Exact Valence Bond Entanglement Entropy and Probability Distribution in the XXX Spin Chain and the Potts Model

J. L. Jacobsen[1,2] and H. Saleur[2,3]

[1]*LPTMS, Université Paris-Sud, Bâtiment 100, 91405 Orsay, France*
[2]*Service de Physique Théorique, CEN Saclay, 91191 Gif Sur Yvette, France*
[3]*Department of Physics, University of Southern California, Los Angeles, California 90089-0484, USA*
(Received 22 November 2007; revised manuscript received 8 January 2008; published 29 February 2008)

We determine exactly the probability distribution of the number N_c of valence bonds connecting a subsystem of length $L \gg 1$ to the rest of the system in the ground state of the XXX antiferromagnetic spin chain. This provides, in particular, the asymptotic behavior of the valence-bond entanglement entropy $S_{\mathrm{VB}} = \langle N_c \rangle \ln 2 = \frac{4 \ln 2}{\pi^2} \ln L$ disproving a recent conjecture that this should be related with the von Neumann entropy, and thus equal to $\frac{1}{3} \ln L$. Our results generalize to the Q-state Potts model.

DOI: 10.1103/PhysRevLett.100.087205 PACS numbers: 75.10.Jm, 03.67.−a, 05.50.+q

Introduction.—The full understanding of quantum critical points in condensed matter physics requires the investigation of specific quantum features such as the entanglement properties (see, e.g., [1] for a review) of the ground state wave functions. Other properties recently considered include the scalar product between ground states corresponding to slightly different values of the coupling [2], and, in a somewhat less general context, the valence-bond entanglement entropy [3,4].

Indeed, it was suggested in [3] that for $SU(2)$ quantum spin systems, the counting of valence-bond spin singlets shared by a subsystem A, and the rest of the system was a useful measure of entanglement, comparable with the von Neumann entanglement entropy (denoted by S_{vN} in what follows), and somewhat easier to study numerically.

We note that in the case of systems admitting infinite randomness fixed points, in one [5–7] as well as in higher [8,9] dimensions, the ground state $|\Omega\rangle$ can be represented as a single valence-bond state, and S_{vN} coincides with the number of singlets that cross the boundary of A times the logarithm of the number of states per site. This quantity we will call valence-bond entanglement entropy, and denote by S_{VB}.

The exact coincidence of S_{vN} and S_{VB} does not hold in general when the ground state is a superposition of valence-bond states. Nevertheless, in the particular case of the XXX antiferromagnetic spin chain, it was suggested in [3] that the two quantities might have the same asymptotic behavior. Recall that in 1D, the von Neumann entanglement entropy diverges logarithmically in the subsystem size with a universal coefficient proportional to the central charge c of the associated conformal field theory. Let $L = |A|$ be the size of the subsystem, and N the size of the whole system, both measured in units of the lattice spacing, with $1 \ll L \ll N$ (as we shall invariably assume in what follows). Then, [10,11]

$$S_{\mathrm{vN}}(A) \overset{a}{=} (c/3) \ln L, \tag{1}$$

where by $\overset{a}{=}$ we denote asymptotic behavior. Calling $N_c(\Omega)$ the number of singlets crossing the boundary of the subsystem, S_{VB} is the average of N_c multiplied by ln2, and thus the observation in [3] amounts to

$$\langle N_c \rangle(\Omega) \overset{a}{\approx} \frac{1}{3 \log 2} \ln L \simeq 0.481 \ln L. \tag{2}$$

In relation with these entanglement considerations, the properties of valence-bond bases have been actively studied recently, in particular, from rigorous [12,13] and probabilistic [14] points of view.

We show in this Letter that the probability distribution of the number of singlets crossing the boundary can be exactly determined for the XXX spin chain as well as for the related Q-state Potts model Hamiltonians. We find that (2) is not quite correct: the exact leading asymptotic behavior is in fact $\langle N_c \rangle(\Omega) \overset{a}{=} \frac{4}{\pi^2} \ln L \simeq 0.405 \ln L$. All other cumulants have similar closed form expressions.

