Boundary effects in the critical scaling of entanglement entropy in 1D systems

Nicolas Laflorencie,1 Erik S. Sørensen,2 Ming-Shyang Chang,1 and Ian Affleck1

1Department of Physics & Astronomy, University of British Columbia, Vancouver, B.C., Canada, V6T 1Z1
2Department of Physics and Astronomy, McMaster University, Hamilton, ON, L8S 4M1 Canada

(Dated: March 23, 2022)

We present exact diagonalization and density matrix renormalization group results for the entanglement entropy of critical spin-1/2 XXZ chains. We find that open boundary conditions induce an alternating term in both the energy density and the entanglement entropy which are approximately proportional, decaying away from the boundary with a power-law. The power varies with anisotropy along the XXZ critical line and is corrected by a logarithmic factor, which we calculate analytically, at the isotropic point. A heuristic resonating valence bond explanation is suggested.

PACS numbers: 03.67.Mn, 05.70.Jk, 75.10.Pq

Introduction — Quantum spin chains have recently acquired the status of paradigmatic systems to investigate and understand the subtle interplay between quantum entanglement and quantum criticality [1, 2, 3, 4, 5]. An important extension to critical and non-critical systems typically have open boundary conditions (OBC). While much theoretical work in this area has focussed on periodic boundary conditions (PBC), experimental systems have not. We present new eect of OBC on quantum entanglement in antiferromagnetic chains.

The entanglement entropy (EE), first introduced by Bennett et al. [6] in a quantum information context, has recently received more attention from a condensed matter point of view since it has been shown to exhibit a universal scaling for some one dimensional (1D) quantum critical points [4, 7, 8]. Defined as the von Neumann entropy of the reduced density matrix $\rho(x)$ of a given subsystem of size $x$ embedded in a larger closed ring of size $L$, a universal scaling is expected at a quantum critical point in the limit $x \gg 1$ and $L \to \infty$: $S(x) = -\text{Tr} \ln \rho = \frac{c}{3} \ln x + s_1$. The prefactor $c$ is the central charge of the associated conformal field theory (CFT) [4, 8]. Defined as $s_1$ a non universal constant related to the ultra-violet cut-off $\Lambda$. The divergence of $S(x)$ with $x$ reflects an interesting property of the reduced density matrix: $\rho(x)$ has a number of non negligible eigenvalues which also diverges with the subsystem size, like $M(x) \sim e^x \sim x^{c/3}$.

This critical scaling has been verified numerically [1, 11] by diagonalizing free-fermion type Hamiltonians for the quantum Ising chain ($c = 1/2$) or the XX chain ($c = 1$). An important extension to critical and non-critical systems with finite size, finite temperature and different boundary conditions has been achieved by Calabrese and Cardy [10]. Using CFT, they showed for instance that for critical systems of finite size $L$ with OBC, the expression for the EE of a subsystem of size $x$ including the open end becomes:

$$S(x, L) = \frac{c}{6} \ln \left( \frac{2L}{\pi} \sin \left( \frac{\pi x}{L} \right) \right) + \ln g + s_1/2,$$

where $\ln g$ is boundary entropy introduced in [8]. (We have corrected factors of 2 in the last 2 terms in Eq. following [10].)

In the following, we investigate the EE for a large class of critical XXZ quantum spin chains of length $L$ with OBC. In addition to confirming the behavior (1), at large $x$, we find an unexpected alternating term in the EE which decays away from the boundary with a power law. The boundary also introduces a slowing decaying alternating term in the energy density. We show numerically that these are proportional. The microscopic origin of the even-odd alternation of the EE will be understood through a qualitative resonating valence bond (RVB) picture.

