Entanglement in quantum critical phenomena

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Quantum phase transitions occur at zero temperature and involve the appearance of long-range correlations. These correlations are not due to thermal fluctuations but to the intricate structure of a strongly entangled ground state of the system. We present a microscopic computation of the scaling properties of the ground-state entanglement in several 1D spin chain models both near and at the quantum critical regimes. We quantify entanglement by using the entropy of the ground state when the system is traced down to L spins. This entropy is seen to scale logarithmically with L, with a coefficient that corresponds to the central charge associated to the conformal theory that describes the universal properties of the quantum phase transition. Thus we show that entanglement, a key concept of quantum information science, obeys universal scaling laws as dictated by the representations of the conformal group and its classification motivated by string theory. This connection unveils a monotonicity law for ground-state entanglement along the renormalization group flow. We also identify a majorization rule possibly associated to conformal invariance and apply the present results to interpret the breakdown of density matrix renormalization group techniques near a critical point.

The study of entanglement in composite systems is one of the major goals of quantum information science [1, 2], where entangled states are regarded as a valuable resource for processing information in novel ways. For instance, the entanglement between systems A and B in a joint pure state $|\Psi_{AB}\rangle$ can be used, together with a classical channel, to *teleport* or send quantum information [3]. From this resource-oriented perspective, the *entropy of entanglement* $E(\Psi_{AB})$ measures the entanglement contained in $|\Psi_{AB}\rangle$ [4]. It is defined as the von Neumann entropy of the reduced density matrix ρ_A (equivalently ρ_B),

$$E(\Psi_{AB}) = -\mathrm{tr}\left(\rho_A \log_2 \rho_A\right), \qquad (1)$$

and directly determines, among other aspects, how much quantum information can be teleported by using $|\Psi_{AB}\rangle$.

On the other hand, entanglement is appointed to play a central role in the study of strongly correlated quantum systems [5, 6, 7], since a highly entangled ground state is at the heart of a large variety of collective quantum phenomena. Milestone examples are the entangled ground states used to explain superconductivity and the fractional quantum Hall effect, namely the BCS ansatz [8] and the Laughlin ansatz [9]. Ground-state entanglement is, most promisingly, also a key factor to understand quantum phase transitions [10, 11], where it is directly responsible for the appearance of long-range correlations. Consequently, a gain of insight into phenomena including, among others, Mott insulator-superfluid transitions, quantum magnet-paramagnet transitions and phase transitions in a Fermi liquid is expected by studying the structure of entanglement in the corresponding underlying ground states.

In the following we analyze the ground-state entanglement near and at a quantum critical point in a series of 1D spin-1/2 chain models. In particular, we consider the hamiltonians

$$H_{XY} = -\sum_{l=0}^{N-1} \left(\frac{a}{2}[(1+\gamma)\sigma_l^x \sigma_{l+1}^x + (1-\gamma)\sigma_l^y \sigma_{l+1}^y] + \sigma_l^z \right) \qquad (2)$$

and

$$H_{XXZ} = -\sum_{l=0}^{N-1} \left(\sigma_l^x \sigma_{l+1}^x + \sigma_l^y \sigma_{l+1}^y + \Delta \sigma_l^z \sigma_{l+1}^z + \lambda \sigma_l^z \right), \qquad (3)$$

which contain both first-neighbor interactions and an external magnetic field, and are used to describe a range of 1D quantum systems [10]. Notice that $H_{XY}(\gamma = 1)$ corresponds to the Ising chain, whereas $H_{XXZ}(\Delta = 1)$ describes spins with isotropic Heisenberg interaction. Both Hamiltonians coincide for $\gamma = \Delta = 0$, where they become the XX model.

