Valence Bond Entanglement Entropy

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We introduce for SU(2) quantum spin systems the Valence Bond Entanglement Entropy as a counting of valence bond spin singlets shared by two subsystems. For a large class of antiferromagnetic systems, it can be calculated in all dimensions with Quantum Monte Carlo simulations in the valence bond basis. We show numerically that this quantity displays all features of the von Neumann entanglement entropy for several one-dimensional systems. For two-dimensional Heisenberg models, we find a strict area law for a Valence Bond Solid state and multiplicative logarithmic corrections for the Néel phase.

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Entanglement is probably the most prominent feature that allows to distinguish quantum from classical systems. While being an inherent ingredient of quantum information processing, the study of entanglement properties of quantum many-body states has recently shed new light on our understanding of condensed matter systems at zero temperature. Over the past few years, various measures of entanglement have been used to investigate quantum phase transitions and states of matter. Amongst them, the von Neumann entanglement entropy (EE) quantifies the bipartite entanglement between two parts of a quantum system. The EE of a quantum state $|\Psi\rangle$ between a part $\Omega$ and the rest of a system is

$$S_{\Omega} = - \text{Tr} \rho_{\Omega} \ln \rho_{\Omega}$$

where $\rho_{\Omega} = \text{Tr}_{\bar{\Omega}} |\Psi\rangle\langle\Psi|$ is the reduced density matrix of $\Omega$ obtained by tracing out the rest of the system $\bar{\Omega}$. An important property of EE is that $S_{\Omega} = S_{\bar{\Omega}}$ and it appears naturally that $S_{\Omega}$ is only related to the common property of $\Omega$ and $\bar{\Omega}$, their boundary: general arguments indeed indicate that $S_{\Omega}$ typically scales with the size of the boundary (area law). For critical systems however, logarithmic corrections can be present. If the critical system is conformal invariant, the amplitude of the logarithmic corrections is related to the central charge of the corresponding conformal field theory (CFT). This has been shown in one dimension (1d) and more recently for some CFT in two dimensions (2d), in which case the coefficient also depends on the geometry of $\Omega$. For systems possessing topological order, other subleading corrections also depend on the topology of $\Omega$. The scaling of the EE with the size of $\Omega$ therefore contains precious informations on the state of the physical system and can be used e.g. to detect criticality. This has been successfully demonstrated in quantum spin systems, which are natural candidates for such studies as they are both of theoretical and experimental relevance in condensed matter.

While many interesting properties of EE have been derived exactly for integrable models or systems with exactly known ground-states (GS), the calculation of EE for general interacting quantum systems is an exacting task. On the practical side, even numerical simulations are difficult. Exact diagonalization is limited to small systems and cannot precisely verify scaling properties and EE is not accessible to Quantum Monte Carlo (QMC) methods. In 1d, EE can be calculated within the DMRG method but this technique is no longer available in higher dimensions. In this Letter, we introduce another measure of entanglement, called Valence Bond Entanglement Entropy (denoted hereafter $S^{VB}$), which is defined for quantum spin systems with SU(2) symmetry. It can be measured efficiently in all dimensions for non-frustrated antiferromagnetic (AF) spin systems via QMC simulations in the Valence Bond (VB) basis. We show that $S^{VB}$, albeit different, captures all features of the von Neumann EE. In particular, it obeys the same scaling properties: for 1d quantum spin systems, we recover CFT predictions. We also investigate the properties of $S^{VB}$ for a 2d Heisenberg model possessing Néel and Valence Bond Solid phases. Our numerical results show that $S^{VB}$ obeys an area law for both phases, with the presence of logarithmic corrections for the Néel phase.
We focus on the AF spin-1/2 Heisenberg Hamiltonian
\[
H = \sum_{ij} J_{ij} S_i \cdot S_j,
\]
which conserves the total spin \( S_T \) of the system. AF interactions \( J_{ij} > 0 \) favor a singlet \( S_T = 0 \) ground-state.

