Critical exponents of one-dimensional quantum critical models by means of MERA tensor network

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An algorithm for optimizing the MERA tensor network in an infinite system is presented. Using this technique we compute the critical exponents of Ising and XXZ model.

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I. INTRODUCTION

Critical phenomena are ubiquitous in science ranging from condensed matter to biological or economic systems. They are associated to scale invariance, a diverging correlation length, and the various correlation functions decay as power law. A key issue in the study of critical systems is the computation of the critical exponents, i.e. the exponents which govern the decay of the correlations. The power of methods like the renormalization group stems from its capability to compute (analytically or numerically) the critical exponents.

In the field of quantum many-body systems important progress has been made recently in one-dimension where a number of tensor network approximations \cite{1,2,3,4,5,6,7,8} of the many-body wave-function allowing an efficient computation of all the relevant observables. The Multi-scale Entanglement Renormalization Ansatz (MERA) introduced by Vidal \cite{8} is particularly appealing since embeds scale invariance typical of critical systems. A method to relate the critical exponents in the MERA tensor network has been very recently put forward by some of us \cite{9} by relating them to the eigenvalues of the MERA transfer matrix.

In the present work we want to apply this method for the computation of the critical exponents of two cornerstone models in quantum statistical mechanics, the Ising and the XXZ model. To this end we provide an algorithm for optimizing the MERA tensor network in an infinite system and then, by employing the results given in \cite{9} we compute the critical exponents.

The paper is organized as follows. In the next section we briefly review the optimization of the MERA tensor network and how to compute the critical exponent. We then proceed with the comparison with the Ising and XXZ model defined in Section III. In Section IV we discuss the results and compare them with the exact known values. The last Section is devoted to the conclusions.

II. MERA OPTIMIZATION

Consider a 1-D translational invariant many-body quantum system at criticality composed of $L = 2^{\ell + 1}$ sites, each of them described by a local Hamiltonian and some nearest neighbor interactions. The global Hamiltonian can then be expressed as $H = \sum_k h_k$, where $k = 1, \cdots, L$ with $L + 1 \equiv 1$ for periodic boundary conditions and where $h_k$ is acting on the three consecutive sites $k - 1, k$, and $k + 1$ (the generalization to longer range interaction is straightforward). In the thermodynamic limit of infinitely many sites the ground state energy per site of the system can thus be computed as

$$E_G := \lim_{L \to \infty} \frac{\min_{\Psi} \langle \Psi | H | \Psi \rangle}{L} = \lim_{L \to \infty} \frac{\min_{\Psi} \sum_{k=1}^{L} \text{Tr}[\rho_k h_k]}{L},$$

where $|\Psi\rangle$ are joint states of the many-body system, and where the last minimization is performed over the sets $\mathcal{B}_\Psi := \{\rho_1, \cdots, \rho_L\}$ whose elements can be obtained as reduced density matrices of some global pure state $|\Psi\rangle$ of the system (specifically $\rho_k$ is the reduced density matrix of $|\Psi\rangle$ that is associated with the sites $k - 1, k$, and $k + 1$). Owing to translational invariance all the addends of the last term of Eq. (1) are equal. Thus without the constraint $\rho_k \in \mathcal{B}_\Psi$ the minimization would be trivial and $E_G$ would coincide with the the ground energy level of the 3-sites Hamiltonian $h_k$. Taking into account the condition $\rho_k \in \mathcal{B}_\Psi$ what makes the calculation of $E_G$ a hard problem to solve: it requires us to minimize the energy of $h_k$ by properly embedding $\rho_k$ in the "environment" formed by the remaining sites of the many-body system.