Osterloh *et al* [12] and Osborne and Nielsen [11] have recently considered the entanglement in the XY spin model, Eq. (2), in the neighborhood of a quantum phase transition. Their analysis, focused on *single-spin* entropies [11] and on *two-spin* quantum correlations [11, 12], suggestively shows that these one- and two-spin entanglement measures are picked either near or at the critical point. Here, alternatively, we undertake the study of the *entanglement between a block of L contiguous spins and the rest of the chain*, when the spin chain is in its ground state $|\Psi_g\rangle$. Thus, the aim in the following is to compute the entropy of entanglement, Eq. (1), for the state $|\Psi_g\rangle$ according to bipartite partitions

parameterized by L,

$$S_L \equiv -\text{tr}\left(\rho_L \log_2 \rho_L\right), \qquad (4)$$

where $\rho_L \equiv \text{tr}_{\bar{\mathcal{B}}_L}|\Psi_g\rangle\langle\Psi_g|$ is the reduced density matrix for $\mathcal{B}_L$, a block of L spins.

The XY model, Eq. (2), is an *exactly solvable* model, in that H_{XY} can be diagonalized by first using a Jordan-Wigner transformation into fermionic modes and by subsequently concatenating a Fourier transformation and a Bogoliubov transformation (see for instance [10]). The calculation of S_L, as sketched below, also uses the fact that the ground state $|\Psi_g\rangle$ of H_{XY} and the corresponding density matrices ρ_L are all *gaussian* states that can be completely characterized by means of certain correlation matrix of second moments.

More specifically, let us introduce two Majorana operators, c_{2l} and c_{2l+1}, on each site $l = 0, \cdots, N-1$ of the spin chain,

$$c_{2l} \equiv \left(\prod_{m=0}^{l-1}\sigma_m^z\right)\sigma_l^x; \quad c_{2l+1} \equiv \left(\prod_{m=0}^{l-1}\sigma_m^z\right)\sigma_l^y. \qquad (5)$$

Operators c_m are hermitian and obey the anti-commutation relations $\{c_m, c_n\} = 2\delta_{mn}$. Hamiltonian H_{XY} can be rewritten as

$$H_{XY} = i\sum_{l=0}^{N-1}\left(\frac{a}{2}\left[\,(1+\gamma)\,c_{2l+1}c_{2l+2}-\right.\right.$$

$$\left.\left.(1-\gamma)\,c_{2l}c_{2l+3}\,\right] + c_{2l}c_{2l+1}\,\right),$$

and can be subsequently diagonalized by canonically transforming the operators c_m. The expectation value of c_m when the system is in the ground state, i.e. $\langle c_m\rangle \equiv \langle\Psi_g|c_m|\Psi_g\rangle$, vanishes for all m due to the $\mathcal{Z}_2$ symmetry $(\sigma_l^x, \sigma_l^y, \sigma_l^z) \to (-\sigma_l^x, -\sigma_l^y, \sigma_l^z)$ $\forall l$ of H_{XY}. In turn, the expectation values

$$\langle c_m c_n\rangle = \delta_{mn} + iB_{mn}, \qquad (6)$$

completely characterize $|\Psi_g\rangle$, for any other expectation value can be expressed, by using Wick's theorem, in terms of $\langle c_m c_n\rangle$. Matrix B reads [13]

$$B = \begin{bmatrix} \Pi_0 & \Pi_1 & \cdots & \Pi_{N-1} \\ \Pi_{-1} & \Pi_0 & & \vdots \\ \vdots & & \ddots & \vdots \\ \Pi_{1-N} & \cdots & \cdots & \Pi_0 \end{bmatrix}, \quad \Pi_l = \begin{bmatrix} 0 & g_l \\ -g_{-l} & 0 \end{bmatrix}, \qquad (7)$$

with real coefficients g_l given, when $N \to \infty$, by

$$g_l = \frac{1}{2\pi}\int_0^{2\pi}d\phi e^{-il\phi}\frac{a\cos\phi - 1 - ia\gamma\sin\phi}{|a\cos\phi - 1 - ia\gamma\sin\phi|}. \qquad (8)$$