Entanglement and the TL algebra.—The 2D classical Q-state Potts model can be defined for arbitrary Q through an algebraic reformulation where Q enters only as a parameter. For this, recall that the transfer matrix in the anisotropic limit gives rise to the Hamiltonian [15]

$$H = -\sum_{i=1}^{N-1} E_i. \tag{3}$$

Here, the E_i are elements of an associative unital algebra called the Temperley-Lieb (TL) algebra, defined by [16]

$$\begin{aligned} E_i^2 &= \sqrt{Q} E_i \\ [E_i, E_j] &= 0 \quad \text{for } |i-j| \geq 2 \\ E_i E_{i\pm 1} E_i &= E_i. \end{aligned} \tag{4}$$

This algebra admits various representations, in particular, for Q integer. In order to discuss valence-bond properties, we will use the loop model representation. Here, the generators act on the following nonorthogonal but linearly

independent basis states. Each basis state corresponds to a pattern of nonintersecting valence bonds (representing a $U_q sl(2)$ singlet; we have set $\sqrt{Q} = q + q^{-1}$) and empty dots. The generator E_i is the operator that projects sites i and $i+1$ onto the singlet. It produces a valence bond between sites i, $i+1$ together with a rearrangement or some other contractions for sites that were contracted with i or $i+1$ before. If i or $i+1$ was an empty dot, it is moved to another position. If both i and $i+1$ were empty, the action of E_i annihilates the state. This gives rise to relations (4).

It is often convenient to represent the basis states using parentheses and dots, such as $\bullet(())()\bullet$. The parentheses must obey the typographical rules for nesting and represent sites paired by a valence bond. The dots must not be inside any of the parentheses, and the projection operator onto the $U_q sl(2)$ singlet for any two dots that are adjacent (when parentheses are ignored) annihilates the state. Thus, those sites are "noncontractible." With these definitions, it is clear that the TL algebra does not mix states with different numbers of noncontractible sites.

For Q generic, the set of basis states with fixed number $2j$ of such sites provides an irreducible representation of TL, of well-known dimension

$$d_j = \binom{N}{N/2+j} - \binom{N}{N/2+j+1} \tag{5}$$

where $N/2 + j$ must be an integer. This dimension coincides with the number of representations of spin j appearing in the decomposition of the product of N spins $1/2$. This is no accident: it is well-known [17] that the uncrossed diagrams are linearly independent and form a basis of the spin j sector in the $sl(2)$ case; the results extend trivially to the $U_q sl(2)$ case with q generic.

When $\sqrt{Q} \geq 0$, the ground state is found in the sector with $j = 0$ for N even (and $j = 1/2$ for N odd). Note that the valence-bond basis is not orthonormal. The simplest way to proceed is thus not to calculate matrix elements of the Hamiltonian H in this basis $\langle w_i|H|w_j\rangle$ but rather to define a nonsymmetric matrix h_{ij} by expressing the action of H on any state as a linear combination of states

$$H|w_i\rangle = \sum_j h_{ij}|w_j\rangle. \tag{6}$$

The matrix h_{ij} is unique due to the linear independence of the states. The eigenvalues and right eigenvectors of h give those of H.