Critical chains with open ends — The Hamiltonian for XXZ quantum spin chains of length $L$ with OBC is

$$H = \sum_{x=1}^{L-1} \left[ \frac{1}{2} (S_x^+ S_{x+1}^- + S_x^- S_{x+1}^+) + \Delta S_x^z S_{x+1}^z \right].$$

The critical regime is achieved for $|\Delta| \leq 1$. The energy density $\langle h_x \rangle = \langle (S_x^+ S_{x+1}^- + S_x^- S_{x+1}^+) / 2 + \Delta S_x^z S_{x+1}^z \rangle$ is independent of $x$ in periodic chains. On the other hand, an open end breaks translational symmetry and the energy density picks up a slowly decaying alternating term or “dimerization”:

$$\langle h_x \rangle = E_U(x) + (-1)^x E_A(x),$$

where $E_A(x)$ becomes non zero near the boundary and decays slowly away from it. We can calculate $E_A(x)$ by Abelian bosonization methods modified by OBC [11]. The low energy effective Hamiltonian is simply that of a free massless relativistic boson, $\phi(x)$ with a boundary condition, $\phi(0) = \text{constant}$. $E_U(x)$ goes to a constant like $1/x^2$ (for all $|\Delta| \leq 1$) but this is not of interest here. The alternating part of $h_x$ is $(-1)^{x+1} \langle \sin(\sqrt{4\pi K} \phi) \rangle$ where $K = \frac{\pi}{2(\pi - \cos^{-1} \Delta)}$ is the Luttinger liquid parameter. Using the standard conformal mapping we obtain in a finite system of length $L$

$$E_A(x, L) \propto \langle \sin(\sqrt{4\pi K} \phi) \rangle \propto \frac{1}{[\frac{\pi}{2(\pi - \cos^{-1} \Delta)}]^{x/2}}.$$
At the Heisenberg [SU(2) invariant] point, $\Delta = 1$, the low energy effective Hamiltonian contains a marginally irrelevant coupling constant, $\lambda$. It leads to a contribution to the scaling dimension of $O(\lambda)$ for most operators $[12, 13]$. The staggered energy density, $\sin \sqrt{2\pi \phi}$ has a scaling dimension $[13]$

$$\gamma = 1/2 + \pi \sqrt{3\lambda} + O(\lambda^2).$$

(5)

This implies $[13]$ that the bulk correlation function $G \equiv \langle h_i h_j \rangle$ decays as $1/|i - j|(|x| - |j|)^{3/2}$. With a boundary, one can derive a renormalization group equation for $E_A(x)$:

$$\frac{\partial}{\partial \ln x} + \beta(\lambda) \frac{\partial}{\partial \lambda} + \gamma(\lambda) E_A(x) = 0,$$

(6)

which is the same as that obeyed by $G(x)$ except that the term $\gamma$ gets replaced by $2\gamma$. (Since we are interested in $E_A(x)$ for $x \gg 1$, the presence of the boundary does not affect the scaling dimension of $\sin \sqrt{2\pi \phi}$. This can be seen from considering the operator product expansion of the marginal operator with $\sin \sqrt{2\pi \phi}$. At short distances, it is unaffected by the boundary. On the other hand, corrections to scaling dimensions of boundary operators due to the marginal operator are affected non-trivially by the boundary condition. See $[13]$.) This implies $E_A(x) \propto 1/\sqrt{|x|(|x|)^{3/4}}$. It is highly non-trivial to include both the log corrections and the finite size effects in $E_A(x, L)$. However, there is a simple result at $x = L/2$. Including the cubic term in the $\beta$-function for the marginal coupling constant, and other higher order corrections, this becomes:

$$E_A(L/2, L) = a_0 \frac{1 + a_2/|\ln(L/a_1)|^2}{\sqrt{|\ln(L/a_1)| + (1/2) \ln \ln(L/a_1)}},$$

(7)

where $a_0$, $a_1$ and $a_2$ are constants. This formula is fit to density matrix renormalization group (DMRG) data, (after extracting uniform and alternating part by fitting both locally to a polynomial using a 5-point formula) in Fig. 1, obtaining excellent agreement. In the same figure we also show $E_A(L/2)$ for the isotropic model with first and second neighbor interactions with $J_2/J_1 = 0.241167$. This model is at the critical point between gapless and gapped spontaneously dimerized phase and the marginal coupling constant, and hence the log corrections are expected to vanish here $[13]$, as is seen in the figure.

