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Entanglement and boundary critical phenomena

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We investigate boundary critical phenomena from a quantum-information perspective. Bipartite entanglement in the ground state of one-dimensional quantum systems is quantified using the Rényi entropy S_α, which includes the von Neumann entropy ($\alpha \to 1$) and the single-copy entanglement ($\alpha \to \infty$) as special cases. We identify the contribution of the boundaries to the Rényi entropy, and show that there is an entanglement loss along boundary renormalization group (RG) flows. This property, which is intimately related to the Affleck-Ludwig g theorem, is a consequence of majorization relations between the spectra of the reduced density matrix along the boundary RG flows. We also point out that the bulk contribution to the single-copy entanglement is half of that to the von Neumann entropy, whereas the boundary contribution is the same.

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Recently much work has been done to understand entanglement in quantum many-body systems. In particular, the behavior of various entanglement measures at or near a quantum phase transition [1] has received a lot of attention [2–9]. These entanglement measures include the von Neumann entropy and the single-copy entanglement, among others. The former is the most studied measure and quantifies entanglement in a bipartite system in the so-called asymptotic regime [10], whereas the latter was recently suggested to quantify the entanglement present in a single copy [9]. For a system in a pure state $|\psi\rangle$ (e.g., the ground state) that is partitioned into two subsystems A and B, the von Neumann entropy is $S_1 \equiv -\mathrm{Tr}_A \rho_A \log_2 \rho_A$ where $\rho_A = \mathrm{Tr}_B |\psi\rangle\langle\psi|$ is the reduced density matrix for A, and the single-copy entanglement is $S_\infty \equiv -\log_2 \lambda_1$, where λ_1 is the largest eigenvalue of ρ_A.

Studies of the von Neumann entropy for quantum spin chains [3–8] have revealed that its dependence on the size ℓ of the block A is very different for noncritical and critical systems. For the former, the von Neumann entropy increases logarithmically with ℓ until it saturates when ℓ becomes of order the correlation length ξ. For the latter, it diverges logarithmically with ℓ, because $\xi = \infty$, and the corresponding $(1+1)$-dimensional field theory becomes invariant under conformal transformations. Conformal field theory (CFT) predicts that the prefactor of the logarithmic term in the entropy scaling is universal and proportional to the so-called central charge c of the theory [6,11]. Furthermore, it has been shown numerically [12] that the entanglement loss along the (bulk) renormalization group (RG) flows, which is consistent with the CFT predictions for the von Neumann entropy [6,11] and with Zamolodchikov's c theorem [13], can be given a more "fine-grained" characterization in terms of the majorization [14] of the reduced density matrix spectra along the RG flow. A theoretical analysis of majorization in these systems also appeared recently [15].

Boundary critical phenomena [16] in one-dimensional (1D) quantum systems (equivalently, 2D classical systems) have attracted a lot of interest, especially in the context of boundary CFT. A closely related subject is the theory of boundary perturbations of certain conformally invariant theories, so-called integrable boundary quantum field theory [17], which is relevant to quantum spin chains with nontrivial boundary interactions, impurities in Luttinger liquids, Kondo physics, tunneling in fractional quantum Hall devices, and open string theory. In these problems, the Affleck-Ludwig g theorem [18], stating that the ground state degeneracy g is nonincreasing along boundary RG flows, is analogous to the c theorem for bulk critical phenomena.

In this Rapid Communication we investigate boundary critical phenomena in quantum spin chains from a quantum-information perspective. Our findings provide insights into the information-theoretic explanation of the boundary entropy and the g theorem characterizing the intrinsic irreversibility due to information loss along boundary RG flows [19]. We choose the Rényi entropy (also known as the α entropy) $S_\alpha = (1-\alpha)^{-1} \log_2 \mathrm{Tr}_A \rho_A^\alpha$ as our entanglement measure, partly motivated by the fact that both the von Neumann entropy and the single-copy entanglement are special cases of the Rényi entropy, corresponding to $\alpha \to 1$ and $\alpha \to \infty$, respectively. Using CFT we derive expressions for the Rényi entropy which include a boundary contribution, and show that a majorization relation underlies an entanglement loss along boundary RG flows (i.e., when a system with a boundary interaction flows from an unstable to a stable fixed point). We support our analytical arguments with numerical density-matrix renormalization group (DMRG) calculations [20,21].

