Valence bond entanglement entropy of frustrated spin chains

Fabien Alet,1,2 Ian P. McCulloch,3 Sylvain Capponi,1,2 and Matthieu Mambrini1,2

1Laboratoire de Physique Théorique, Université de Toulouse, UPS (IRSAMC), F-31062 Toulouse, France
2CNRS, LPT (IRSAMC), F-31062 Toulouse, France
3School of Physical Sciences, The University of Queensland, Brisbane, QLD 4072, Australia

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We extend the definition of the recently introduced valence bond entanglement entropy to arbitrary SU(2) wave functions of $S = 1/2$ spin systems. Thanks to a reformulation of this entanglement measure in terms of a projection, we are able to compute it with various numerical techniques for frustrated spin models. We provide extensive numerical data for the one-dimensional $J_1 - J_2$ spin chain where we are able to locate the quantum phase transition by using the scaling of this entropy with the block size. We also systematically compare with the scaling of the von Neumann entanglement entropy. We finally underline that the valence-bond entropy definition does depend on the choice of bipartition so that, for frustrated models, a “good” bipartition should be chosen, for instance according to the Marshall sign.

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I. INTRODUCTION

Entanglement is a fundamental notion of quantum mechanics, that has over the recent years gained popularity as a way to provide new insights in the quantum many-body problem. From the condensed matter point of view, one of the most interesting promises of the study of entanglement properties is the possibility to automatically detect the nature of quantum phases and of quantum entanglement properties. We finally underline that the valence bond entropy definition does depend on the choice of bipartition so that, for frustrated models, a “good” bipartition should be chosen, for instance according to the Marshall sign.

Alternatively, it is possible to define for certain quantum spin systems, a different quantifier of entanglement through the use of the Valence Bond (VB) representation. The key idea is that for two quantum spins $1/2$ at sites $i$ and $j$, the singlet state (or VB) $|\Psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow_i \downarrow_j \rangle - |\downarrow_i \uparrow_j \rangle)$ is maximally entangled. It can therefore be used as a nat-
ural unit of entanglement (in the quantum information community, the entanglement is often measured in units of singlets). Consider now a VB state where an even number \( N \) of spins 1/2 are coupled pairwise in singlets, and divide the spins in two arbitrary sets \( \Omega \) and \( \Omega' \). It is simple to see that the von Neumann entropy \( S^{vN} \) is equal to the number of VBs shared between \( \Omega \) and \( \Omega' \) (i.e. where one of the two spins is located in \( \Omega \) and the other in \( \Omega' \)), times the constant \( \ln(2) \). This constant is just the von Neumann entropy of a single spin in a VB. In other words, every singlet that crosses the boundary between \( \Omega \) and \( \Omega' \) contributes \( \ln(2) \) to the von Neumann entropy. The picture is very appealing as it provides a simple geometrical interpretation of entanglement, a quantity which is not always easy to grasp intuitively. This argument of course is only exact for the case of VB states, which are simple factorized states. However, it can be shown, and we will describe this in detail below, that the picture holds for all singlet states. This is an important property as most antiferromagnetic systems have a singlet finite size ground-state.

In general, the resulting Valence Bond Entanglement Entropy (VB EE) \(^{11,12}\) is different from the von Neumann entropy, except for the case of VB states where they coincide. There are however several points of interest for this alternative description: (i) it fulfills all desired properties of an entropy\(^ {12}\) (ii) the VB EE can be easily computed through QMC methods in the VB basis\(^ {13}\), offering the possibility to study \( d > 1 \) systems, (iii) the scaling properties of the VB EE display several interesting features.

Concerning the scaling (with system size) of the VB EE, it has been shown first numerically and then analytically that for critical systems in 1d, the VB EE scales logarithmically with block size \( S^{VB} \propto x \ln(x) \) (here and in the following the symbol \( \propto \) denotes proportionality up to a constant). On the other hand, \( S^{VB} \) converges to a constant for gapped systems. The same scaling behavior is displayed by the von Neumann EE. The only difference comes from the prefactor of the log divergence: while the numerical estimation of \( \gamma \) was first reported\(^ {12}\) to be consistent with \( c/3 \) (as for vN EE), the analytical results of Ref.\(^ {15}\) indicate that the two quantities are different for Heisenberg spin chains \( \gamma = 4 \ln(2)/\pi^2 \neq 1/3 \), even though the numerical value of \( \gamma \approx 0.279 \) is very close to 1/3 (\( c = 1 \) for the Heisenberg chain). We will comment on the numerical validation of the exact value \( \gamma = 4 \ln(2)/\pi^2 \) at a later stage of this paper.

