Quantum Information and Computing 2021-2022

Final Project
XXZ Quantum Heisenberg Model

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Outline

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- The Heisemberg chain is a 1D spin model, allowing to display how spin-spin interaction can lead to collective behaviours, having magnetism as the most famous one.
- In particular, the spin-1/2 XXZ Heisenberg model represents a milestone in the quantum information field, since each of the two-states spins can represent a qubit.
- The spin-1/2 XXZ model is also an optimal playground to investigate quantum phase transitions, superconductivity and entanglement.
- In this work, after a theoretical overview on the model, the property of the exact eigenvalues and eigenstates in different anysotropy regimes are studied. To get to the thermodynamic limit, at which quantum phase transitions are analyzed, the infinite-Density Matrix Renormalization Group algorithm is exploited. Finally, the entanglement entropy is computed and obtained results are compared with the Conformal Field Theory (CFT) prescription.

Outline

- the spin-1/2 XXZ Heisenberg chain with **nearest-neighbours** only coupling, in **open boundary conditions**, is described by the Hamiltonian $\hat{H}_N : \mathbb{C}^{d^N} \to \mathbb{C}^{d^N}, \quad d = 2$:

$$\hat{H}_N = -\sum_{i=1}^{N-1} J \left[\hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y\right] + J_z \hat{S}_i^z \hat{S}_{i+1}^z$$

$$= -J \left[\sum_{i=1}^{N-1} \hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y + \Delta \hat{S}_i^z \hat{S}_{i+1}^z\right] \text{[3]}$$

  where J is the strength of the flip-flop interaction, J_z is the strength of the Ising interaction and $\mathbf{\Delta = J_z/J}$ is the **anisotropy** parameter
- the notation used implies that

$$\hat{S}_i^j \hat{S}_{i+1}^j = \mathbb{1}_1 \otimes \cdots \otimes \mathbb{1}_{i-1} \hat{S}_i^j \otimes \hat{S}_{i+1}^j \otimes \mathbb{1}_{i+2} \cdots \otimes \mathbb{1}_N$$

  where

$$\hat{S}^j = \hat{\sigma}^j/2 \quad \text{for j=x,y,z,}$$

  with $\hat{\sigma}^{x,y,z}$ being the Pauli matrices
- the natural basis for the system is given by the eigenvectors of $\hat{S}^z$:

$$S^z |\uparrow\rangle = \frac{1}{2} |\uparrow\rangle, \quad |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$S^z |\downarrow\rangle = -\frac{1}{2} |\downarrow\rangle, \quad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

- the sign of the nearest neighbour coupling **J** determines whether the behaviour is **ferromagnetic**, with all spins aligned along the z axis or **anti-ferromagnetic**, with flipped nearest neighbour spins.
- anyway, performing the trasformation $\hat{S}_x \to -\hat{S}_x$, $\hat{S}_y \to -\hat{S}_y$ on half the sites leaves the algebra unchanged but flips J[2]. Then, it is the sign of $\mathbf{\Delta} = \frac{\mathbf{J_z}}{|\mathbf{J}|}$ that determines **the nature of the coupling**:$\Delta > 0$: ferromagnetic, $\Delta < 0$: anti-ferromagnetic
- the effect of the flip-flop term in the Hamiltonian is to interchange up and down spins and then to move perturbations throughout the chain[3]

$$J\left[\hat{S}_n^x \hat{S}_{n+1}^x + \hat{S}_n^y \hat{S}_{n+1}^y\right] |\uparrow_n \downarrow_{n+1}\rangle = \frac{J}{2} |\downarrow_n \uparrow_{n+1}\rangle$$

  and has no effect on couples of aligned spins
- the Ising terms favors couples of aligned spins

$$\hat{S}_n^z \hat{S}_{n+1}^z |\uparrow_n \uparrow_{n+1}\rangle = -\frac{J}{4} |\uparrow_n \uparrow_{n+1}\rangle$$

