Valence Bond Entanglement and Fluctuations in Random Singlet Phases

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The ground state of the uniform antiferromagnetic spin-1/2 Heisenberg chain can be viewed as strongly fluctuating liquid of valence bonds, while in disordered chains these bonds lock into random singlet states on long length scales. We show that this phenomenon can be studied numerically, even in the case of weak disorder, by calculating the mean value of the number of valence bonds leaving a block of \(L\) contiguous spins (the valence bond entanglement entropy) as well as the fluctuations in this number. Results are obtained for a class of models which include the Heisenberg chains as special cases.

The set of valence-bond states — states in which localized spin-1/2 particles are correlated in singlet pairs said to be connected by valence bonds — provides a useful basis for visualizing singlet ground states of quantum spin systems. For example, the ground state of the uniform one-dimensional nearest-neighbor spin-1/2 antiferromagnetic (AFM) Heisenberg model (the prototypical spin-liquid state [1]) can be viewed as a strongly fluctuating liquid of valence bonds with a power-law length distribution. This intuitive picture reflects the long-range spin correlations in this state, as well as the existence of gapless excitations created by breaking long bonds.

Valence-bond states also play a key role in describing the physics of random spin-1/2 AFM Heisenberg chains. For these systems, it was shown by Fisher [2], using a real space renormalization group (RSRG) analysis, that on long length scales the ground state is described by a single valence-bond state known as a random singlet state. This single valence-bond state should be viewed as a caricature of the true ground state, which will certainly exhibit bond fluctuations on short length scales. In fact, it is natural to expect that, when measured on these short length scales, a fluctuating random singlet state would be difficult to distinguish from the uniform Heisenberg ground state, particularly in the limit of weak disorder.

In valence-bond Monte Carlo (VBMC) simulations [3] valence-bond states are used to stochastically sample singlet ground states of quantum spin systems. One of the appealing features of VBMC is that if one imagines viewing the sampled valence-bond states over many Monte Carlo time steps the resulting “movie” would correspond closely to the intuitive resonating valence bond picture described above. For random Heisenberg chains (and related models) VBMC should therefore provide a useful method for directly studying the phenomenon of random singlet formation on long length scales, while at the same time capturing the short-range fluctuations which will always be present.

With this motivation, we present here results of VBMC studies for a class of models which include the uniform and random spin-1/2 AFM Heisenberg chains. To define these models we first specify their relevant Hilbert spaces. It is well known that the set of \emph{non-crossing} valence-bond states (see Fig. 1(a)) form a complete linearly independent basis spanning the total spin 0 Hilbert space of a chain of spin-1/2 particles [4]. We denote the singlet projection operator acting on neighboring sites \(i\) and \(i+1\) by \(\Pi_i^0\), which, for spin-1/2 particles, can be expressed as \(\Pi_i^0 = \frac{1}{2} - \vec{S}_i \cdot \vec{S}_{i+1}\) (taking \(\hbar = 1\)). Figure 1(b) shows two representative examples of \(\Pi_i^0\) acting on a non-crossing valence-bond state. For spin-1/2 particles, the parameter \(d\) appearing in Fig. 1(b) is equal to 2; however, in principle, \(d\) can take any value, (of course if \(d \neq 2\) the Hilbert space no longer describes spin-1/2 particles).

Of particular interest are the cases \(d = 2\cos \frac{\pi}{k}\) where \(k\) is a positive integer [5]. For these values of \(d\), when \(k\) is finite, the non-crossing states are no longer linearly independent and the Hilbert space dimensionality of \(N\) sites can be shown to grow asymptotically as \(d^N\) with \(d < 2\). The \(k \to \infty\) limit then corresponds to the case of ordinary spin-1/2 particles with \(d = 2\) for which the Hilbert space dimensionality grows as \(2^N\).

One consequence of the reduced Hilbert space dimensionality for finite integer \(k\) is that it changes the entanglement entropy associated with a valence bond. The entanglement entropy of a subsystem \(A\) of a larger system consisting of parts \(A\) and \(B\) is defined to be the von Neumann entropy, \(S^N\), of the reduced density matrix \(\rho_A\) obtained by tracing out the degrees of freedom in region \(B\), thus \(S^N = -\text{Tr}[\rho_A \log_2 \rho_A]\). With this defi-
nition, an ordinary singlet formed by two spin-1/2 particles, with one spin in region $A$ and the other in region $B$, will have $S_{VN} = 1$. However, when $d = 2 \cos \frac{\pi}{2 + \ell}$, it was shown in [6] that if there are $M$ valence bonds connecting sites in region $A$ with sites in region $B$, then, in the $M \gg 1$ limit, because the dimensionality of the traced out Hilbert space grows as $d^M$, $S_{VN} \simeq M \log_2 d$ and the entanglement per bond is $\log_2 d$.