In two dimensions, the situation seems slightly different. For gapped spins systems, the VB EE was shown\(^ {12,13,14} \) to fulfill a strict area law \( S^{VB} \propto x \) (with \( x \) the linear size of the boundary between \( \Omega \) and \( \Omega' \)). The same scaling is expected on general grounds for \( S^{VN} \). In the case of the ground-state of the 2d Heisenberg model displaying Néel order with gapless excitations, the VB EE displays a multiplicative logarithmic correction to the area law\(^ {12,13,16} \): \( S^{VB} \propto x \ln(x) \). There is no equivalent calculation (analytical or numerical) for the von Neumann EE of the 2d Heisenberg model, for the reasons described above. However, recent DMRG calculations\(^ {13} \) on N-leg ladders and QMC computations of the Renyi entropy of the 2d Heisenberg model\(^ {14} \) suggest that the vN EE displays no such multiplicative logarithmic and that the Néel ground-state fulfills strictly an area law \( S^{vN} \propto x \). This can be seen negatively as the scaling of the VB EE does not match the one of the vN EE, showing its limits to discuss the adherence of the vN EE to the area law in higher dimensions. One should note however that the VB EE is able to distinguish between a gapless and a gapped state, which the vN EE cannot -, one of the main original and practical motivations of studying entanglement in condensed-matter systems. As a side remark, we also note that the VB EE can be used to characterize shared information in the different context of stationary states of stochastic models\(^ {15} \).

In this paper, we investigate the properties of the VB EE using a different approach. The original VB EE definition\(^ {12} \) is intimately related to the fact it is possible to consistently define\(^ {16} \) a VB occupation number able to quantify the presence/absence of a SU(2) dimer on a given bond for any singlet state. Note that the definition only depends on the chosen bipartition of the lattice into two subsets, in spite of the VB basis overcompleteness. We derive in Sec.\(^ {11} \) an alternative but equivalent definition of the VB occupation number which is free of any VB basis formulation. This allows to define the VB EE in the practical \( S_x \) basis, and its computation through different numerical schemes (such as Exact Diagonalization or DMRG) than the VB QMC method used in previous works. Being now able to compute the VB EE for frustrated systems, we study in Sec.\(^ {13} \) both vN and VB EE for the \( J_1-J_2 \) spin chain, using DMRG techniques. We discuss and compare how the scaling of both entropies can detect the critical phase (for small \( J_2 \)) and the quantum critical point that separates it from the dimerized gapped phase present at large \( J_2 \). We also discuss the importance of the Marshall sign present in the ground-state wave function when comparing the two entropies. We finish with a discussion in Sec.\(^ {15} \) on the usefulness of the approach, as well as on the further possibilities open by the \( S_x \) representation of VB occupation numbers.

II. VB FREE FORMULATION OF THE VB EE

A. VB occupation number as a projection

Original formulation — In this paragraph we recall some definitions and results on VB occupation number\(^ {15} \). Choosing a bipartition of the \( N \)-site lattice into two equal sized subsets \( A \) and \( B \), the bipartite VB subspace is generated by all the bipartite VB states

\[
|i, j \rangle = \bigotimes_{(i,j) \in D} \langle i, j |, \quad (1)
\]

where \( |i, j \rangle \) is a SU(2) dimer state and \( D \) is a dimer cov-
ering of the system. For any bond \((i, j)\) such as \(i \in A\) and \(j \in B\) the VB occupation number in the state \(|\varphi_D\rangle\) is defined as:

\[
n_{(i,j)}(|\varphi_D\rangle) = \begin{cases} 1 & \text{if } (i,j) \text{ belongs to } D, \\ 0 & \text{otherwise}. \end{cases}
\]

The bipartite VB manifold is overcomplete: all bipartite VB states are singlet \((S = 0)\) states but their number \((N/2)\) is much larger than the singlet subspace dimension \(2^N\). As a consequence, a given linear combination of bipartite VB states \(|\Psi\rangle = \sum_D \lambda_D |\varphi_D\rangle\) can be rewritten in many alternative linear combinations \(|\Psi\rangle = \sum_D \mu_D |\varphi_D\rangle\) with \(\lambda_D \neq \mu_D\). This point requires to reconsider the extension of Eq. \((2)\) for linear combinations of bipartite VB states since the identity \(\sum_D \lambda_D n_{(i,j)}(|\varphi_D\rangle) = \sum_D \mu_D n_{(i,j)}(|\varphi_D\rangle)\) is not obviously granted. It is nevertheless possible to prove that \(n_{(i,j)}\) is linear \(19\) in \(|\varphi_D\rangle\) which provides an intrinsic definition of \(n_{(i,j)}(|\Psi\rangle)\) despite the bipartite VB manifold overcompleteness.

**Projection (VB states)** — We give here an alternative but equivalent definition of the VB occupation number which \(i\) is explicitly independent of the way the state is decomposed in the overcomplete bipartite VB basis, \(ii\) is valid for any spin \(S\) and \(iii\) will be shown to be more versatile for numerical computations. The spin-\(S\) dimer is defined as the two-site singlet state:

\[
|i,j\rangle_S = \frac{1}{\sqrt{2S+1}} \sum_{s_z = -S}^{S} (-1)^{s_z} | -s_z, +s_z \rangle
\]

We define the reference state:

\[
| R_S \rangle = | -S, +S, \ldots, -S, +S \rangle
\]

where the state is written in the \(\otimes \hat{S}_z\) eigenstates basis and ordered such as \(A\) and \(B\) sites appear in alternating order. In particular \(| R_{1/2} \rangle\) is nothing but the Néel state. As already noticed \(13\) for \(S = 1/2\), the reference state has an equal overlap with all bipartite VB states: \(| R_S \rangle |\varphi_D\rangle\) does not depend on the bipartite dimer covering \(D\). This property is established by a direct evaluation from Eq. \((3)\) and Eq. \((4)\) showing \(| R_S \rangle |\varphi_D\rangle = 1/(2S+1)^{N/4}\).