- then, the two states in which all spins are aligned are always an eigenstate of the Hamiltonian, but whether in the ferromagnetic coupling they coincide with the ground-state, this does not hold when the coupling is anti-ferromagnetic

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Eigenvalues and eigenvectors for $N = 3$

- **Ferromagnetic phase**: $\Delta = 10$
  - degenerate ground states: $|\uparrow\uparrow\uparrow\rangle\,, \quad |\downarrow\downarrow\downarrow\rangle$
  - 1^{st} excited states:

$$0.7\,|\uparrow\downarrow\downarrow\rangle + 0.13\,|\downarrow\uparrow\downarrow\rangle + 0.7\,|\downarrow\downarrow\uparrow\rangle\,, \quad 0.7\,|\downarrow\uparrow\uparrow\rangle + 0.13\,|\uparrow\downarrow\uparrow\rangle + 0.7\,|\uparrow\uparrow\downarrow\rangle$$

$$0.71\,|\downarrow\uparrow\uparrow\rangle - 0.71\,|\uparrow\downarrow\downarrow\rangle\,, \quad 0.71\,|\uparrow\uparrow\downarrow\rangle - 0.71\,|\downarrow\uparrow\uparrow\rangle$$

  - 2^{nd} excited states:

$$-0.1\,|\uparrow\uparrow\downarrow\rangle + 0.99\,|\uparrow\downarrow\uparrow\rangle - 0.1\,|\downarrow\uparrow\uparrow\rangle\,, \quad 0.1\,|\uparrow\downarrow\downarrow\rangle - 0.99\,|\downarrow\uparrow\downarrow\rangle + 0.1\,|\downarrow\downarrow\uparrow\rangle$$

- **Anti-ferromagnetic phase**: $\Delta = -10$
  - degenerate ground states:

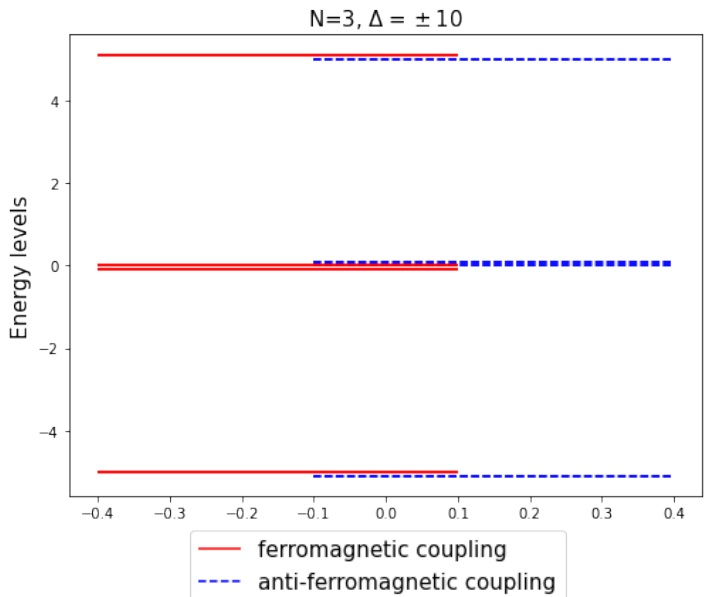
$$0.1\,|\uparrow\uparrow\downarrow\rangle + 0.99\,|\uparrow\downarrow\uparrow\rangle\, 0.1\,|\downarrow\uparrow\uparrow\rangle\,, \quad -(0.1\,|\uparrow\downarrow\downarrow\rangle + 0.99\,|\downarrow\uparrow\downarrow\rangle + 0.1\,|\downarrow\downarrow\uparrow\rangle)$$