Consider a 1D lattice of interacting spins with lattice spacing a. Let L be the total length of the system, and let the two subsystems A and B be blocks of consecutive spins of length ℓ and $L-\ell$, respectively. Then CFT predicts that for an infinite spin chain at criticality

$$S_\alpha = \frac{c}{6}(1+\alpha^{-1}) \log_2 \frac{\ell}{a} + c'_\alpha \qquad (1)$$

where c is the central charge and c'_α is a nonuniversal constant [6]. For a semi-infinite spin chain with the block A

starting at the origin where a boundary interaction is applied, we have instead

$$S_\alpha = \frac{c}{12}(1+\alpha^{-1})\log_2\frac{2\ell}{a} + \frac{1}{2}c'_\alpha + S_b. \qquad (2)$$

Here $S_b = \log_2 g$ is the boundary entropy [18], with $g = \langle B|0\rangle$, where $|B\rangle$ is the so-called boundary state [22–24] and $|0\rangle$ is the ground state. We emphasize that, compared with the corresponding expression for S_1 in Ref. [6], there is an extra factor 1/2 in front of c'_α and S_b in Eq. (2).

The corresponding Rényi entropies for finite L are found from Eqs. (1) and (2) by standard conformal mappings [23]. As a result, the Rényi entropy for periodic boundary conditions (PBCs) [open boundary conditions (OBCs)] is given by replacing $\ell/a \to (L/\pi a)\sin \pi\ell/L$ in Eq. (1) [Eq. (2)]. For the OBC case we have assumed that the BCs on the left and right ends are identical; otherwise one would have to consider the complicating effects of so-called boundary-condition-changing operators.

From these results one sees that the contribution of the bulk universal part to the single-copy entanglement S_∞ is always half of that to the von Neumann entropy S_1, thus extending the conclusion in Ref. [9] for the XX chain ($c=1$) to all conformally invariant critical systems. However, we stress that the contribution of the boundary entropy to S_α does not depend on α.

The details of the CFT derivation of the above results (which makes use of CFT expressions for $\mathrm{Tr}_A\rho_A^\alpha$ from Ref. [6]) will be given elsewhere. Here we will instead present a heuristic argument to justify Eqs. (1) and (2). The central charge c measures the (effective) number of gapless excitations. It also describes the way a specific system reacts to the introduction of a macroscopic length scale into the system [23]. Therefore, when the entire (infinite) system is partitioned into a block of length ℓ and its environment, one may expect that the Rényi entropy S_α depends only on c and ℓ/a with some short distance cutoff a, e.g., the lattice spacing for quantum spin chains. Because both the Rényi entropy and the central charge are additive, one can see [25] that the Rényi entropy must be linear as a function of the central charge, i.e., $S_\alpha = c f_\alpha(\ell/a) + h_\alpha$, with f_α a universal function and h_α a nonuniversal (i.e., model-dependent) function. The specific form of the function f_α may be determined by calculating the Rényi entropy for any exactly solvable model, for instance the massless Dirac fermion field as done in Ref. [8] for PBCs, thus confirming Eq. (1). The calculation may be extended to the massless Dirac fermion with a conformally invariant boundary condition, leading to the conclusion that h_α consists of the nonuniversal bulk part $(1/2)c'_\alpha$ and the universal boundary part S_b. The bulk universal part of Eq. (2) and its counterpart for finite L result from the substitution $c \to c/2$, $\ell \to 2\ell$ and $L \to 2L$ in Eq. (1) and its corresponding counterpart, due to the fact that one may "unfold" the system of a finite size L by identifying left movers at position x ($x = ja$, with j labeling lattice sites) with right movers at $-x$ so that the resulting system consists of only right movers subject to PBCs and with the system size scales ℓ and L doubled and the number of gapless degrees of freedom halved. The factor 1/2 in front of c'_α in the second bulk term in Eq. (2) also originates from this halving of the number of gapless degrees of freedom.