Since all entries h_{ij} are (strictly) positive, the Perron-Frobenius theorem implies that the ground state $|\Omega\rangle$ expands on the basis states with positive coefficients [18]

$$|\Omega\rangle = \sum \lambda_w |w\rangle, \qquad \lambda_w > 0. \tag{7}$$

We define the number of valence bonds N_c connecting the subsystem to the outside as the number of unpaired parentheses in the subsystem. We are here interested in its mean value

$$\langle N_c\rangle(\Omega) = \frac{\sum_w \lambda_w N_c(w)}{\sum_w \lambda_w} \tag{8}$$

and more generally in the probability distribution

$$p(N_c) = \frac{\sum_{w:N_c(w)=Nc} \lambda_w}{\sum_w \lambda_w}. \tag{9}$$

Below, we establish the leading asymptotic behavior of $\langle N_c\rangle$ (and the higher cumulants) in the scaling limit $1 \ll L \ll N$. Note that the TL formulation shows relationship between the Potts Hamiltonian when $\sqrt{Q} = 2\cos\frac{\pi}{k+2}$, with k integer, and the interacting anyons (coming in $k+1$ species) Hamiltonian in [19]. The valence-bond entanglement entropy can be defined for these models as well, and, in the sector of vanishing topological charge, coincides with the one we are studying.

Mapping onto a boundary problem.—The wave function in the ground state of a Hamiltonian with periodic (or free) boundary conditions [20] can be obtained as the path integral of the equivalent Euclidian theory on a infinite half cylinder (or annulus), denoted C_- (or A_-). To translate this in statistical mechanics terms, note that if we consider the square lattice with axial (or diagonal) direction of propagation [cf. Figure 1], the Hamiltonian belongs to a family of commuting transfer matrices describing the Q-state Potts model with various degrees of anisotropy. The ground state of all these transfer matrices is given by $|\Omega\rangle$. Let us choose for instance the particular case where the Potts model is isotropic, with coupling constant $e^K = 1 + \sqrt{Q}$. Now the ground state $|\Omega\rangle$ can be obtained by applying a large number of times the transfer matrix on an arbitrary initial state, corresponding to boundary conditions at the far end of C_- (or A_-). Clearly, by the mere definition of the transfer matrix, this means that the coefficients of the ground state $|\Omega\rangle$ on the basis states $|w\rangle$ are, up to a common proportionality factor, equal to the parti-

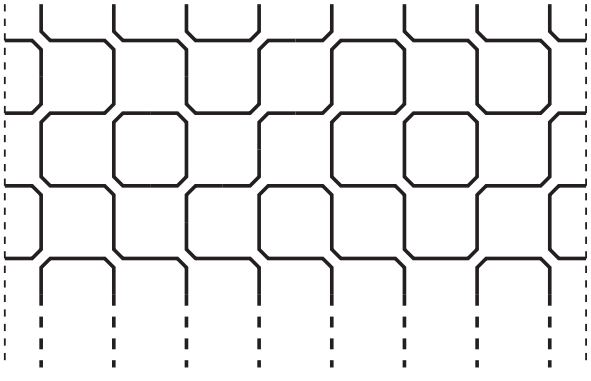

FIG. 1. Loop representation of the periodic TL algebra (with $N = 8$) on the infinite half cylinder C_-. The basis state corresponding to the upper rim is $\bullet(())()\bullet$.

tion function of the 2D statistical system on C_- (or A_-) with boundary conditions specified by $|w\rangle$.

We must now study such partition functions. We move immediately to the limit $N \to \infty$. We then have a system in the half plane, which, in the geometrical description, corresponds to a gas of fully packed self and mutually avoiding loops with fugacity $\sqrt{Q}$ in the bulk, with arcs ending up on the boundary. To go to the continuum limit, it is convenient to transform this model into a solid-on-solid model [21]. This is done by orienting the loops and arcs, which are then interpreted as domain walls between two regions where the height variables—denoted by Φ in what follows—differ by a fixed amount taken by convention equal to $\pm\pi$. The loop fugacities can then be made into a local interaction as follows. Parametrize $\sqrt{Q} = 2\cos\pi e_0$ with $0 \le e_0 < 1$ [22] and introduce complex weights $\exp(\pm \frac{i\pi e_0}{4})$ for the left and right turns. Since on the square lattice the number of left (n_L) minus the number of right (n_R) turns equals ± 4, this gives closed loops the correct weight $\sqrt{Q}$. It is known that in the continuum limit, the dynamics of the SOS height variables turns into the one of a free bosonic field [21], with a coupling constant g that is a known function of Q, viz. $g = 1 - e_0$.