  - 1^{st} excited states

$$0.71\,|\uparrow\uparrow\downarrow\rangle - 0.71\,|\downarrow\uparrow\uparrow\rangle\,, \quad 0.71\,|\downarrow\uparrow\uparrow\rangle - 0.71\,|\uparrow\downarrow\downarrow\rangle$$

$$0.7\,|\uparrow\downarrow\downarrow\rangle - 0.13\,|\downarrow\uparrow\downarrow\rangle + 0.7\,|\downarrow\downarrow\uparrow\rangle\,, \quad 0.7\,|\downarrow\uparrow\uparrow\rangle - 0.13\,|\uparrow\downarrow\uparrow\rangle + 0.7\,|\uparrow\uparrow\downarrow\rangle$$

  - 2^{nd} excited states: $|\uparrow\uparrow\uparrow\rangle\,, \quad |\downarrow\downarrow\downarrow\rangle$



Effect of the interplay between the Ising and the flip-flop term on the eigenvalues

- When looking at the diagonal terms in the Hamiltonian $E_{zz} = [2p - (L-1)]J\Delta/4$, they appears to form bands determined by the number of pairs p of (anti)aligned spins
- On the other hand, the eigenvalues distribution is strongly affected by the anysotropy Δ: when $\Delta < 1$ the flip-flop term is able to couple inter and intra-bands states, leading to loss of band structures. When $\Delta \gg 1$ the flip-flop term just broadens each band[3].

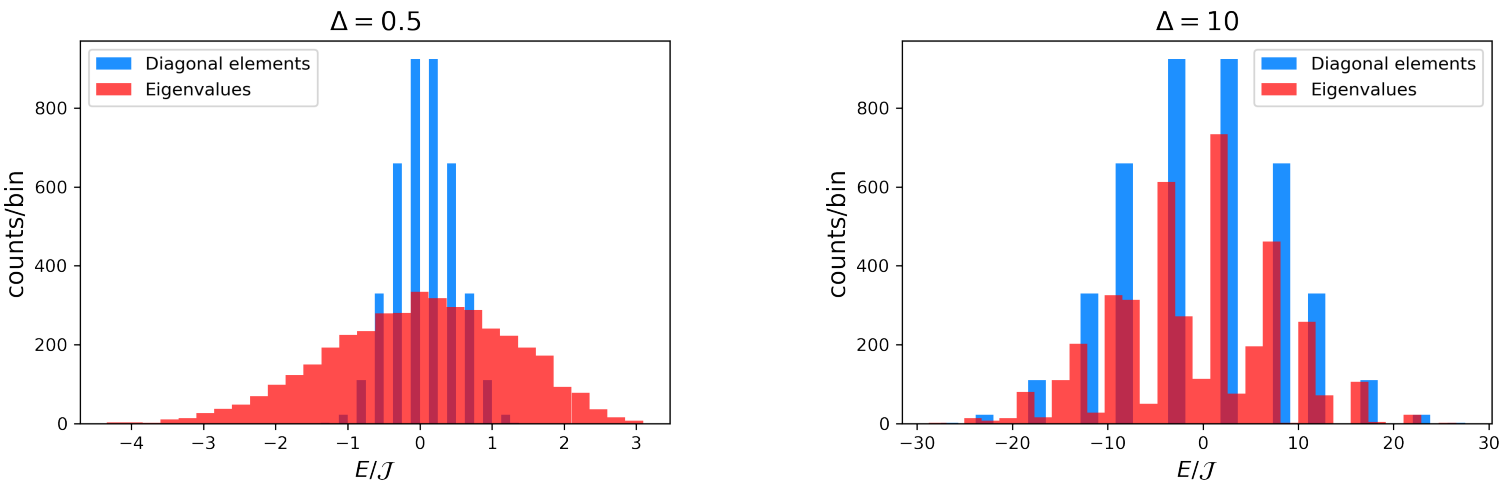


Figure: Diagonal elements (blue) and eigenvalues (red) for a system with $N = 12$ in $\Delta = 0.5$ (right) and $\Delta = 10$ regime

