Exact valence bond entanglement entropy and probability distribution in the XXX spin chain and the Potts model

Jesper Lykke Jacobsen, Hubert Saleur

To cite this version:
Jesper Lykke Jacobsen, Hubert Saleur. Exact valence bond entanglement entropy and probability distribution in the XXX spin chain and the Potts model. 2007. hal-00189664

HAL Id: hal-00189664
https://hal.science/hal-00189664
Preprint submitted on 21 Nov 2007

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
Introduction. Entanglement is a central concept in quantum information processing, as well as in the study of quantum phase transitions. One of the widely used quantum information processing, as well as in the study of quantum phase transitions. One of the widely used entanglement measures is the von Neumann entanglement entropy. In the case of systems admitting infinite randomness fixed points, in one and higher dimensions [8, 9] dimensions, the ground state of the isotropic spin chain, namely (2) with $c = 1$. In other words, the observation of [10] was that

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

Apart from this, the valence bond basis has been actively studied recently, in particular from rigorous [12, 13] and probabilistic [14] points of view.

Studying entanglement entropy from a geometrical point of view seems particularly appealing in view of the quantum dimer model of Rokhsar and Kivelson [15] and its many recent generalizations. Indeed, Henley [16] has shown that for any classical statistical mechanics model equipped with a discrete state space and a dynamics satisfying detailed balance, there is a corresponding quantum Hamiltonian whose ground state $|\Omega\rangle$ is precisely the classical partition function. Of particular interest are then statistical mechanics models in which the microscopic degrees of freedom directly define the valence bonds. This is the case for a certain class of lattice models of loops, to be studied below.
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 (3) is not quite correct: the exact leading asymptotic behaviour is in fact $\langle N_c \rangle_{\Omega} \approx \frac{1}{4} \ln L + 0.405 \ln L$. All other cumulants have similar closed form expressions.

**Entanglement and the TL algebra.** The 2D classical $Q$-state Potts model can be defined for $Q$ non integer 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 \[ H = -\sum_{i=1}^{N-1} e_i \] (4)

Here the $e_i$ are elements of an associative unital algebra called the Temperley-Lieb (TL) algebra, defined by

\[ e_i^2 = \sqrt{Q} e_i \]

\[ [e_i, e_j] = 0 \text{ for } |i-j| \geq 2 \]

\[ e_i e_{i+1} e_i = e_i \] (5)

The ground state of $H$ depends on the representation of the algebra. For our purpose, it is natural to use the loop model representation, where the generators act on the following non-orthogonal but linearly independent basis states. Each basis state corresponds to a pattern of $N$ parentheses and dots, such as $(\cdot)(\cdot)(\cdot)$. The parentheses must obey the typographical rules for nesting, and the dots must not be inside any of the parentheses. These rules imply that the $(\cdot)$ pairs consist of one even and one odd site, and that dots are alternately on even and odd sites. We start by convention with an odd site on the left. Note that we have used an open chain for convenience, but that a periodic chain can be considered as well. This rules imply that the $(\cdot)$ pairs consist of one even and one odd site, and that dots are alternately on even and odd sites. We start by convention with an odd site on the left. Note that we have used an open chain for convenience, but that a periodic chain can be considered as well. This requires the introduction of an additional generator $e_N$ coupling the $N^{th}$ and first site, and in the graphical representation, parentheses can now be paired cyclically so $(\cdot)(\cdot)(\cdot)$ is now a valid pattern. This is shown in Fig. 1.

One can interpret these states in terms of spin $1/2$ by associating with each pair of nearest parentheses $(\cdot)$ a $U_q sl(2)$ singlet $(\sqrt{Q} = q + q^{-1})$ so a valence bond can be drawn between the two corresponding sites. (Note that the generator $e_i$ is nothing but the operator that projects sites $i$ and $i + 1$ onto the singlet.) For the dots, the state \[ \langle \Omega \rangle = \sum_{j} h_{ij} |w_j\rangle \] (7)

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 words with positive coefficients \[ |\Omega\rangle = \sum_{w} \lambda_w |w\rangle, \quad \lambda_w > 0 \] (8)

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

\[ \langle N_c \rangle_{\Omega} = \frac{\sum_{w} \lambda_w N_c(w)}{\sum_{w} \lambda_w} \] (9)

