Parity Effects in the Scaling of Block Entanglement in Gapless Spin Chains

Pasquale Calabrese,[1] Massimo Campostrini,[1] Fabian Essler,[2] and Bernard Nienhuis[3]

[1]*Dipartimento di Fisica, dell'Università di Pisa and INFN, 56127 Pisa, Italy*
[2]*The Rudolf Peierls Centre for Theoretical Physics, Oxford University, Oxford OX1 3NP, United Kingdom*
[3]*Institute for Theoretical Physics, Universiteit van Amsterdam, 1018 XE Amsterdam, The Netherlands*

We consider the Rényi α entropies for Luttinger liquids (LL). For large block lengths ℓ, these are known to grow like $\ln\ell$. We show that there are subleading terms that oscillate with frequency $2k_F$ (the Fermi wave number of the LL) and exhibit a universal power-law decay with ℓ. The new critical exponent is equal to $K/(2\alpha)$, where K is the LL parameter. We present numerical results for the anisotropic *XXZ* model and the full analytic solution for the free fermion (*XX*) point.

PACS numbers: 64.70.Tg, 03.67.Mn, 05.70.Jk, 75.10.Pq

Luttinger liquid (LL) theory describes the low-energy (large-distance) physics of gapless one-dimensional models such as quantum spin chains and correlated electron models. It corresponds to a conformal field theory (CFT) with central charge $c = 1$ and is known to provide accurate predictions for universal properties of many physical systems. LL theory has been applied successfully to recent experiments on carbon nanotubes [1], spin chains [2], and cold atomic gases [3]. A much studied example of a lattice model that gives rise to a LL description at low energies is the spin-1/2 Heisenberg *XXZ* chain

$$H = -\sum_{j=1}^{L}[\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y + \Delta\sigma_j^z\sigma_{j+1}^z]. \quad (1)$$

Here, σ_j are Pauli matrices at site j, and we have imposed periodic boundary conditions. Recent years have witnessed a significant effort to quantify the degree of entanglement in many-body systems (see, e.g., [4] for reviews). Among the various measures, the entanglement entropy (EE) has been by far the most studied. By partitioning an extended quantum system into two subsystems, the EE is defined as the von Neumann entropy of the reduced density matrix ρ_A of one of the subsystems. The leading contribution to the EE of a single, large block of length ℓ can be derived by general CFT methods [5–7]. The case of a subsystem consisting of multiple blocks requires a model dependent treatment, but the EE can still be obtained from CFT [8]. On the other hand, little is known with regard to corrections to the leading asymptotic behavior. In the following, we consider the Rényi entropies

$$S_\alpha = \frac{1}{1-\alpha}\ln\text{Tr}\rho_A^\alpha, \quad (2)$$

which give the full spectrum of ρ_A [9] and are fundamental for understanding the scaling of algorithms based on matrix product states [10–12]. We note that S_1 is the von Neumann entropy and S_∞ gives minus the logarithm of the maximum eigenvalue of the reduced density matrix

(known as single copy entanglement [13,14]). According to CFT, in an infinite gapless one-dimensional model, a block of length ℓ has entropies [5–7]

$$S_\alpha^{\text{CFT}}(\ell) = \frac{c}{6}\left(1 + \frac{1}{\alpha}\right)\ln\ell + c_\alpha', \quad (3)$$

where c is the central charge and c_α' a nonuniversal constant. In a finite system of length L, the block length ℓ in (3) should be replaced with the chord distance $D(\ell, L) = \frac{L}{\pi}\sin\frac{\pi\ell}{L}$. In many lattice models, the asymptotic scaling is obscured by large oscillations proportional to $(-1)^\ell$. Some typical examples are shown in Fig. 1, where we plot $S_\alpha(\ell, L)$ for $\alpha = 1, 2, \infty$ for the *XXZ* model at $\Delta = -1/2$ as obtained by density matrix renormalization group (DMRG) computations. While S_1 is smooth, $S_{\alpha\neq1}$ is seen to exhibit large oscillations. For $\alpha = \infty$, in particular, it is difficult to recognize the CFT scaling behavior (3). While such oscillations have been observed in several examples [15,16] and can be seen to arise from strong antiferromagnetic correlations, a quantitative understanding of these features was until now lacking. We show that these oscil-
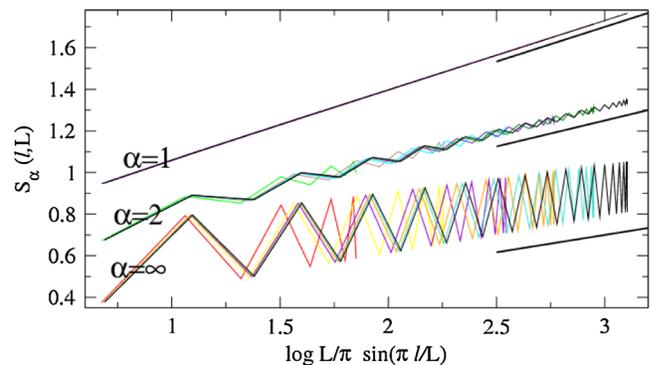
FIG. 1 (color online).   Parity effects in Rényi entropies in the *XXZ* model at $\Delta = -1/2$. $S_\alpha(\ell, L)$ for several L and $\alpha = 1, 2, \infty$. The straight lines indicate the asymptotic slopes $(1 + \alpha^{-1})/6$.

