Spin-resolved entanglement spectroscopy of critical spin chains and Luttinger liquids

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Abstract. Quantum critical chains are well-described and understood by virtue of conformal field theory. Still, the meaning of the real space entanglement spectrum—the eigenvalues of the reduced density matrix—of such systems remains elusive in general, even when there is an additional quantum number available such as the spin or particle number. In this paper, we explore in detail the properties and structure of the reduced density matrix of critical XXZ spin-$\frac{1}{2}$ chains. We investigate the quantum/thermal correspondence between the reduced density matrix of a $T = 0$ pure quantum state and the thermal density matrix of an effective entanglement Hamiltonian. Using large scale DMRG and QMC simulations, we investigate the conformal structure of the spectra, the entanglement Hamiltonian, and temperature. We then introduce the notion of spin-resolved entanglement entropies, which display interesting scaling features.

Keywords: entanglement in extended quantum systems (theory)
1. Introduction

Entanglement is a key concept to understand the quantum correlations at play in several condensed matter systems [1]. The central object after a real space bipartition of a quantum system in a pure state $|\Psi\rangle$ is its reduced density matrix (RDM)

$$\hat{\rho}_A = \text{Tr}_B |\Psi\rangle\langle\Psi|,$$

where $A$ is the subsystem and $\text{Tr}_B$ is the partial trace performed over the degrees of freedom of the rest of the system. Because it is at the core of the density matrix renormalization group (DMRG) algorithm [2], entanglement has received a great deal of attention over the past decade [3–10]. A quite natural quantity to study is the so-called Rényi entanglement entropy (EE)

$$S_q = \frac{1}{1-q} \text{Tr} \left[ \hat{\rho}_A^q \right],$$

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Figure 1. Bipartition of the system into region $A$ (red) with length $\ell$ and the remainder $L-\ell$, where $L$ is the total length of the system. Depicted are situations for periodic boundary conditions (a) and open boundary conditions (b).

which in the limit $q \to 1$ yields the von Neumann EE

$$S_1 = -\text{Tr} \left( \hat{\rho}_A \ln \hat{\rho}_A \right).$$

Rényi EEs have been intensively investigated for one-dimensional systems, both analytically [5, 11, 12] and numerically [4, 13]. Most importantly, a central result for a clean critical chain is its universal scaling behavior with the length $\ell$ of a subsystem [1]

$$S_q(\ell) = c \frac{1+q}{6B} \ln \ell + \cdots,$$

where $B = 1$ for periodic boundary condition (PBC), and $B = 2$ for open boundary conditions (OBC) (see figure 1). The universal character of $S_q$ appears in the prefactor $c$, which is the central charge of the underlying conformal field theory (CFT). The dots in equation (4) correspond to subleading corrections [13,14].

For non critical chains, EEs do not grow with $\ln \ell$ but instead saturate with the correlation length $\sim \ln \xi$ [5]. That is, away from a critical point, the EEs approach a constant value. In past years, multi-interval entanglement entropy [15, 16] as well as various other measures of entanglement have also been studied [17–24].

Recently, it was suggested by Li and Haldane [25] that not only should quantities that depend on $\hat{\rho}_A$ such as the EEs $S_q$ be considered, but that the structure of the reduced density matrix $\hat{\rho}_A$ itself should also be investigated. They analyzed the spectrum of the reduced density matrix $\hat{\rho}_A$ for several fractional quantum Hall states (note that they did not consider a real-space cut but instead an orbital cut). Writing

$$\hat{\rho}_A = \exp \left( -\beta \mathcal{H}_E \right),$$

dubbed entanglement spectrum. Note that in the above definition, the inverse entanglement temperature is $\beta = 1$. Li and Haldane showed that the low-lying levels in the entanglement spectrum exhibit the same state counting as elementary quasi-hole excitations of fractional quantum Hall states. They further claimed that the entanglement spectrum can be used to detect fingerprints of the topological order associated with the fractional quantum Hall states [25]. Soon after, Calabrese and Lefevre studied the entanglement spectrum associated with a real space cut (as shown in figure 1) in case of a critical free-fermion chain [26]. As one of their central results, they found the distribution of the entanglement levels. They further pointed out that generalization to other critical chains involves the parameters of the corresponding CFT. More recently, a correspondence between the low-lying part of the ES and the energy spectrum of a boundary CFT was
proposed, providing the opportunity to extract the boson compactification radius directly from the ES [27].