We now address the implications of these CFT predictions for models of semi-infinite quantum spin chains. We first consider the $S=1/2$ transverse Ising chain in a boundary magnetic field, described by

$$H_{\text{Ising}} = -\sum_{j=0}^{\infty}(S_j^x S_{j+1}^x + hS_j^z) + h_b S_0^x. \qquad (3)$$

Here h is the transverse bulk magnetic field, and h_b is the boundary magnetic field. We set $h=1/2$ so that the model is bulk critical with central charge $c=1/2$. The second model is the $S=1/2$ XXZ chain, for which

$$H_{XXZ} = \sum_{j=0}^{\infty}(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z) + h_b S_0^x. \qquad (4)$$

Here Δ denotes the anisotropy and h_b is the (transverse) boundary magnetic field. The model is bulk critical with central charge $c=1$ for $-1 < \Delta \leqslant 1$.

For both models, the points $h_b=0$ and $h_b=\pm\infty$, corresponding to the free and fixed conformally invariant BCs, are boundary critical fixed points; the former is unstable and the latter is stable. A boundary magnetic field $h_b > 0$ is generally a relevant perturbation of the free BC $h_b=0$, and generates a boundary RG flow of h_b towards the fixed point $h_b=\infty$. For $0 < h_b < \infty$, the conformal invariance is lost, and the competition between boundary ordering and bulk criticality introduces a crossover length $\zeta \propto h_b^{d-1}$ [26], where $d<1$ is the scaling dimension of the relevant boundary perturbation, characterizing its behavior under scale transformations. For the Ising model, $d=1/2$, and for the XXZ model, $d=2\pi R^2$, where $R=\sqrt{(1/2\pi)-(1/2\pi^2)\arccos\Delta}$ is the compactification radius. Furthermore, for both models, g for fixed BC is less than g for free BC, which implies that the Rényi entropy is less for fixed than for free BC. This is also consistent with the g theorem [18], which states that g decreases along boundary RG flows. For the transverse Ising model, $g=1$ (free) and $g=1/\sqrt{2}$ (fixed) [22]; for the XXZ model, $g=\pi^{-1/4}(2R)^{-1/2}$ (free) and $g=\pi^{1/4}R^{1/2}$ (fixed) [26]. We emphasize that, even away from boundary critical points, Eq. (2) is still valid for $\ell > \zeta$, due to bulk criticality.

H_{XXZ} reduces to the isotropic XXX model for $\Delta=1$ ($R=1/\sqrt{2\pi}$). This case is special, because the boundary perturbation is marginal ($d=1$). In fact, $g=2^{-1/4}$ for both free and fixed BC. The line from $h_b=0$ to $h_b=\infty$ is a line of fixed points; there is no RG flow since g is the same everywhere along the line, as follows from the equivalence to a free scalar boson field with a dynamical boundary interaction [27].

To check the CFT predictions, we analyze quasiexact DMRG results. Figure 1 shows the entanglement in the bulk critical transverse Ising model (3) for PBCs and OBCs with different boundary fields h_b. For OBCs, the chain size is $L=800a$ and the number of retained block states is $M=140$. For PBCs we use the DMRG variant described in Ref. [28], i.e. a true PBC matrix product state, with $L=80a$ and matrix

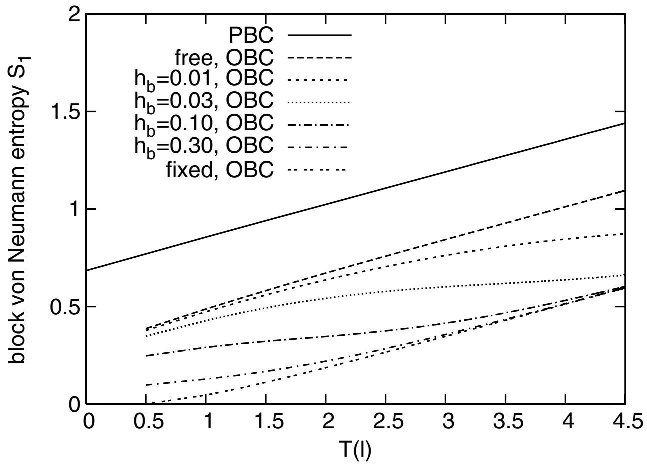

FIG. 1. Bipartite entanglement for the bulk critical transverse Ising model, quantified by the von Neumann entropy S_1 of the reduced density matrix. The block size ℓ is given as $T(\ell)$ (see text) which allows for a direct check of the CFT predictions (1) and (2). The fit yields the predicted boundary entropies.