For any bipartite VB state \(|\varphi_D\rangle\) and for any bond \((i,j)\) such as \(i \in A\) and \(j \in B\) we are going to show that:

\[
n_{(i,j)}(|\varphi_D\rangle) = -\frac{(2S+1)^{N/4}}{2S} \langle R_S | \hat{S}_i^+ \hat{S}_j^- | \varphi_D \rangle.
\]

Indeed, we have:

\[
\hat{S}_i^+ \hat{S}_j^- | R_S \rangle = (2S)|i,j\rangle_S \ldots -S + 1, S - 1, \ldots \rangle
\]

If the bond \((i,j)\) is occupied, \(|\varphi_D\rangle = \ldots \otimes |i,j\rangle_S \otimes \ldots \) and a simple inspection of Eq. \((3)\) shows that \(\langle R_S | \hat{S}_i^+ \hat{S}_j^- | \varphi_D \rangle = -(2S)/(2S+1)^{N/4}\) and hence \(n_{(i,j)}(|\varphi_D\rangle)\) as defined in Eq. \((5)\) is 1. On the other hand, \(|\varphi_D\rangle = \ldots \otimes |i,k\rangle_S \otimes |l,j\rangle_S \ldots \) if the bond \((i,j)\) is unoccupied. The total \(S_z\) component on any occupied bond of a VB state is 0. Thus any eigenstate of \(\hat{S}_i^+ \hat{S}_j^- (or \hat{S}_i^- \hat{S}_j^+ with a non-zero eigenvalue is then orthogonal to \(|\varphi_D\rangle\). It is salient from Eq. \((6)\) that \(| \hat{S}_i^+ \hat{S}_j^- | R_S \rangle = +\hat{S}_i^+ \hat{S}_j^- | R_S \rangle\) and \(| \hat{S}_i^- \hat{S}_j^+ | R_S \rangle = -\hat{S}_i^- \hat{S}_j^+ | R_S \rangle\). Hence \(n_{(i,j)}(|\varphi_D\rangle)\) as defined in Eq. \((5)\) is 0 in this case.

Finally, it is easy to see that if both \(i\) and \(j\) sites are located in the same subset \(A\) or \(B\), the definition Eq. \((5)\) also ensures that \(n_{(i,j)} = 0\) which is always true (independently of \(|\varphi_D\rangle\)) as no dimer is allowed on such a non-bipartite bond.

Let us mention some of the advantages of definition Eq. \((5)\) as an alternative to Eq. \((2)\). First of all, it is explicitly linear in \(|\varphi_D\rangle\) which ensures that its extension to arbitrary linear combination of bipartite VB states can be consistently defined. As stated before, in the case of \(S = 1/2\), the subspace of bipartite VB states is a basis of the total singlet sector, ensuring that a dimer occupation number can be defined for any \(S = 1/2\) singlet. This is not true anymore for general spin \(S\): bipartite spin-S VB states do not form a basis of spin-\(S\) singlets. However it can be shown that they form a basis of the subset of spin-S singlets that are also \(SU(4N)\) singlets \(21\) (with \(N = 2S + 1\)) so that Eq. \((5)\) can be useful in that context.

**Projection (VB states superpositions)** — Using Eq. \((5)\), the occupation number for an arbitrary linear combination of bipartite VB states \(|\Psi\rangle = \sum_D \lambda_D |\varphi_D\rangle\) is defined as:

\[
n_{(i,j)}(|\Psi\rangle) = -\frac{N(2S+1)^{N/4}}{2S} \langle R_S | \hat{S}_i^+ \hat{S}_j^- | \Psi \rangle,
\]

where \(N\) is a normalization constant. It would be tempting to take \(N = 1/\langle |\Psi\rangle |\Psi\rangle\). However \(n_{(i,j)}\) is designed to measure the number of dimers (0 or 1) on bond \((i,j)\) and for any VB state a given site \(i \in A\) is dimerized with another site on sublattice \(B\). Hence the normalization condition writes:

\[
\sum_{j \in B} n_{(i,j)}(|\Psi\rangle) = 1.
\]

This condition enforces:

\[
N = \frac{1}{\sum_D \lambda_D} = \frac{1}{(2S+1)^{N/4} \langle R_S | |\Psi\rangle},
\]

and

\[
n_{(i,j)}(|\Psi\rangle) = \frac{1}{2S} \langle R_S | \hat{S}_i^+ \hat{S}_j^- | |\Psi\rangle.
\]

Contrary to Eq. \((2)\), this last expression is explicitly independent of the linear combination chosen to expand \(|\Psi\rangle\) on the overcomplete bipartite VB manifold as it only involves projections of \(|\Psi\rangle\). Since Eq. \((7)\) does not give
any prominent role to the bipartite VB basis to express \(|\Psi\rangle\), it will allow numerical computations outside the VB QMC scheme such as with Exact Diagonalization and DMRG (see Sec. II B).