For gapped (spin) chains, the investigation of the ES has led to the discovery that in certain phases all entanglement levels are two-fold degenerate [28]. In the meantime, this degeneracy has been interpreted as one of the hallmarks of symmetry protected topological (SPT) phases [29,30]. In topologically trivial phases, this degeneracy is absent. Of course, there are natural degeneracies in the ES when a conserved U(1) current is present such as particle number or z-component of spin $S_z$. For instance, if the Hamiltonian commutes with $S_z$ of the total system, then the reduced density matrix $\hat{\rho}_A$ and the spin operator $S^z_A$ of subsystem $A$ must commute as well,

$$[S^z_A, \hat{\rho}_A] = 0.$$  

As a consequence, each entanglement level $\xi_1$ associated with a finite $S^z_A \neq 0$ must have a partner $\xi_2 = \xi_1$ associated with $-S^z_A$ (provided the spin inversion symmetry is preserved by the Hamiltonian). If even the full SU(2) symmetry is preserved by the Hamiltonian, then the SU(2) multiplet structure is also present in the ES. The degeneracies due to spin multiplet structure (or, similarly, particle conservation) are present in both critical and gapped systems.

The presence of a conserved U(1) current also links to another interesting quantity. The variance or fluctuations of spin or particle number, respectively, defined for a bipartite subsystem $A$, behave as a measure of entanglement [18]. It has been pointed out recently that the EEs and these bipartite fluctuations share various properties [18,31,32]. In the case of free fermions, exact relations between the Renyi EEs and the full set of charge cumulants have been established [18,33,34]. In certain cases, bipartite fluctuations can be even used to measure the entanglement spectrum of quantum Hall states [35].

Nonetheless, general knowledge of the entanglement spectrum and its implications in critical chains is rather limited, even when an additional quantum number such as spin or particle number is available. To shed more light on this quantity, in the following, we investigate the entanglement spectrum of the XXZ spin chain as a paradigm of critical chains with conserved $S^z$ quantum number. We aim to analyze the different subspaces associated with values of $S^z$. We also consider entanglement entropies, which are restricted to fixed $S^z$, dubbed spin-resolved EEs, and study their scaling behavior.

The paper is organized as follows. In section 2, we analyze the reduced density matrix and the entanglement Hamiltonian of the XXZ spin chain in detail, compare the results with predictions from the literature, and eventually consider the spin-resolved density matrix. Our findings are substantiated with large scale DMRG and QMC simulations. In section 3, we elaborate further on the CFT-related properties of the ES. Then, we discuss spin resolved entanglement entropies and conclusions in section 4.

2. Reduced density matrix and entanglement Hamiltonian for critical XXZ chains

We begin from the one-dimensional $S = \frac{1}{2}$ XXZ model, governed by the following Hamiltonian

$$H_{XXZ} = \sum_{i=1}^{L+1-B} \left( S^x_i S^x_{i+1} + S^y_i S^y_{i+1} + \Delta S^z_i S^z_{i+1} \right) ,$$  

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where $B = 1$ or $2$ accounts for boundary conditions, defined in equation (4). This model displays critical correlations for $-1 < \Delta \leq 1$ with a continuously varying Luttinger liquid parameter

$$K_{\text{LL}} = \frac{1}{2 \arccos(-\Delta)/\pi}.$$  

(9)

Following the setups sketched in figure 1, when a critical XXZ chain is cut into two parts ($A$ of length $\ell$ and the remainder), the leading term of Rényi entanglement entropies is given by equation (4), with a central charge $c = 1$, as verified numerically, for instance, in [4, 13, 36, 37]. While the knowledge of $S_q$ is fully relevant for the characterization of entanglement properties of a given system, it does not reveal the complexity of the reduced density matrix itself, and it is expected that much more information can be obtained from the eigenvalues of the reduced density matrix, i.e. the entanglement spectrum.

2.1. Block diagonal RDM and distribution of eigenvalues

2.1.1. Eigenvalues distribution: DMRG results and finite size effects. In the following, we analyze numerical data for the XXZ spin chain obtained within the density matrix renormalization group (DMRG) [2, 38]. Apart from the fact that the DMRG method is probably the most powerful technique for one-dimensional quantum systems at zero temperature, it features another major advantage for the study of quantum entanglement in many-body systems: the reduced density matrix is the key quantity (and not the wavefunction or the Green’s function) that is calculated and optimized permanently. That is, whenever one applies the DMRG method to a problem, its entanglement entropies and entanglement spectrum is immediately known—without any extra computational costs.

All DMRG results presented in this paper are computed with OBC and for system sizes ranging from $L = 100$ to $L = 2000$ lattice sites. We consistently performed 10 DRMG sweeps and kept the discarded entropy below $10^{-14}$.

From Calabrese and Lefevre (CL) [26], we expect the mean number of eigenvalues larger than a given $\lambda$ to be

$$n(\lambda) = I_0\left(b \ln(\lambda_{\text{max}}/\lambda)\right),$$

(10)

where $I_0$ is the modified Bessel function of the first kind, $\lambda_{\text{max}}$ is the largest eigenvalue, and $b = -\ln \lambda_{\text{max}}$. DMRG results are shown in figure 2. It is very interesting to notice that the CL formula works remarkably well for the XX point (corresponding to free fermions). However, we observed some significant deviations for interacting cases $\Delta \neq 0$. Such deviations have already been observed, for instance, in [39, 40]. In particular, for attractive $\Delta < 0$, $n(\lambda)$ underestimates the analytical prediction [40]. Conversely, for repulsive interaction, $\Delta > 0$, $n(\lambda)$ overestimates the CL-curve. While we are dealing with already very large systems (up to $L = 2000$ sites), it is still possible to face finite size effects, which apparently change sign with the sign of anisotropy and are much smaller for $\Delta = 0$.