lations obey the universal scaling law

$$S_\alpha(\ell) - S_\alpha^{\mathrm{CFT}}(\ell) = f_\alpha \cos(2k_F\ell)|2\ell \sin k_F|^{-p_\alpha}, \quad (4)$$

where p_α is a universal critical exponent equal to $2K/\alpha$. Here, K is the LL parameter, k_F is the Fermi momentum, and f_α is a nonuniversal constant. In a finite system, the block length ℓ in (4) is replaced by the chord distance, and f_α is multiplied by a *universal* scaling function $F_\alpha(\ell/L)$, that in general depends on the parity of L. We note that in zero magnetic field (half-filling), we have $k_F = \pi/2$, and the oscillating factor in (4) reduces to $(-1)^\ell$ as observed. While we establish (4) for the particular case of the Heisenberg *XXZ* chain (1), where the LL parameter is given by $K = \pi/(2 \arccos\Delta)$, we expect the scaling form to be universal because it is related to the low-energy excitations of the model and is therefore encoded in the continuum LL field theory description. Recent results for the entanglement entropy confirm these expectations [17].

XX model.—This case corresponds to $\Delta = 0$ in (1). The LL parameter and exponent in (4) are $K = 1$ and $p_\alpha = 2/\alpha$, respectively. The computation of the Rényi entropies can be achieved by exploiting the Jordan-Wigner mapping to free fermions, which reduces the problem to the diagonalization of an $\ell \times \ell$ correlation matrix (see [18] for details). Jin and Korepin (JK) showed [19] that Rényi entropies can be obtained by the following contour integral encircling the segment $[-1, 1]$ of the real axis

$$S_\alpha(\ell) = \frac{1}{2\pi i} \oint e_\alpha(\lambda) \frac{d \ln D_\ell(\lambda)}{d\lambda} d\lambda. \quad (5)$$

Here, $D_\ell(\lambda)$ is the determinant of a $\ell \times \ell$ Toeplitz matrix and $e_\alpha(\lambda) = \frac{1}{1-\alpha} \ln[(\frac{1+\lambda}{2})^\alpha + (\frac{1-\lambda}{2})^\alpha]$. In [19], the Fisher-Hartwig formula was used to determine the asymptotic scaling of the Rényi entropy with ℓ, which agrees with the CFT formula (3). Here, we employ the *generalized* Fisher-Hartwig conjecture [20] in order to go beyond the results of [19] and determine the subleading corrections. The terms in the asymptotic expansion of the determinant relevant for calculation of the Rényi entropy can be cast in the form

$$\frac{D_\ell(\lambda)}{D_\ell^{\mathrm{JK}}(\lambda)} = 1 + e^{-2ik_F\ell} L_k^{-2[1+2\beta(\lambda)]} \frac{\Gamma^2(1 + \beta(\lambda))}{\Gamma^2(-\beta(\lambda))}$$
$$+ e^{2ik_F\ell} L_k^{-2[1-2\beta(\lambda)]} \frac{\Gamma^2(1 - \beta(\lambda))}{\Gamma^2(\beta(\lambda))}, \quad (6)$$

where D_ℓ^{JK} is the result of [19], $2\pi i\beta(x) = \ln[(1 + x)/(1 - x)]$, and $L_k = |2\ell \sin k_F|$. The calculation of the integral in (5) is now straightforward. One expands $\ln D_\ell$ in (6) in powers of L_k, determines the discontinuity across the cut $[-1, 1]$, changes the integration variable from λ to $-i\beta(\lambda)$, and finally obtains the leading behavior from the poles closest to the real axis (details will be reported elsewhere [21]). The resulting asymptotic expression is valid at fixed α, in the limit $\ln L_k \gg \alpha$. The final result is given by Eq. (4) with

$$f_\alpha = \frac{2}{1 - \alpha} \frac{\Gamma^2((1 + \alpha^{-1})/2)}{\Gamma^2((1 - \alpha^{-1})/2)}. \quad (7)$$

We note that $f_1 = 0$, and therefore no oscillating corrections for the Von-Neumann entropy are predicted, in agreement with numerical observations.