From Eqs. (7)-(8) we can extract the entropy S_L of Eq. (4) as follows. First we compute the correlation matrix of the state ρ_L for block $\mathcal{B}_L$, namely $\delta_{mn} + i(B_L)_{mn}$, where

$$B_L = \begin{bmatrix} \Pi_0 & \Pi_1 & \cdots & \Pi_{L-1} \\ \Pi_{-1} & \Pi_0 & & \vdots \\ \vdots & & \ddots & \vdots \\ \Pi_{1-L} & \cdots & \cdots & \Pi_0 \end{bmatrix} \qquad (9)$$

is constructed by eliminating $2(N-L)$ contiguous columns and rows from B, those corresponding to the $N-L$ traced-out spins. Let $V \in SO(2L)$ denote an orthogonal matrix that brings B_L into a block-diagonal form, that is

$$\tilde{B}_L = VB_LV^T = \oplus_{m=0}^{L-1}\nu_m\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad \nu_m \geq 0. \qquad (10)$$

Then the set of $2L$ Majorana operators $d_m \equiv \sum_{n=0}^{2L-1}V_{mn}c_n$, obeying $\{d_m, d_n\} = 2\delta_{mn}$, have a block-diagonal correlation matrix $\langle d_m d_n\rangle = \delta_{mn} + i(\tilde{B}_L)_{mn}$. Therefore, the L fermionic operators $b_l \equiv (d_{2l}+id_{2l+1})/2$, obeying $\{b_m, b_n\} = 0$ and $\{b_m^\dagger b_n\} = \delta_{mn}$, have expectation values

$$\langle b_m\rangle = 0, \quad \langle b_m b_n\rangle = 0, \quad \langle b_m^\dagger b_n\rangle = \delta_{mn}\frac{1+\nu_m}{2}. \qquad (11)$$

Eq. (11) indicates that the above fermionic modes are in a *product* or *uncorrelated* state, that is

$$\rho_L = \varrho_0 \otimes \cdots \otimes \varrho_{L-1}, \qquad (12)$$

where ϱ_m denotes the mixed state of mode m. The entropy of ρ_L is a sum over the entropy $H_2((1+\nu_m)/2)$ of each mode $[H_2(x) = -x\log_2 x - (1-x)\log_2(1-x)$ is the binary entropy] and thus reads

$$S_L = \sum_{m=0}^{L-1}H_2(\frac{1+\nu_m}{2}). \qquad (13)$$

For arbitrary values of (a, γ) in H_{XY} and in the thermodynamic limit, $N \to \infty$, one can evaluate Eq. (8) numerically, diagonalize B_L in Eq. (9) to obtain ν_m and then evaluate Eq. (13). The computational effort grows only polynomially with L and produces reliable values of S_L for blocks with up to several tens of spins. However, further analytical characterization is possible in some cases, which speeds the computation significantly. For instance, for the XX model with magnetic field, $\gamma = 0$ and $1/a \in [-1, 1]$, one obtains $g_0 = \phi_a/\pi - 2$ and $g_l = 2\sin(l\phi_a)/l\pi$ for $l \neq 0$, where $\phi_a = \arccos(1/a)$, from which S_L can be numerically determined. We obtain, up to $L = 100$ spins,

$$S_L^{XX} \approx \frac{1}{3}\log_2(L) + k_1(a), \qquad (14)$$

where $k_1(a)$ depends only on a. For the Ising model with critical magnetic field, $\gamma = 1, a = 1$, one finds $g_l = -2/l$

for odd l and $g_l = 0$ for even l and, for up to $L = 100$ spins,

$$S_L^{Ising} \approx \frac{1}{6}\log_2(L) + k_2, \qquad k_2 \approx \pi/3. \qquad (15)$$

Finally, for the Ising model with magnetic field, $\gamma = 1$, and for a close to 1, Kitaev has obtained an analytical expression for the entropy of half of an infinite chain [15]. To use this result in our setting we need to double its value because the entropy resides near the boundary. Thus we get

$$S_{N/2}^{Ising} \approx \frac{1}{6}\log_2\frac{1}{|1-a|}. \qquad (16)$$

The XXZ model, Eq. (3), cannot be analyzed using the previous method. Instead we have used the Bethe ansatz [16] to exactly determine, through a numerical procedure, the ground state $|\Psi_g^{(20)}\rangle$ of H_{XXZ} for a chain of up to $N = 20$ spins, from which $S_L^{(20)}$ can be computed. Recall that in the XXZ model the non-analyticity of the ground-state energy characterizing a phase transition occurs already for a finite number N of spins in the chain, since it is due to level-crossing. It turns out that, correspondingly, already for $N = 20$ spins one can observe a distinct, characteristic behavior of $S_L^{(20)}$ depending on whether the values (Δ, λ) in Eq. (3) belong to a critical regime.

