Scaling of entanglement support for iTEBD algorithm

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Abstract: We present the results obtained by using the iTEBD algorithm in the Ising and Heisenberg models as well as in the AKLT model. By modifying the external field parameter, in the Ising case, and the anisotropy parameter, in the Heisenberg case, we can observe quantum phase transitions in their ground states. In the AKLT model we study its generalization to find its phase transition. To study these transitions, we analyse the entanglement of the system near the critical point in order to find scaling laws.

I. INTRODUCTION

Entanglement plays an important role in distinguishing the nature of quantum versus classical systems. It is directly responsible for the appearance of long-rage correlations in the quantum critical phenomena which are the core of the quantum phase transitions. In contrast with classical phase transitions, which are driven by thermal fluctuations, these phase transitions occur at absolute zero temperature, and they are induced in the ground state of the system by changing an external parameter or an interaction coupling constant. They can be identified by a point of nonanalicity of the ground state energy caused by a level-crossing where an excited state becomes the ground state. However, if the system is finite the energy of the ground state will be an analytic function and it is possible to locate phase transition by finding a minimum of the energy gap between the two energy levels. Because entanglement is the heart of the study of strongly correlated quantum systems, finding out how entangled is the system we can identify the transition.

Entanglement also connects quantum information theory to the traditional quantum many-body systems, for example, topological systems such as fractional quantum Hall effect [1], topological insulators [2], graphene [3] or quantum teleportation [4]. Because of that, many figures of merit are used to measure the entanglement, such as purity or the entropy [5]. In this work it will be used the entropy of entanglement as a figure of merit. We need first to recall the basic construction of the Schmidt decomposition for any state in a bipartite Hilbert space $\mathcal{H} = \mathcal{H}_{\rm A} \otimes \mathcal{H}_{\rm B}$ [5]:

$$|\psi\rangle = \sum_{\alpha=1}^{\chi_A} \lambda_\alpha |\varphi_\alpha\rangle_A |\varphi_\alpha\rangle_B \tag{1}$$

where $\sum_\alpha |\lambda_\alpha|^2 = 1$ and ${}_A\langle\varphi_\alpha|\varphi_\beta\rangle_A = {}_B\langle\varphi_\alpha|\varphi_\beta\rangle_B = \delta_{\alpha\beta}$. The amount of entanglement between systems A and B can be quantified in terms of the von Neumann entropy of part A (or B):

$$S(\rho_A) = -\sum_\alpha \lambda_\alpha^2 \log_2 \lambda_\alpha^2 = S(\rho_B) \tag{2}$$

An important parameter in the present study is $\chi_A \equiv \mathrm{rank}(\rho_A)$, which is the Schmidt rank. We use the parameter $\chi \equiv \max_A \chi_A$ (the maximal Schmidt rank over all possible bipartite splittings A:B of the n system qubits) as a parameter to quantify the entanglement.

The paper is organized as follows. The tool that has been used to simulate and compute our results is presented in Section II, the infinite Time Evolution Block Decimation algorithm (iTEBD), which consists of an evolution on a family of relevant Tensor Networks states, e.g. Matrix Product States (MPS), for a given quantum Hamiltonian. In Section III we explain the approximations used to identify and classify the phase transitions. In order to validate these approximations, in Section IV are studied two known models: Ising and Heisenberg 1-d spin-1/2 chains. Finally, in Section V the AKLT model is discussed. We summarize our results in Section VI.

II. THE ITEBD ALGORITHM

In the many-particles studies finding an exact solution can be often too hard or impossible to compute. If we are talking about quantum systems the difficulty increases as a consequence that the Hilbert space grows exponentially with the number of particles. However, in the last years some classical strategies have been developed and they have given quite accurate results.

Tensor Network (TN) methods [6] have become increasingly popular to simulate strongly correlated systems. In these methods the wave functions of the system is described by a network of interconnected tensors. There are several examples of TN implementations, one of the most famous is Density Matrix Renormalitzation Group (DMRG)[7], introduced by Steve White in 1992 and the reference of these methods for the last 20 years to simulate 1d quantum lattice systems. Other examples are Projected Entangled-Pair States (PEPS) [8], to describe the evolution of systems of two and higher spacial dimensions, or Multi-scale Entanglement Renormalization Ansatz (MERA) [9], to describe systems with a topological order. Behind DMRG algorithm and other

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examples of TN methods there is the Matrix Product State (MPS) [10], an example of TN state. It consists to represent the coefficients of a quantum state as a product of matrices. Using the canonical form and the decomposition in Eq. 1 of a MPS, we finally can describe the system's wave function as [11]

$$|\Psi\rangle = \sum_{\{i\}}\sum_{\{\alpha\}} \left(\Gamma^{[1]i_1}_{\alpha_1}\lambda^{[1]}_{\alpha_1}\Gamma^{[2]i_2}_{\alpha_1\alpha_2}\lambda^{[2]}_{\alpha_2}\dots\lambda^{[N-1]}_{\alpha_{N-1}}\Gamma^{[N]i_N}_{\alpha_{N-1}}\right) |i_1\dots i_N\rangle \quad (3)$$

The Γ tensors correspond to changes of basis between the different Schmidt basis. In the case of an infinite MPS with one-site translational invariance [12], the canonical form corresponds to have just one Γ and one vector λ describing the whole state.

