Entanglement renormalization of anisotropic XY model

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Abstract – The renormalization group flows of the one-dimensional anisotropic XY model are obtained by different multiscale entanglement renormalization ansatz schemes. It is shown that the optimized disentangler removes the short-range entanglement by rotating the system in the parameter space spanned by the anisotropy and the magnetic field. It is understood from the study that the disentangler reduces the entanglement by mapping the system to another one in the same universality class but with smaller short-range entanglement. The phase boundary and corresponding critical exponents are calculated using different schemes with different block sizes, look-ahead steps and truncation dimensions. It is shown that a larger truncation dimension leads to more accurate results and that using a larger block size or look-ahead step improves the overall calculational consistency.

The real-space renormalization-group (RSRG) [1] revolving around the coarse-graining and rescaling transformation, has been proven to be a very useful tool in the understanding of the critical phenomena and the quantum many-body system, whose difficulty lies in the exponential growth of the Hilbert space with the system size. The original RSRG, introduced by Wilson based on the block spin idea [2], addresses the problem by dividing the system into blocks and truncating the block Hilbert space to a subspace spanned by a few eigenstates of the lowest energies [1]. Later, White suggested that one should consider the interplay between the block and its environment in the truncation and promoted the density matrix renormalization group (DMRG) [3]. In DMRG algorithm, the states to be retained are the eigenstates with the largest eigenvalues of the reduced density matrix of the ground state of the block and its environment [3]. Since the reduced density matrix measures the entanglement between the block and its environment, it is later understood that the performance of DMRG depends on the entanglement in the ground state [4]. Unfortunately, near the quantum critical point, the ground state has large entanglement and hence one needs large truncated dimensions to get accurate results. To solve this problem, Vidal proposed a new entanglement renormalization ansatz (MERA) [5,6], by introducing an additional unitary transformation \( U \), the disentangler, which acts on the boundary of the adjacent blocks to remove the short-range entanglement (SRE) before performing the coarse-graining. MERA has been shown to be a successful numerical scheme in a lot of different physics systems, such as one-dimensional [6] and two-dimensional quantum spin system [7], interacting Fermions [8], boundary critical phenomena [9]. Using scale-invariant MERA and some modest truncation dimensions, the critical exponents for different systems are obtained with remarkable accuracy [5]. Several digest of accuracies in the critical exponents for various models have been achieved [5]. The success of MERA is mainly attributed to the presence of the disentangler, which was introduced to remove the entanglement. In ref. [5] it is shown numerically that disentangler can indeed reduce the entanglement entropy of the block. However, there is no analytical form for the disentanglers. Except for the numerical evidences in ref. [5], there is no analytical understanding on how the disentanglers affect the system. Given the central role that disentanglers play in MERA, it is of interest to obtain further insight into how they work by obtaining some analytical forms for the disentanglers. In order to do so, we apply MERA to study the one-dimensional (1D) anisotropic XY chain (AXY) under a transverse field. As we can see below, AXY model is mapped into itself under some restricted MERA

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transformation. Thus the 1D AXY model provides a platform for one to analytically understand how the disentanglers work. It should be pointed out that, our goal here is not to solve this model as accurate as possible by increasing the truncation dimension, but to understand how the disentanglers work by comparing the results from different MERA schemes. In doing so, we only use small truncation dimensions, such as 2 or 4.

The Hamiltonian of AXY is defined as $H = \sum_i H_i$, with [10]

$$H_{i+1} = -\frac{J}{2}[(1 + \gamma)S^x_i S^x_{i+1} + (1 - \gamma)S^y_i S^y_{i+1}] - \frac{h}{2}(S^z_i + S^z_{i+1}),$$

(1)

where $i$ is the site index, $S^\alpha = \sigma^\alpha/2(\alpha = x, y, z)$ are the spin components represented by the Pauli matrix $\sigma^\alpha$, $J$, $\gamma$ and $h$ stand for the interaction strength, anisotropy of the interaction and transverse field, respectively. In the limits of $\gamma = 0$ and 1, the model becomes the XY model and the Ising model in a transverse field (ITF), respectively. The model is exactly solvable by using the Jordan-Wigner and Fourier transformations [11].

The ground state of AXY in the regime $0 < \gamma \leq 1$ belongs to the quantum Ising model universality class [11]. The system exhibits three critical lines at $x_c(\gamma) = h_c(\gamma)/J = \pm 1$ and $y_c = 0$. The ground state of the system is in the ferromagnetic phase when the magnetic field is weak ($|x| = |h/J| < 1$), while in the paramagnetic phase when the field is strong ($|x| = |h/J| > 1$).

At the critical field, the system undergoes a quantum phase transition (QPT). Due to its exact solvability and rich physics, AXY and its special case ITF have been extensively studied to understand the nature of QPT, especially the role of the entanglement in QPT [12]. It also provides a test field for new numerical schemes [13]. The phase diagrams and the critical exponents of AXY and ITF have been obtained using exact diagonalization [11], various RSRG and DMRG schemes [13]. In this paper, we study these models by using different MERA schemes.