Note that this expression is potentially singular if \(|R_S\rangle\) is orthogonal to \(|\Psi\rangle\). As an example, let us consider a one-dimensional spin-1/2 chain with \(N = 4p\) sites (where \(p\) is an integer). If we denote \(S\) the spin inversion symmetry \(S^z \to -S^z\) and \(T\) the translation symmetry, any \(q = \pi\) singlet state \(|\Psi\rangle\) will transform as \(S|\Psi\rangle = |\Psi\rangle\) and \(T|\Psi\rangle = -|\Psi\rangle\). Consequently, \(S T |\Psi\rangle = -|\Psi\rangle\). On the other hand, if the bipartition \(ABAB\ldots\) is chosen, the reference state given in Eq. (4) is obviously invariant under \(S T\). As a consequence, \(|\Psi\rangle\) and \(|R_S\rangle\) are orthogonal and Eq. (10) cannot be used.

This issue, which is a direct consequence of the normalization defined by Eq. (9), suggests that the bipartition and hence \(|R_S\rangle\) (see Eq. (4)) may not be chosen regardless of \(|\Psi\rangle\). More generally, normalizing a state by the sum of its coefficients in an expansion like in Eq. (9), requires a careful inspection of its nodal structure or equivalently of its Marshall sign which in turn dictates an appropriate bipartition for the reference state. We will further discuss this issue in Sec. III C.

VB EE — Using Eq. (10), the VB EE measuring the entanglement between \(\Omega\) or \(\bar{\Omega}\) in a state \(|\Psi\rangle\) can be expressed as,

\[
S^\text{VB}_{\Omega}(|\Psi\rangle) = \ln 2 \times \sum_{(i,j) \text{ such as } i \in \Omega, j \in \bar{\Omega}} n_{(i,j)}(|\Psi\rangle),
\]

where the spatial sums run over all possible locations of VBs, that is over all sites \(i\) in \(\Omega\) and all sites \(j\) in \(\bar{\Omega}\). Since we know that \(n_{(i,j)} = 0\) whenever \(i\) and \(j\) belong to the same subset \(A\) or \(B\), we can restrict the summation only to the non-vanishing cases.

VB EE for one-dimensional periodic systems — We finally make a remark on the behavior of \(S^\text{VB}_{\Omega}\) for translation-invariant one-dimensional systems. When \(\Omega\) is a linear segment of size \(2n\) (with \(n\) integer) we find that

\[
S^\text{VB}(2n) = \frac{1}{2} \left[ S^\text{VB}(2n-1) + S^\text{VB}(2n+1) \right],
\]

which means graphically that \(S^\text{VB}\) is made of linear segments. Let us propose an easy graphical proof of this statement. Consider a VB configuration and let us compare VB EE for different blocks obtained by adding two extra sites \(R\) and \(L\) at each end of a \((2n-1)\)-sites block \(B\) (see Fig. 1). Since the VB EE is a well defined quantity, we can choose to work in the complete non-crossing basis \(\Omega, \bar{\Omega}\) where VB do not cross according to some one-dimensional ordering of the sites. Since the \(2n-1\) block has an odd number of sites, it is clear that \(R\) and \(L\) cannot be connected by a singlet. Then, we can consider all possible cases: (i) \(R\) is connected to \(B\) but not \(L\), or vice-versa; (ii) neither \(R\) nor \(L\) are connected to \(B\); (iii) both \(R\) and \(L\) are connected with \(B\). These cases are shown in Fig. 1 and from the figure, it is straightforward to check that \(S^\text{VB}(B) + S^\text{VB}(B + R + L) = S^\text{VB}(B + R) + S^\text{VB}(B + L)\). As a conclusion, if periodic boundary conditions are used so that the entropy only depends on the number of sites of the block, we deduce Eq. (12).

B. Numerical computations

From now on, we focus on the case of \(S = 1/2\) systems.

With Exact Diagonalization — We use the Lanczos algorithm in order to compute the ground-state of large 1d chains\(\text{\cite{19}}\). We also implement lattice translations as well as fixing the total \(S^z\) quantum number in order to reduce the Hilbert space size so that we can solve systems up to \(N = 32\) sites. Once the wavefunction is obtained in the symmetrized basis, one can easily compute its overlap with the reference state, which gives the denominator of Eq. (10). In order to compute its numerator, we need to apply the operator \(\hat{S}^+_i \hat{S}^-_j\) for all pairs of sites \((i, j)\) with \(i\) in the selected block and \(j\) outside (let us remind that we can restrict ourselves to the case where \(i\) and \(j\) belong to different subsets). In this case, it turns out that it is simpler to apply this spin operator on the reference state, since it reduces to a swap operator for spins 1/2. Finally, in order to compute the VB EE, and since we are using translation symmetry, we have to make an average over all the positions of the block on the chain.

With DMRG — The calculation of the VB entanglement entropy is straightforward, utilizing matrix product techniques to calculate the overlap between the ground-state and the reference state \(N = \langle \uparrow \downarrow \uparrow \ldots \downarrow |\Psi\rangle\), and the expectation value \(P = \langle \uparrow \downarrow \uparrow \ldots \downarrow |P|\langle \uparrow \downarrow \uparrow \ldots \downarrow |\Psi\rangle\) where \(P = \sum_{i,j} S^+_i S^-_j + S^z_i S^z_j\) has a simple representation as a Matrix Product Operator, using the techniques

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III. RESULTS FOR THE $J_1$-$J_2$ SPIN CHAIN

A. Model and simulation details

We now present numerical results for the frustrated $J_1$-$J_2$ spin chain. $|\Psi\rangle$ in Eq. (10) is taken as the ground-state of the $S = 1/2$ Hamiltonian:

$$H = \sum_{i=1}^{L} J_1 S_i \cdot S_{i+1} + J_2 S_i \cdot S_{i+2}$$

where we set $J_1 = 1$ and will vary $J_2$. The physics of this spin chain is well understood: for $J_2$ smaller than the critical value $J_2^c \approx 0.241167$ (Ref. [20]), the system displays antiferromagnetic quasi-long range order, with algebraically decaying spin correlations. For $J_2 > J_2^c$, the system is located in a gapped dimerized phase which spontaneously breaks translation symmetry. We will study both VB and vN EE entropies in this system in both phases.