The infinite Time Evolution Block Decimation algorithm (iTEBD) allows to simulate unitary evolution and to compute the ground state of $1d$ quantum lattice system in the thermodynamic limit. This quantum system is described by an infinite MPS. Let us consider an infinite array of sites in 1-d, where $|\Psi\rangle$ denotes a pure state of the lattice. Given an initial state $|\Psi_0\rangle$, the iTEBD algorithm simulates the evolution according to H – a Hamiltonian with nearest neighbour interactions – in imaginary time [13].

$$|\Psi_\tau\rangle = \frac{\exp(-H\tau)|\Psi_0\rangle}{\|\exp(-H\tau)|\Psi_0\rangle\|} \quad (4)$$

The exponential is expanded through a Suzuki-Trotter decomposition [14] as a sequence of small two-site non-unitary gates U^{AB} and U^{BA} acting, respectively, on the qubit $[n, n+1]$ and $[n-1, n]$.

III. FINITE χ SCALING

For one-dimensional quantum chains at zero temperature it is generally known that the entanglement entropy of a system saturates away from criticality whereas it scales logarithmically when the system becomes quantum-critical, that is, when the correlation length diverges. We expect at the critical point a description of the ground state of the Hamiltonian in terms of a finite χ blurs a phase transition smooth. For instance, the diverging correlation length is replaced by a peak for the value of ξ_χ at some value of the local order parameter and should be dictated by the scaling relation $\xi_\chi \sim \chi^\kappa$. Thus, the *finite χ scaling* of a half-infinite chain shows

$$S \simeq \frac{c}{6}\log\xi_\chi \quad (5)$$

where c is the central charge associated with the universality class of the quantum phase transition. It is shown in [18] that the value of exponent κ for an infinite size algorithm could be estimated as

$$\kappa = \frac{6/c}{\sqrt{12/c}+1} \quad (6)$$

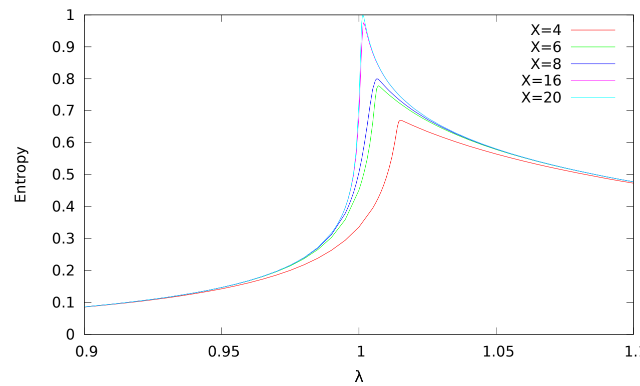

FIG. 1: Ising model entropy as a function of the external field λ for different Schmidt ranks χ. It is easy to identified the phase transition, where the entropy presents a maximum. The critical point shifts to $\lambda = 1$ as χ increases. The maximum grows up following an scaling law as we can see in Fig. (2). Theoretically, $S = 1$ when $\lambda = 0$ due to the system is a $|GHZ\rangle$, but because the structure of the algorithm there is a break on the symmetry and the probabilities of the initial states are not equiprobables, causing a null initial value for the entropy.

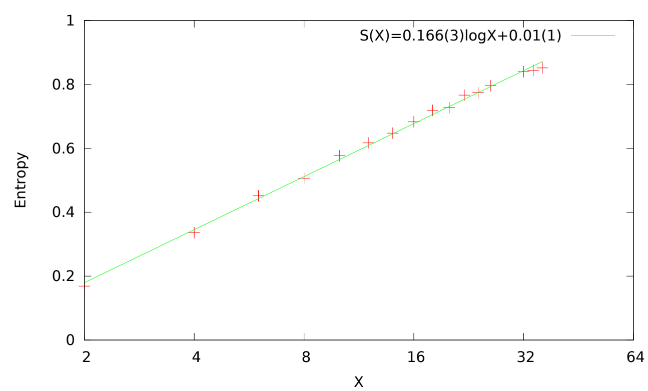

FIG. 2: Entropy as a function of $\log_2\chi$ at $\lambda = 1$ in the Ising model. The scaling law for the Ising model predicts that the entropy is proportional to $\log_2\chi$ with a constant of $1/6$, which is very similar to the result obtained.