The class of Hamiltonians studied here are all characterized by the parameter $d$ and have the form

$$H = -\sum_i J_i \Pi_i^0, \quad (1)$$

with $J_i > 0$. For $d = 2$ these models correspond to spin-1/2 AFM Heisenberg chains with $J_i$ equal to the exchange energy associated with spins $i$ and $i + 1$. For general $d$, if the $J_i$’s are uniform ($J_i = J$) the Hamiltonians [1] can be viewed as 1+1 dimensional quantum Potts models obtained by taking the asymmetric limit of the transfer matrix of the $Q$-state Potts models with $Q = d^2$ [7]. For $d \leq 2$ the uniform models are all gapless, and for the special values $d = 2 \cos \frac{\pi}{k+2}$ they correspond to a sequence of conformally invariant Andrews-Baxter-Forrester (ABF) [8] models with central charges $c_k = 1 - 6/(k+1)(k+2)$ [9]. Physically, these ABF models can be thought of as describing chains of interacting non-Abelian particles described by $su(2)_k$ Chern-Simons-Witten theory, believed to be relevant for certain quantum Hall states [10]. The known universal entanglement scaling of conformally invariant 1+1 dimensional systems [11] then implies that the entanglement entropy of a block of $L$ contiguous sites, $S^N_{VL}$, in the ground states of these models will scale logarithmically for $L \gg 1$ as $S^N_{VL} \simeq \frac{d}{\ell} \log_2 L$ [12].

When the $J_i$’s are random, the Hamiltonians [1] can no longer be solved exactly. However, the RSRG approach of Fisher [2] can be straightforwardly applied for all $d \geq \sqrt{2}$ [8] with the result that the ground states all flow to the same infinite randomness fixed point [12] — one for which the bond strength distribution is the same as that of the fixed point of the random Heisenberg chain [2]. For this fixed point, Refael and Moore [13] have shown that if $n_L$ is the number of valence bonds leaving a given block of size $L$ (see Fig. 1(c)), then, in the $L \gg 1$ limit, $\bar{n}_L \simeq \frac{\ln L}{3} \simeq \frac{\ln \ell}{3} \log_2 L$, where the overbar denotes a disorder average over random singlet states produced by the RSRG. This logarithmic scaling is a direct consequence of the inverse-square distribution of valence bond lengths characteristic of random singlet states [14].

Multiplying $\bar{n}_L$ by the entanglement per bond of $\log_2 d$ then yields the RSRG result for the asymptotic scaling of the entanglement entropy for the random ABF models, which is again logarithmic and has the form $S^N_{VL} \simeq \bar{n}_L \log_2 d \simeq \frac{d}{\ell} \log_2 L$ [6] [13].

In VBMC the ground states of the Hamiltonians [1] are projected out by repeatedly applying $-H$ to a particular non-crossing valence-bond state $|\alpha\rangle$. The result of this projection after $n$ iterations is,

$$(-H)^n |\alpha\rangle = \sum_{i_1, \cdots, i_n} J_{i_1} \cdots J_{i_n} \Pi_{i_1}^0 \cdots \Pi_{i_n}^0 |\alpha\rangle.$$  \quad (2)

The properties of the projection operators shown in Fig. 1(b) imply that $\Pi_{i_1}^0 \cdots \Pi_{i_n}^0 |\alpha\rangle = \lambda_{i_1, \cdots, i_n} |\alpha\rangle$ where $|\alpha\rangle$ is a non-crossing-valence-bond state with the same norm as $|\alpha\rangle$ and $\lambda_{i_1, \cdots, i_n} = d^{-m}$ where $m$ is the number of times a projection operator acts on two sites which are not connected by a valence bond when projecting $|\alpha\rangle$ onto $|\alpha\rangle$. This projection thus leads to an expression for the ground state $|\psi\rangle$ which becomes exact in the limit of large $n$ (in our simulations we find it is sufficient to take $n = 20N$ where $N$ is the number of sites) and has the form

$$|\psi\rangle = \sum_\alpha w(\alpha) |\alpha\rangle,$$  \quad (3)

where $w(\alpha) = J_{i_1} \cdots J_{i_n} \lambda_{i_1, \cdots, i_n}$. In VBMC the valence-bond states $|\alpha\rangle$ contributing to $|\psi\rangle$ are sampled with probability $w(\alpha)$ by updating the sequence of projection operators $(i_1, \cdots, i_n)$ using the usual Metropolis method [3].

