Logarithmic divergence of the block entanglement entropy for the ferromagnetic Heisenberg model

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Recent studies have shown that logarithmic divergence of entanglement entropy as a function of the size of a subsystem is a signature of criticality in quantum models. We demonstrate that the ground-state entanglement entropy of n sites for the ferromagnetic Heisenberg spin-$\frac{1}{2}$ chain of the length L in a sector with fixed magnetization y per site grows as $\frac{1}{2}\log_2[n(L-n)/L]C(y)$, where $C(y)=2\pi e\left(\frac{1}{4}-y^2\right)$.

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I. INTRODUCTION

Recently it has been argued, on the example of the exactly solvable antiferromagnetic Heisenberg spin-$\frac{1}{2}$ chain

$$H_{XXZ} = J\sum_{i=1}^{\infty} (\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \Delta\sigma_i^z\sigma_{i+1}^z), \quad (1)$$

that for a critical (gapless) quantum system [for the XXZ model when Δ belongs to the interval $(-1,1)$], the entanglement entropy of a block of n spins diverges logarithmically as $\gamma\log_2 n$, while for noncritical systems (Δ outside the above-mentioned interval), it converges to a constant finite value [1–3]. This property was interpreted in the framework of conformal field theory [4] associated with the corresponding quantum phase transition and the prefactor γ of the logarithm related to the central charge of the theory $c=3\gamma$ (for the XXZ model this gives $\gamma=\frac{1}{3}$).

The aim of this paper is to show that the entanglement entropy of a block of spins in the ground state of the antiferromagnetic XXZ model (1), at the point $\Delta=-1$ grows *faster* than for other critical points $-1<\Delta\leqslant 1$, namely as $\gamma\log_2 n$ with the logarithmic prefactor $\frac{1}{2}\leqslant\gamma\leqslant 1$.

Our approach uses the permutational invariance of the ground state of Eq. (1) at $\Delta=-1$, thus allowing us to compute the entanglement entropy exactly for blocks of arbitrary size and system of arbitrary length. To this regard, we remark that by performing the transformation which overturns each second spin along the chain (we assume the length of the chain even), the Hamiltonian (1) for $\Delta=-1$ reduces to the isotropic Heisenberg ferromagnet (2). Since this transformation does not change the entropy of entanglement, one can compute the block entropy of the antiferromagnetic Heisenberg chain at $\Delta=-1$ directly from that of the isotropic ferromagnetic model. It is worth noting that, in contrast with critical points $-1<\Delta\leqslant 1$, the point $\Delta=-1$ cannot be studied by means of conformal field theory since this point is not conformal invariant [4], the ground state being infinitely degenerated at $\Delta=-1$ [5]. We also note that, in contrast with the critical region $-1<\Delta\leqslant 1$ of the antiferromagnetic Heisenberg chain, at the point $\Delta=-1$ all spin-spin correlations vanish in the thermodynamic limit and only correlations due to the constraint of fixed magnetization are present. Finally, we wish to point out that besides the Heisenberg model and models of interacting bosons [6], our results naturally apply to all permutationally invariant states and in particular to eta pairing states of fermionic lattice models of interest for high T_c superconductivity. It is well known, indeed, that eta-pairing states of the Hubbard model can be mapped into the ground-state sector of fixed magnetization of the ferromagnetic spin-$\frac{1}{2}$ isotropic Heisenberg model [10] and, therefore, all derived formulas for entanglement entropies apply to these states as well.