With the local complex turn weights, arcs will get the weight $\sqrt{Q_b} = 2\cos\frac{\pi e_0}{2}$ since for them $n_L - n_R = \pm 2$ [23]. Although no such boundary weight appeared in the initial lattice model and partition function, we note that for the fully packed loop model we are interested in, the number of arcs touching the boundary is just $N/2 - j$, a constant, so the arc weight is immaterial. We take it to be precisely $\sqrt{Q_b}$ to complete the mapping. The SOS model then sees Neumann boundary conditions on the boundary, and the height correlator becomes, in the continuum and infinite size limit [23]

$$\langle \Phi(x)\Phi(x')\rangle_N = -\frac{1}{g}\ln|x - x'|^2. \tag{10}$$

Let us now single out a segment of length L on this boundary and count the number of arcs connecting this segment to the rest of the boundary. To do this, we insert a pair of so-called vertex operators, one at each a extremity of the segment, $V_\pm = \exp[i(\pm e_1 + e_0/2)\Phi]$, and we evaluate their correlation function. The insertion does not affect the arcs encircling the whole interval L since the weight of oriented arcs is modified from $e^{\pm i\pi e_0/2}$ to $e^{\pm i\pi e_0/2}e^{\mp i\pi e_0} = e^{\mp i\pi e_0/2}$, thus giving the same sum $\sqrt{Q_b}$ over orientations. But for loops connecting the inside to the outside, the weight is now $w = 2\cos\pi e_1$. The boundary dimension of the fields $V_\pm$ is, using the propagator

$$h = \frac{4e_1^2 - e_0^2}{4g}, \tag{11}$$

and we have

$$\langle V_+(0)V_-(L)\rangle = \frac{\sum_{\mathcal{C}}(\sqrt{Q})^{N_L}(\sqrt{Q_b})^{N_{nc}}w^{N_c}}{\sum_{\mathcal{C}}(\sqrt{Q})^{N_L}(\sqrt{Q_b})^{N_{nc}+N_c}} \propto L^{-2h} \tag{12}$$

where $\mathcal{C}$ denotes all the allowed configurations, N_L is the number of loops in the bulk, N_c the number of arcs connecting the segment to the rest of the boundary, and N_{nc} the number of remaining arcs. We can then find the average number of loops separating two given points by taking a derivative with respect to w and setting $w = \sqrt{Q_b}$ in the end. Using the correspondence between these parameters and e_1, e_0 as well as Eq. (11) for h leads to our main result

$$\langle N_c\rangle(\Omega) \overset{a}{=} \frac{e_0}{\pi(1-e_0)}\frac{2\cos(\pi e_0/2)}{\sin(\pi e_0/2)}\ln L. \tag{13}$$

For the XXX chain ($e_0 = 0$), this reads $\langle N_c\rangle \overset{a}{=} \frac{4}{\pi^2}\ln L \approx 0.405\ln L$, while for bond percolation ($Q = 1$ or $e_0 = 1/3$), we have $\langle N_c\rangle \overset{a}{=} \frac{\sqrt{3}}{\pi}\ln L \approx 0.551\ln L$. The slope becomes 1 exactly as $e_0 \to 1$, or $\sqrt{Q} \to -2$. We note that the result for the XXX case is close but definitely different from the one proposed in [3].

It is amusing to observe that one can exactly interpret the valence bond as singlet contractions for an ordinary supergroup in the case $Q = 1$, by taking a lattice model where the fundamental three-dimensional representation of $SU(2/1)$ and its conjugate alternate. The Hamiltonian is again (3), but this time the E_i are projectors onto the singlet in $3 \otimes \bar{3}$. The effective central charge for this spin chain is $c_{\text{eff}} = 1 + \frac{9}{\pi^2}[\text{arccosh}(3/2)]^2 \simeq 1.845$, and extending the argument suggested in [3] for the XXX case gives a slope of $\frac{c_{\text{eff}}}{3\ln 3} \simeq 0.559$, even closer to the exact result (13).