The results of the computation of S_L for the spin chains (2) and (3) can be summarized as follows.

Non-critical regime. For those values (a, γ) or (Δ, λ) for which the models are non-critical, the entropy of entanglement S_L either vanishes for all L [*e.g.* when a sufficiently strong magnetic field aligns all spins into a product, unentangled state] or grows monotonically as a function of L until it reaches a *saturation* value S_{max}. For instance, in the infinite Ising chain the saturation entropy S_{max} is given by Eq. (16). As shown in Fig. (1), S_L often approaches S_{max} already for a small number L of spins.

Critical regime. Instead, critical ground-states are characterized by an entropy S_L that diverges logarithmically with L,

$$S_L \approx \frac{c + \bar{c}}{6}\log_2(L) + k, \qquad (17)$$

with a coefficient given by the holomorphic and antiholomorphic *central charges* c and $\bar{c}$ of the conformal field theory that describes the universal properties of the phase transition [17], see Fig. (2). This expression was derived by Holzhey, Larsen and Wilczek [18] for the *geometric entropy* (analogous of Eq. (4) for a conformal field theory), and our calculation confirms it for several critical spin chains. Thus, the critical Ising model corresponds to a free fermionic field theory, with central charges $c_f = \bar{c}_f = 1/2$, whereas the rest of critical
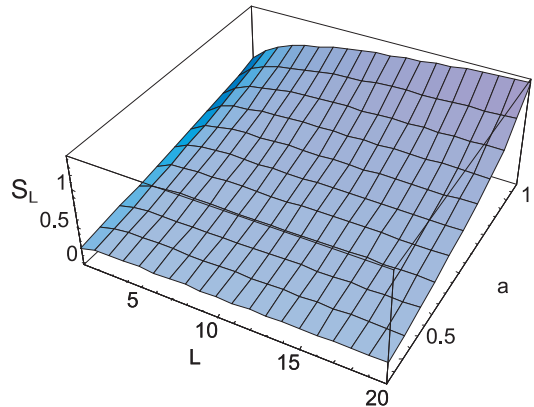

Figure 1: Non-critical S_L for the Ising model, $H_{XY}(\gamma = 1)$ in Eq. (2), as a function of the size L of the spin block (left axis) and parameter a (right axis). The finite correlation length governing non-critical phenomena translates into a finite *entanglement length*, that is, a finite value of L for which adding new spins to a block does not increase its entanglement with the rest of the chain. Such an *entanglement length* (which scales as the correlation length) diverges only at the critical point $a = 1$. Scaling arguments also imply that the entropy surface is given by $\log[Lf(L|1-a|)]$. For any given a, the saturation value for the entropy is given by Eq. (16).

regimes in (2) and (3) are described by a free bosonic field theory, $c_b = \bar{c}_b = 1$ (cf. Eqs. (14) and (15)). In particular, the marginal deformation $0 < \gamma \leq 1$ for $a = 1$ shows scaling for every γ with universal coefficient $c = \bar{c} = 1/2$. It is possible to compare the subleading correction between two different values of γ. The behavior we obtain is described by

$$\lim_{L\to\infty}[S_L(\gamma = 1) - S_L(\gamma)] = -\frac{c + \bar{c}}{6}\log_2\gamma . \qquad (18)$$

The singular behavior at $\gamma = 0$ is the signature of the fact that that point belongs to the abrupt change of universality class for the XX model.

The above characterizations motivate a number of observations, that we move to discuss.