The requirement that $\ln L_k \gg \alpha$ implies that the asymptotic behavior is only reached for very large block lengths, e.g., at $\alpha = 10$, we need $L_k \gg 20\,000$. In the preasymptotic regime, there are several sources of corrections. First, the integral is no longer dominated by the poles closest to the real axis, which leads to power-law corrections of the form $L_k^{-2m/\alpha}$ (with integer m), which oscillate as $e^{\pm i2k_F\ell}$. Corrections with different oscillatory behavior arise from the higher order terms in the expansion of $\ln D_\ell(\lambda)$ in powers of L_k. The first correction is proportional to $e^{\pm i4k_F\ell}$, the next to $e^{\pm i6k_F\ell}$, etc. In zero magnetic field, where $k_F = \pi/2$, the leading term is proportional to $(-1)^\ell$ while the second does not oscillate. Hence, there is a subleading constant background in addition to the leading oscillatory behavior. In the limit $\alpha \rightarrow \infty$, all these terms become of the same order so that we need to resum the entire series that arises from expanding $\ln D_\ell(\lambda)$ and then carrying out the λ integral. In the zero magnetic field case, we thus obtain

$$S_\infty(\ell) - S_\infty^{\mathrm{JK}}(\ell) = \begin{cases} \frac{\pi^2}{12} \frac{1}{\ln b L_k} & \ell \text{ odd,} \\ -\frac{\pi^2}{24} \frac{1}{\ln b L_k} & \ell \text{ even.} \end{cases} \quad (8)$$

Here, the constant $b \approx 7.1$ has been fixed by summing certain contributions to all orders in $1/(\ln L_k)$ and agrees well with numerical results [22].

Numerical results for the XX model can be obtained by diagonalizing the correlation matrix both infinite and finite systems. We first present the results for infinite systems. We consider only the model in zero magnetic field and plot the quantity

$$d_\alpha(\ell) \equiv S_\alpha(\ell) - S_\alpha^{\mathrm{CFT}}(\ell) \quad (9)$$

where the value for the constant contribution c'_α in $S_\alpha^{\mathrm{CFT}}(\ell)$ is taken from [19]. According to Eq. (4) for $k_F = \pi/2$, $d_\alpha(\ell) \simeq (-)^\ell (2\ell)^{-p_\alpha} f_\alpha$. In Fig. 2, we compare the absolute value of $d_\alpha(\ell)$ for $\alpha = 2, 5, 20, \infty$ and block sizes ℓ up to 4000 sites to our asymptotic results (4) and (8). For $\alpha = 2$, the curves for odd and even ℓ are practically indistinguishable (the line corresponding to the analytical result is invisible under the data points). For $\alpha = 5$, we still obtain power laws with the exponent $p_5 = 2/5$, but the curves are not as symmetrical as for $\alpha = 2$ because subleading corrections become visible. Increasing α further, the deviations of $d_\alpha(\ell)$ for $\ell < 4000$ from the asymptotic behavior become quite pronounced. This is shown in Fig. 2 for the case $\alpha = 20$, where the leading asymptotic result (straight line) is seen to be a poor approximation to $d_\alpha(\ell)$ for even ℓ. Including the subleading corrections gives curves perfectly covered by data in Fig. 2. The last panel in Fig. 2 shows the
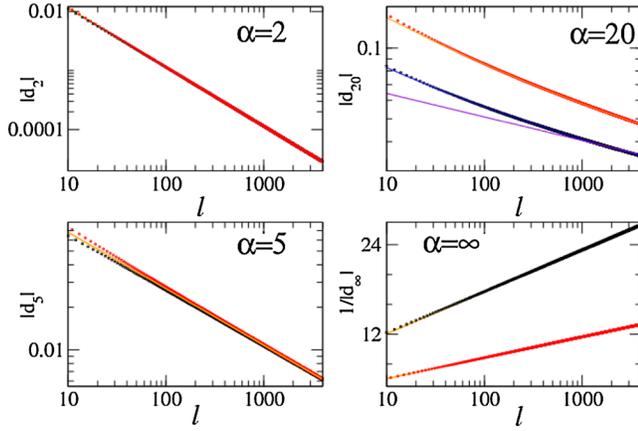
FIG. 2 (color online). Corrections to scaling $d_\alpha(\ell) = S_\alpha(\ell) - S_\alpha^{\mathrm{CFT}}(\ell)$ for the XX model and four different values of α. Red circles and black squares correspond to even and odd ℓ, respectively.