To study the interplay between the Ising and the flip-flop term on the eigenvectors structure, the chosen metric is the **Inverse Participation Ratio**[3]:

$$IPR = \frac{1}{\sum_{k=1}^{D} |a_k^{(j)}|^4},$$

being $a_k^{(j)}$ the projection of the j_{th} eigenvector on the k_{th} orthonormal basis element:

$$\left|\psi^{(j)}\right\rangle = \sum_{k=1}^{D} a_k^{(j)} \left|\phi_k\right\rangle$$

The IPR is proportional to the **number of basis vectors** participating in the energy eigenvectors and then it gives an indication on how spread the eigenvectors are:

- it exhibits **low** values when the eigenvector is **localized** in the chosen basis, i.e. in our case the quantum computation basis
- its extent grows when the eigenvector is **spread** in the chosen basis

With this premises set, in our case, IPR is an indicator on how much eigenvectors are oriented **along z** and we expect it to be deeply influenced by Δ.

The represented graphs report the trend of the average value over all eigenvectors of IPR in the ferromagnetic coupling (left) and in the anti-ferromagnetic one (right) as a function of Δ. The maximum of the distribution is reached around 0, when the system is in the XY disordered phase and converges towards minimum when increasing the anysotropy, reflecting the fact that alignment along z is favoured in this condition.

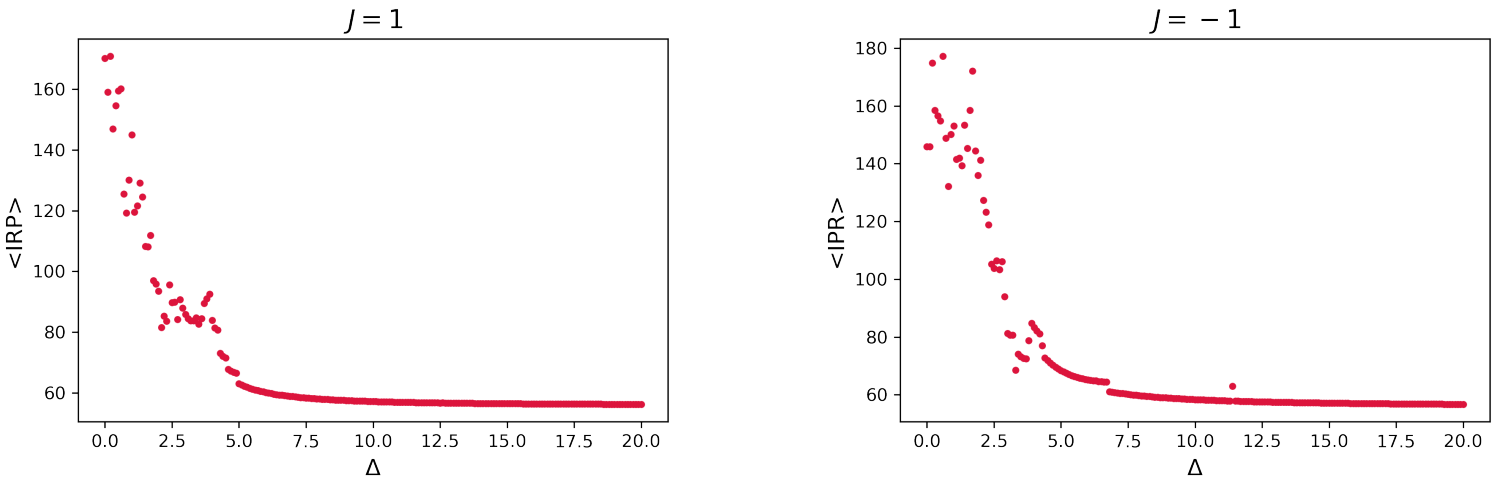


Figure: Inverse participation ratio varying Δ in respectively ferromagnetic and anti-ferromagnetic coupling

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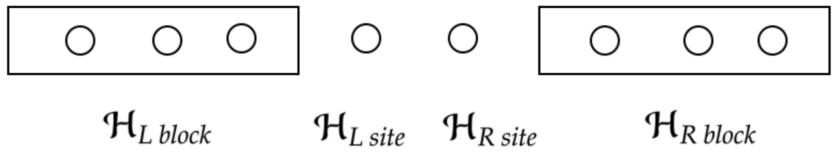