Given any observable $O$ with expectation values $O(\alpha) = \langle \alpha | O | \alpha \rangle / \langle \alpha | \alpha \rangle$ in the non-crossing-valence-bond states $|\alpha\rangle$, VBMC can be used to compute the average $\langle O \rangle = \sum_\alpha w(\alpha) O(\alpha) / \sum_\alpha w(\alpha)$ for any state $|\psi\rangle$ of the form (3), provided $w(\alpha) \geq 0$. In what follows, angle brackets will always denote this average, though it should be noted that $\langle O \rangle$ will in general not be equal to $\langle \psi | O | \psi \rangle / \langle \psi | \psi \rangle$, both because the valence-bond states are nonorthogonal and because the weight factors $w(\alpha)$ are amplitudes and not probabilities. One such averaged quantity is the valence-bond entanglement entropy, $S^B_{VL}$, which, for the uniform Heisenberg chain, is defined to be equal to $\langle n_L \rangle$, the average number of valence bonds leaving a block of size $L$ [13] [10]. To generalize $S^B_{VL}$ to the ABF models with $d = 2 \cos \frac{\pi}{k+2}$ it is natural to multiply $\langle n_L \rangle$ by the asymptotic entanglement per bond of $\log_2 d$. For this choice, provided $n_L \gg 1$, $S^B_{VL}$ will be equal to $S^N_{VL}$ for any single valence-bond state. We therefore take $S^B_{VL} = \langle n_L \log_2 d \rangle$.

While $S^B_{VL}$ is easy to compute numerically by VBMC, for a general superposition of valence-bond states it will not be equal to $S^N_{VL}$. Nonetheless, VBMC simulations [13] [10] [17] of the uniform AFM Heisenberg chain with $N \simeq 100$ spins have shown numerically that $S^B_{VL}$ grows logarithmically with $L$, in the same fashion as the von Neumann entanglement $S^N_{VL}$. To characterize this log scaling it is convenient to introduce an effective valence-bond central charge, $c_{VB}$, defined so that $S^B_{VL} \simeq \frac{c_{VB}}{1} \log_2 L$ in the limit $L \gg 1$.

In addition to showing log scaling of $S^B_{VL}$, previous VBMC simulations of the uniform AFM Heisenberg chain
have given results consistent with $c^{\text{VB}}$ being close to $[16]$, or even possibly equal to $[15]$, 1, the value of the true central charge for the uniform $d = 2$ model. However, Jacobsen and Saleur $[18]$ were able to determine the exact asymptotic scaling of $\langle n_L \rangle$ analytically for all $d \leq 2$, and while their results confirmed the log scaling of $S_L^{\text{VB}}$ for $L \gg 1$, they also showed that for $d = 2$ the coefficient for this scaling does not correspond to $c^{\text{VB}}$ being equal to one, but rather $c^{\text{VB}} = 12 \ln 2/\pi^2 \approx .843$.

Figure 2(a) shows our VBMC results for $S_L^{\text{VB}}$ for $k = 2, 3$ and $\infty$ (corresponding to $d = \sqrt{2}, \phi$ and 2, respectively, where $\phi$ is the golden mean) for periodic systems with $N = 1024$ sites. The solid lines show the exact asymptotic scaling found by Jacobsen and Saleur $[18]$ which clearly agree with our numerical results for $L \gg 1$. Note that for the case $k \to \infty$ it is necessary to consider fairly large values of $L$ before entering the scaling regime, whereas for $k = 2$ and 3 the scaling begins at relatively small $L$. This fact may account for the initial numerical difficulty in determining $c^{\text{VB}}$ for $d = 2$ using small systems (see, however, $[17]$). Presumably, the reason finite size effects become more pronounced as $d$ approaches 2 is because this is a critical value (for $d > 2$ the uniform models acquire a gap $[27]$).

For random Heisenberg chains $S_L^{\text{VB}}$ was first computed numerically by Alet et al. $[15]$. Following the same procedure as these authors, we compute $S_L^{\text{VB}}$ by determining $\langle n_L \rangle$ for particular realizations of disorder and then disorder averaging. For the random ABF models we again multiply by the entanglement per bond, and thus take $S_L^{\text{VB}} = \langle n_L \rangle \log_2 d$ (here again the overbar denotes disorder average). Figure 2(b) shows log plots of our results for $S_L^{\text{VB}}$ for random chains, again for $k = 2, 3$ and $\infty$ and $N = 1024$. The solid lines show the scaling predictions of Refael and Moore $[13]$ for $S_L^N$ based on the RSRG which clearly agree with our numerical results. As pointed out by Alet et al. $[15]$, the fact that $S_L^{\text{VB}}$ and $S_L^N$ show the same scaling for $L \gg 1$ is to be expected if, as predicted by the RSRG, on long length scales the ground states of the random models are dominated by a single valence-bond state.