Strong finite size effects are indeed responsible for the observed deviation, as displayed in figure 3 for the SU(2) Heisenberg point $\Delta = 1$. There, $n(\lambda)$ are plotted for all available sizes $L = 100, \ldots, 1500$, and infinite size extrapolations are performed for seven values of $n$. As shown in the inset of figure 3, the convergence to the thermodynamic limit is logarithmically slow $\sim 1/\ln L$. Nevertheless, the CL expression (red curve) gives a very
Figure 2. Distribution of eigenvalues $n(\lambda)$ obtained from DMRG for various anisotropies $\Delta$ for system sizes $L \geq 1500$ with OBC and partitions at $L/2$. The CL expression is from the Calabrese–Lefevre [26] equation (10).

Figure 3. Finite size convergence of $n(\lambda)$ towards the Calabrese–Lefevre formula equation (10). DMRG data for $\Delta = 1$. Error bars reflect the uncertainty due to vertical jumps in the $n(\lambda)$ curves. Inset: logarithmic convergence to the thermodynamic limit where the lines are linear fits.

good description of the DMRG data once the thermodynamic limit is taken. We repeated the same analysis for $\Delta = -0.5$ and $-0.9$ (data not shown here) and also numerically found a logarithmic convergence to the CL expression but with an opposite sign. Our data suggest that the prefactor of the $1/\ln L$ correction has the sign of $\Delta$ and, as shown in figure 2, vanish at the free-fermion point $\Delta = 0$. An analytical understanding of such finite size effects is needed and certainly calls for further work.
Figure 4. Weights of the eigenvalues of the RDM $\hat{\rho}_A$ shown for four different values of the Ising anisotropy $\Delta$. DMRG results for $L = 1500$ sites with OBC are displayed as a map showing the individual eigenvalues $\lambda_i$ for each sector $S^z_A = \pm m$ in a logarithmic scale (see legend). Only eigenvalues larger than $\lambda_{\text{min}} = 10^{-9}$ have been kept, with $N_\lambda$ the total number of such states. For each couple $(m, \Delta)$, we show above the circles (whose radii materialize the $\lambda_i$) the number of states in this subsector and the total weight $p_m$ (see text).

2.1.2. Spin-resolved RDM. We now turn to the internal structure of the RDM of the XXZ chain, which is block diagonal, with each block corresponding to the subsystem magnetization $S^z_A = 0, \pm 1, \pm 2, \cdots, \pm \ell/2$. Therefore, each sector can be diagonalized separately, $S^z_A = \pm m$. The spin inversion symmetry yields only $m \geq 0$ that can be considered. The size $D(m, \ell)$ of each $m$-sector is exponentially large with $\ell$ for finite $m$:

$$D(m, \ell) = \frac{\ell!}{(\ell - m)!(\ell + m)!} \approx 2^\ell \sqrt{\frac{2}{\pi \ell}} \exp\left(-\frac{4m^2}{\ell}\right), \quad (m \ll \ell).$$

Nevertheless, the power of DMRG allows access to ground-state properties and, particularly important for our present purpose, entanglement estimates with a very high precision by keeping only a very small number of eigenstates of the RDM, as compared to the exponentially large $D(m, \ell)$ (see appendix).

In figure 4, we present a map of the eigenvalues of the RDM for four representative values of the Ising anisotropy $\Delta = 1, 0, -0.5, -0.9$, for chains of length $L = 1500$ with OBC. Here, only states with weight $\lambda > 10^{-9}$ were retained\(^3\). Interestingly, while the

\(^3\) There is no physical or numerical reason for this; for practical reasons only we omit entanglement levels $\lambda < 10^{-9}$ as these are beyond any accuracy dealt with in this analysis.

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number of kept state $N_{\lambda}$ does varies little with $\Delta$, the spin-resolved structure turns out to be qualitatively different across the critical regime. Indeed, at the Heisenberg point, 33% of the states lie in the $m = 0$ sector with a weight 0.73, and there is no left state for $m > 3$. Conversely, close to the ferromagnetic point at $\Delta = -0.9$, the $m = 0$ sector represents a total weight of 0.35 with only 15.7% of the states, but one can find states up to $m = 7$. Note that if the distribution of the eigenvalues was uniform, from equation (11), for $L = 1500$ sites, a weight of only 2% would be obtained for the $m = 0$ sector and 1.8% for $m = 7$.