The paper is organized as follows. In Sec. II, we introduce the model and study the general properties of the reduced density matrix for the ferromagnetic ground states. In particular, we formulate and demonstrate a theorem which gives the analytical expression of the eigenvalues of the reduced density matrix for arbitrary sizes of the system and value of the magnetization. In Sec. III, we use this theorem to compute the entanglement entropy of a block of size n in the finite system of total length L for two specific choices of the ground-state sector. Taking the limit of large subsystem sizes, we derive analytical expressions for the entanglement entropy $S_{(n)}$ of a block of spins of size n in the ferromagnetic ground state, both for $n, L\gg 1$ and for $n\gg 1$, $L=\infty$. As a result, we obtain that in the ground-state sector with a fixed value of S^z, the block entanglement entropy grows as $S_{(n)}=1/2\log_2[n(L-n)/L]$ for large n, while in the ground-state sector in which all the S^z components of the spin multiplet are equally weighted, $S_{(n)}=\log_2(n+1)$ for arbitrary n and L. Finally, in Sec. IV, we discuss and summarize the main results of the paper.

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II. REDUCED DENSITY MATRIX FOR THE FERROMAGNETIC HEISENBERG MODEL

We consider the ferromagnetic Heisenberg model with nearest-neighbor interaction,

$$H_{XXX} = -J\sum_{i=1}^{L}\left(\vec{\sigma}_i\vec{\sigma}_{i+1} - 3I\right), \tag{2}$$

where σ are Pauli matrices, $J>0$ denotes the exchange constant, and L is the number of spins (we assume periodic boundary conditions $L+1\equiv 1$). As is well known, the ground state of Eq. (2) belongs to a multiplet of total spin $S=L/2$ and is degenerate with respect to $S^z=-L/2,-(L/2)+1,\ldots,L/2$. In the sector with a fixed number N of spins down, i.e., with a fixed $S^z=N-(L/2)$, the ground state is obtained by the action of the rising operator $S^+=\Sigma_i\sigma_i^+$ on the vacuum state with all spins down,

$$|\Psi_L^N\rangle \sim (S^+)^N|\downarrow\downarrow\cdots\downarrow\rangle. \tag{3}$$

All eigenfunctions (3) correspond to the same ground-state energy $E=0$ of the XXX model (2). The structure of the state (3) is given by

$$|\Psi(L,N)\rangle = \frac{1}{\sqrt{C_N^L}}\sum_P |\underbrace{\uparrow\uparrow\cdots\uparrow}_{N}\underbrace{\downarrow\downarrow\cdots\downarrow}_{L-N}\rangle, \tag{4}$$

where the sum is taken over all possible distributions of N spins on L sites and the binomial coefficient $C_N^L=L!/N!(L-N)!$ takes care of the normalization. Note that Eq. (4) is also a ground state for the model of interacting bosons [6], while for the partially asymmetric exclusion process ASEP [7] with N particles hopping with hard-core exclusion on a closed chain of the length L, Eq. (4) represents a steady-state vector.

We will be interested in the ground-state entanglement (von Neumann) entropy $S_{(n)}$ of a block of n (not necessarily contiguous) spins

$$S_{(n)} = -tr(\rho_n\log_2\rho_n) = -\sum \lambda_k\log_2\lambda_k, \tag{5}$$

where ρ_n is the reduced density matrix of the block, obtained from the density matrix ρ of the whole system by tracing out external degrees of freedom $\rho_{(n)}=tr_{(L-n)}\rho$ (notice that due to the permutational symmetry of the ground state, $S_{(n)}$ does not depend on the particular choice of the block but only on its size n). In Eq. (5), λ_k are the eigenvalues of the reduced density matrix which are all real, non-negative, and sum up to 1: $\Sigma\lambda_k=1$.