**Definition** — It is well-known that any singlet state can be expressed in the VB basis, where spins couple pairwise in singlets \( |\uparrow \downarrow \rangle - |\downarrow \uparrow \rangle / \sqrt{2} \). The VB basis is overcomplete (there are more VB coverings than the total number of singlets). Another basis is the bipartite VB basis \[14\], where the system is decomposed into two sets (for instance different sublattices for a bipartite lattice) such that two spins forming a singlet necessarily belong to different sets. This basis is smaller, but still overcomplete. In a given bipartition of sites and bipartite VB state \( |\Psi\rangle \) such as the ones in Fig. 1, consider a subsystem \( \Omega \) (shaded area in the figure). We define the Valence Bond Entanglement Entropy of this state as:
\[
S^\text{VB}_\Omega(|\Psi\rangle) = \ln(2), n^\text{c}_\Omega(|\Psi\rangle)
\]
where \( n^\text{c}_\Omega(|\Psi\rangle) \) is the number of singlets that cross the boundary of \( \Omega \) (i.e. singlets with one and only one constituting spin within \( \Omega \). The constant \( \ln(2) \) is used to match the EE for a unique singlet. In general, the GS of the Hamiltonian \( H \) is not a single VB state. For a linear combination \( |\Psi\rangle = \sum_i a_i |\Psi_i\rangle \) with \( |\Psi_i\rangle \) bipartite VB states, we define \( S^\text{VB}_\Omega(|\Psi\rangle) = \sum_i a_i S^\text{VB}_\Omega(|\Psi_i\rangle) / \sum_i a_i \). An estimate of \( S^\text{VB}_\Omega \) for the GS of \( H \) can then be obtained by using the Projector QMC method recently proposed by Sandvik \[13\], which precisely works in a bipartite VB basis (as soon as \( H \) is not frustrated). In this method, the GS is sampled by applying \( H^* \) stochastically (with \( n \) sufficiently large) to an initial VB state \( |\Psi_0\rangle \) in order to obtain a projected state \( |\Psi_n\rangle \). In this process, \( |\Psi_n\rangle \) appears a number of times proportional to its coefficient in the GS wave function. The GS estimate of \( S^\text{VB}_\Omega \) is obtained by Monte Carlo-averaging \( S^\text{VB}_\Omega(|\Psi_n\rangle) \) over the projected states obtained in all Monte Carlo steps.

**Bipartite basis and overcompleteness** — At first glance, \( S^\text{VB}_\Omega \) seems ill-defined as the bipartite VB basis is overcomplete. \( |\Psi\rangle \) can indeed be rewritten as a linear combination of other states for which \( S^\text{VB}_\Omega \) could be different. However, \( S^\text{VB}_\Omega \) turns out to be conserved in any linear combination between the bipartite VB states. Via an algebraic representation of the singlet wave function, it can be indeed shown that for any linear relation \( \sum_i c_i |\Psi_i\rangle = 0 \) between the bipartite VB states \( |\Psi_i\rangle \), we have \( \sum_i c_i S^\text{VB}_\Omega(|\Psi_i\rangle) = 0 \) for all \( \Omega \) \[15\]. Another issue is the choice of the bipartite basis: in the general case, \( S^\text{VB} \) does depend on the precise choice of bipartition. However, if \( |\Psi\rangle \) satisfies a Marshall sign criterion \[16\], a genuine bipartition where all \( a_i > 0 \) exists and should be taken. Not all singlet states satisfy this, but this is the case for e.g. the GS of \( H \) on bipartite lattices \[16\]. In practice, the QMC method is efficient only for bipartite \( H \) (when all \( a_i > 0 \)) and the Marshall condition is not a restriction. This implies that \( S^\text{VB}_\Omega \) is a well-defined quantity for any singlet wave function satisfying the Marshall criterion and that it can easily be measured (e.g. graphically as in Fig. 4) for any bipartite VB state.