On one hand, the result shown in figure 4 is not so surprising since the magnetic correlations of the spin chain $\langle S_i^z S_{i+r}^z \rangle$ are dominated by antiferromagnetic quasi-order $\sim (-1)^r/r^2 K_{LL}$ for $\Delta > 0$ whereas the ferromagnetic component $\sim 1/r^2$ dominates the other regime $\Delta < 0$. On the other hand, as far as entanglement properties are concerned, we expect universality for both the entanglement entropy equation (4) and the spectra equation (10) across the full critical regime. Nevertheless, microscopic details of the RDM, in particular the spin-resolved structure, are a key feature that we now study in detail.

2.2. Entanglement Hamiltonian and entanglement temperature

2.2.1. Quantum/thermal mapping. To gain a better understanding of the RDM structure, it is very instructive to investigate the entanglement Hamiltonian. Interestingly, it was recently argued [27] that the entanglement spectrum of $\hat{\rho}_A$ can be directly related to the energy spectrum of an open XXZ chain. We thus expect the RDM of subsystem $A$ to be written as the following thermal density matrix:

$$\hat{\rho}_A = \exp \left( -\beta_{\text{ent.}} \mathcal{H}_{\text{XXZ}}^{\text{obc}} \right),$$

where $\mathcal{H}_{\text{XXZ}}^{\text{obc}}$ is the Hamiltonian of an open XXZ chain equation (8) ($B = 2$) with an energy shift such that the free energy is $\propto \ln Z = 0$. The inverse entanglement temperature $\beta_{\text{ent.}} = 1/T_{\text{ent.}}$ can be determined directly from the fact that the entanglement entropy of subsystem $A$ must exactly match the thermal entropy of the effective Hamiltonian at temperature $T_{\text{ent.}}$, which is true for any Rényi order $q$.

In the low temperature regime $1 \gg T/u \gg 1/\ell$, the extensive part of the thermal Rényi entropies of an XXZ chain of length $\ell$ (boundary conditions do not change this leading behavior) is [41]

$$S_q^{\text{th}} = \frac{\pi c}{6u} \left( 1 + \frac{1}{q} \right) \ell T.$$  (13)

When identified with the $S_q(\ell)$ equation (4), it yields the entanglement temperature

$$T_{\text{ent.}} = \frac{u \ln(\ell/\ell_0)}{B \pi \ell},$$  (14)

with $B = 1$ (resp. $B = 2$) for PBC (resp. OBC). Note that this result could also be obtained from the bipartite fluctuation of magnetization [18,31]

$$C_2(\ell) = K_{LL}/(B \pi^2) \ln(\ell/\ell_0),$$  (15)

which, in the thermal ensemble, is simply the Curie constant of the entanglement Hamiltonian $\chi_T = (K_{LL} T)/(u \pi)$ and equally leads to the same entanglement temperature equation (14). Note that the above scalings are only the leading part, with subdominant terms ignored.
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2.2.2. Partition function of the entanglement Hamiltonian. The Hamiltonian of an open critical XXZ chain, when irrelevant operators are ignored, is equivalent to a free boson model whose partition function at inverse temperature \( \beta \) is known \([42,43]\):

\[
Z(\ell, \beta) = \zeta(\ell, \beta) \sum_{m=-\ell}^{\ell} \exp\left(-\beta \frac{\pi u}{2K_{LL}} m^2\right), \tag{16}
\]

where \( \zeta(\ell, \beta) = \prod_{n=1}^{\infty} \left[2 \sinh \left(\frac{\pi u}{4\ell T} n\right)\right]^{-1} \). From this expression, we immediately see that the weights \( p_m \) of the sectors with \( S_z = \pm m \) have a Gaussian distribution with a variance \( \sigma^2 = \left(\frac{K_{LL}\ell T}{u\pi}\right) \).

2.3. Numerical results

2.3.1. DMRG. We find that DMRG data are in very good agreement with the predicted Gaussian distribution for \( p_m \) equation (17), as displayed in figure 5 where \( p_m(\ell = L/2) \) has been computed for the XXZ chain at \( \Delta = -0.9 \) (OBCs imposed) for various chain lengths \( L = 100, \ldots, 2000 \). Gaussian fits yield a Gaussian variance \( \sigma^2_g \), which agrees perfectly with the second cumulant \( C_2 = \sum_m m^2 p_m - (\sum_m mp_m)^2 = C_2(\ell) \), which is nothing but the bipartite fluctuation of a magnetization equation (15) for which the scaling is well-known \([18,31]\), as displayed in equation (15). This leads to

\[
p_m(\ell) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{m^2}{2\sigma^2}\right), \tag{17}
\]

with variance \( \sigma^2 = \sum_m m^2 p_m - (\sum_m mp_m)^2 = C_2(\ell) \), which is nothing but the bipartite fluctuation of a magnetization equation (15) for which the scaling is well-known \([18,31]\), as displayed in equation (15). This leads to

\[
p_m(\ell) = \sqrt{\frac{B\pi}{2K_{LL} \ln(\frac{\ell}{\ell_0})}} \exp\left(-\frac{B\pi^2 m^2}{2K_{LL} \ln(\frac{\ell}{\ell_0})}\right). \tag{18}
\]