The density matrix ρ for a degenerate ground state is given by

$$\rho = \sum_{N=0}^{L}\alpha_N|\Psi(L,N)\rangle\langle\Psi(L,N)|, \quad \sum\alpha_N = 1, \tag{6}$$

where $\alpha_0,\alpha_1,\ldots,\alpha_L$ is a set of non-negative coefficients. Denoting the reduced density matrix in a fixed sector with N spins up by $\rho_n(N)$,

$$\rho_n(N) = \mathrm{tr}_{(L-n)}|\Psi(L,N)\rangle\langle\Psi(L,N)|, \tag{7}$$

where $|\Psi(L,N)\rangle$ is given by Eq. (4), one can write the general reduced density matrix as

$$\rho_n = \sum_{N=0}^{L}\alpha_N\rho_n(N). \tag{8}$$

In the following, we consider two choices for the coefficients $\{\alpha_i\}$:

$$\text{(a)}\quad \alpha_i = \delta_{iN}, \tag{9}$$

$$\text{(b)}\quad \alpha_0 = \alpha_1 = \cdots = \alpha_L = \frac{1}{L+1} \tag{10}$$

(the analysis for arbitrary $\{\alpha_i\}$ proceeds in a similar manner). The choice (a) corresponds to the case when a small anisotropy singles out a sector with N spins up resulting in a pure state of a global system; see Eqs. (4) and (6). The choice (b) corresponds to an equilibrated density matrix (i.e., with all components of the ground-state multiplet equally weighted) which preserves the SU(2) invariance of the Hamiltonian (2) (this case is equivalent to infinite temperature). Using the general property of the entropy of composite systems, $S_{(n)}=S_{(L-n)}$, and its invariance with respect to the inversion of all spins, we can restrict the analysis, without losing generality, to the case $n\leqslant L/2$, $N\leqslant L/2$. The computation of the block entanglement entropy is drastically simplified by the following.

Theorem. The eigenvalues of the reduced density matrix $\rho_n(N)$ of a block of n spins in the sector with N spins up in the ground state of the ferromagnetic Heisenberg model (2) are given by

$$\lambda_k(L,n,N) = \frac{C_k^nC_{N-k}^{L-n}}{C_N^L}, \quad k = 0,1,\ldots,\min(n,N). \tag{11}$$

The proof of the theorem follows from the decomposition of $\rho_n(N)$ with respect to the symmetric orthogonal subspaces of the system of n spins, classified by the integer $k=0,1,\ldots,\min(n,N)$ giving the number of spins up in the block,

$$\rho_n(N) = \sum_{k=0}^{\min\{n,N\}} c_k|\psi(n,k)\rangle\langle\psi(n,k)|. \tag{12}$$

Here $|\psi(n,k)\rangle$ denotes the symmetric state with k spins up among n spins,

$$|\psi(n,k)\rangle = \sum_P |\underbrace{\uparrow\uparrow\cdots\uparrow}_{k}\underbrace{\downarrow\downarrow\cdots\downarrow}_{n-k}\rangle \tag{13}$$

and c_k is the corresponding probability $c_k=C_{N-k}^{L-n}/C_N^L$ (notice that C_{N-k}^{L-n} is the number of states with k spin up in the block of n spins and C_N^L is the total number of states). Expression (12) can be rewritten as

$$\rho_n(N) = \sum_{k=0}^{\min\{n,N\}} \lambda_k \rho_n(k), \tag{14}$$

where $\rho_n(k)$ is the density matrix of the state $|\psi(n,k)\rangle$ and the coefficients $\lambda_k = C_k^n C_{N-k}^{L-n} / C_N^L$ sum up to 1, $\Sigma\lambda_k = 1$. From this it follows that $\rho_n(N)$ is the density matrix associated with the ensemble of orthogonal pure states $\{\lambda_k, \rho_n(k)\}$ and therefore it has a block diagonal form, each block having only one nonzero eigenvalue λ_k which coincides with the expression (11). This concludes the proof of the Theorem.

We remark that the specific case $N=n=L/2$ was also considered in Ref. [8]. Having found the eigenvalues of $\rho_n(N)$, one can easily compute the entanglement entropy $S_{(n)}$ for arbitrary L, n, and N. This will be done in the next section.