Figure 3 shows our VBMC results for $c^{\text{VB}}$ for both uniform and random models for different values of $d$. For the uniform models Fig. 3 also shows the exact values of $c^{\text{VB}}$ which follow from the analytic results of Jacobsen and Saleur $[18]$ as well as the true central charges $c_k$ of the ABF models with $d = 2 \cos \frac{\pi}{k+2} [19]$. For the random models the $d$ dependence of $c^{\text{VB}}$ is seen to be entirely due to the entanglement per bond, reflecting the fact that the
FIG. 4: (Color online) Log-linear plots of bond fluctuations as a function of block size \( L \) for both uniform and random chains with \( k \to \infty \) (upper panel) and \( k = 2 \) (lower panel). For uniform chains these fluctuations grow logarithmically with \( L \) in agreement with the analytic results of \([13]\) (solid lines), indicating that bonds are strongly fluctuating on all length scales. For random chains the fluctuations saturate, signaling the formation of a random singlet phase in which the bonds have locked into a particular random singlet configuration on long length scales. The parameter \( u \) (defined in the text) is a measure of the disorder strength and the results clearly show that the saturation length scale grows with decreasing \( u \). Results are for periodic chains with \( N = 1024 \) sites and for random models are self-averaged over all blocks for 100 disorder samples.

The expectation that for random chains the \( L \gg 1 \) scaling of \( S^\text{VB}_{2L} \) should be the same as that of \( S^\text{N}_{2L} \) is based on the assumption that the valence bonds lock into a particular random singlet state on long length scales. This assumption is in turn based on the RSRG approach which, although it can be shown to capture the long distance properties of the fixed point exactly \([2]\), is still an approximate method. It is clearly desirable to have a direct numerical demonstration that the valence bonds are indeed locking into a particular random singlet state on long length scales.

To provide such a demonstration we calculate the fluctuations in \( n_L \). To be precise, we first compute the quantity \( \langle n^2_L \rangle - \langle n_L \rangle^2 \) for a particular block of size \( L \) and a particular realization of disorder, and then perform a disorder average. The quantity we compute is thus \( \sigma^2_L \). For this choice of averaging \( \sigma^2_L \) has the property that, in an idealized random singlet phase for which the ground state is a single non-crossing valence bond state, \( \sigma^2_L \) would vanish, even though the number of bonds leaving a given block would be different for different realizations of disorder.

For the uniform models with \( d \leq 2 \) Jacobsen and Saleur \([18]\) have also determined the asymptotic scaling of \( \sigma^2_L \) (in this case there is, of course, no disorder average). They find that, like \( \langle n_L \rangle \), \( \sigma^2_L \) scales logarithmically with \( L \), and they were again able to obtain exact analytic results for the coefficients of the log. This log scaling characterizes the expected strong fluctuations of valence bonds on all length scales in the uniform models.

For random models there will be strong valence bond fluctuations on length scales up to a certain length \( l \), beyond which the bonds should lock into a random singlet phase. In this case one expects \( \sigma^2_L \) to not differ much from its value for the uniform case when \( L \ll l \), but for \( L \gg l \) the fluctuations should saturate. This saturation is due to the fact that, once the block size \( L \) becomes much larger than the fluctuation length \( l \), the fluctuations which occur outside of a distance \( l \) from the two boundaries of the block will not change the number of bonds leaving the block, and hence will not contribute to \( \sigma^2_L \).

Figure 4 shows log plots of our results for \( \sigma^2_L \) for the case \( k \to \infty \) (corresponding to the Heisenberg chain, with \( d = 2 \)) and \( k = 2 \) (corresponding to the \( Q = 2 \) Potts model, i.e. the critical transverse field Ising model, with \( d = \sqrt{2} \)). For the uniform models our results confirm the log scaling and exact coefficients found by Jacobsen and Saleur \([18]\). For the random models the \( J_i \)'s are taken to be uniformly distributed in the interval \([1-u, 1+u]\), where \( u \) is a measure of disorder strength, and we observe that \( \sigma^2_L \) saturates on a length scale which grows as \( u \) decreases. We believe the observation of this saturation, which indicates a finite fluctuation length scale \( l \), together with the log scaling of \( \langle n_L \rangle \), which indicates a power-law distribution of valence bond lengths, provides a direct numerical proof of random singlet phase formation in these models.

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[19] It is interesting to note that while $c_{VB}$ and $c_k$ are not equal for the uniform ABF models, they are close in magnitude. This is primarily due to the fact that the entanglement per bond, $\log_d$, is equal to $c_k$ for $k = 2$ and $k \to \infty$, and very close to $c_k$ for $k > 2$. 