Valence Bond and von Neumann Entanglement Entropy in Heisenberg Ladders

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Introduction.– Entanglement has arisen in condensed matter physics as a new paradigm for the study of correlations in a system. Measurements of entanglement between separate subregions, chiefly using entropic quantities, have an advantage over traditional two-point correlation functions in that they encode the total amount of information shared between two subregions without the possibility of missing "hidden" correlations [1]. Such hidden correlations may occur in some quantum groundstates, in particular the important example of spin liquid states, where two-point correlation functions decay at large lengthscales. However, it is well known that a type of topological order may exist in spin liquids, which may be quantified in a "topological entanglement entropy", a property of the groundstate wavefunction [2, 3]. This and other entropic measures are typically discussed in the context of the von Neumann entanglement entropy, which for a system bipartitioned into two regions A and B, quantifies the amount of entanglement of A with B as

$$S_A^{\mathrm{VN}} = -\mathrm{Tr}[\rho_A \ln \rho_A]. \quad (1)$$

Here, the reduced density matrix $\rho_A = \mathrm{Tr}_B|\psi\rangle\langle\psi|$ is obtained by tracing out the degrees of freedom associated with the region B.

The von Neumann (VN) entanglement entropy (EE) has a well-defined and oft-studied set of analytical properties in interacting quantum systems. In one dimension (1D), exact analytical results are known from conformal field theories (CFT); they show that, away from special critical points, the VN EE between A and B scales according to the size of the boundary. This so-called *area law* is also believed to hold in many groundstates of two dimensional (2D) interacting quantum Hamiltonians, although few exact results are available [4]. Of particular importance, the existence of an area law has consequences in the rapidly-advancing field of computational quantum-many body theory: it is known that if the groundstate of a one-dimensional Hamiltonian satisfies an area law, then this state is well approximated by a Matrix Product State (MPS). Tensor-network extension of such MPS states are the basis for a new promising class of numerical algorithms that may push our abilities to simulate two-dimensional (2D) quantum systems past that allowed by quantum Monte Carlo (QMC) technologies, which are hampered by the notorious fermionic sign problem. However, it is believed that 2D states which lend themselves to accurate approximation by such methods must also obey an area law.

Thus the question of an area law in the groundstates of 2D quantum systems is of utmost important for the development of new simulation techniques. Paradoxically, it is also a quantity that is difficult to measure in 2D systems, due to the fact that QMC techniques (currently the only scalable method capable of unbiased 2D simulations) do not have direct access to the groundstate wavefunction $|\psi\rangle$, required to construct the VN EE. In response to this, several authors [5, 6] has recently introduced the concept of *valence bond* (VB) entanglement entropy, defined for an SU(2) symmetric spin system as

$$S_A^{\mathrm{VB}} = \ln(2) \cdot N_A, \quad (2)$$

where N_A is the number of EPR spin singlets $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$ crossing the boundary between regions A and B. Unlike the VN EE, the VB EE can be accessed very easily in the valence-bond basis projector QMC method recently proposed by Sandvik [7]. As demonstrated in Refs. [5, 6], the VB EE has many properties in common with the VN EE, in particular the relationship $S_A = S_B$, and the fact that $S_A^{VB} = 0$ for regions "un-entangled" by valence bonds. Further, a comparison of the scaling of the VB EE for a (critical) 1D spin 1/2 Heisenberg chain shows good agreement with analytical results known from conformal field theory (CFT), which we discuss more below. What is particularly striking about the results presented in Refs. [5, 6] is the extension of their work to the 2D isotropic Heisenberg model, which displays a *multiplicative* logarithmic correction to the area law. This multiplicative log correction was attributed to algebraically decaying correlations [6] and gapless modes [5]. If this property were to be shared by the VN EE, it could have the consequence that the 2D Neel groundstate can not be approximated by a tensor-network, and therefore not amenable to simulation techniques based on the MPS framework