III. EXACT ENTANGLEMENT ENTROPY OF FERROMAGNETIC GROUND STATES

A. Case (a)

To obtain an analytical expression for $S_{(n)}$, from the exact expression [Eqs. (5) and (11)], we observe that for blocks of large size, $n \gg 1$, the dominant contribution to the sum (5) comes from the eigenvalues λ_k with large k. In this case, one can approximate the binomial coefficients in Eq. (11) by the normal distribution, see, e.g., Ref.[9],

$$C_n^m p^m q^{n-m} \approx \frac{1}{\sqrt{2\pi npq}} \exp\left(-\frac{(m-np)^2}{2npq}\right), \quad npq \gg 1, \tag{15}$$

where $0<p<1$, $q=1-p$. Using this approximation, and defining $p=N/L$, the eigenvalues (11) can be written as

$$\lambda_k(L,n,N) = \frac{C_k^n p^k q^{n-k} C_{N-k}^{L-n} p^{N-k} q^{L-n-N+k}}{C_N^L p^N q^{L-N}} \approx \frac{1}{n}\frac{1}{\sqrt{2\pi\alpha}} \exp\left(-\frac{\left(\frac{k}{n}-p\right)^2}{2\alpha}\right),$$

where $\alpha = pq(L-n)/nL$. Substituting this expression into Eq. (5) and replacing the sum with an integral, we obtain

$$S_{(n)}(p) \approx \int_0^1 R\left(\log_2 \frac{R}{n}\right) dx,$$

$$R = \frac{1}{\sqrt{2\pi\alpha}} \exp\left(-\frac{(x-p)^2}{2\alpha}\right).$$

For large n, the limits of the integral can be extended to include the whole real axis, after which the result of the integration gives

$$S_{(n)}(p) \approx \frac{1}{2}\log_2(2\pi epq) + \frac{1}{2}\log_2 \frac{n(L-n)}{L}. \tag{16}$$

Notice that this approximate result is valid for $npq \gg 1$ and in the limit $npq \to \infty$ it becomes exact. From the analytical expression (16), the following properties can be easily derived: (i) $S_{(n)}(p) = S_{(n)}(1-p)$, (ii) $S_{(n)}(p) = S_{(L-n)}(p)$, (iii) $\partial S_{(n)}(p)/\partial n = 0$ only at $n=L/2$, (iv) $\partial S_{(n)}(p)/\partial p = 0$ only at $p=\frac{1}{2}$, (v) $S_{(n)} \times (p)$ is a monotonically increasing function of the total length L. In Fig. 1, we compare the exact entropy of finite systems, as computed from exact expressions Eqs. (5) and (11), with the analytical expression (16), from which we see that there is an excellent agreement also for small values of npq. In the thermodynamic limit $L\to\infty$, $N/L \to p$ the eigenvalues (11) reduce to

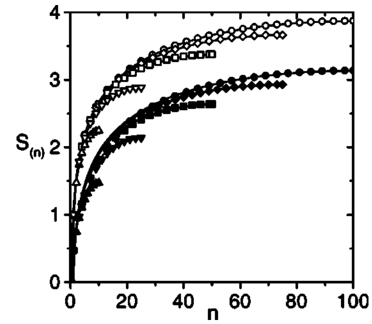

FIG. 1. Entanglement entropy as obtained from the exact expressions Eqs. (5) and (11), as a function of the block size n and for $L=20$ (up triangles), 50 (down triangles), 100 (squares), 150 (diamonds), and 200 (circles). Filled (empty) symbols correspond to $p=1/10$ ($p=1/2$). Continuous curves represent the analytical expression in Eq. (16). For $n>L/2$, $S_{(n)} = S_{(L-n)}$ (not shown).

$$\lambda_k = C_n^0 p^n, C_n^1 p^{n-1} q, \ldots, C_n^n q^n, \tag{17}$$

and the corresponding entanglement entropy is obtained from Eq. (16) as

$$S_{(n)}(p) \approx \frac{1}{2}\log_2(2\pi epq) + \frac{1}{2}\log_2 n. \tag{18}$$