Interestingly, one can compare the above expression for \( p_m(\ell) \) with the relative size of each subsector \( m \) given by equation (11) by \( D_m(\ell)/2^\ell \approx \sqrt{\frac{2\pi}{\ell}} \exp(-4m^2/\ell^2) \). Both display Gaussian distributions but with quite different variances.

The same analysis can be repeated for other values of the anisotropy \( \Delta \), as shown in figure 6. The Gaussian distribution equation (17) correctly describes \( p_m \), as displayed in figure 6(c) for \( L = 1500 \) and \( \Delta = -0.9, -0.5, 0, 1 \). Again one can extract both the second cumulant \( C_2 \) and the variance \( \sigma^2_g \) obtained from a fit to the Gaussian form equation (17). This is plotted in figure 6(a), where both quantities scale with \( \ln L \). Note, however, that the almost perfect agreement observed for \( \Delta = -0.9 \) becomes gradually less good as \( \Delta \)
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Figure 5. DMRG results for the weights $p_m(L/2)$ per sector of the RDM for the XXZ chain at $\Delta = -0.9$ and OBC, shown for various chain lengths $L$ with a bipartition (figure 1(b)) at $L/2$. Full lines are fits to the Gaussian form equation (17) with a Gaussian variance $\sigma_g^2$ displayed in the inset (green circles), where the second cumulant $C_2(L/2)$ is also shown (black stars). Both are fitted to the form equation (15) with $B = 2$, $\ell_0 = 0.416$ and $K_{LL} = 3.476$ (black line) for $C_2$ and $\ell_0 = 0.391$, and $K_{LL} = 3.458$ (green line) for $\sigma_g^2$. Note that data for $L = 1500$ are the same as the map in figure 4.

increases, which is expected since irrelevant and boundary corrections increase [43, 44]. Nevertheless, the prefactor of the log behavior can be extracted and is plotted in figure 6(b) versus $\Delta$, where it compares quite well to the exact expression for the Luttinger exponent equation (9).

This validates the open XXZ chain as the correct entanglement Hamiltonian with an entanglement temperature given by equation (14). One can also compare DMRG with quantum Monte Carlo computations at both zero and finite temperature, as we now do.

2.3.2. Quantum Monte Carlo approach. A similar study can be done using quantum Monte Carlo (QMC) simulations. While a direct access to the individual eigenvalues $\lambda_i^{(m)}$ of the RDM is practically out of reach within QMC [41, 45], one can nevertheless very efficiently sample the diagonal of the reduced density matrix, as recently introduced in a series of papers [46–48]. With the RDM as block diagonal with respect to $m$, one can also compute with QMC the trace for each sector, and thus access $p_m$. Contrary to DMRG, PBC do not introduce additional computational costs to QMC calculations. Moreover, one can also access finite temperature physics and DMRG is the most efficient for $T = 0$ ground-state properties (although efficient finite-$T$ DMRG algorithms are available). We exploit finite-$T$ QMC calculations below and directly compare the distributions $p_m$ at $T = 0$ for bipartite systems to finite-$T$ $p_m$ for the entanglement Hamiltonian.
Figure 6. DMRG results for the weights $p_m(L/2)$ per sector $m$ of the RDM for the XXZ chain with OBC at $\Delta = -0.9, -0.5, 0, 1$ shown in panel (c) for $L = 1500$ sites. Full lines are fits to the Gaussian form equation (17) with a Gaussian variance $\sigma_g^2$ displayed in panel (a) (red symbols) together with the second cumulant $C_2$ (black symbols). Panel (b) shows the Luttinger liquid exponent $K_{LL}$ extracted from either the second cumulant equation (15) (black diamonds) or from a Gaussian variance, assuming equation (17) (red diamonds), with both compared to the exact expression equation (9). Note again that data are the same as the map in figure 4.

Bipartition at zero temperature. We first present $T = 0$ QMC results for PBC (setup (a) in figure 1) with a bipartition at $\ell = L/2$ for the same anisotropy $\Delta = -0.9$ as previously analyzed for DMRG data. As shown in figure 7, the Gaussian behavior equation (18) is again nicely reproduced with a variance perfectly described by $C_2(\ell) = (K_{LL}/\pi^2) \ln(\ell/\ell_0)$. Fits are performed either versus $m$ for fixed length $L$ (main panel of figure 7 and left in table 1) or versus $L$ for fixed magnetization $m$ (inset of figure 7 and right in table 1). The agreement with the exact value of the Luttinger liquid parameter $K_{LL}$ is again excellent.