- Right and left **blocks** with $\mathcal{H}_{block} : \mathcal{C}^m \times \mathcal{C}^m$
- Right and left **single sites** with $\mathcal{H}_{site} : \mathcal{C}^d \times \mathcal{C}^d$

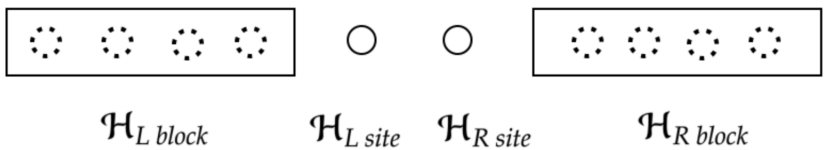
$$\hat{H} = \hat{H}_L \otimes \mathbb{1}_{m\times d} + \mathbb{1}_{m\times d} \otimes \hat{H}_R + \hat{H}_{int}$$
$$\hat{H}_L = \hat{H}_{L_{block}} \otimes \mathbb{1}_d + \mathbb{1}_m \otimes \hat{H}_{L_{site}} + \hat{H}_{int_{block-site}}$$
$$\hat{H}_L = \mathbb{1}_d \otimes \hat{H}_{R_{block}} + \hat{H}_{R_{site}} \otimes \mathbb{1}_m + \hat{H}_{int_{block-site}}$$

- compute the **ground-state** $|\psi_G\rangle$ and the correspondent **density matrix** $\rho = |\psi_G\rangle \langle\psi_G|$
- obtain the **reduced density matrix** for the left (right) sub-system and diagonalize it: $\rho_L = Tr_R \rho = \sum_1^{m\cdot d} w_i |w_i\rangle \langle w_i|, \quad \sum w_i = 1, \quad w_i \geq 0$
- obtain a **projector** $P_L : \mathcal{C}^{m\cdot d} \times \mathcal{C}^m$ from the first m ordered eigenvectors $w_1 \geq w_2 \geq \cdots \geq w_{m\cdot d}$

- perform **truncation**

$$H_{L_{block}} = P_L^{\dagger} H_L P_L$$
$$H_{int_{block-site}} = P_L^{\dagger} H_{int_{block+1-site}} P_L$$

- after this first step the total hamiltonian $\hat{H}$ represents an enlarged system, in which **single sites have been incorporated in blocks**



- after each step both of the two blocks represent a system with an additional degree of freedom: 'virtual' number of spins **grows linearly** with iteration number

$$N_{virtual} = 2(N_0 + N_{iteration})$$

From the behaviour of the ground-state energy per spin $e_G = E_G/(N-1)$, **three different phases**, and the correspondent phase transitions, can be recognised[5]:

- $\Delta < -1$: **anti-ferromagnetic phase**, with two degenerates ground states of couples of anti-aligned spins
- $\Delta > 1$: **ferromagnetic phase**, in which the system is in one of the two degenerates ground-states, displaying all the spins aligned either up or down, breaking the $\mathbb{Z}_2$ symmetry
- $-1 < \Delta < 1$: **XY paramagnetic phase**. In this phase no axial symmetry is found and the system is in a gapless critical phase