In Fig. 2, we plot the exact entanglement entropy of a block of size $1 \le n \le 1000$ in an infinite chain (5) and (17), versus the limiting expression (18) for different filling p. We see that the analytic formula (18) gives a good approximation even for a small finite number of sites n in the block. For very small p the convergence is slower (see the lowest graph

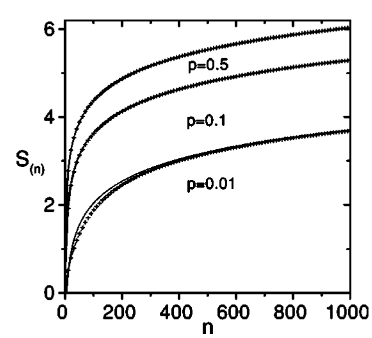

FIG. 2. Entanglement entropy as function of a block size n, for different values of $p=\frac{1}{100}, \frac{1}{10}, \frac{1}{2}$. Comparison of exact formula (points) with the limiting expression (18) (continuous curves).

in Fig. 2) because the validity of formula (15) crucially depends on the value of *npq*.

Thus, for case (a) we conclude that the block entanglement entropy of the ferromagnetic ground state grows logarithmically with n, as for critical quantum systems, but with a different prefactor, i.e., as $\frac{1}{2}\log_2 n$ rather than $\frac{1}{3}\log_2 n$ predicted in Ref. [3].

B. Case (b)

In this case, the eigenvalues of the reduced density matrix are given by

$$\lambda_k = \frac{C_n^k}{L+1}\sum_{N=n-k}^{L-k}\frac{C_{L-n}^{N-n+k}}{C_L^N} = \frac{1}{n+1}, \quad k=0,1,\ldots,n \tag{19}$$

and are independent on k and on the size of the system L. The entanglement entropy is obtained as

$$S_{(n)} = \log_2(n+1), \quad n=1,2,\ldots,L. \tag{20}$$

Equations (11), (16), (18), (19), and (20), corresponding to the cases (a) and (b) considered above, are the main results of the paper.

IV. DISCUSSION AND CONCLUSION

In discussing the above results we remark that, due to the permutational invariance of the ground state, for any choice of the density matrix (8) the reduced density matrix for a block of size n has exactly $n+1$ nonzero eigenvalues (see the theorem) in the ground state. This implies the upper bound for the entropy $S_{\max}(n)=\log_2(n+1)$, which is achieved in the case of a thermally equilibrated density matrix [case (b)]. The lower bound of logarithmic growth $S_{(n)} \sim \frac{1}{2}\log_2 n$ is achieved for the "anisotropic" choice corresponding to a pure state (6) of the whole system [case (a)]. For a generic choice of the coefficients $\{\alpha_N\}$ in Eqs. (6) and (8), $S_{(n)}$ will grow as $\gamma \log_2 n$ with $\frac{1}{2} \leqslant \gamma \leqslant 1$.

We also note that Eq. (20) is a monotonically increasing function of n, attaining maximum for the whole system $n=L$, while in the case of pure state the maximum is achieved for a block of half-system size $n=L/2$. This feature is related to the fact that the ground state of a ferromagnet is highly degenerate and the total system for the choice (10) is in the maximally mixed state.

Another remark concerns the origin of the logarithmic prefactor $\gamma=\frac{1}{2}$ in formula (18). Apparently γ is not related to any central charge since $\Delta=-1$ is not a conformal point. We find that in our case the prefactor γ is related to the spin s per site, i.e., one can show that for a ferromagnetic spin s chain (i.e., with on-site spin s), the block entanglement entropy in the ground-state sector grows like $S_{(n)} \simeq \text{const} + s\log_2 n$ (details will be presented elsewhere).

We also remark that it would be of great interest to generalize Eqs. (16) and (20) to the case of nonzero temperature where excited states have to be taken into account. Work in this direction is in progress.

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