Critical and non-critical ground states contain structurally different forms of quantum correlations. Non-critical ground-state entanglement corresponds to a weak, *semi-local* form of entanglement driven by the appearance of a length scale, *e.g.* a mass gap. Indeed, for any L, the reduced density matrix ρ_L is supported on a small, bounded subspace of the Hilbert space of the L spins, and can be obtained by diagonalizing the hamiltonian corresponding to the block $\mathcal{B}_L$ and only a few extra *neighboring* spins, as skillfully exploited in White's density matrix renormalization group (DMRG) techniques [19]. We note here that a bounded rank for ρ_L (relatedly, a saturation value for S_L) is instrumental for the success of DMRG schemes, where only of a finite number
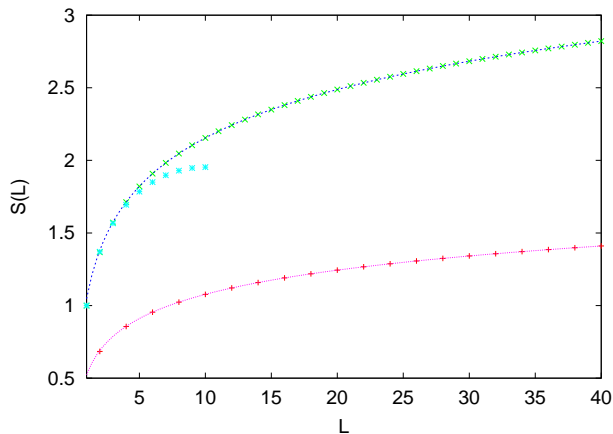
Figure 2: Numerical calculation of critical entanglement S_L for 1D spin chains. Points $(+)$ come from an infinite Ising chain with critical magnetic field, $H_{XY}(a = 1, \gamma = 1)$ in Eq. (2), and corresponds to $S_L^{Ising} \approx \log_2(L)/6 + k_2$. Curve $(\times)$ comes from an infinite XX spin chain without magnetic field, $H_{XY}(a = \infty, \gamma = 0)$ in Eq. (2), and corresponds to $S_L^{XX} \approx \log_2(L)/3 + k_1$. Thus the growth in L of entanglement in the XX model, asymptotically described by a free boson, is twice that in the Ising model, corresponding to a free fermion, $S_{L+1}^{XX} - S_L^{XX} \approx 2(S_{L+1}^{Ising} - S_L^{Ising})$. Finally, curve $(*)$ comes from a XXX chain of 20 spins without magnetic field, $H_{XXZ}(\Delta = 1, \lambda = 0)$ in Eq. (3). These finite-chain results, obtained using the Bethe ansatz, combine the logarithmic behavior $(L = 1, \cdots, 5)$ of a free boson field theory with a finite-size saturation effect $(L = 6, \cdots, 10)$. We have added the lines $\frac{c+\bar{c}}{6}[\log_2(L) + \pi]$ both for bosons and fermions to highlight their remarkable agreement with the numerical diagonalization.

of eigenvectors of ρ_L can be kept. Critical bound-state entanglement corresponds, on the contrary, to a stronger form of entanglement, one that embraces the system at all length scales simultaneously. DMRG techniques have reportedly failed to reproduce quantum critical behavior [20] and we may, in view of Eq. (17), be in a position to understand why. Indeed, the divergent character of S_L is just one particular manifestation of the fact that the number of relevant eigenvectors of ρ_L unboundedly grows with L. If, as is the case in DMRG schemes, only a finite number of levels can be considered, then a sufficiently large L will always make the computation of ρ_L impossible (arguably, even in an approximate sense) by using such schemes. This strongly suggests that overcoming the above difficulties necessarily requires techniques that do not attempt to reproduce the critical behavior of the ground state through a local, real space construction.

Another remarkable, far-reaching fact is that, as mentioned below Eq. (17), our results coincides with entropy computations performed in conformal field theory. There, a *geometric* or *fine-grained* entropy analogous to Eq. (4) but for a continuous field theory has been considered by several authors, including Srednicki

[21], Callan and Wilczek [22], Holzhey et al [18] and Fiola et al [23]. Thus, starting from non-relativistic spin chain models, and by performing a microscopic analysis of a relevant quantity in quantum information, we have obtained a universal scaling law for entanglement that is in full agreement with previous findings in the context of, say, black-hole thermodynamics in 1+1 dimensions [18, 23].