**RVB picture** — This modulation in $\langle h_x \rangle$ can be interpreted as an alternation of strong and weak bonds along the chain. Indeed, the boundary spin at $x = 1$ will have a strong tendency to form a singlet pair with its only partner on the right hand side. On the other hand the spin located at $x = 2$ will be consequently less entangled with its right partner at $x = 3$ since it already shares a strong entanglement with its left partner. This tendency towards dimer formation over odd bonds induced by OBC can be naively depicted through the simple valence bond solid state:

$$|\Psi\rangle = \frac{1}{2L/2} \otimes_{x=1}^{L/2} [\uparrow_{2x-1} \downarrow_{2x} - \downarrow_{2x-1} \uparrow_{2x}].$$

(8)

(This is the exact ground state of the Majumdar-Ghosh model with a second neighbor coupling obeying $J_2/J_1 = 1/2$.) In such a state, the EE of a finite subsystem alternates between $\ln 2$ if the interface between the subsystem and the rest of the chain cuts a singlet bond and 0 otherwise. More generally, we may write any singlet state as a linear combination of all valence bond states (with no bonds crossing each other). It is trivial to calculate the EE for a simple state corresponding to any particular valence bond configuration, such as the one drawn in Fig. 2. It is given exactly by $S(x) = N(x) \ln 2$, where $N(x)$ is the number of valence bonds crossing the link $x$ between sites $x$ and $x + 1$. Since one may think, in a renormalization group sense, of the ground state of the random-bond Heisenberg model as consisting of a single valence bond configuration $[15]$, this leads $[15]$ to an interesting prediction for the EE. Unfortunately, the non-random critical case, where the ground state involves an

![FIG. 1: $E_A(L/2, L)$ computed by DMRG (keeping $m = 512$ states) at the SU(2) point up to $L = 1000$ for the nearest neighbor model $J_2/J_1 = 0$ (c) and at the critical point $J_2/J_1 = 0.241167$ (□) (a). Full lines are fits, indicated on the main panel. Zooms on large L regions are showed in (b) and (c): (b) absence of log corrections for $J_2/J_1 = 0.241167$; (c) excellent agreement between Eq. (7) and DMRG.](image1)

![FIG. 2: A particular valence bond state. The number of valence bonds crossing each link, $N(x)$, is given.](image2)
incfinite sum over different valence bond configurations, including bonds of arbitrary length, appears more difficult. Nevertheless, it seems plausible that the enhanced tendency towards valence bonds on odd links induced by a boundary will translate into an alternating term in the EE.

Numerical results for the entropy—It is well known that when the Ising exchange term $\Delta = 0$, using a Jordan-Wigner mapping, the XXZ Hamiltonian \( \mathcal{H}_{XX} \) is equivalent to a free fermion Hamiltonian

\[
\mathcal{H}_{XX} = \frac{J}{2} \sum_{x=1}^{L-1} \left[ \Psi_x^\dagger \Psi_{x+1} + \Psi_{x+1}^\dagger \Psi_x \right],
\]

which can be solved in momentum space. The computation of the EE in this non-interacting case can be easily achieved numerically for very large systems since it only requires diagonalization of an \( L \times L \) matrix (see Ref. \[16\] for some details). We first report results from exact diagonalizations of the free fermion Hamiltonian \( \mathcal{H}_{XX} \) with \( L = 2000 \) sites. In Fig. 3 we superimpose both PBC and OBC cases. In the PBC situation, as predicted in Ref. \[2\], the entropy is very well described by the following expression

\[
S_{\text{PBC}}(x, L) = \frac{c}{3} \ln \left( \frac{L}{\pi} \sin \left( \frac{\pi x}{L} \right) \right) + s_1,
\]

with \( c = 1 \) and \( s_1 \approx 0.726 \). On the other hand, the open chain does not obey the expression \( \mathcal{H} \), but as expected from the RVB picture presented above, an alternating term is found, as is visible in the lower inset of Fig. 3. Indeed, the strong odd bond - weak even bond picture agrees qualitatively with an enhanced (reduced) entropy for subsystems cutting an odd (even) bond. We thus define the uniform and alternating parts of the EE for large \( x \):

\[
S(x, L) = S_U(x, L) + (-1)^x S_A(x, L),
\]

where both \( S_U(x, L) \) and \( S_A(x, L) \) are expected to be slowly varying functions for \( x \gg 1 \). Interestingly, for the XX case, \( S_A(x, L) \) is found to decay slowly like a power-law,

