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 partitioned into two regions A and B, quantifies the amount of entanglement of A with B as

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

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 the utmost importance 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

$$S_A^{\mathrm{VB}} = \ln(2) \cdot \mathcal{N}_A, \tag{2}$$

where $\mathcal{N}_A$ 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 is 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.– We consider the spin 1/2 Heisenberg Hamiltonian, given by

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

where the sum is over nearest-neighbor sites. Geometries studied are 1D chains, and multi-leg ladders with length L and number of legs n. 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. 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, allowing easy calculation of Eq. 1. The density matrix is of course truncated in the usual DMRG algorithm, so care must be taken to ensure that enough of the eigenvalue spectrum is included to converge the VN EE to sufficient accuracy; typically the number of states required is larger then that needed to converge the energy alone.

The VB EE can be calculated using the valence-bond basis QMC proposed by by Sandvik in 2005 [7]. The valence-bond basis QMC algorithm that we use is the simple single-projector method, 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 chains. We employ both open (OBC) and periodic (PBC) boundary conditions with both DMRG and QMC, in order to study the VN and VB entanglement entropies (PBCs typically have poorer convergence properties with standard DMRG and more states must be kept in the algorithm). Figure 1

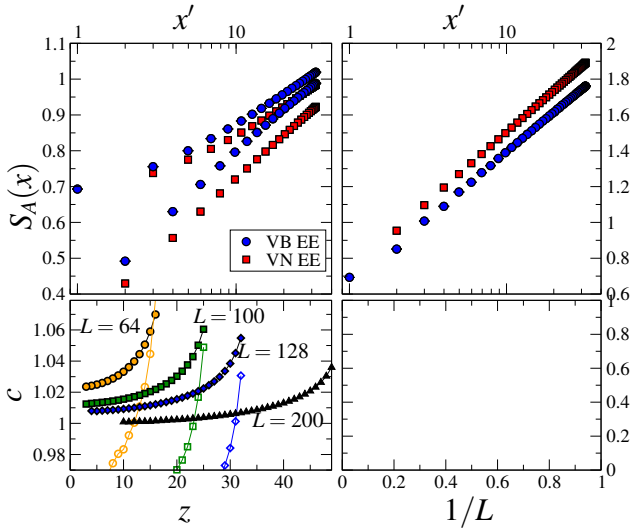

FIG. 1: (color online) Upper plots: the valence bond (VB) and von Neumann (VN) entanglement entropies for a 100-site 1D Heisenberg chain with (left) open boundary conditions and (right) periodic boundary conditions. Lower plots show the central charge c; for OBC (left), the central charge is illustrated for the VN EE (closed symbols) and the VB EE (open symbols) for system sizes L=64 (circles), L=100 (squares), L=128 (diamonds) and L=200 (triangles) as a function of the number 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. At right, the central charge as a function of inverse system size, for PBC.

illustrates simulation results in both cases, where the bipartition between regions A and B are defined via the length $1 \le x \le L$ along the chain. In the upper panels of Fig. 1, the two entanglement entropies are plotted to versus conformal distance x', defined in the OBC case as $x' = 2L/\pi \sin(\pi x/L)$ and in the PBC as $x' = L/\pi \sin(\pi x/L)$ (**check**) [8]. This allows one to compare the simulation results to exact result from conformal field theory (CFT) in the limit of infinite chains. Namely, from CFT the VN EE is known to obey $S_A^{VN} = c/3 \ln(x') + S_1$ in the PBC case, and $S_A^{VN} = c/6 \ln(x') + \ln(g) + S_1/2$ in the OBC case, where S_1 is a model-dependent constant, g is Ludwig and Affleck's universal boundary term, and c is the central charge of the CFT.

In Refs. [5, 6], VB EE calculated from QMC was compared to this CFT result, and a good fit to a central charge of $c = 1$ was found for both cases. In Fig. 1 we compare this result to the VN EE calculated from the DMRG. 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. In Fig. 1 (a), 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 num-

ber 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).

In Fig. 1 (b), the VN and VB entropies are also seen to diverge, however in this case the VN EE is greater than the VB EE. **CENTRAL CHARGE FIGURE?**

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

Area law in multi-leg ladders.– Given the ground state of a quantum many-body system in 2D, the question of whether the entanglement entropy fulfills and "area" (boundary) law is in general a difficult one to answer. However from a simulation perspective this question is of utmost importance, since tensor-network generalization of MPS techniques, such as PEPS, produce states that satisfy the area law by construction. Thus in order to simulate, for example, the Néel groundstate of the 2D Heisenberg model accurately with such methods depends critically on whether or not the entanglement entropy of the Néel state obeys an area law. Refs. [5, 6] examined this issue using the VB EE, and found clear multiplicative logarithmic corrections to the area law in the Néel state, which was tentatively attributed to gapless Goldstone modes and algebraically decaying correlations.

We can address this question using our data for the VB and VN EE alluded to in the above section on multi-leg ladders. That is, we chose a lattice geometry such that subregion A is rectangular, cutting a multi-leg ladder cleanly across a rung, such that the "area" separating region A and B is equivalent to the number of legs in the ladder N. We chose this area A to contain contain $2N^2$ sites ...**Matt: do we want to spell out the argument involving the sum over quasi-1D modes? I think we will have room**.

Fig. 3 illustrates the simulation results for N-leg ladders. Plotting S_A/N versus N on a log scale, one sees that we reproduce the multiplicative logarithmic correction to the VB area-law, in agreement with Refs. [5, 6]. However, the linear slope is not present in the plot of the VN EE data from the DMRG, which convincingly approaches a constant for large N. Clearly, the VN EE suggests that the area law is indeed obeyed in the Néel groundstate, leading one to conclude that the multiplicative logarithmic correction is an artifact of the VB EE.

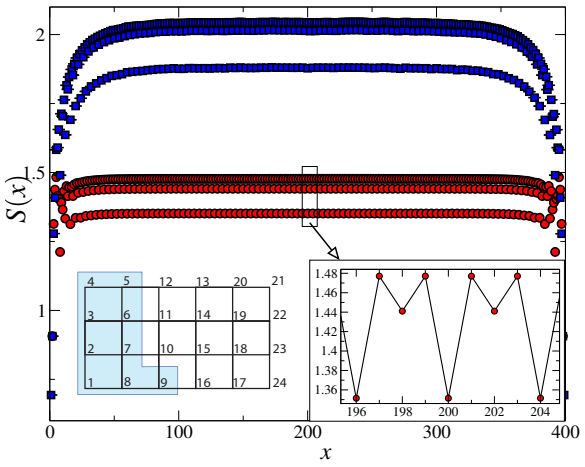

FIG. 2: (color online)

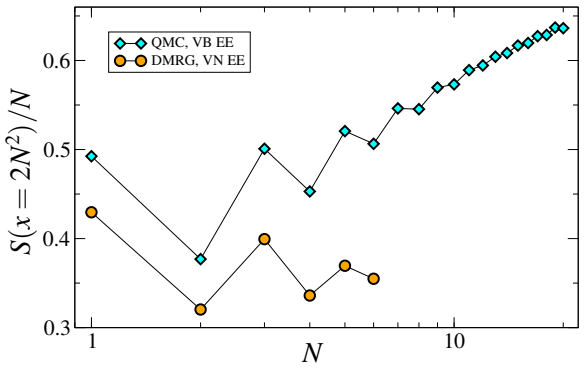

FIG. 3: (color online) The VB and VN entanglement entropies (taken such that the region A includes $2N^2$ sites) normalized by N, the number of legs. All ladders have 100 sites per leg.

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