and more generally in the probability distribution

\[ p(N_c) = \frac{\sum_{w} \lambda_w N_c(w) = N_c \lambda_w}{\sum_{w} \lambda_w} \] (10)
Below we establish the leading asymptotic behaviour 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 \( \sqrt{Q} = 2 \cos \frac{\pi c_0}{4} \), with \( k \) integer, and the interacting anyons (coming in \( k + 1 \) species) hamiltonian in [3]. 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 certain hamiltonian with periodic (free) boundary conditions [24] can be obtained as the path integral of the equivalent Euclidian theory on an infinite half cylinder (annulus), denoted \( C_- \) (or \( A_- \)). To translate this in statistical mechanics terms, note that if we consider the square lattice with axial (diagonal) direction of propagation [cf. Fig. 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 \( \langle \Omega \rangle \). Let us chose for instance the particular case where the Potts model is isotropic, with coupling constant \( e^{K} = 1 + \sqrt{Q} \). Now the ground state \( \langle \Omega \rangle \) 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 \( \langle \Omega \rangle \) on the words \( |w\rangle \) are (up to a common proportionality factor) equal to the partition 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 loops with fugacity \( \sqrt{Q} \) in the bulk, with half loops ending up with open extremities on the boundary. To go to the continuum limit it is convenient to transform this loop model into a solid-on-solid model [13]. For this parametrize \( \sqrt{Q} = 2 \cos \pi c_{0} \) with \( 0 \leq c_{0} < 1/2 \) [24]. Give to all the loops an orientation, and introduce complex weights \( \exp (\pm \frac{i \pi e_{0}}{2}) \) 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 \( \pm 4 \), this gives closed loops the correct weight \( \sqrt{Q} \).

Meanwhile, loops ending on the boundary will get, with this construction, the weight \( \sqrt{Q}_{b} = 2 \cos \frac{3 \pi c_{0}}{2} \) since for them \( n_{L} - n_{R} = \pm 2 \) [20]. 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 it does not matter: the number of open loops touching the boundary is just \( N/2 - j \), a constant.

Introducing this boundary loop weight allows complete mapping to the SOS model (or free six-vertex model). Now it is known that in the continuum limit, the dynamics of the SOS height variables turns into the one of a free bosonic field [14]. In a renormalization scheme where loops carry a constant height step \( \Delta \Phi = \pm \pi \), the propagator of the field evaluated at two points \( x, x' \) on the boundary reads, in the infinite size limit [2]

\[
(\Phi(x)\Phi(x'))_{N} = -\frac{1}{g} \ln |x - x'|^{2}
\]

where \( g = 1 - e_{0} \). Here the subscript \( N \) indicates Neumann boundary conditions, corresponding to the presence of loop extremities on the boundary.

Let us now single out a segment of length \( L \) on this boundary and attempt to count the number of loops connecting this segment to the rest of the boundary. To do this we insert a pair of vertex operators, one at each a extremity of the segment, \( V = \exp [i (\pm e_{1} + e_{0}/2) \Phi] \). These operators do not affect the loops encircling the whole interval \( L \) since they modify the weight of such loops from \( e^{\pm i \pi c_{0}/2} \) to \( e^{\pm i \pi c_{0}/2} e^{\pm i \pi c_{0}} = e^{\pm i 2 \pi c_{0}/2} \), thus giving the same sum \( \sqrt{Q}_{b} \). But for loops connecting the inside to the outside, the weight is now \( w = 2 \cos \pi c_{1} \). The boundary dimension of the fields \( V \) is, using the propagator

\[
h = \frac{4 e^{2} - e_{0}^{2}}{4 g}
\]

so their two-point function decays as \( L^{-2h} \). We can then find the average number of loops separating two given points by taking appropriate derivatives, and setting \( e_{1} = e_{0}/2 \) in the end. This leads to our main result

\[
\langle N_{c} \rangle (\Omega) \approx \frac{e_{0}}{\pi (1 - e_{0})} \frac{2 \cos (\pi e_{0}/2)}{\sin (\pi e_{0}/2)} \ln L
\]

For the XXX chain \( (e_{0} = 0) \) this reads \( \langle N_{c} \rangle \approx \frac{1}{\sqrt{2}} \ln L \approx 0.465 \ln L \), while for bond percolation \((Q = 1 \text{ or } e_{0} = 1/3)\) we have \( \langle N_{c} \rangle \approx \frac{\pi}{4} \ln L \approx 0.551 \ln L \). 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 [10].

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 [10], but this time the \( e_{1} \) are projectors onto the singlet in \( 3 \otimes 3 \). The effective central charge for the this spin chain is \( c_{eff} = 1 + \frac{\pi}{3} \left[ \text{arcosh}(3/2) \right]^{2} \approx 1.845 \), and extending the argument suggested in [10] for the XXX case gives a slope of \( \frac{\pi e_{0}}{\sqrt{3}} \approx 0.559 \), 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 \( \langle N_{c} \rangle \). 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 \( C_{k} = \left( e_{k}/\pi^{k} \right) \ln L \), with,
in the XXX case (top) and the \( Q = 1 \) case (bottom):

\[
\begin{align*}
  c_1 &= \begin{cases} 
  4 & /3 \\
  2(2\pi/3 - 9) & 8/3
  \end{cases} \\
  c_2 &= \begin{cases} 
  16/15 & 8(5\pi/3 - 27)
  \end{cases}
\end{align*}
\]

(14)

(15)