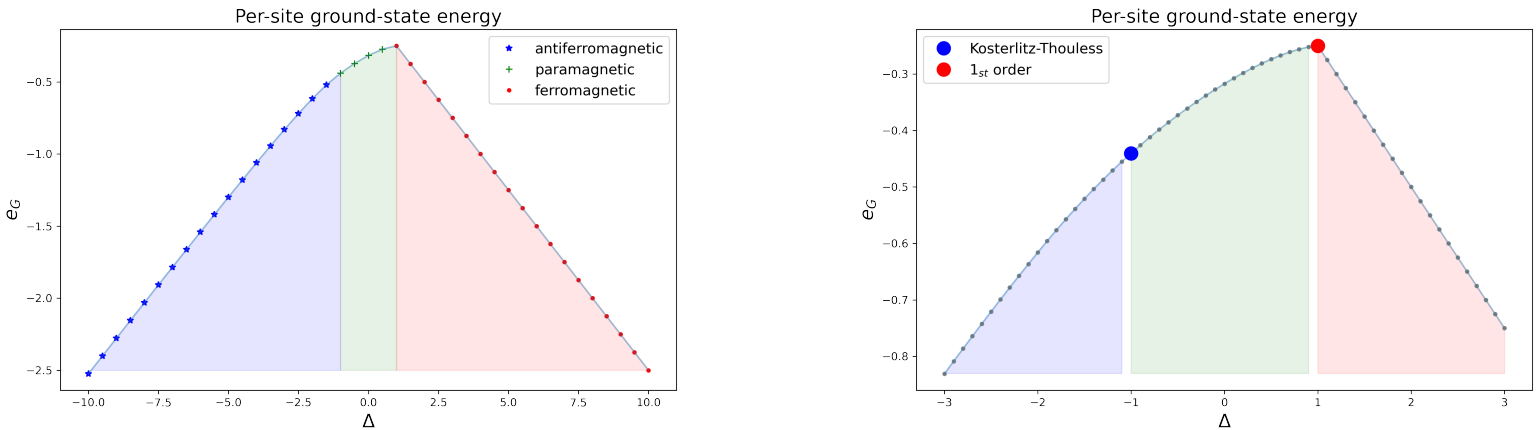


Figure: Per-site ground state energy across the three phases

- at $\boldsymbol{\Delta = -1}$ there is a **Kosterlitz-Thouless infinite order**[4] quantum phase transition from the gapped anti-ferromagnetic regime to the gapless (and so, as said, critical) paramagnetic one
- at $\boldsymbol{\Delta = 1}$ there is a **first-order** phase transition from the critical phase to the ferromagnetic Ising one. It can be clearly recognise when looking at the trend of ground state energy first derivative