Finite temperature. It is also instructive to test the validity of the quantum/thermal mapping equation (12) by simply comparing $p_m$ for a bipartite system (XXZ with PBC) at $T = 0$ with an open chain of length $\ell$ at finite temperature $T_{ent} = u \ln(\ell/\ell_0)/(\pi \ell)$. We take $L = 256$ and $\ell = 128$, with an anisotropy $\Delta = -0.9$, yielding $\ell_0 = 0.61$ from table 1. Using the exact Bethe Ansatz expression for the velocity of excitations $u = \pi \sqrt{1 - \Delta^2}/(2 \arccos \Delta)$, we fix the entanglement temperature for this particular
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Figure 7. Zero temperature QMC results for the weights $p_m(L/2)$ per sector of the RDM for the XXZ chain at $\Delta = -0.9$ and PBC, shown for various chain lengths $L$ with a bipartition (figure 1(b)) at $L/2$. Full lines are equation (18) with $B = 1$ and $K_{LL}$ and $\ell_0$ are fit parameters displayed below in table 1.

Table 1. Parameters used to fit the QMC data $p_m(L/2)$ shown in figure 7 to the form equation (18), either versus $m$ at fixed $L$ (left) or versus $L$ at fixed $m$ (right). The exact value of the Luttinger liquid parameter for anisotropy $\Delta = -0.9$ is $K_{LL} = 3.4827$.

| $L$  | $K_{LL}$ | $\ell_0$ | $m$  | $K_{LL}$ | $\ell_0$ |
|------|---------|---------|------|---------|---------|
| 32   | 3.511   | 0.63    | $\pm 1$ | 3.5     | 0.63    |
| 64   | 3.519   | 0.64    | $\pm 2$ | 3.48    | 0.6     |
| 128  | 3.485   | 0.61    | $\pm 3$ | 3.5     | 0.63    |
| 256  | 3.479   | 0.61    | $\pm 4$ | 3.51    | 0.66    |
| 512  | 3.48    | 0.61    | $\pm 5$ | 3.52    | 0.68    |
| 1024 | 3.48    | 0.62    | $\pm 6$ | 3.54    | 0.72    |
|      |         |         | $\pm 7$ | 3.65    | 0.89    |

situation to $\beta_{ent.} = 339.412$, with no adjustable parameters. The comparison, shown in figure 8, nicely validates the quantum/thermal correspondence.

3. Conformal spectrum and spin resolved entanglement entropies

Now that the relative weights of spin-resolved sectors of the RDM and the quantum/thermal mapping are well understood, we turn to the internal structure of the entanglement spectrum. Recently studied by Läuchli in [27], we provide here further
Figure 8. QMC results for the weights $p_m$ computed for XXZ chains with anisotropy $\Delta = -0.9$. (•) $L = 256$, PBC, and $T = 0$ with a bipartition at $\ell = 128$. (◦) $\ell = 128$, OBC, and $T = T_{\text{ent.}}$ equation (14).

demonstration that it is directly related to the energy spectrum of an open XXZ chain. We then discuss some consequences for the spin-resolved entanglement entropies.

3.1. Conformal spectrum from DMRG

Conformal field theory predicts [49] the following low-energy spectrum for an open XXZ chain of $\ell$ sites:

$$E^m_0 - E^0_0 = \frac{\pi u}{2K_{\text{LL}}\ell} m^2,$$

(19)

where $m$ is the $S^z$ quantum number, $E^0_0$ the GS energy, $u$ the velocity of excitations, and $K_{\text{LL}}$ the Luttinger liquid parameter. Such low-energy levels can be identified with the $q = \infty$ $m$-resolved entropies

$$S_{\infty}^{(m)} = -\ln \lambda_{\text{max}}^{(m)},$$

(20)

provided the energy spectrum is correctly normalized. From the above definition of the RDM equation (12), and using the entanglement temperature equation (14), the entropy is simply related to the above energy by $S = E/T_{\text{ent.}}$, and thus equation (19) becomes

$$S_{\infty}^{(m)}(\ell) - S_{\infty}(\ell) = \frac{B\pi^2}{2K_{\text{LL}}\ln(\ell/l_0)} m^2,$$

(21)

where $S_{\infty} = -\ln \lambda_{\text{max}}$ is the single copy entanglement [17].

We successfully checked this quadratic $m$ dependence using DMRG simulations for the XXZ model with OBC (setup (b) in figure 1) $\ell = L/2$ for various chain lengths $L = 100, \ldots, 2000$. Indeed, figure 9 shows the entanglement spectrum $-\ln(\lambda_i/\lambda_{\text{max}})$ versus the spin quantum number $m$ of subsystem $A$ for an Ising anisotropy $\Delta = -0.5$. The
Figure 9. Spin-resolved entanglement spectrum from DMRG calculations. OBC results for XXZ chains at $\Delta = -0.5$ and various lengths $L$, as indicated on the plot. The lower part of the spectrum is fitted to the quadratic form equation (21).