Results for $J_2 \leq 0.5$ were obtained with DMRG. We used samples with $L = 64, 128$ and $192$ and periodic boundary conditions in order to avoid dimerization effects in the entanglement entropy (Ref. [22,27]), which complicate the finite-size analysis. Up to $m = 192$ SU(2) states (roughly corresponding to 4000 usual U(1) states) have been kept for the largest samples. A long warm-up procedure has been used, by performing between 10 and 50 sweeps each time $m$ was increased by 50. Convergence has been checked by ensuring that the energy does not change significantly on more than 20 sweeps for the last value of $m$. Truncation error per site and variance per site $(H-E)^2/L$ were always at most $10^{-10}$ for the largest systems. For these periodic boundary conditions, a two-sites version of the DMRG algorithm has been used. We will essentially present results for the largest $L = 192$ chains, but will occasionally show data for smaller $L$ when a discussion of finite-size effects is necessary.

Prior to calculating the scalar products with the reference state, we use the Wigner-Eckart theorem to project the SU(2) ground state to U(1), thus giving direct access to the axis-dependent spin vector operators.

Later in the paper, we will present results for $J_2 > 0.5$ which were obtained with ED for chains of length up to $L = 32$. For large values of $J_2$, the DMRG algorithm has more difficulties to converge, even for small samples - a fact which has already been reported (Ref. [29]). Also, some intrinsic difference shows up in the definition of the VB EE in this case due to the rapid vanishing of the Marshall sign in the ground-state wave function. In that situation, the analysis of the definition as well as meaning of the VB EE is different and will be discussed in Sec. IIIIC.

We finally note that the vN EE of the ground-state of this spin chain was studied previously (Ref. [30]) albeit on smaller systems, with ED techniques. As we will see later, the use of large systems is necessary to locate precisely the quantum phase transition at $J_2^c$.

B. Results for $J_2 \leq 0.5$

We will present in this section results obtained for vN and VB entanglement entropies in parallel. We first present raw data for both entropies as a function of the block size $x$ for different values of $J_2$ in Fig. 2. Data are shown only for $x \in [0, L/2]$ (we have checked that curves are symmetric around $L/2$). Both sets of curves show a similar behavior: on the scale of the figure, one can distinguish between curves which converge to a constant (for $J_2 \geq 0.4$) and those which grow slowly but steadily with $x$. The difference between the two entropies appears on the former cases, where curves for different $J_2$ appear more shifted for VB. The shift also exists for $S^{vN}$ but is smaller (see zoom around $x \sim L/2$ in the inset of the figure).

One should also note the clear dimerization of both entropies for large $J_2$: this is naturally expected at the Majumdar-Ghosh (Ref. [29]) point $J_2 = 1/2$ where $S^{VB}$ and $S^{vN}$ are strictly equal to 0 for even $x$ and $\ln(2)$ for odd $x$. Note that this dimerization effect comes from the intrinsic dimerized nature of the ground state in this region, and not from the boundary conditions as in Ref. [27].

Let us concentrate now on the upper beam of curves, for $J_2 \leq 0.35$. From conformal invariance of the ground-state in the critical phase, the use of the conformal block length $x' = L/\pi \sin(\pi x/L)$ should be useful for systems with periodic boundary conditions: in the critical phase, vN EE should scale as $S^{vN} = c_2/3 \ln(x') + K_1$ whereas $S^{VB} = \gamma_2 \ln(x') + K_2$.

Fig. 3 displays both entropies versus $x'$ in a log-linear scale. All curves seem at first glance linear with approximately the same slope, except for $J_2 = 0.35$ where a crossover to a constant regime can be identified: this is well visible for $S^{vN}$ in the figure, but is also the case for $S^{VB}$ when zoomed in.

We fit the curves to a form $S^{vN} = c_{2\text{eff}}/3 \ln(x') + K_1$ and $S^{VB} = \gamma_{2\text{eff}} \ln(x') + K_2$ within the window $x' > 10$. Fits are excellent and lead to $c_{2\text{eff}}$ (respectively $\gamma_{2\text{eff}}$) very close to the CFT prediction $1$ (resp. $4 \ln(2)/\pi^2$) in the critical phase. The values of the fitted $c_{2\text{eff}}$ and $\gamma_{2\text{eff}}$ are displayed in the left insets of Fig. 3 as obtained for the three different samples sizes $L$ used in this study. The finite-size effects are found to be small on both quantities.

Several remarks are in order at this stage:

(i) The finite size dependence of the fitted values indicate that $J_2 = 0.35$ is clearly not in the critical regime as we already guessed from a visual inspection of curves.