Accordingly, we can evaluate the central charge without computing the correlation length

$$S = \frac{c\kappa}{6}\log\chi = \frac{1}{\sqrt{12/c}+1}\log\chi \quad (7)$$

IV. VALIDATION OF THE MODEL: QUANTUM ISING AND HEISENBERG SPIN CHAINS

In this section we present the validation of the *finite χ scaling* from the known models of quantum Ising model and Heisenberg model. Both describe a one-dimensional chain of $s = 1/2$ spins interacting with the nearest neighbours.

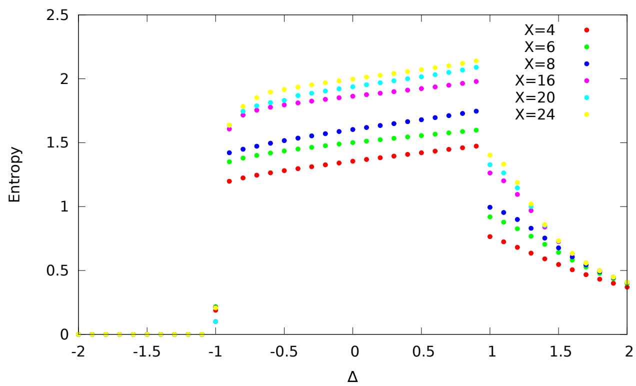

FIG. 3: Entropy as a function of the anisotropy parameter Δ for different Schmidt ranks χ in Heisenberg model. For $\Delta > 1$ the system is in the Neel phase, for $\Delta < -1$ the system is in the ferromagnetic Ising phase and when $-1 < \Delta < 1$ the system is critical. We can identify the two critical points for $\Delta = -1$ and for $\Delta = 1$, where there is a significant jump in the entropy.

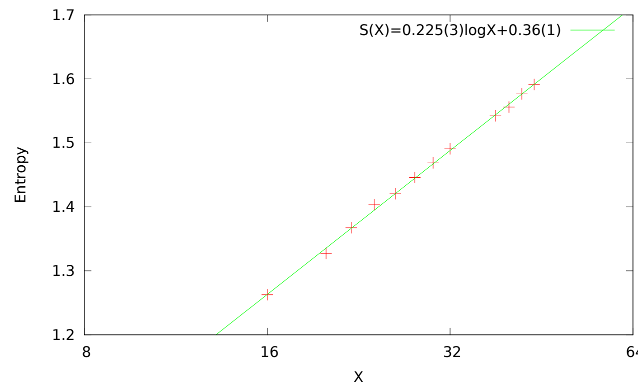

FIG. 4: Entropy as a function of $\log_2 \chi$ for the Heisenberg model with $\Delta = 1$. Fitting the data we can obtain the value of the exponent κ from the proportional constant, similarly as we have done with the Ising model. The κ value obtained is 1.35(2).

The Ising model is described by the Hamiltonian

$$\mathcal{H} = \sum_i \left(\sigma_i^x \sigma_{i+1}^x + \lambda \sigma_i^z\right) \tag{8}$$

where σ_i^x and σ_i^z are the Pauli matrices acting on the i-th spin and λ is the value of the external magnetic field that will be our order parameter.

The phase transition of this model is driven by λ. For small λ the x-magnetization dominates the state of the system – the spins tend to be oriented according to x-direction – but as λ grows, the transverse field in z-direction is taking relevance until overcomes the internal field. At that point, the system undergoes a phase transition and the system goes from a paramagnetic behaviour to ferromagnetic behaviour: initially, the spins are oriented in a randomly way, but after certain value of λ, spins are oriented in the direction of the external field.

The critical point is given when $\lambda^* = 1$ [15]. In Fig.1 we plot the entropy as a function of λ for different Schmidt rank χ . The entropy increases with lambda until the critical point λ^* from which decreases. We see how the entropy peak increases and shifts to $\lambda = 1$ as χ grows. Conformal field theory (CFT) sets a value of the central charge $c = 1/2$ for the Ising model, so from the relation (6) we expect to find a κ approximately closer to 2. In Fig. 2 it is shown the proportionality between the entropy and $\log \chi$ at criticality and the value for the exponent κ obtained is

$$\kappa \simeq 2.00(2) \tag{9}$$

We can also validate the relation (7) from the Heisenberg model. The model that is presented here corresponds with the XXZ and it is similar to the standard Heisenberg model but introducing an anisotropy in z-direction:

$$\mathcal{H} = \sum_i \left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z\right) \tag{10}$$

The parameter Δ describes the anisotropy of the system. In this model exists two phase transitions, for $\Delta = -1$ and for $\Delta = 1$. For $\Delta > 1$ the system is in the Neel phase which spontaneously breaks the lattice translation symmetry and the ground states are two-fold degenerate. For $\Delta < -1$ the system is in the ferromagnetic Ising phase which spontaneously breaks the spin reflection symmetry. When $-1 < \Delta < 1$ the system is in the gapless critical XY phase [17]. We expect to find an entanglement scaling law like in the case of the Ising model but with another value for the central charge; $c = 1$. The value of exponent κ that we find for $\Delta = 1$ is

$$\kappa \simeq 1.35(2) \tag{11}$$

which is close to the expected value that we obtain from (6) ($\kappa \simeq 1.34$).

