27] respectively. The interplay between an area law for noncritical parameters and a logarithmic correction for critical parameters can be captured by assuming $\bar{\mathcal{N}}_L = aL + bL\log(L)$, i.e., $\bar{\mathcal{N}}_L/L = a + b\log(L)$, where $\bar{\mathcal{N}}_L$ now regards a square block of linear size L. The estimator satisfies an area law in the valence bond phase, as seen in Fig. 4(b) for different lattice sizes.

For uniform couplings ($J'/J = J''/J = 1$), the ground state of the square lattice is in a Néel phase in the thermodynamic limit. Finite size scaling of the entanglement estimator reveals a logarithmic correction to the area law [Fig. 4(a)]. This is interesting as the considered point does not correspond to a critical point of this model. The result is, however, not surprising as the Néel phase, while or-

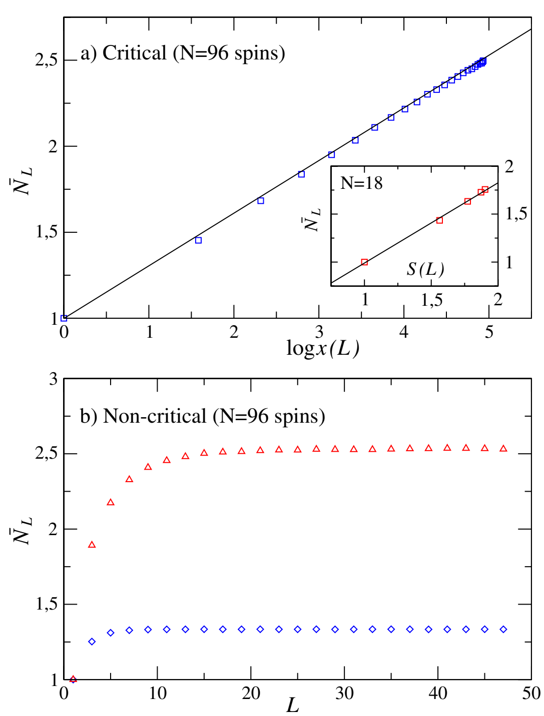

FIG. 3 (color online). (a) Scaling of $\bar{\mathcal{N}}_L$ for the critical chain with respect to the effective length $x(L)$. Inset: Comparison of the estimator and exact entanglement for the same partitions in a small system. (b) Saturation of $\bar{\mathcal{N}}_L$ for noncritical systems: diamonds—dimerized chain ($J'/J = 0.5$); triangles—spin ladder.

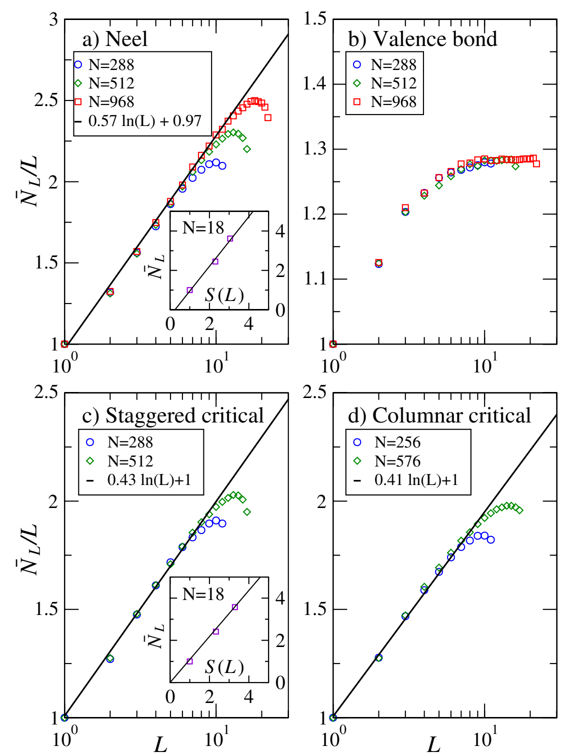

FIG. 4 (color online). Scaling of the entanglement estimator per boundary area on the two-dimensional square lattice. Shown are data points for $J'/J = 1.0$, 6.0, 2.46, and $J''/J = 1.91$. Insets: The estimator versus exact entanglement for small systems.

dered, is gapless with algebraically decaying correlations [28].

On tuning toward the critical points, the contribution due to the logarithmic term smoothly decreases from its Néel value. Nevertheless, logarithmic corrections to the scaling of $\bar{\mathcal{N}}_L$ are also present around the respective critical points of both considered models [Fig. 4(c) and 4(d)]. The critical coefficients governing the area law violations are almost equal, presumably because both critical points belong to the same universality class [25]. The results show that the average number of bonds crossing a large boundary is smaller than in the Néel state. This is consistent with the increase of order, *viz.* as argued in Ref. [18] antiferromagnetic order must be associated with longer range singlets in the resonating valence bond description.

It is worth emphasizing that the relation of the entanglement estimator and true entanglement in the interesting two-dimensional cases, for a small system, is similar to those proved in the one-dimensional case [Fig. 4(a) and 4(b)—insets; results are for $L = 1, 2, 3$] [29]. The valence bond phase is characterized by the formation of local singlets on the strong bonds and so the entanglement must manifestly satisfy an area law.

In conclusion, we have introduced a novel, intuitive estimator of block entanglement entropy having the relevant scaling properties. In two dimensions, this estimator predicts logarithmic corrections to the area law for block entanglement in the Néel (noncritical) phase as well as at criticality. These results are relevant to the identification of systems that can be simulated by new variational techniques based on ansatz states (see Ref. [6]) satisfying the area law. Our estimator is useful in Heisenberg systems, where entanglement cannot be directly evaluated numerically or analytically due to the complexity of the associated ground states.

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Note added.—Recently, it was brought to our attention that an approach equivalent to the one presented here has been independently undertaken in Ref. [30], where 1D cases and the columnar lattice in the Néel and valence bond phase have been studied yielding results in agreement with those presented here.

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