**Entanglement properties** — \( S^\text{VB}_\Omega \) is in general different from EE (this can be seen by computing exactly both quantities on a small system). However, \( S^\text{VB} \) share many properties with EE: (i) \( S^\text{VB}_\Omega \) is a sub-additive quantity: \( S^\text{VB}_\Omega \leq S^\text{VB}_{\Omega_1} + S^\text{VB}_{\Omega_2} \), (ii) \( S^\text{VB}_\Omega = \max_{\text{singlets}} \) as in Fig. 4 for any bipartite VB state: this is the case in the thermodynamic limit for the Majumdar-Ghosh spin chain \[17\] or for the Random Singlet phase \[18\] of disordered spin chains where one VB state essentially dominates \[4\]. Finally, we note that \( S^\text{VB} \) offers a simple geometrical interpretation of entanglement properties of a quantum spin state: \( \Omega \) is entangled with the rest of the system if there are singlets in between these two parts.

In the rest of this paper, we will show that \( S^\text{VB} \) captures both qualitative and quantitative features of the EE. \( S^\text{VB} \) can be calculated for all systems that can be simulated with the VB QMC method, in particular all spin-1/2 AF Heisenberg-like models on bipartite lattices in all dimensions, including models with multiple-spin interactions \[13\]. We first start with 1d models, where all the characteristics of the EE are recovered with high precision. We then present results on entanglement properties of 2d AF Heisenberg models.

**1d systems** — We first consider 1d uniform AF Heisenberg chains where the GS is known to be critical, with algebraic decay of spin correlations. For systems of finite size \( L \) with periodic boundary conditions (PBC), CFT predicts that the EE of a block of spins of size \( x \) scales (for large \( x \)) as \( S(x) = c/L \) \( x \) \( \ln(x/L) + S_0 \), where \( x' = L/\pi \sin(\pi x/L) \) is the conformal distance, the central charge \( c = 1 \) and \( S_0 \) a non-universal constant \[3\]. Fig. 2a displays \( S^\text{VB}(x) \) for a 1d uniform chain of size \( L = 128 \) and the resulting curve is well fitted by the form \( S^\text{VB}(x) = c_{\text{eff}}/3 \ln(x') + S_0 \) with \( c_{\text{eff}} = 1 \), in full agreement with CFT predictions for EE.

Now we turn to uniform AF Heisenberg chains with open boundary conditions (OBC). For a segment of size \( x \) starting at the open boundary, the CFT prediction for EE is \( S(x) = c/6 \ln(x') + S_1 \) with \( c = 1 \) and \( S_1 \) another constant related to \( S_0 \) \[3\]. Our results (see Fig. 2b) for \( S^\text{VB}(x) \) for an \( L = 128 \) open chain also clearly follow this scaling form. We also recover the alternating term found for the EE of open Heisenberg chains \[11\], as can be seen from the two distinct odd-even sets of points in Fig. 2a.

We next consider an alternating Heisenberg spin chain, where the coupling is \( 1+\delta \) (respectively \( 1-\delta \)) for all even (resp. odd) bonds. This system is non-critical with a finite correlation length for all \( \delta \neq 0 \) and the EE \( S(x) \) of
We conclude this section by showing results on the scaling form with a prefactor $\gamma_{\text{eff}} = 0.6(1)$, in agreement with the RSRG prediction for the average EE. Actually, the average in the thermodynamic limit is dominated by a single VB state, we expect $S_{\text{VB}}$ and $S$ to coincide. This is however difficult to check numerically because of the finite $L$ and the small number of random samples used in the simulations. This also accounts for the small discrepancy in our numerical estimate of $\gamma_{\text{eff}}$ with respect to the RSRG prediction (note that a fit forcing $\gamma_{\text{eff}} = \ln(2)$ is also of good quality as seen in Fig. 2d).