Numerical calculations. We have computed the distribution \([13]\) numerically by exactly diagonalizing the transfer matrix, for periodic chains of size up to \( N_{\text{max}} = 32 \). The cumulants \( C_k \propto \ln L \) of \( p(N_c) \) obey a very simple finite size scaling (FSS) form, where \( \ln L \) has to be replaced by \( \frac{\pi}{6} \ln \sin \frac{\pi}{L} \); this follows from standard formulas for two-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. 3 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 \( |\Omega| \) implies that all \( \lambda_k \) in (8) are integers. This allows to obtain \( p(N_c) \) exactly for finite \( L \) and \( N \leq N_{\text{max}} \). Using this, we can in some cases conjecture \( p(N_c) \) for any value of \( N \) [2]. In particular we have established that

\[
N_{c} = (N^2 - L^2)p_k(N^2) \prod_{n=0}^{N/2-1} (N^2 - (2n+1)^2)^{N-n/2}
\]

(16)

where \( p_k \) is a polynomial of degree \( k = \frac{1}{2}(N + 4)(N - 2) \) 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. As already argued in \([14]\), \( S_{\text{VB}} \) is a measure of entanglement which seems as good qualitatively as \( S_{\text{NC}} \), and easier to obtain numerically. We have shown in this Letter that it is also possible to tackle it analytically in the 1D case. The results are less easily expressed than for \( S_{\text{NC}} \) (which is proportional to \( c \)) . On the other hand, they fit considerably more naturally within the transfer matrix and Coulomb gas formalism. It remains to be seen what happens for other models, and whether in particular a c-theorem of sorts is obeyed for \( S_{\text{VB}} \).

Acknowledgments. We thank F. Alet for helpful exchanges, and for pointing out Ref. [18]. This work was supported by the European Community Network ENRAGE (grant MRTN-CT-2004-005616) and by the Agence Nationale de la Recherche (grant ANR-06-BLAN-0124-03).

1. C. Holzhey, F. Larsen and F. Wilczek, Nucl. Phys. B 424, 44 (1994).
2. P. Calabrese and J. Cardy, J. Stat. Mech. P06002 (2004).
3. P. Martin, Potts models and related problems in statistical mechanics, World Scientific, Singapore (1991).
4. P. Martin and H. Saleur, Comm. Math. Phys. 158, 155 (1993).
5. G. Refael and J.E. Moore, Phys. Rev. Lett. 93 260602 (2004).
6. G. Refael and J.E. Moore, cond-mat/0703038.
7. R. Santachiara, J. Stat. Mech. L06002 (2006).
8. Y.C. Lin, F. Igloi and H. Rieger, Phys. Rev. Lett. 99, 147202 (2007).
9. R. Yu, H. Saleur and S. Haas, cond-mat/07103840.
10. F. Alet, S. Capponi, N. Laflorencie and M. Mambrini, Phys. Rev. Lett. 99, 117204 (2007).
11. R.W. Chhajlany, P. Tomczak and A. Wojcik, Phys. Rev. Lett. 99, 167204 (2007).
12. M. Mambrini, 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. D.S. Rokhsar and S.A. Kivelson, Phys. Rev. Lett. 61, 2367 (1988).
16. C.L. Henley, J. Phys.: Cond. Matt. 16, S891 (2004).
17. K. Chang, I. Affleck, G. Hayden and Z. Soos, J. Phys. C 1, 153 (1989).
18. A. Feiguin, S. Trebst, A.W.W. Ludwig, M. Troyer, A. Kitaev, Z. Wang and M.H. Freedman, Phys. Rev. Lett. 98, 160409 (2007).
19. B. Nienhuis, in C. Domb and J.L. Lebowitz (eds.), Phase Transitions and Critical Phenomena, vol. 11 (Academic, London, 1987).
20. I.K. Kostov, B. Ponsot and D. Serban, Nucl. Phys. B 683, 309 (2004).
21. J.L. Jacobsen and H. Saleur, to be published.
22. The scale of (4) affects the sound velocity and is important when studying the scaling of gaps. But it does not matter when dealing with entanglement issues.
23. Note that the scalar product of a state \( |w\rangle \) with itself is equal to \( \sqrt{Q^{N/2}} \) for all \( w \), so there is no need to consider “normalized” basis words.
24. The boundary conditions at large \( N \) are not expected to affect the leading behaviour of \( S_{\text{VB}} \).
25. When \( \sqrt{Q} < 0 \) (i.e. \( \frac{1}{2} < e_0 < 1 \)) the true ground state has

\[
\frac{4}{\sqrt{3\pi}} c_2 = \begin{cases} 
  8/3 & 2(2\pi/3 - 9) \\
  8(5\pi/3 - 27)
  \end{cases}
\]

\[
\lim_{Q \to 2} P(N_c) = e^{-\ln L} \frac{(\ln L)^{N_c}}{N_c!}
\]
spin $j > 0$. Nevertheless, we continue to let $|\Omega\rangle$ denote the $j = 0$ ground state. Numerical studies then indicate that (8) holds even for $\sqrt{Q} < 0$, if $N$ is large enough.