A solution can be found by adopting the so called Multi-scale Entanglement Renormalization Ansatz (MERA) \cite{8}, which, similarly to the matrix product state decomposition \cite{1,2,3,4,5,6,7,8}, assumes a specific representation of the many-body state $|\Psi\rangle$. In particular according to this ansatz the wave function of an $L$ sites many-body system is expressed in terms of $O(L \log_2 L)$ tensors of two different species (i.e. the type-(\(\frac{\ell}{2}\)) disentangler tensors $\chi$ and type-(\(\frac{\ell}{2}\)) isometry tensors $\lambda$) which are connected to form a multi-layer structure which admits efficient contraction rules (see Fig. I — we refer the reader to Ref. \cite{8} for details). Specifically, following Ref. \cite{9} we will restrict the minimization to states $|\Psi\rangle$ which can be expressed (or at least approximated) by homogeneous MERAs, in which all the disentangler $\chi$ and all the isometry $\lambda$ entering the tensor network are identical. Under these conditions it has been shown \cite{9} that the
thermodynamic limit \( L \to \infty \) of \( |\Psi\rangle \) can be characterized in terms of a transfer super-operator (the QuMERA map \( \Phi \)) that is determined by the \( \chi \)'s and the \( \lambda \)'s that forms the MERA \cite{10}. In particular the reduced density matrix \( \rho_k \) of \( |\Psi\rangle \) can be computed as the (unique) eigenvector \( \rho_k^* \) of the MERA transfer super-operator (QuMERA map) \( \Phi \) associated with the unitary eigenvalue, i.e.

\[
\Phi(\rho_k^*) = \rho_k^* .
\] (2)

This means that Eq. (1) can now be expressed as

\[
E_G = \min_{\Phi} \text{Tr}[\rho_k^* h_k] ,
\] (3)

where the minimization is performed over the set of all possible QuMERA channels \( \Phi \) – the equivalence being guaranteed by the stationary condition \cite{2}. Equation (3) achieves two fundamental goals: i) it allows us to directly address the thermodynamic limit, ii) it guarantees the possibility of reconstructing a many-body joint state \( |\Psi\rangle \) associated with the three sites local density operator \( \rho_k^* \) (this is the MERA state corresponding to the QuMERA channel \( \Phi \)). In other words, exploiting the above derivation the constrained energy minimization problem \cite{1} corresponds to minimize the functional

\[
F(\Phi, \rho) = \text{Tr}[\Phi(\rho) h] + \mathcal{L} \|\Phi(\rho) - \rho\|,
\]

where \( \mathcal{L} \) is a Lagrange multiplier. This is the main result of this paper and as we will show in the following, this allows us to compute the thermodynamic ground state energy employing a number of steps which do not depend upon the system size (the limit \( L \to \infty \) being already included in the QuMERA description). Once the transfer operator has been found via minimization, as shown in \cite{3}, the long range properties (critical exponents) can be easily computed.

A. Minimization

The problem of finding the ground state properties have been reformulated in terms of the minimization of the quantity \cite{3} with the additional constraint \cite{2}. To solve it we proceed with an iteration procedure starting from an initial guess \( \Phi_0 \) and \( \rho_0^* \) for the QuMERA channel \( \Phi \) and its associated eigenvector \( \rho^* \). Specifically, all the \( \chi \) and \( \lambda \) tensors entering in the definition of the transfer super-operator \( \Phi \) are given by an initial guess \( \chi_0 \) and \( \lambda_0 \) which we optimize by varying each of them one at the time. In this framework the problem is reduced to perform the following minimizations

\[
\min_{\chi} \{ \text{Tr} \left[ (\lambda_0 \chi \lambda_0 \chi_0) \rho_0^*(\lambda_0 \chi \lambda_0 \chi_0) h \right] \} ,
\] (4)

where the tensors are contracted following rule given in Fig. 1 (here we specialize in the case of the optimization of \( \chi \), while keeping fix the initial guess for \( \lambda_0 \) and \( \rho_0^* \)). Possible strategies to solve such minimization have been presented in \cite{11} where unconstrained quadratic optimization have been considered. This approach is not longer applicable in our case where the homogeneity constraint adopted to deal with the translational invariance of the system, forces all the \( \chi \)'s and \( \lambda \)'s entering in Eq. (1) to be identical while transforming the minimization in a non-quadratic optimization problem. To cope with this we approach Eq. (4) by computing at each step the linearized gradient on a basis for the tensors belonging to the MERA, while alternating moving from the \( \chi \)'s to the \( \lambda \)'s. Once the gradient is computed we move the tensor in a random direction whose signs in a given basis (going forward or backward along a given direction) are defined by the gradient’s ones as in Ref. \cite{12}.