V. THE AKLT MODEL

The AKLT model was proposed to simplify the description of quantum spin chains formed by particles with spins greater than 1/2. It consist in combine spin-1/2 particle and projected them into a total spin that interest us to define the chain, for example, for a spin-1 chain we projected two spin-1/2 first neighbours in a triplet state while stuck in a singlet state the second neighbours as shown in Fig.5. This model is an special case of the Hamiltonian

$$\mathcal{H} = \sum_i \left(S_i \cdot S_{i+1} + \beta \left(S_i \cdot S_{i+1}\right)^2\right) \tag{12}$$

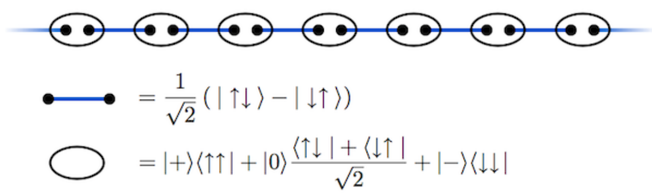

FIG. 5: Ground state of AKLT Hamiltonian. The solid points represent spin-1/2 which are put into singlet states. The lines connecting the spin-1/2 are the valence bonds indicating the pattern of singlets. The ovals are projection operators which bond together two spin-1/2 into a single spin 1.

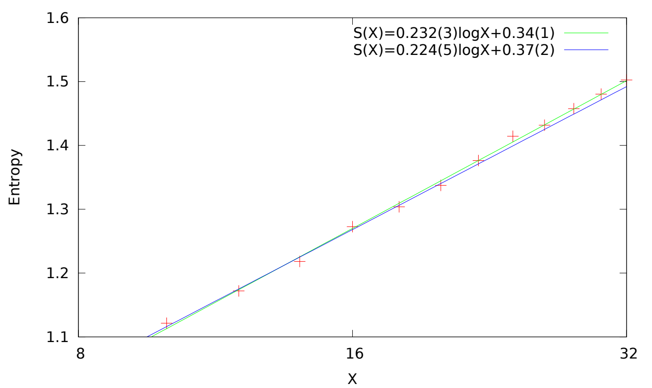

FIG. 6: Entropy as a function of $\log_2 \chi$ for the AKLT model with $\beta = 1$. Blue line corresponds to the fitting $\chi = [10 : 22]$ and the model presents a central charge $c \simeq 1.00(3)$, as the Heisenberg model. Green line corresponds to the $\chi = [10 : 32]$ fitting and the value of the central charge obtained is $c \simeq 1.09(2)$.

where S_i are the spin-1 matrices. When $\beta = 1/3$ we have the standard AKLT model where the second part of Eq. 12 corresponds to the projected spin-1 operator. The ground state of this Hamiltonian is called Valence Bond Solid (VBS) and can be described with spin-1/2 matrices [20].

The model with $\beta = 0$ corresponds to the standard Heisenberg model which have a unique massive ground state as $\beta = 1/3$ case. When $\beta = 1$ the model has an exact SU(3) symmetry and it is very likely massless [19]. We find a transition when $\beta = 1$ and the entropy seems to scale with χ as Heisenberg model, but if we consider greater χ's the slope increases (Fig. 6). If the model is massless the system has scaling invariance and the correlation length is infinite, but because we have done a finite approximation, the correlation length is finite although increases with χ. The system tends to reproduce the scaling invariance when $\chi \to \infty$, as expected.

VI. CONCLUSIONS

The amount of entanglement supported by the MPS approximation is limited by the size χ of the matrices that form the ansatz. We have studied numerically this issue in the cases of Ising and Heisenberg models and found that at criticality the entropy approaches to its exact value obeying scaling laws in χ. Both presents the central charge value predicted by the CFT confirming the considered approximations in Sec. III.

In the study of a generalization of AKLT model we have found, as expected, a transition when β parameter is equal to 1: the system goes from a unique massive ground state to a massless ground state. The correlation length is finite but increases with χ, so in the limit $\chi \to \infty$ tends to be infinite as CFT describes.

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