2d systems — The previous section showed the precise agreement between the VB entanglement entropy $S_{\text{VB}}$ and the true EE $S$ in both quantitative and qualitative respects for 1d systems. This gives us confidence that $S_{\text{VB}}$ is a good observable to quantify entanglement also in larger dimensions $d$. This is an important point as the VB QMC simulations (and therefore the calculation of $S_{\text{VB}}$) can easily be extended to higher $d$. Note at this stage that only few results are available on entanglement properties in high $d$: exact results have been derived for free fermions [22, 23], bosons [20, 24] and some exactly solvable spin models [25], but EE has never been calculated numerically for large $d > 1$ systems to our best knowledge [26]. At present time, the connection between the area law and the precise nature of the ground-state (range of correlations, presence of a gap) is not fully understood for $d > 1$ (see a discussion in Ref. 24a).

We now investigate 2d Heisenberg systems and calculate $S_{\text{VB}}$ for a square subsystem $\Omega$ of linear size $x$ (such as the one in Fig. 1), for $L \times L$ samples with PBC up to $L = 64$. In particular, we consider a model of coupled dimers in two dimensions depicted in the inset of Fig. 3, where dimers (with intra-dimer exchange $\lambda_2$) are coupled with an inter-dimer exchange $\lambda$. The physics of this model is well-understood [27]: at low $\lambda$, the system is in a dimerized Valence Bond Solid (VBS) phase whereas the case $\lambda = 1$ corresponds to the Néel phase of the isotropic 2d Heisenberg model. The system undergoes a quantum phase transition between these two states at $\lambda_c = 0.52337(3)$ [27]. Fig. 3 displays the average Valence Bond entanglement entropy divided by the linear size $S_{\text{VB}}(x)/x$ for the point $\lambda = 0.2$ located in the VBS phase. All the curves for different $L$ saturate for large enough $x$, indicating that the Valence Bond entanglement entropy obeys an area law $S_{\text{VB}}(x) \propto x$, as expected for a gapped phase. For the isotropic case $\lambda = 1$ located in the Néel phase, $S_{\text{VB}}(x)/x$ does not saturate, and the curve is actually well-fitted by a log form, as exemplified by the log-linear scale of Fig. 3b. Our numerical results therefore indicate that the Valence Bond entanglement entropy scales as $S_{\text{VB}}(x) \propto x \ln(x)$ in the Néel phase. Multiplicative logarithmic corrections have also been found for the EE of fermions [22, 23]. They
are tentatively attributed here to the Goldstone modes present in the Néel phase, which also make for the algebraic transverse spin correlations. Scaling of $S^{\text{VB}}$ at the critical point $\lambda_c$ is currently under investigation.

To summarize, we have proposed the Valence Bond entanglement entropy as a new measure of entanglement for SU(2) quantum spin systems. $S^{\text{VB}}$ offers a powerful tool to quantitatively investigate the deep connection between VB physics and the amount of entanglement present in spin systems, although its precise connection to EE needs further studies. Several questions then arise, pointing for instance towards $d \geq 2$ exotic phases (such as RVB spin liquids) and quantum critical points (as in Ref. 19), which should hopefully exhibit striking valence bond entanglement features. Finally, in the absence of a Marshall sign rule (as for some frustrated systems) where $S^{\text{VB}}$ depends on the choice of a bipartite basis, the usefulness of $S^{\text{VB}}$ has to be clarified.

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FIG. 3: (Color online) $S^{\text{VB}}/x$ versus distance $x$ for 2d quantum spin systems: (a) 2d AF dimerized Heisenberg model ($\lambda = 0.2$), (b) 2d AF Heisenberg model ($\lambda = 1$) (log-linear scale). Solid line is a fit to a logarithmic divergence form. Inset: Illustration of the coupled-dimer model. Simulation parameters are $n = 30L^2$ for $L \leq 32$, $n = 20L^2$ for $L > 32$.

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