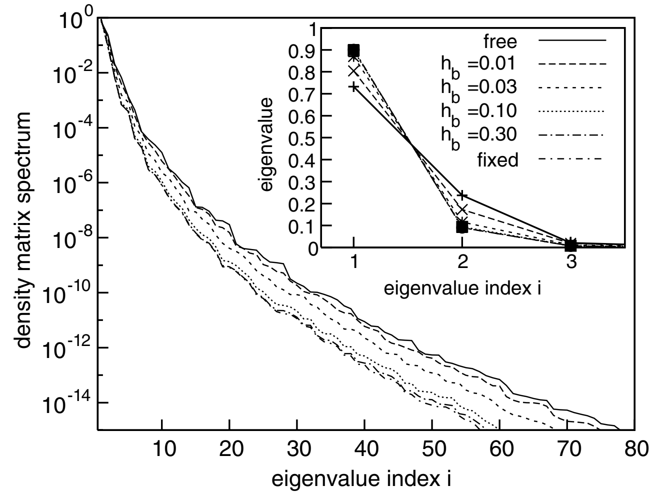

FIG. 2. Eigenvalue distributions for the reduced density matrix of a block of size $\ell=128a$ in the bulk critical transverse Ising model (3) for various values of the boundary magnetic field h_b. The quasiexact DMRG results confirm the majorization relation along the boundary field RG flow (see text). The inset displays the first three eigenvalues and shows that the crossing of the spectra occurs at $i^*=1$.

dimension $D=24$ (corresponding to $\approx D^2$ retained block basis states). The maximum truncated density matrix eigenvalues are in the numeric noise ($<10^{-16}$). The block size ℓ is shown as $T(\ell)$, with $T_{\rm PBC}(\ell)=\log_2(\frac{L}{\pi a}\sin\frac{\pi\ell}{L})$ and $T_{\rm OBC}(\ell)=\frac{1}{2}\log_2(\frac{2L}{\pi a}\sin\frac{\pi\ell}{L})$, appropriate for a linear fit of the finite L counterparts of (1) and (2). The fits for PBCs, free OBCs, and fixed OBCs yield the predicted central charge ($c=0.500,0.502,0.498\approx 1/2$) and boundary entropies ($S_b^{\rm free}=-0.003\approx 0$, $S_b^{\rm fixed}=-0.497\approx\log_2 1/\sqrt{2}$), which can be read off from the differences of the axis intercepts. The curves for nonzero h_b converge for large ℓ to the fixed BC curve (the smaller the value of h_b, the larger the crossover length ζ). This implies that the boundary entropy for any nonzero h_b is the same as that for fixed BCs, consistent with the explicit construction of boundary states in Ref. [17].

Let us now turn to the topic of majorization relations. We first recall the definition of majorization [14]. Consider two probability distributions $\lambda\equiv\{\lambda_i\}$ and $\mu\equiv\{\mu_i\}$ whose elements are ordered such that $\lambda_1\geqslant\lambda_2\geqslant\cdots\geqslant\lambda_r$, and similarly for μ. We say that λ is majorized by μ, written $\lambda\prec\mu$, if $\Sigma_{i=1}^k\lambda_i\leqslant\Sigma_{i=1}^k\mu_i$ for $k=1,\ldots,r-1$ and $\Sigma_{i=1}^r\lambda_i=\Sigma_{i=1}^r\mu_i$ (=1). Here the probability distributions are formed by the eigenvalues of the reduced density matrix ρ_A, and r is the Schmidt rank. An elementary result [14] states that $\lambda\prec\mu$ if and only if $\phi(\lambda)\geqslant\phi(\mu)$ for all Schur-concave functions ϕ [29]. In fact, the Rényi entropy is Schur concave for any index α. Therefore it is necessary (but not sufficient) for the Rényi entropy for all indices α to be monotonic with some system parameter (ℓ or h_b) for the corresponding spectra of the reduced density matrix to be subject to a majorization relation.