FIG. 3 (color online). Corrections to scaling in the finite length XX model for odd L. $F_2(x)$ and $F_\infty(x)$ ($x = \ell/L$) obtained from 69 different systems with lengths in the range $17 \leq L \leq 4623$ exhibit perfect data collapse.

result in the $\alpha = \infty$. The numerical results are seen to be in perfect agreement with Eq. (8).

We now turn to finite systems. We numerically determined the quantity [recall that $D(\ell, L) = \frac{L}{\pi} \sin\frac{\pi\ell}{L}$]

$$F_\alpha(\ell/L) = [S_\alpha(\ell, L) - S_\alpha^{\mathrm{CFT}}(\ell, L)]f_\alpha^{-1}D(\ell, L)^{2/\alpha}, \quad (10)$$

[for $\alpha = \infty$, we multiply by $\ln bD(\ell, L)$] for a variety of values of α and system sizes ranging from $L = 17$ to $L = 4623$. We observe that there is data collapse for any L on two scaling functions for ℓ odd and even, respectively. Results for the cases $\alpha = 2, \infty$ and odd L are shown in Fig. 3. The quality of the collapse is impressive considering that there are no adjustable parameters and that the plots contain millions of points ranging over 3 orders of magnitude in both ℓ and L. For $\alpha = 2$, we observe that $F_2(x) = \pm \cos\pi x$ (these are shown as continuous curves in Fig. 3). We currently have no analytical derivation of this scaling function. For other values of α, we obtain similar data collapse, but the quality decreases with increasing α, indicating the presence of other corrections. For even L, we obtain different scaling functions—$F_\alpha(x)$ then is almost constant (see below).

XXZ model and DMRG.—To characterize the *XXZ* model in the gapless phase with $-1 \leq \Delta < 1$, we performed extensive DMRG calculations at finite L. We used the finite-volume algorithm keeping $\chi = 800$ states in the decimation procedure. This rather large value of χ is required to obtain a precise determination of the full spectrum of the reduced density matrix in the case of periodic boundary conditions. The data we have used in our analysis can be considered as numerically exact. Hence, the main limitation as compared to the XX case is the relatively small value of L accessible by DMRG (we considered $21 \leq L \leq 81$ for odd L and $20 \leq L \leq 80$ for even L). Another complication stems from the fact that the value of the constant contribution c_α^l to the Rényi entropy is not known analytically for $\Delta \neq 0$ [23]. We obtain it by fitting
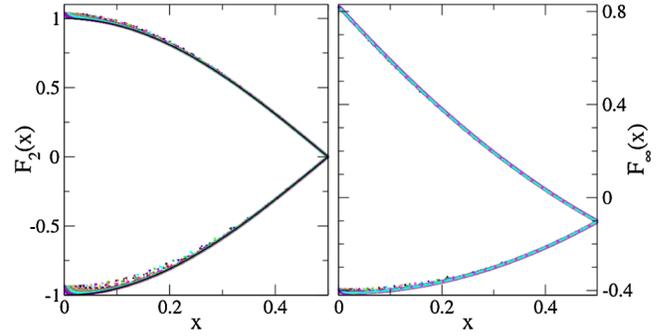
our numerical data. The results are shown in Fig. 4. The data for $\Delta = 0$ is in good agreement with the exact results of [19] (full line), establishing the correctness of our fitting procedure and the reliability of DMRG. The multiplicative constant $c_\alpha = e^{(1-\alpha)c_\alpha'}$ in the moments of the density matrix $\mathrm{Tr}\rho_A^\alpha = c_\alpha \ell^{c/6(\alpha - 1/\alpha)}$ in Fig. 4 shows an exponential decay with α, except for α very close to 1. Hence, c_α can essentially be absorbed into a rescaled block length ℓ as was pointed out in [9,24].