Of course, by taking higher derivatives of the two-point function of the vertex operators, one can access the higher moments of (9). In fact, the two-point function itself is nothing but the characteristic function of $p(N_c)$, although carrying out the Fourier transform in general is somewhat cumbersome. We will content ourselves here by giving the first few cumulants $\mathcal{C}_k = (c_k/\pi^k)\ln L$, with, in the XXX case (top) and the $Q = 1$ case (bottom):

$$c_1 = \begin{cases} 4 \\ \sqrt{3}\pi \end{cases} \qquad c_2 = \begin{cases} 8/3 \\ 2(2\pi\sqrt{3} - 9) \end{cases} \qquad c_3 = \begin{cases} 16/15 \\ 8(5\pi\sqrt{3} - 27) \end{cases} \tag{14}$$

together with the observation that, as $\sqrt{Q} \to -2$, the probability distribution becomes Poissonian:

$$\lim_{\sqrt{Q}\to -2} P(N_c) = e^{-\ln L}\frac{(\ln L)^{N_c}}{N_c!}. \tag{15}$$

Numerical calculations.—We have computed the distribution (9) numerically by exactly diagonalizing the transfer matrix, for periodic chains of size up to $N_{\max} = 32$. The cumulants $\mathcal{C}_k \propto \ln L$ of $p(N_c)$ obey a very simple finite size scaling (FSS) form, where $\ln L$ has to be replaced by $\frac{N}{\pi} \times \ln(\sin\frac{L\pi}{N})$; this follows from standard formulas for two-

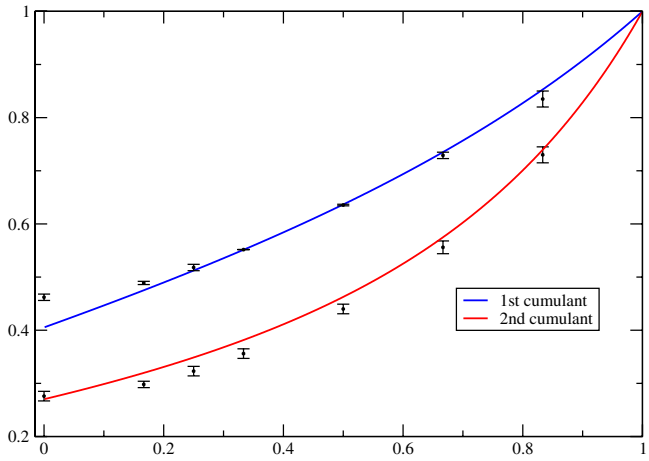

FIG. 2 (color online). Comparison between exact and numerically determined values of the slopes c_1 and c_2, shown as functions of the parameter e_0.

point functions of our vertex operators V. Precise values of the slopes c_k can then be extracted from a careful analysis of the residual FSS effects. As shown in Fig. 2, they agree well with our analytical results, except for $Q \to 4$, where we expect logarithmic FSS corrections.

For $Q = 1$, the combinatorial nature of $|\Omega\rangle$ implies that all λ_w in (7) are *integers*. This allows to obtain $p(N_c)$ *exactly* for finite L and $N \leq N_{\max}$. Using this, we can in some cases conjecture $p(N_c)$ for any value of N [24]. In particular, we have established that

$$\langle N_c \rangle = (N^2 - L^2) p_k(N^2) \prod_{n=0}^{N/2-1} [N^2 - (2n+1)^2]^{n-N/2} \tag{16}$$

where p_k is a polynomial of degree $k = \frac{1}{8}(N+4)(N-2)$ in N^2. This exact FSS form allows to obtain for the slope $c_1 = 0.5517 \pm 0.0003$, in very precise agreement with the value 0.551329 from (13).