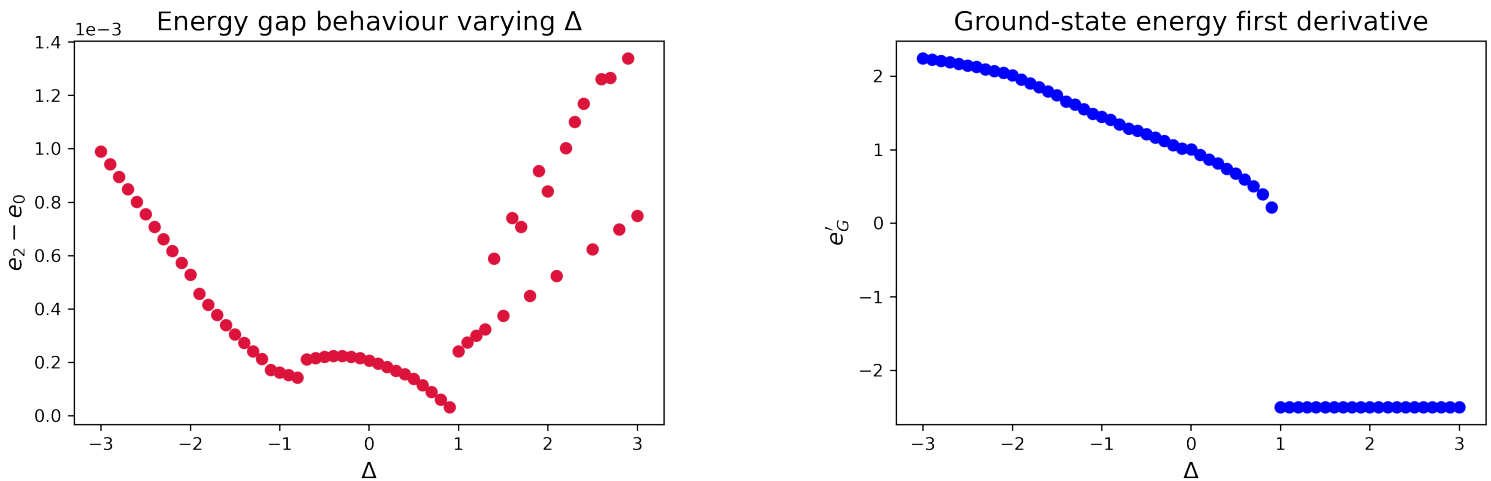


Figure: Energy gap (left) and ground state energy first derivative (right) varying Δ

Outline

- if a **bi-partite** system $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ is in a **pure state** $\rho = |\psi\rangle \langle\psi|$, then the **Von Neumann Entropy** of one of its two sub-systems, its a good measure of entanglement

$$S = -Tr\rho_A \ln \rho_A,$$

  where ρ_A is the reduced density matrix of sub-system A

$$\rho_A = Tr_B \rho$$

- In our case, it is considered the entanglement entropy of a **sub-chain** of length n with the rest of the $L - n$ spins chain.
- Entanglement entropy allows to identify **critical points and phase transitions**. When considering a 1D system in periodic boundary conditions at its ground state, in the critical region the **entropy diverges logarithmically** as[1], [6]:

$$S = \frac{c}{3} \log\left(\frac{L}{\pi a} \sin\left(\frac{\pi n}{L}\right)\right) + c_1'$$

- $\Delta = 0.5$, in the critical region
- $c_1' = 0.7305$ as obtained from conformal field theory (CFT)
- fitting function: $\frac{1}{3}\log\left(\sin\left(\frac{\pi n}{L}\right)\right) + c_1'$
- $\sigma(L = 10) = 7.0 \cdot 10^{-2}, \quad \sigma(L = 11) = 4.4 \cdot 10^{-2} \quad \sigma(L = 12) = 2.0 \cdot 10^{-2}$