Having obtained the constant contribution c_α', one can determine the universal scaling functions $F_\alpha(x)$. We present results for both even and odd L and a number of representative values of α and Δ in Fig. 5. We find that the data collapse is very good for all cases. This is remarkable given the limited system sizes accessible by DMRG. We note that, as expected, the data collapse becomes poor in the vicinity of the two isotropic points $\Delta = \pm 1$. At $\Delta = -1$, there is a marginal operator (see, e.g., [15]) that gives rise to well-known logarithmic corrections to scaling for
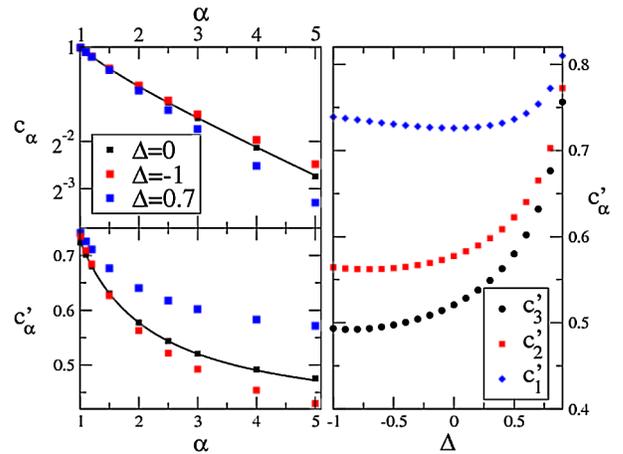
FIG. 4 (color online). Left: The additive constant in the Rényi entropies c_α' (bottom) and the multiplicative constant c_α for the moments $\mathrm{Tr}\rho_A^\alpha$ (top in log scale) as function of α at fixed Δ. The drawn lines are the exact values for $\Delta = 0$. Right: c_α' as function of Δ at fixed α.
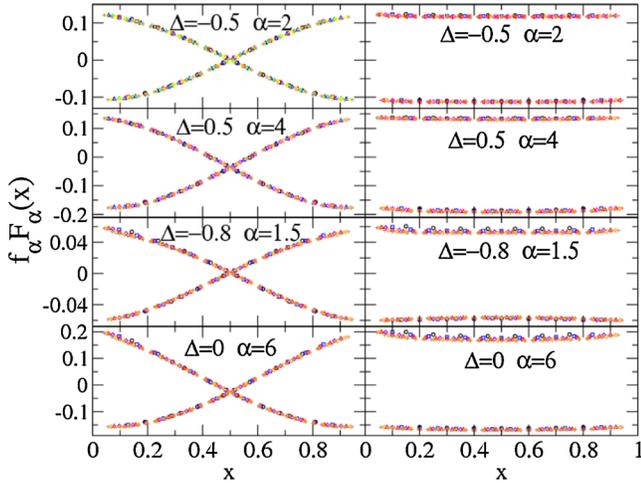
FIG. 5 (color online). Universal scaling function $f_\alpha F_\alpha(x)$ (where $x = \ell/L$) for the *XXZ* chain for several values of α and Δ. Left: Several α and Δ for odd L. Right: even L. In the latter case, $F_\alpha(x)$ is practically independent on x.

correlation functions. In the ferromagnetic limit $\Delta \to 1$, the model loses conformal invariance (the dispersion relation becomes quadratic) and is no longer described by a LL. Hence, none of the results presented here is expected to hold.

The critical Ising chain has no strong antiferromagnetic correlations, and we therefore expect the corrections to scaling to be nonoscillatory. It is easy to see that this is indeed the case. Igloi and Juhasz [25] showed that the EEs of the XY chain can be expressed in terms of the EEs of two Ising chains. At the quantum critical point, this relation reads $S_\alpha^{XX}(2\ell, 2L) = 2S_\alpha^I(\ell, L)$, where S_α^I refers to the critical Ising chain. This implies that the Rényi entropies in the Ising chain are just one half of the corresponding entropies in a *XX* chain of twice the block length and twice the system size. As both ℓ and L are even, our results for the *XX* model imply that the corrections to scaling are nonoscillatory and decay as $\ell^{-2/\alpha}$. This agrees with numerical computations.

Conclusions.—In this Letter, we considered the Rényi entropies for the critical spin-1/2 Heisenberg *XXZ* chain with periodic boundary conditions. By a combination of analytic and numerical techniques, we computed oscillating corrections to scaling which are expected to be universal. These are parametrized in terms of the Luttinger parameter K and the Fermi momentum k_F. We argued that our results hold generally for Luttinger liquids. In the case of open boundary conditions, a similar relationship is expected to hold, but with the replacement $K \to K/2$ (see also [15]). It would be interesting to prove this at least in the special case of free fermions. Finally, we would like to comment on our results in light of a recent proposal [8], that one way of distinguishing between different theories with the same central charge is to consider the entanglement of multiple blocks. Our results establish that it is

sufficient to consider a single block once one takes into account the universal subleading oscillatory corrections.

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