(ii) It is quite interesting to note that both $\gamma_{2\text{eff}}$ and $c_{2\text{eff}}$ are not strictly equal to the predicted values for low $J_2$ (including $J_2 = 0$) but are getting closer monotonously to the theoretical predictions when increasing $J_2$. This effect can clearly be seen for $\gamma_{2\text{eff}}$, but also exist (even if...
(iii) The values closest to $1$ and $4\ln(2)/\pi^2$ are found to be precisely at $J_2 = 0.241167$. The fitted $c_{\text{eff}}$ is smaller than $1$ for $J_2 = 0.30$, and $\gamma_{\text{eff}}$ is smaller than $4\ln(2)/\pi^2$ for $J_2 \geq 0.241167$.

The two former points lead to the following interpretation: given the existence of dangerously irrelevant operators in the critical phase (but not at $J_2^c$), we expect that they could influence the effective value of the central charge and $\gamma$ as measured from a fit of EE on finite systems (they should not in the thermodynamic limit). The strength of their influence decreases as one approaches the critical point where they vanish. This scenario sounds plausible for $\gamma$: indeed in the field-theoretical description of the Heisenberg chain, $\gamma$ is related to the coupling constant of the free boson field whose numerical
determination is known to suffer from log corrections due to dangerously irrelevant operators. A similar effect has been recently predicted for the effective central charge in presence of marginally irrelevant operators with the prediction that $c_{\text{eff}} < c$. Raw fits of the form $S^\text{vN} = c_{\text{eff}}/3\ln(x') + K_1$ appear to give a value of $c_{\text{eff}}$ slightly larger than 1 (in all cases less than 1%). We find however that the simultaneous fits of $c_{\text{eff}}$ and $K_1$ actually affect the determination of $c_{\text{eff}}$. A more precise fitting procedure along the lines of Ref. 31 produce values of $c_{\text{eff}} < 1$ in agreement with Ref. 30. Details of such a precise estimation of $c_{\text{eff}}$ are left for a future study (we checked that a similar analysis for $\gamma_{\text{eff}}$ does not affect the results displayed in Fig. 3).

The analysis above explains why first simulations of the unfrustrated Heisenberg chain (at $J_2 = 0$) indicate that the scaling of the VB EE was identical to the one of vN EE: indeed the fitted value of $\gamma_{\text{eff}} \sim 0.310$ is closer to $1/3$ than to $4 \ln(2)/\pi^2 \approx 0.281$. We note that the transfer matrix estimates of $\gamma_{\text{eff}}$ also display such a small discrepancy for the Heisenberg chain. The numerical results of Ref. 15 for other spin chains not suffering from these log corrections appear to be in much better agreement with the analytical predictions, confirming this scenario.

Actually, the vanishing of these log corrections appear as a way to detect on finite systems the quantum critical point $J_2^c$ through the log scaling of $S^\text{VB}$ (and possibly $S^\text{vN}$), as long as the exact values $\gamma = 4 \ln(2)/\pi^2$ and $c = 1$ are known. If these values were not available, it would be more difficult to judge on the extent of the critical phase. Indeed from the sole quality of the fits, data at $J_2 = 0.25$ and $J_2 = 0.30$ (which are theoretically located in the gapped phase) are compatible with a critical scaling. This is certainly due to the small simulation length used $L$ with respect to the large correlation length close to $J_2^c$.

Finally, we discuss the behavior of the constants $K_1$ and $K_2$. Both constants are non-universal and are a priori not related. The fitted value of $K_1$ is shown in the right inset of Fig. 3 and displays a non-monotonous behavior (especially at small $J_2$). This non-monotonous behavior can also directly be seen on the raw $S^\text{vN}$ data at $L/2$ (inset of Fig. 2). On the other hand, and this can be noticed without a fit, the constant $K_2$ for $S^\text{VB}$ decreases monotonously with $J_2$.

The final transformation which summarizes these results consists in directly subtracting the expected exact value from both entanglement entropies. Fig. 4 displays $S^\text{vN} - 1/3\ln(x')$ and $S^\text{VB} - \gamma\ln(x')$ versus $x'$. Curves should saturate to the constants $K_1$ and $K_2$ respectively, which they do (except obviously for $J_2 = 0.35$) on this scale. Zooming in, one observes that all curves for $S^\text{vN}$ grow in a very smooth way, except for $J_2 = 0.30$ which actually decreases with $x'$ (for $S^\text{VB}$ all curves for $J_2 \geq 0.241167$ tend to decrease when increasing block size $x'$). This is in correspondence with the fitted $c_{\text{eff}} < 1$ for this value of $J_2$. The flattest curves are observed for $J_2 = 0.241167 \sim J_2^c$ and $J_2 = 0.25$ for both entropies, in agreement with our previous observations.

C. Results for $J_2 > 0.5$

Knowing the nodes and the signs of all coefficients of a correlated wavefunction is a difficult task. Indeed, such an information could allow to design a sign-free QMC algorithm as well as help on building variational wavefunctions. In this context, one can define the so-called Marshall-Perls sign

$$s(|\Psi\rangle) = \sum_i (-1)^N a_i^\dagger a_i$$

(14)
where the sum runs over the $|\psi_i\rangle$ basis states and with the wavefunction given by $|\Psi\rangle = \sum a_i |\psi_i\rangle$. $N^B$ counts the number of up spins on the $B$ sublattice so that obviously, $s$ depends on the choice of bipartition.