In this paper, we compare the VB EE calculated by valence-bond QMC to the VN EE accessible through large-scale density-matrix renormalization group (DMRG) measurements on the Heisenberg model on multi-leg ladder geometries. We show that in 1D, contrary to initial results presented in Refs. [5, 6], the CFT central charge calculated by scaling the VN EE (confirmed with DMRG to converge to $c = 1$) does not converge to the expected result when calculated by scaling the VB EE. On multi-leg ladders, it becomes clear that the VB EE is always greater than the VN EE, a trend which grows rapidly with the number of legs N. Finally, a comparison of the area law defined by bisecting the multi-leg ladders shows a clear logarithmic correction for the VN EE, $S_A^{VB}/N = N \ln N$ (in agreement with Refs. [5, 6]), however for data up to $N = 7$, the VN EE as calculated by DMRG convincingly shows a scaling of $S_A^{VB}/N = N$, the expected area law.

Model and Methods.– The spin 1/2 Heisenberg hamil-

tonian is given by

$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \qquad (3)$$

where the sum is over nearest-neighbor sites on a ladder with length L and legs n. Many properties of this model on open-boundary ladders with n legs has been exhaustively studied. Of importance, it is known that a spin gap exists for even-n ladders in the limit of $L \to \infty$, whereas odd-n ladders behave somewhat more like quasi-1D systems with spin $n/2$ and, from Haldane's conjecture, are therefore gapless.

We employ two complementary numerical techniques in our study of EE on ladder geometries, namely the valence-bond basis QMC and DMRG, both of which give *unbiased* approximations to the ground state of the Hamiltonian at zero temperature, and results from both of which can be compared directly to one another. Of interest to us are the two definitions of entanglement entropy; the VN EE is naturally accessible through the DRMG "sweeping" algorithm, which converges the groundstate wavefunction of a finite-size system by calculating the reduced density matrix between a "system" and "environment" (subregions A and B), the size of each of which are systematically grown or reduced in the usual DMRG sweep. The reduced density matrix ρ_A is calculated at each sweeping step, therefore the VN EE is immediately available for geometries illustrated in Fig. 2. In this paper, we label the regions A by the largest lattice site x contained therein.

The valence-bond basis QMC algorithm that we use is the simple single-projector method proposed by Sandvik in 2005 [7], with lattice geometries constructed to match those given by the DMRG algorithm. The ground state of the system is projected out by repeated application of a list of bond operators on nearest neighbor sites of the ladder. A number of bond operators (r) are changed each step and the change is accepted with a probability depending on the number of nearest neighbor bonds in the resulting valence bond states. Measured quantities such as energy or valence bond entanglement entropy are then calculated by a weighted average over all the valence bond states obtained by this procedure.

One-dimensional chain.– We consider first the case of a one-dimensional Heisenberg chain, limiting ourselves to a discussion of the system with open boundary conditions (OBC), in order to retain the maximal efficiency of the DMRG, which is known to have poorer convergence properties under periodic boundary conditions (PBC). For the isotropic OBC chain with Hamiltonian Eq. (3) with some interior point subdividing the region A of length x from the remainder of the system, the von Neumann entropy is known from conformal field theory (CFT) to obey $S_A^{VN} = c/6 \ln(x') + S_1$, where $c = 1$ is the central charge, and $x' = L/\pi \sin(\pi x/L)$ is the conformal distance [8]. In Ref. [5], VB EE calculated from QMC was