Once the optimization of the \( \chi \) and the \( \lambda \) have been performed and a new QuMERA channel \( \Phi_1 \) is defined, the stability constraint \cite{2} have to be fulfilled. Hence, we replace \( \rho_0^* \) with a new guess \( \rho_1^* \) from the eigenvector of the eigenproblem \( \Phi_1 (\rho_1^*) = \rho_1^* \), which can be addressed by using some smart eigen-problem solvers as the Lanczos or Davidson algorithms. The latter approach is favorable also due to the presence of a “good guess” \( \rho_0^* \) for the new eigenvector \( \rho_1^* \). The result presented in the next sections are obtained using this second method. We can then proceed again in optimizing another tensor belonging to the transfer super-operator up to the desired convergence. Notice that this procedure is not guaranteed to converge to the optimal minimum, however in general gives good results.

III. THE MODELS

The models we consider are defined through the Hamiltonian

\[
H = -\frac{J}{2} \sum_j [(1 + \gamma) \sigma_j^x \sigma_{j+1}^x + (1 - \gamma) \sigma_j^y \sigma_{j+1}^y + \Delta \sigma_j^z \sigma_{j+1}^z + 2 b \sigma_j^z] ,
\] (5)
where $\sigma_i^\alpha$ ($\alpha = x, y, z$) are the Pauli matrices of the $i$-th spin. The constants $J$, $\Delta$, $\gamma$ and $b$ respectively characterize the interaction strength between neighboring spins, the anisotropy parameter along $z$ and in the $xy$ plane, and an external transverse magnetic field. The Hamiltonian $[5]$ has a very rich structure $[13]$. We consider the two cases:

- the Ising-model in a transverse field. Here one has $\Delta = 0$ and $\gamma = 1$. The model presents a critical point at $|b| = 1$.

- the $XXZ$ anisotropic Heisenberg model. Here one has $b, \gamma = 0$ and $\Delta$ generic. In this case the Hamiltonian $[5]$ is critical for $-1 \leq \Delta \leq 1$ while it has ferromagnetic or anti-ferromagnetic order for $\Delta > 1$ or $\Delta < -1$ respectively.

The exact critical exponents, related to the correlation functions

$$\langle \sigma_i^\alpha \sigma_{i+t}^\alpha \rangle - \langle \sigma_i^\alpha \rangle \langle \sigma_{i+t}^\alpha \rangle \sim r^{-\nu_\alpha},$$

are given by

- Ising model ($\gamma = 1, \Delta = 0$)

  $\nu_z = 2, \quad \nu_x = 0.25, \quad \nu_y = 2.25,$

- $XXZ$ model ($\gamma = 0, |\Delta| \leq 1$)

  $\nu_x = \nu_y = 1/\nu_z = 1 - \arccos(\Delta)/\pi.$

We are going to compare our numerical results against these values.

**IV. RESULTS**

The algorithm we developed for solving the minimization of Eq. (3) requires to store order of $O(m^6)$ tensors with $m$ being the dimension of the indexes of the $\chi$s and $\lambda$s, their multiplication ($O(m^{10})$ operations) and their diagonalization. As for the t-MERA $[14]$ this is “reasonable” up to $m = 4, 6$.

We first concentrate on the Ising model, where we have obtained an energy convergence to the exact energy per site of the ground state at the thermodynamic limit of the order of $\delta E = 10^{-4}$. In Fig. 2 we report (in decreasing order) the modulus of eigenvalues of the QuMERA map $\Phi$ found by means of the minimization strategy we represented in the last section. As discussed in $[9]$ we expect the first eigenvalue ($\kappa = 1$) to be non-degenerate as the $\Phi$ should be mixing. The subsequent eigenvalues instead express the critical exponents of the system via the relation:

$$|\kappa_\alpha^l| = 2^{-\nu_\alpha/2}.$$  

The dashed red lines of the Figure report the theoretical expectations of the eigenvalues. The result is good, the first one is exact up to the machine precision, while the others have numerical errors of the order of $\delta|\kappa| \sim 10^{-4}, 10^{-2}, 10^{-2}$.

The results obtained for the Ising model are very promising, however it is well known that the Ising model...
V. CONCLUSIONS

This paper presents a recursive algorithm for optimizing the MERA tensor description of the ground state $|\Psi_G \rangle$ of a critical many-body Hamiltonian in the thermodynamic limit of infinitely many sites. It is based on the results of Ref. [9] which established a connection between $|\Psi_G \rangle$ and the transfer super-operator of the MERA network that approximates it.

While completing the writing of the present manuscript we became aware of a work by Pfeifer, Evenbly and Vidal (arXiv:0810.0580v1) employing a modified MERA tensor network representation seems to lead to a more efficient evaluation of the critical exponents.

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