The lower branch is precisely $S_{\infty}^{(m)}(\ell) - S_{\infty}(\ell)$, which fits perfectly to a parabola $\propto m^2$. The prefactor of this quadratic form is studied in figure 10 where, plotted against $\ln L$, a very good agreement is found with equation (21). This is also the case for other values of the Ising anisotropy $\Delta$. According to equation (21), we expect the slope to be $K_{LL}/\pi^2$, which compares very well with the exact result for the XXZ model equation (9), as demonstrated in the inset of figure 10.

At this stage, it is interesting to remark that the curvature of the energy levels of equation (19) is controlled by the uniform susceptibility $\chi_0 = K_{LL}/u\pi$ such as

$$E_0^m - E_0^0 = m^2/2\chi_0.$$  \hfill (22)

Similarly, the quadratic entanglement spectrum

$$S_{\infty}^{(m)} - S_{\infty} = m^2/2C_2,$$  \hfill (23)

is controlled by the bipartite fluctuations of magnetization $C_2$.

3.2. Consequences for the spin resolved entanglement entropies

An important emerging question concerns the individual scalings of the spin-resolved von-Neumann entropies in each magnetization block $m$, defined by

$$S_1^{(m)} = -\sum_i \lambda_i^{(m)} \ln \lambda_i^{(m)}.$$  \hfill (24)

The sum over the sectors $m$: $\sum_m S_1^{(m)} = S_1$ obeys the usual universal log scaling with the sub-system size $\ell$ equation (4). It is thus natural to ask whether some kind
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Figure 10. DMRG results for the inverse curvature of the lower branch of the entanglement spectrum shown for various XXZ anisotropies versus the chain length \( L \). Solid lines are fits to the logarithmic scaling from equation (21) from which \( K_{LL} \) is extracted, and are shown in the inset against \( \Delta \) (symbols) and compared to the exact expression equation (9) (black curve).

of universality may also emerge from individual blocks, regarding their spin-resolved entanglement entropies.

For the \( q = \infty \) Rényi index, we have just seen that

\[
S_{\infty}(m)(\ell) = S_{\infty}(\ell) + \frac{m^2}{2C_2(\ell)},
\]

\[
= \frac{c}{6B} \ln(\ell/\ell_0) + \frac{B\pi^2}{2K_{LL} \ln(\ell/\ell_1)} m^2,
\]

where \( \ell_0 \) and \( \ell_1 \) are natural length scales of order 1. From equation (25), we see that for finite \( m \) sectors, the leading scaling is \( \propto c \ln \ell \) with additional slowly decaying corrections \( \sim 1/\ln \ell \). However, consequences for the scaling of \( S_1(m) \) are not obvious. We can nevertheless try to make a conjecture. Using the Jensen inequality [50], we have \( H_q \geq H_{q'} \) if \( q > q' \), where \( H_q = (\ln \sum_i x_i^q)/(1 - q) \) are normalized Rényi entropies such that \( \sum_i x_i = 1 \). This yields the following inequality for the spin-resolved entanglement entropies:

\[
S_1(m) \geq p_m S_{\infty}(m).
\]

One can use the following ansatz for the SREE:

\[
S_1(m)(\ell) = \frac{c_{\text{eff}}(m, \ell)}{3B} \ln(\ell/\ell_0),
\]

with

\[
\sum_m c_{\text{eff}}(m, \ell) = 1.
\]
Figure 11. (a) SREE $S_{1}^{(m=0)}$ plotted versus the size $L$ for four values of the Ising anisotropy, as indicated on the plot. From the apparent log scaling of $S_{1}^{(m=0)}$, we extract the ‘effective central charge’, defined in equation (27), plot it against $L$, and compare it to $\alpha_\Delta p_0(L)$ (full lines) with prefactors: $\alpha_1 \simeq 0.66, \alpha_0 \simeq 0.65, \alpha_{-0.5} \simeq 0.6, \alpha_{-0.9} \simeq 0.45$. (b) $c_{\text{eff}}$ is plotted against $p_m$ for sectors $m = 0, 1, 2, 3$ (different colors) and different anisotropies (different symbols). Inset: same as in a log–log scale.