\[
S_A^{XX}(x, L) \sim \frac{1}{x} \sin \left( \frac{\pi x}{L} \right),
\]

which has the same exponent as the alternating part of the energy density \( E_A \), as follows from Eq. \( \mathcal{H} \) using the correct value \( K = 1 \), for the XX model. It turns out that both the alternating part of the EE \( S_A \) and \( E_A \), defined by Eq. \( \mathcal{H} \), are nearly proportional at large \( x \) with a proportionality constant of \( \pi/2 \):

\[
S_A(x, L) = (-\pi/2) E_A(x, L) + O(1/x^2).
\]

from ED at \( \Delta = 0 \) are also shown for \( L = 2000 \). Dashed lines are linear fits of the form \( \mathcal{H} \), which is also \( \propto 1/[L \sin(\pi x/L)] \). This is included in the fit in Fig. 4.

FIG. 3: Results from exact diagonalization of XX chains with \( L = 2000 \) spins 1/2. EE \( S(x, 2000) \), plotted vs the subsystem size \( x \) in PBC (upper symbols) and OBC (lower symbols); the insets show zooms around the chain center. The full lines are fits: Eq. \( \mathcal{H} \) with \( s_1 = 0.726067 \) for the PBC case whereas in the OBC case, some uniform and staggered terms \[0.05(1-x)^{0.25} \] have been added to Eq. \( \mathcal{H} \).

FIG. 4: Linear behavior of the alternating part of the EE, \( S_A \) as a function of the alternating energy density, \( -E_A \), both computed using DMRG on critical open XXZ chains of size \( 200 \leq L \leq 1000 \) for a few values of the anisotropy \( \Delta \). Data from ED at \( \Delta = 0 \) are also shown for \( L = 2000 \). Dashed lines are linear fits of the form \( S_A = -\alpha E_A \) (see text). The inset \( \mathcal{H} \) is a zoom close to 0, showing data for \( \Delta = -3/4 \) and \( -1/2 \). The inset \( \mathcal{H} \) shows the prefactor \( \alpha \) vs \( \Delta \) extracted from the numerical data (circles), for a larger set of values of \( \Delta \), which is compared with \( \pi/2v = \mu/\sin \mu, \mu = \cos^{-1} \Delta \).

Based on DMRG data obtained on critical open chains of size \( 200 \leq L \leq 1000 \), we find this proportionality is
still true even when $\Delta \neq 0$ where the decaying behavior of $E_A$ is controlled by $K$. More precisely, plotting $S_A$ as a function of $-E_A$ for various values of the anisotropy $\Delta$ in Fig. 4 we find a linear relation $S_A = -\alpha E_A$ with a prefactor perfectly described by $\alpha = \mu/\sin \mu$, as shown in the inset of Fig. 4 with $\mu = \cos^{-1} \Delta$. We note that the spin-wave velocity for the XXZ model is given by $v = \pi (\sin \mu)/(2\mu)$ so that we may write this relation as

$$S_A = -(\pi a^2/2v)E_A,$$

(13)

where we have introduced the lattice spacing, $a$, to make the EE a dimensionless quantity ($E_A$ has dimensions of energy per unit length.). We emphasize that Eq. (13) even holds for the Heisenberg model with $\alpha = 1$ where we find both $E_A(L/2, L)$ and $S_A(L/2, L)$ display the same logarithmic corrections, Eq. (13), as shown in Fig. 4. The sum $E_A(L/2, L) + S_A(L/2, L)$ is found to rapidly decay as a power-law, with a power $\simeq 2.59$ (see Fig. 5). Interestingly, for the $SU(2)$ invariant model with $J_1 = 1$ and $J_2 = 0.241167$, again linearity is observed, but with a prefactor $\alpha \simeq 1.001689$ not related to the spin velocity, $v$, which we have determined to be $v \approx 1.16992$. Hence, Eq. (13) does not hold in this case. In Fig. 4 we also show the sum $E_A(L/2, L) + \alpha S_A(L/2, L)$, for this model, which decays rapidly with a power $\simeq 2.56$.