For non-frustrated Heisenberg model, it can be shown that the ground-state has $s = 1$ with the natural choice of bipartition. Frustration will spoil this result, although the sign may not drop suddenly (see for instance 1d or 2d $J_1 - J_2$ model). On left panel of Fig. 5 we present ED data for the frustrated Heisenberg chain. With the natural $AB$ bipartition, the Marshall sign stays extremely close to 1 for $0 \leq J_2 \leq 0.5$ but starts to deviate substantially beyond. Since the ground-state oscillates between having momentum 0 and $\pi$, we plot both values of $s$.

Fig. 6 shows ED data for various entropies. In particular, since $S^{VB}$ depends on the choice of bipartition, one may wonder what to choose. Usually, one is guided by the Ising solution: for small $J_2/J_1$, it is natural to choose a $ABAB...$ bipartition, while for large $J_2/J_1$, the system will behave as two decoupled Heisenberg chains with twice as large lattice spacing, meaning that bipartition should be of the form $AABB...$. The Marshall sign for this $AABB$ partition is presented in the right panel of Fig. 5.

Of course, the intermediate region with maximal frustration has no preferred bipartition. Moreover, since the ground-state oscillates between $q = 0$ and $q = \pi$, we plot both entropies. Still, as can be seen from its definition Eq. (11), $S^{VB}$ is only defined when the overlap between the ground-state and the classical Néel state is finite. Unfortunately, the $ABAB$ Néel state has no projection in the singlet $q = \pi$ sector as it is invariant by a combination of lattice translation and spin reversal. However, for $AABB$ bipartition, we can compute $S^{VB}$ for both lowest $q = 0$ and $q = \pi$ states and it turns out that data are very similar (sometimes they cannot be distinguished on the scale of Fig. 6), although states are quite different (see their Marshall sign in Fig. 5).

By comparing Fig. 6 and Fig. 5, we observe that when the Marshall sign is too small, $S^{VB}$ behaves much better and follows the same trend as $S^{VN}$, that is both converge to a constant for large enough block size. In fact, for large $J_2/J_1$ where the Marshall sign becomes again close to 1 for the $AABB$ choice, we observe that both entropies become more and more similar.

### IV. Discussion

In this paper, we studied the behavior of the Valence Bond Entanglement Entropy of the frustrated $J_1-J_2$ spin chain, and offered a direct comparison with the von Neumann entropy. Numerical DMRG calculations indicate that both entropies scale logarithmically with block size in the critical phase, and converge in the gapped dimerized phase of this model. The study of the VB EE has been made possible in this frustrated model through a formulation of valence bond occupation number, which extends this notion out of the Valence Bond basis.
We now discuss several interests of studying entanglement in quantum spin systems through a valence bond measure, and point out some open issues.

First, as based on the example of the $J_1$-$J_2$ model, the scaling of $S^{\text{VB}}$ with the block size allows to differentiate critical from gapped phases in one dimension, similarly to $S^{\text{vN}}$. Moreover, the knowledge of the exact prefactor of the log scaling permits a relatively precise determination of the quantum critical point at $J_2^c$ with finite-size data (this is however due to the vanishing of log corrections at this particular point, a non-generic feature). Note that this knowledge can be useful as the scaling of $S^{\text{VB}}$ might now be used to characterize uniquely the unknown phase of a new model. $S^{\text{VB}}$ can be computed for the Q-states Potts model using the loop language of Ref. [14] and there, the prefactor of the logarithmic scaling depends on $Q$ and is therefore indeed different for the different critical points encountered in the Potts model.

This is similar to the scaling of $S^{\text{vN}}$ which allows the determination of the central charge - the knowledge of which entirely determines the CFT at play for minimal models.

It is possible to compute $S^{\text{VB}}$ directly in the thermodynamic limit using the infinite-size algorithm iDMRG [33] or iTEBD [34]. In this formulation, the number of basis states in the calculation controls the spectrum transfer matrix of the system, which gives a scaling of the correlation length $\xi \propto m^\kappa$ at criticality, where $\kappa$ is a function of the central charge [35]. However, the effective boundary condition for the transfer matrix, and hence the form of the corrections to scaling of the entropies $S^{\text{VB}}$ and $S^{\text{vN}}$, will be different to the case of periodic boundary conditions, and we leave this analysis for a future study. Besides, knowing the corrections to scaling induced on a finite system by marginally irrelevant operators is interesting by itself (see for instance Ref. [36]).

In dimension higher than 1, it was already demonstrated [12,13,15] that the scaling of $S^{\text{VB}}$ discriminates between gapped and gapless phases. Since numerical calculations are possible in $d > 1$ with QMC VB method [13], it would be of high interest to perform a systematic study of the scaling of $S^{\text{VB}}$ in different phases of quantum spin models. Several questions are in order: for instance, do the multiplicative log corrections observed for the 2d Heisenberg model have a physical interpretation? Are prefactors of the scaling of $S^{\text{VB}}$ universal within a phase or at a quantum critical point [33], as observed in 1d?

We note that the techniques described here for calculating the VB entanglement entropy can easily be applied to higher dimensional tensor network algorithms such as PEPS [35], where the necessary scalar products are similarly easily computed. This opens the door to studies of the VB entanglement entropy for frustrated 2D systems.