While there is no simple argument for the precise form of the ‘effective central charge’ $c_{\text{eff}}(m, \ell)$, the relation between $S_1$ and the single copy entanglement $S_\infty = S_1/2$ for critical chains leads us to make a conjecture, following equation (26):

$$S_1^{(m)}(\ell) \overset{?}{=} 2p_m S_\infty.$$  

This would mean that the ‘effective central charge’ $c_{\text{eff}}(m, \ell) \approx p_m(\ell)$ slowly goes to zero with system size. We checked this conjecture against DMRG results, as shown in figure 11(a) for the $m = 0$ sector and $\Delta = 1, 0, -0.5, -0.9$. The left panel of figure 11(a) shows $S_1^{(m=0)}(L)$ in a log-linear scale from which, according to the ansatz equation (27), the ‘effective central charge’ $c_{\text{eff}}(m = 0, L)$ is extracted and plotted in the right panel of figure 11(a). We find that $c_{\text{eff}}(m = 0, L)$ slowly decays with $L$, in qualitative agreement with the decay of $p_0(L)$ (equation (17)). Indeed, the values of $c_{\text{eff}}(L)$ compare relatively well to $\alpha_\Delta p_0(L)$ with prefactors $\alpha_1 \simeq 0.66, \alpha_0 \simeq 0.65, \alpha_{-0.5} \simeq 0.6, \alpha_{-0.9} \simeq 0.45$. However, this scaling becomes less good for the other sectors $m \neq 0$, as seen in panel (b) of figure 11, where the linear behavior $c_{\text{eff}}(m, \ell) \sim p_m(\ell)$ does not appear to be valid, at least for the sizes considered here.

Therefore, based on our finite size data, we cannot conclude the validity of the proposed log scaling equation (27) or regard the putative ‘effective central charge’ $c_{\text{eff}}(m, \ell)$. Further studies are necessary to capture the scaling features of the spin-resolved entanglement entropies.

4. Conclusions

To elucidate the structure, properties, and meaning of the real space entanglement spectrum we investigated the XXZ spin half chain in the critical Luttinger liquid...
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regime. Particular emphasis was placed on the presence of the additional spin quantum number associated with spin conservation. We further elaborated on the quantum/thermal correspondence between the entanglement spectrum of a $T = 0$ pure quantum state and the thermal density matrix of an effective entanglement Hamiltonian at a finite entanglement temperature $T_{\text{ent}} \sim \ln(\ell)/\ell$. This allowed us to identify a direct correspondence between the entanglement spectrum of an XXZ chain with the energy spectrum of an open XXZ chain. In the second part of the paper, we have introduced entanglement entropies for each individual block of the reduced density matrix associated with the spin quantum number of the subsystem, dubbed spin-resolved entanglement entropies. We proposed the scaling behavior with the subsystem length of these new entropies. Within the process of exploring the spin-resolved properties of the reduced density matrix and the entanglement spectrum in general, various interesting questions have arisen which remain to be clarified:

(a) In figure 2, we show the eigenvalue distribution of the reduced density matrix for the XXZ chain and compare it to the analytical prediction of Calabrese and Lefevre [26]. While the free fermion case $\Delta = 0$ agrees very well, interacting cases ($\Delta \neq 0$) show a significant deviation from the Calabrese–Lefevre result. Finite size extrapolation revealed that the leading correction is $\sim 1/\ln L$. Surprisingly, this correction seems to change its sign with the sign of the Ising anisotropy $\Delta$. At the free fermion point, we did not find any log-correction, which suggests the correction is of the form $\sim \Delta/\ln L$. Analytical understanding of such a finite-size correction is desirable.

(b) For the introduced spin-resolved entanglement entropies, we made the conjecture $S^{(m)}_1(\ell) = 2p_mS_\infty = c_{\text{eff}}(m, \ell)/(3B)\ln(\ell/\ell_0)$, implying that the spin-resolved entanglement entropies are controlled by an effective central charge $c_{\text{eff}}(m, \ell) \sim 1/\sqrt{\ln(\ell/\ell_1)}$, which slowly goes to zero with system size. Although we used very large-scale DMRG and QMC numerical simulations, we could not draw a firm conclusion regarding this point. Better analytical understanding is needed, probably within the framework of conformal field theory. A possible calculation would be to compute the low temperature behavior of the thermal entropy of the entanglement Hamiltonian within each magnetization sector.

Finally, it would be very interesting to extend these ideas of spin-resolved entanglement spectra and entropies to other strongly correlated systems as well as to higher dimensional systems [47, 48, 51].

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Figure A1. Comparison between DMRG and ED for $S_1(\ell = L/2)$ of an open XX chain of length $L = 2000$ sites.

Appendix. DMRG convergence

As exemplified in figure A1, for a $L = 2000$ open XX chain, when keeping only eigenvalues $\lambda > 10^{-9}$, the von Neumann entropy of a half chain $S_1 = -\sum_{i=1}^{N_\lambda} \ln \lambda_i$ (with $\lambda_1 > \lambda_2 > \cdots$) converges very rapidly with the number $N_\lambda$. In figure A1, we observe that the lowest 20 entanglement levels are sufficient to reach the exact value of $S_1$ within 1% accuracy. In the inset of figure A1, the difference between the exact result and the DMRG data as a function of $N_\lambda$ is shown, further substantiating the good convergence behavior.

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