The above connection has a number of implications to be exploited. For instance, Srednicki [21] has obtained the behavior of entropy in 2+1 and 3+1 dimensional conformal field theories. For a region $\mathcal{R}$ in 2 or 3 spatial dimensions, the entropy of $\mathcal{R}$ is proportional to the size $\sigma(\mathcal{R})$ of its boundary,

$$S_{\mathcal{R}} \approx \kappa \sigma(\mathcal{R}). \qquad (19)$$

That is, the entropy per unit of boundary area, κ, is independent of the size of $\mathcal{R}$. [This is in sharp contrast with the same quantity in 1D, where the boundary consists of two points and $S_{\mathcal{R}}/\sigma(\mathcal{R})$ diverges logarithmically with the length L of $\mathcal{R}$]. Accordingly, Eq. (19) also describes the critical ground-state entanglement of 2D and 3D spin lattices.

Also the fact that the entropy of entanglement for 1D critical spin chains, Eq. (17), matches well-known conformal field theory parameters carries an extra bonus. The coefficient in control of the divergent behavior of S_L at critical points is the central charge, which is subject to Zamolodchikov's c-theorem [24]. The c-theorem states that the central charges associated to the ultraviolet and infrared end points of renormalization group flows, labeled by C_{UV} and C_{IR}, obey the inequality $C_{UV} > C_{IR}$ for unitary theories. This powerful result establishes an irreversible arrow as renormalization group transformations are performed. The translation of this idea to the quantum information setting is that entanglement decreases along renormalization group flows. An infrared theory carries less global entanglement than the ultraviolet theory where it flowed from. The c-theorem seems natural as renormalization group transformations integrate out short distance degrees of freedom, accompanied with their quantum correlations. Yet, it is not at all trivial due to, first, the infinite degrees of freedom (needing regularization) existing in a quantum field theory and, second, the rescaling step in the renormalization group transformation. It is noteworthy, then, that entanglement decreases both (*i*) under the *local operations and classical communication* and (*ii*) along *renormalization group trajectories*. The former case corresponds to *local manipulation* of an entangled system while the second is made out of a block-spin transformation followed by a *rescaling* of the system. Both actions do reduce quantum correlations and become irreversible [24, 25].

One more remark. From Eqs. (8)-(9) the complete spectrum of ρ_L can be extracted. The 2^L eigenvalues are

given by

$$\lambda_{x_1 x_2 \cdots x_L} = \prod_{m=0}^{L-1} \frac{1 + (-1)^{x_m} \nu_m}{2}, \quad x_m = 0, 1 \ \forall m. \quad (20)$$

This allows us to look in more detail to the reshuffling of the ground state as more sites are incorporated in the block $\mathcal{B}_L$. Every time a new spin is added, the amount of local surprise due to quantum correlations with the rest of the chain increases, and so does the entropy. But critical quantum correlations entangle every single subset of the system, and the way they are reordered is far more subtle than the relation hinted by entropy arguments. We have numerically verified that also a majorization relation [26] holds for the ground-state reduced density matrices of the infinite XY spin chain, namely

$$\vec{\lambda}_{L+2} \prec \vec{\lambda}_L \quad \forall L, \quad (21)$$

where the jump in steps of two is forced by the subtleties of the microscopic model. Thus, a critical ground state orderly redistributes weights, so as to accommodate for the new correlations, according to a detailed, exponentially large set of inequalities as contained in Eq. (21). In this sense, majorization may be a signature –admittedly a very refined one– of conformal invariance.

But the majorization counterpart in the continuum conformal field theory is not yet known. Perhaps, then, the correspondence between concepts of quantum information science and conformal field theory, between critical ground-state entanglement and geometrical entropy, can also be exploited in the reverse direction.

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