Conclusions.—We have shown in this Letter that it is possible to tackle analytically many statistical properties of valence-bond entanglement in the 1D case, thus disproving the conjecture in [3], providing benchmarks for future numerical studies, and opening the way to, in particular, combinatorial studies. It is our hope that S_{VB} might turn out to be useful to distinguish, in particular, the various critical points with vanishing central charge appearing in the recent studies of supersymmetric spin chains [24].

We thank F. Alet for helpful exchanges and for pointing out Ref. [19]. This work was supported by the European Community Network ENRAGE (Grant No. MRTN-CT-2004-005616), by the Agence Nationale de la Recherche (Grant No. ANR-06-BLAN-0124-03), and by the ESF Network Program INSTANS.

[1] J. L. Latorre, J. Phys. A **40**, 6689 (2007); L. Amico, R. Fazio, A. Osterloh, and V. Vedral, arXiv:quant-ph/0703044 [Rev. Mod. Phys. (to be published)].
[2] P. Zanardi and N. Paunkovic, Phys. Rev. E **74**, 031123 (2006).
[3] F. Alet, S. Capponi, N. Laflorencie, and M. Mambrini, Phys. Rev. Lett. **99**, 117204 (2007).
[4] R. W. Chhajlany, P. Tomczak, and A. Wojcik, Phys. Rev. Lett. **99**, 167204 (2007).
[5] G. Refael and J. E. Moore, Phys. Rev. Lett. **93**, 260602 (2004).
[6] G. Refael and J. E. Moore, Phys. Rev. B **76**, 024419 (2007).
[7] R. Santachiara, J. Stat. Mech. (2006) L06002.
[8] Y. C. Lin, F. Igloi, and H. Rieger, Phys. Rev. Lett. **99**, 147202 (2007).
[9] R. Yu, H. Saleur, and S. Haas, arXiv:cond-mat/0709.3840.
[10] C. Holzhey, F. Larsen, and F. Wilczek, Nucl. Phys. B **424**, 443 (1994).
[11] P. Calabrese and J. Cardy, J. Stat. Mech. (2004) P06002.
[12] M. Mambrini, arXiv:cond-mat/0706.2508.
[13] K. S. D. Beach and A. W. Sandvik, Nucl. Phys. B **750**, 142 (2006).
[14] A. W. Sandvik, Phys. Rev. Lett. **95**, 207203 (2005).
[15] The scale of (3) affects the sound velocity and is important when studying the scaling of gaps. But it does not matter when dealing with entanglement issues.
[16] P. Martin, *Potts Models and Related Problems in Statistical Mechanics* (World Scientific, Singapore, 1991).
[17] K. Chang, I. Affleck, G. W. Hayden, and Z. G. Soos, J. Phys. Condens. Matter **1**, 153 (1989).
[18] Note that the scalar product of a state $|w\rangle$ with itself is equal to $\sqrt{Q}^{N/2-j}$ for all w, so there is no need to consider "normalized" basis states.
[19] A. Feiguin, S. Trebst, A. W. W. Ludwig, M. Troyer, A. Kitaev, Z. Wang, and M. H. Freedman, Phys. Rev. Lett. **98**, 160409 (2007).
[20] The boundary conditions at large N are not expected to affect the leading behavior of S_{VB}.
[21] B. Nienhuis, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, London, 1987), Vol. 11.
[22] When $\sqrt{Q} < 0$ (i.e. $\frac{1}{2} < e_0 < 1$), the true ground state has spin $j > 0$. Nevertheless, we continue to let $|\Omega\rangle$ denote the $j = 0$ ground state. Numerical studies then indicate that (7) holds even for $\sqrt{Q} < 0$, if N is large enough.
[23] I. K. Kostov, B. Ponsot, and D. Serban, Nucl. Phys. B **683**, 309 (2004).
[24] J. L. Jacobsen and H. Saleur (to be published).