MERA can be understood as a quantum circuit or renormalization group (RG) transformation [5,6,14]. Here we briefly summarize MERA from the RG point of view. For more technique details, one is refereed to refs. [5,6,14].

As demonstrated in fig. 1, the system is divided into blocks of $n$ sites, with the $j$-th block composed of sites from $(jn + 1)$-th to $(j + 1)n$-th. The RG transformations are performed by applying a series of disentanglers $U_j$ and isometries $W_j$ on these blocks. When the system is invariant under the translation transformation, the disentanglers $U_j$ and isometries $W_j$ can be chosen to be the same $U$ and $W$ for each block. The coarse-graining is implemented by the isometries, which apply on a $n$-site block and maps the Hilbert space on the block into a new space on a coarse-grained site. The new Hilbert space is truncated to a subspace of dimension $\chi$ that is small enough for one to carry out the calculation, but large enough to represent the system faithfully. The disentangler applies on the two boundary sites of the two neighboring blocks and maps the Hilbert space on these two sites into another two-site space. The purpose of the disentangler is to remove SRE so that one can use small $\chi$ to get accurate results even in the critical regime. The application of the disentangler $U_j$ and the isometry $W_j$ lifts the system on the original sites to a new system on the coarse-grained sites. Under this transformation, Hamiltonian terms composed of local operators are mapped into another local Hamiltonian. Especially, after the application of the disentanglers, the two-body Hamiltonian terms $H_{jn,jn+1}^{(0)}$ are mapped into $H_{jn,jn+1}^{(0)} = U^\dagger H_{jn,jn+1} U$, while the Hamiltonian terms $\sum_{i=(j+1/2)n}^{(j+1)n-1} H_i^{(0)}$ are mapped into $H_{j,j+1}^{(1)} = W_j^\dagger W_{j+1} H_{j,j+1} W_j W_{j+1}^\dagger$.

Here $H_{jn,jn+1}^{(0)}$ is the Hamiltonian term $H_i$ defined in eq. (1). By comparing the properties of the Hamiltonian of the original system $H_i^{(0)}$ and the corresponding coarse-grained version $H_i^{(1)}$, one can get the renormalized parameters that define the coarse-grained system. Repeating the process on the coarse-grained systems by using other sets of $U$ and $W$ one then gets a well-defined RG flow.

In order to target the ground state, we assume that the ground state takes the form of the block mean-field state [15] after $\tau$-layer coarse-graining,

$$|\Phi^{(\tau)}\rangle = \Pi_j |\phi_j^{(\tau)}\rangle,$$

(2)

where $|\phi_j^{(\tau)}\rangle$, whose form does not depend on $j$, is a wave function defined on the $j$-th block at the $\tau$-th coarse-grained layer. In MERA’s language, we use translational invariant MERA, but set the truncation dimension of the top $[(\tau+1)-th]$ layer isometry to be 1. The disentanglers and isometries corresponding to this block mean-field state are optimized by the algorithm for the translational
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invariant MERA presented in ref. [6]. For the coarse-grained Hamiltonian to have same symmetries as the original one, the disentanglers and the isometries are chosen to preserve the spatial reflection symmetry and global parity symmetry [16]. It should be noted that even though we might use more than one layer of coarse-graining to obtain the ground state in the form of eq. (2), the RG flow is solely determined by the disentangler \( U \) and isometry \( W \) at the first layer. Once we have \( U \) and \( W \), we can use them to construct the eigenoperators and the corresponding eigenvalues of the RG transformation [17]. At fixed points, the eigenvalue \( \lambda \) relates to the critical exponent as \(-\ln(\lambda)/\ln(n)\). By studying the forms of the eigenoperators, one is able to connect the corresponding eigenvalues to the critical exponents. For example, at the critical point, the Hamiltonian is itself an eigenoperator of the RG transformation. Once one finds the eigenoperator which has same form as the Hamiltonian, one then obtains critical exponent \( z \) from the corresponding eigenvalue. Similarly, one can obtain the critical exponents \( \nu \), corresponding to eigenoperators \( S_i \otimes S_j \rightarrow S_i \otimes S^\prime_j \), and \( \beta \), corresponding to the transverse magnetization \( S_z \). The error mainly comes from the truncation error due to the finite truncation dimension \( \chi \) and the uncertainty of the fixed-point position, which in our calculation is determined to three digit accuracy. Our RG scheme is similar to the Born-Oppenheimer RG scheme used in ref. [15] with multiple look-ahead steps. However, we do not need to introduce some artificial parameters to describe the slow mode, which is nothing but the effect of the inter-block interaction and is naturally and self-consistently taken into account in MERA scheme. Like the original Born-Oppenheimer RG scheme, \( \tau \) can be viewed as look-ahead step. The scale-invariant MERA [5,6] used to study the critical system can be seen as an approximation of infinite look-ahead steps. In the following we will discuss the results for different MERA schemes, such as with/without disentangler, different block size \( n \), look-ahead step \( \tau \). For simplicity, the schemes are denoted by a string “n\( \tau \)x\( Z \)”, where \( n \) is the block size, \( \tau \) is the look-ahead step, \( x \) can be 1 for the simple block mean-field state or \( \infty \) for the scale-invariant scheme. \( Z \) is “D” or “I” for schemes with or without disentangler, respectively.