Our study on frustrated systems also sheds lights on the importance of a good physical choice for the bipartition used in the definition of the VB EE, and its relation to the existence of a Marshall sign rule (or a large Marshall sign) in the wave-function under study. When the Marshall sign is exactly or close to 1, the vanishing of the corrections to scaling of the entropies $S^{\text{VB}}$ and $S^{\text{vN}}$ would be of high interest to perform a systematic study. Since numerical calculations are possible in $d > 1$ with QMC VB method [13], it would be of high interest to perform a systematic study of the scaling of $S^{\text{VB}}$ in different phases of quantum spin models. Several questions are in order: for instance, do the multiplicative log corrections observed for the 2d Heisenberg model have a physical interpretation? Are prefactors of the scaling of $S^{\text{VB}}$ universal within a phase or at a quantum critical point [33], as observed in 1d?

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1 P. Calabrese, J. Cardy, and B. Doyon, J. Phys. A 42, 500301 (2009).
2 M. Srednicki, Phys. Rev. Lett. 71, 666 (1993) ; J. Eisert, M. Cramer and M.B. Plenio, Rev. Mod. Phys. 82, 277 (2010).
3 C. Holzhey, F. Larsen, and F. Wilczek, Nucl.Phys.B 424, 443 (1994); G. Vidal, J.I. Latorre, E. Rico and A. Kitaev, Phys. Rev. Lett. 90, 227902 (2003); J.I. Latorre, E. Rico
4. E. Fradkin and J.E. Moore, Phys. Rev. Lett. 97, 050404 (2006).
5. J.-M. Stéphan, S. Furukawa, G. Misguich and V. Pasquier, Phys. Rev. B 80, 184421 (2009).
6. M. Cramer, J. Eisert, M. B. Plenio and J. Dreissig, Phys. Rev. A 73, 012309 (2006).
7. T. Barthel, M.-C. Chung and U. Schollwöck, Phys. Rev. A 74, 022329 (2006).
8. M.M. Wolf, Phys. Rev. Lett. 96, 010404 (2006); D. Gioev and I. Klich, ibid 96, 100503 (2006).
9. E. Fradkin and J.E. Moore, Phys. Rev. Lett. 97, 050404 (2006).
10. M. Mambrini, Phys. Rev. B 77, 134430 (2008).
11. G. Rumer, E. Teller and H. Weyl : Nachr. Gott., Math. physik. Klasse, 499 (1932). See also H. N. Temperley and E. H. Lieb, Proc. Roy. Soc. Lond. A. 322, 251-280 (1971) and R. Saito J. Phys. Soc. Japan 59, 482-491 (1990).
12. K. S. D. Beach, F. Alet, M. Mambrini and S. Capponi, Phys. Rev. B 80, 184401 (2009).
13. See for instance N. Laflorange and D. Poilblanc, Lect. Notes Phys. 645, 227 (2004) and references therein.
14. I.P. McCulloch, J. Stat. Mech. P10014 (2007).
15. R.W. Chhajlany, P. Tomczak, A. Wójcik, and J. Richter, Phys. Rev. A 75, 032340 (2007).
16. W. Marshall, Proc. R. Soc. London Ser. A 232, 48 (1955); E.H. Lieb and D.C. Mattis, J. Math. Phys. 3, 749 (1962).
17. S. Eggert, Phys. Rev. B. 54, R9612 (1996).
18. N. Laflorange, E.S. Sørensen, M.-S. Chang and I. Affleck, Phys. Rev. Lett. 96, 100603 (2006).
19. S.R. White and I. Affleck, Phys. Rev. B 54, 9862 (1996).
20. C.K. Majumdar and D.K. Ghosh, J. Math. Phys. 10, 1388 (1969); ibid 1399 (1969).
21. J. Cardy and P. Calabrese, J. Stat. Mech. P04023 (2010).
22. J.C. Xavier, Phys. Rev. B 81, 224404 (2010).
23. P. Calabrese, private communication.
24. E.H. Lieb, T.D. Schultz, and D.C. Mattis, Ann. Phys. (NY) 16, 407 (1961).
25. J. Richter, N.B. Ivanov, and K. Retzlaff, Europhys. Lett. 25, 545 (1994).
26. I. P. McCulloch, arXiv:0804.2509 (unpublished).
27. G. Vidal, Phys. Rev. Lett. 98, 070201 (2007).
28. F. Pollmann, S. Mukerjee, A. M. Turner and J. Moore, Phys. Rev. Lett. 102, 255701 (2009).
29. F. Verstraete and J. I. Cirac, cond-mat/0407066; F. Verstraete, M. M. Wolf, D. Perez-Garcia, and J. I. Cirac, Phys. Rev. Lett. 96, 226001 (2006).
30. V. Murg, F. Verstraete and J. I. Cirac, Phys. Rev. B 79, 195119 (2009).
31. G. Refael and J.E. Moore, Phys. Rev. Lett. 93, 260602 (2004).
32. H. Tran and N.E. Bonesteel, arXiv:0909.0038 (unpublished).
33. V. Pasquier and H. Saleur, Nucl. Phys. B 330, 523 (1990).
34. M. Oshikawa, D. Schwandt, and F. Alet, unpublished.