The CFT results (1) and (2) show that at (both bulk and boundary) criticality the Rényi entropy increases monotonically with the block size ℓ (for this to hold for a finite chain of length L, ℓ must be less than $L/2$). In particular, the largest eigenvalue $\lambda_1=2^{-S_\infty}$ of ρ_A decreases with increasing ℓ. This indicates that $\rho_{A'}\prec\rho_A$ if the block A is a sub-block of A' [30]. Indeed, the majorization relation follows from the fact that any two eigenvalue distributions, corresponding to two different block sizes, only cross once when the eigenvalues λ_i are plotted versus the eigenvalue index i. That is, an index i^* exists, such that λ_i decreases with increasing ℓ for $i\leqslant i^*$, and λ_i increases with increasing ℓ for $i>i^*$. The uniqueness of this crossing is guaranteed by the fact that the eigenvalue distribution follows $\lambda_i\propto q^{\beta_i}$ for both bulk and boundary conformal theories, apart from degeneracies n_i. Here $q=\exp(2\pi i\tau)$ for conformal theories and $q=\exp(-\pi\delta)$ for boundary conformal theories [31], and β_i are integers related to the scaling dimensions of the descendant operators. The conformal invariance requires that both τ and δ should be proportional to $1/\ln(\ell/a)$. The discreteness of n_i and β_i ensures that they do not change when the block size ℓ is varied (for finite L, ℓ must be restricted to even or odd values if the model has a parity effect).

Next, we consider the behavior of the Rényi entropy along boundary RG flows. By combining our CFT results with the g theorem, it follows that the Rényi entropy decreases (more precisely, does not increase) along a boundary RG flow. In particular, the largest eigenvalue λ_1 of ρ_A increases along the boundary RG flow. Furthermore, one may argue that along the boundary RG flow, the eigenvalues of ρ_A take the same form $\lambda_i\propto q^{\beta_i}$ as at the conformally invariant fixed point at the end of the flow, except that the dependence of q on ℓ is different (again, the discreteness of the degeneracies n_i and β_i ensures that they remain the same along the flow). However, for any nonzero h_b, the bulk criticality requires that the dependence $\delta\sim 1/\ln(\ell/a)$ is recovered for $\ell>\zeta$. It then follows that there is one and only one crossing for the eigenvalue distributions versus i along the boundary RG flow. More precisely, an index i^* exists, such that λ_i increases for $i\leqslant i^*$, and decreases for $i>i^*$ along the flow. This in turn implies the majorization relation.

A rough estimate for the crossing index i^* can be obtained from the CFT predictions for the largest eigenvalue λ_1. This gives $i^* \sim \ell^{c/6}$ for PBCs and $i^* \sim \ell^{c/12}$ for OBCs. Thus the block size ℓ must be sufficiently large to observe that the crossing occurs at $i^* > 1$. For instance, to see that the second largest eigenvalue decreases with increasing ℓ, ℓ should at least be $1800a$ for the semi-infinite *XX* chain, as estimated from the exact solution [32]. DMRG calculations of the reduced density matrix spectra show majorization along boundary RG flows, where eigenvalues down to $\sim 10^{-15}$ are considered. Figure 2 shows the crossing point i^* of the spectra in the bulk critical transverse Ising model with block size $\ell = 128a$ and various values of the boundary field h_b. The crossing of the spectra occurs here at $i^* = 1$.

For the Heisenberg *XXX* model ($\Delta = 1$) the Rényi entropy does not depend on the boundary magnetic field: $\partial S_\alpha / \partial h_b = 0$. These constraints (of which there is an infinite number, one for each α) imply that the spectra of ρ_A do not vary with h_b. Therefore the presence of a line of fixed points here amounts to the statement that all of these critical points share the same eigenvalue distribution, so there is no boundary RG flow.

In conclusion, we have investigated the interrelations between the boundary entropy, the Affleck-Ludwig *g* theorem, and entanglement in quantum spin systems with boundary interactions. The intrinsic irreversibility along boundary RG flows, as embodied in the Affleck-Ludwig *g* theorem, is connected with the majorization relation solely characterized by the ground state itself. The results also bring new insights into our understanding of 2D classical statistical mechanical systems. In fact, the majorization relations for the density submatrix [33,34] spectra of the transfer matrix eigenvectors corresponding to the largest eigenvalue are still preserved in 2D classical systems, even if it does not make sense to speak of quantum entanglement for classical cases.

Recently, work [35] appeared that reached the same conclusion as us regarding the connection between the von Neumann entropy and the single-copy entanglement for bulk conformal theories.

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