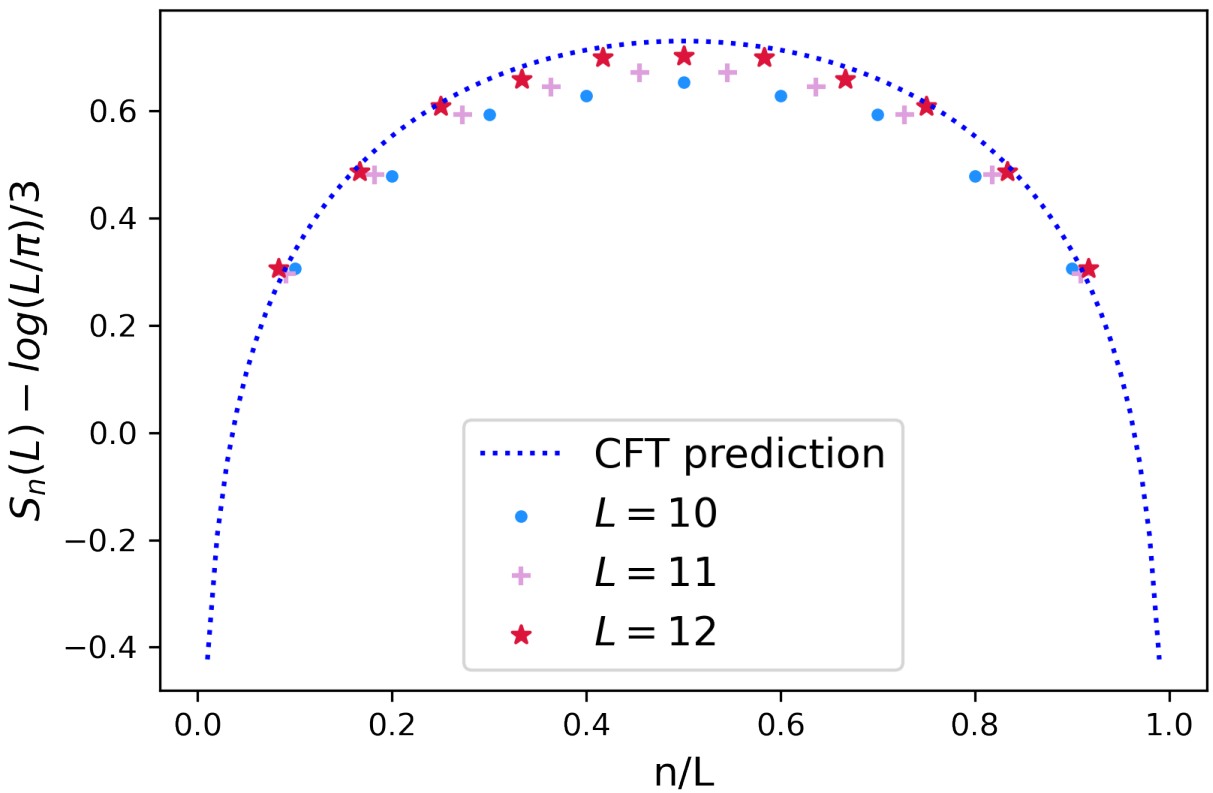


Figure: $S_n(L)$ for L=10, 11, 12 and CFT prediction for XXZ chain in PBC at $\Delta = 0.5$

Thanks for the attention!

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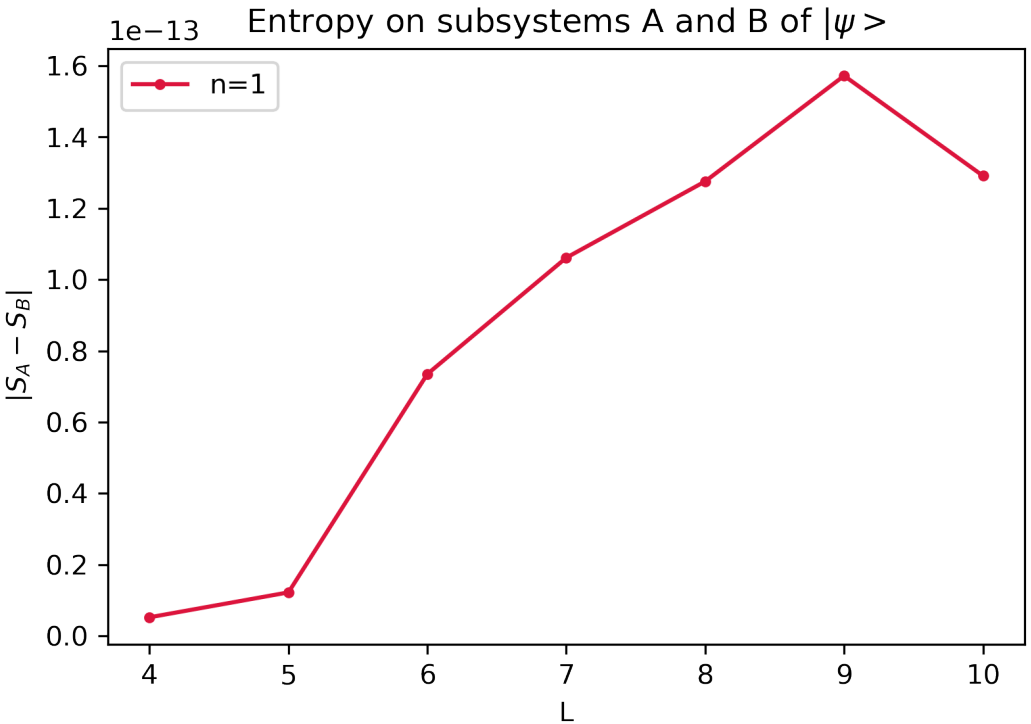
Entropy on subsystems A and B of $|\psi>$
1e−13
n=1
$|S_A - S_B|$
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
4
5
6
7
8
9
10
L

References

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