Conclusion — We emphasize that this alternating term in $S(x, L)$ is universal and should not be regarded as a correction due to irrelevant operators. First of all, it is not a “correction”, since it is alternating. Secondly, it decays with the same power law as $E_A(x, L)$ which is seen to be a property of the fixed point, not the irrelevant operators. (However, for the Heisenberg model, $\Delta = 1$, the log factor in $E_A(x, L)$ is due to the marginally irrelevant operator.) The presence of a universal alternating term in $S(x, L)$ is connected with the antiferromagnetic nature of the Hamiltonian (not appearing, for example, in the quantum Ising chain [14]) and does not seem to follow from the general CFT treatment in [2]. An analytic derivation of this phenomena remains an open problem.

Acknowledgements — We are grateful to J. Cardy for interesting discussions. N.L. acknowledges I. Peschel for correspondence. I.A. also wishes to thank S. Eggert for discussions about $E_A$. This research was supported by NSERC (all authors), the CIAR (I.A.) CFI (E.S.) and SHARCNET (E.S.). Numerical simulations have been performed on the WestGrid network and the SHARCNET facility at McMaster University.

### References

[1] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. 90, 227902 (2003).
[2] P. Calabrese and J. Cardy, J. Stat. Mech. 06 (2004) 002.
[3] A. Osterloh, L. Amico, G. Falci, and R. Fazio, Nature (London) 412, 608 (2002).
[4] T. J. Osborne and M. A. Nielsen, Phys. Rev. A 66, 32110 (2002).
[5] G. Refael and J. E. Moore, Phys. Rev. Lett. 93, 260602 (2004); N. Laflorencie, Phys. Rev. B, 72, 140408(R) (2005).
[6] C. H. Bennett, H. J. Bernstein, S. Popescu, and B. Schumacher Phys. Rev. A 53, 2046 (1996).
[7] C. Holzhey, F. Larsen and F. Wilczek, Nucl. Phys. B, 424, 443 (1994).
[8] However, the constant contribution has been exactly evaluated analytically for a critical XX chain: see [13].
[9] I. Affleck and A.W.W. Ludwig, Phys. Rev. Lett. 67, 161 (1991).
[10] H.-Q. Zhou, T. Barthel, J. Fjaerestad and U. Schollwöck, cond-mat/0511732.
[11] S.W. Tsai and J. B. Marston, Phys. Rev. B 62, 5546, (2000).
[12] J. Cardy, J. Phys. A Math. Gen. 19, L1093 (1986).
[13] I. Affleck, D. Gepner, H.J. Schulz, and T. Ziman, J. Phys. A Math. Gen. 22, 511 (1989); S. Eggert, Phys. Rev. B54, R9612 (1996).
[14] C. K. Majumdar and D. K. Ghosh, J. Math. Phys. 10, 1399 (1969).
[15] D. S. Fisher, Phys. Rev. B 50, 3799 (1994).
[16] M.-C. Chung and I. Peschel, Phys. Rev. B 64, 064412 (2001).
[17] B.-Q. Jin and V. E. Korepin, J. Stat. Phys. 116, 79 (2004).
[18] I. Affleck and S. Qin, J. Phys. A32, 7815 (1999).
[19] V. Barzykin and I. Affleck, J. Phys. A Math. Gen. 32, 867 (1999).
[20] This velocity has been estimated from DMRG data using the finite size scaling of the ground state energy $E_0(L) = e_0L + e_1 - \frac{\pi}{2\mu} + O(L^{-2})$ on open chains up to $L = 500$. 

![Fig. 5: Comparison between the alternating part of EE $S_A$ and $E_A$ [Eq. (6)] from DMRG with $m = 512$ states, for Heisenberg models. Power-law decay of $S_A(L/2, L) + \alpha E_A(L/2, L)$ drawn in a log-log plot, with $\alpha = 1$ for the nearest neighbor chain ($J_2 = 0$) and $\alpha = 1.00169$ at the critical second neighbor coupling $J_2 = 0.241167$. Lines are power-law fits: $\sim L^{-2.56}$ for $J_2 = 0.241167$ and $L^{-2.59}$ for $J_2 = 0.$](image-url)