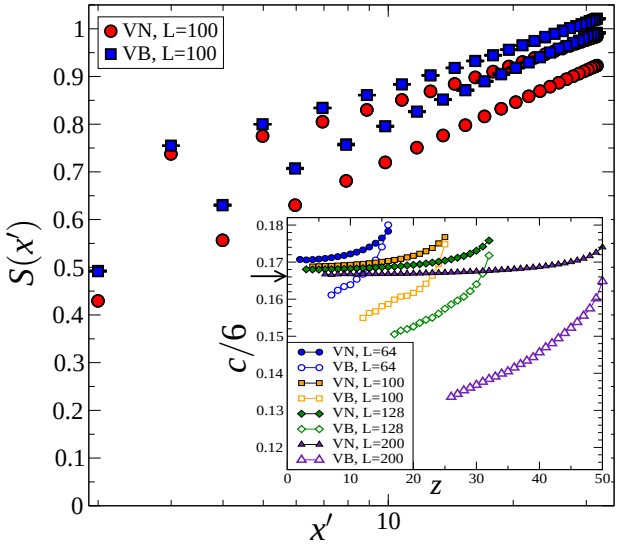

FIG. 1: (color online) Main: The valence bond (VB) and von Neumann (VN) entanglement entropies for a 1D Heisenberg chain with 100 sites. The horizontal axis x' is the conformal distance, as described in the text. Inset: coefficient of a linear regression fit of the data to the form $c/6 \ln(x')$, as a function of data points included in the fit, z. Here, z is systematically decreased by removing points from the *outside* ends of the open-boundary chain. The arrow, at $c/6 = 1/6$, is the analytical result from CFT [8].

compared to this CFT result, and a good fit to a central charge of $c = 1$ was found. In Fig. 1 we compare this result to the VN EE calculated from the DRMG. We stress that the QMC and DMRG results are on the same geometry and Hamiltonian, and reproduce the same ground state energies; the remaining figures in the paper can be considered as exact comparisons between the VB and VN EE as calculated with the two methods. In Fig. 1 (main), both the VN and VB EE are seen to split into two branches, the lower corresponding to an even number of lattice sites in the *system* A, and the upper corresponding to an odd number of sites in A. This reflects a well-known "dimerization" effect induced by the open system boundaries [9]. A regression fit of the lower branch to the form $c/6 \ln x'$ (inset) shows excellent convergence of the VN EE to the central charge predicted by CFT, $c = 1$, once finite-size effects and the proximity of the data to the open boundaries is taken into account. In contrast, the VB EE fit deviates significantly from the CFT result for larger system sizes, give $c > 1$ when all or most data is included in the fit, and $c < 1$ as data is systematically excluded from the fit (data closest to the open boundary is removed first).

Multi-leg ladders.– Moving away from the one dimensional chain, one can add "legs" to the lattice in a systematic way.

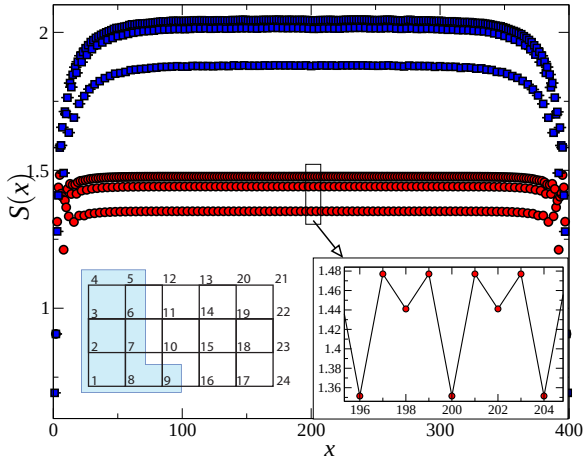

FIG. 2: (color online)

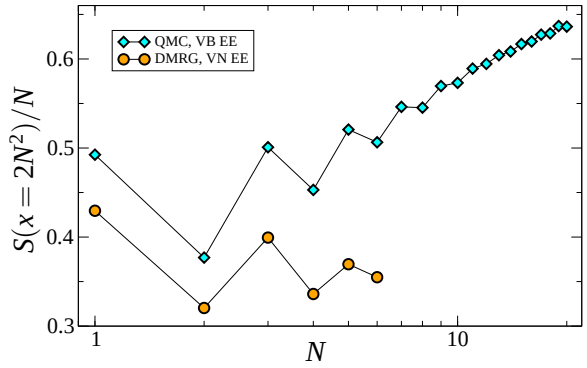

FIG. 3: (color online) The VB and VN entanglement entropies (taken such that the region A includes $2N^2$ sites) normalized by N, the number of legs. All ladders have 100 sites per leg.

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