We first focus on the simplest case when only two states, one with even parity and the other with odd parity, are retained so that we can track the RG flow analytically. Under the restriction of symmetry requirement, the disentangler takes the form of \( U = U_E + U_O \) with \( U_E \) and \( U_O \) applying on the even and odd parity subspace, respectively. For the disentangler acts on sites 0 and 1, \( U_E \) and \( U_O \) take the following two possible forms:

\[
U_E = \begin{cases} 
\cos \theta & (1 + \sigma_0^x \sigma_1^x) + i \sin \theta & (\sigma_0^+ \sigma_1^y + \sigma_0^- \sigma_1^y), \\
\cos \theta & (\sigma_0^x \sigma_1^x) + i \sin \theta & (\sigma_0^+ \sigma_1^y - \sigma_0^- \sigma_1^y), 
\end{cases}
\]

\[U_O = (1 - \sigma_0^+ \sigma_1^+)/2 \text{ or } (\sigma_0^- \sigma_1^y + \sigma_0^+ \sigma_1^y)/2.\]  

The disentangler keeps the form of the AXY Hamiltonian \( H_{i,i+1} \) on the boundary sites unchanged, but maps the anisotropy \( \gamma \) and magnetic field \( x \) as

\[
\gamma' = \gamma \cos 2\theta + x \sin 2\theta, \\
x' = -\gamma \sin 2\theta + x \cos 2\theta.
\]

That is, it rotates the vector \((\gamma, x)\) in the parameter space by \(2\theta\). Since SRE depends on these parameters [12,18], it is possible for the disentangler to remove the inter-block entanglement by a suitable rotation. It is noted that even if one starts from the ITF model in which \( \gamma = 1 \), the application of non-identity disentangler makes it become the general AXY model with \( \gamma \neq 1 \). This is quite different from the previous RSRG schemes for ITF where the RG transformations do not change the form of the ITF Hamiltonian. The change from ITF to AXY should not affect the calculation of the critical properties since the anisotropy is an irrelevant term and AXY belongs to the same universality class for the whole regime \( 0 < \gamma \leq 1 \).

To see the effect of the disentangler on SRE, we use the concurrence of the ground state of the two-qubit system [18,19] composed of the spins on the two adjacent sites as an estimation of SRE. Note that we choose the concurrence to measure SRE because of its simplicity. Other definitions, such as entanglement entropy, can also be chosen to serve the purpose since the concurrence is monotonically related to them [19] in the two-qubit system. It is known that the concurrence \( C \) of the two-qubit system stays at 1 for \( \eta = \sqrt{\gamma^2 + x^2} < 1 \) and decreases as \( \gamma/\eta \) when \( \eta \) is larger than one. At exactly \( \eta = 1 \), the concurrence is \(\gamma/2\) which is a local minimum when \( x < \gamma^2(4 - \gamma)/(2 - \gamma)^2 \) [18]. Strictly speaking, this concurrence can only measure the entanglement of the isolated two-qubit system and should not be regarded as the exact SRE between the two boundary spins. Nevertheless, it provides some qualitative information of SRE and the simple form enables one to understand the role of disentangler analytically. In fig. 2, we plot the
concurrency of the ground state of the two-qubit system after the application of the disentangler for different magnetic fields and anisotropies. For comparison, we also plot the concurrency of the original and coarse-grained two-qubit system. The figure clearly shows that the disentangler indeed reduces the SRE. Analytically, the optimized $\theta$ is larger than zero when $\eta < 1$ and approaches to negative values when $\eta$ becomes larger than 1. When $\eta = 1$, the optimized $\theta$ is about 0. One can see from these results that, the optimized disentangler reduces SRE by mapping the system to a new one of the same universality class but with smaller entanglement.

In fig. 3, we present the flows in the parameter space under RG transformation and the phase boundary defined by the flows. It is seen that the system has three critical lines at $\gamma = 0$, $x \leq 1$, and $0 < \gamma \leq 1$, $x = x_c(\gamma)$ that divide the parameter space $-1 \leq \gamma \leq 1$ and $-\infty < x < \infty$ into four parts (since the diagram is symmetrical under $x \rightarrow -x$ and $\gamma \rightarrow -\gamma$, only one part is shown in the figure). Starting from $\gamma > 0$, $x > x_c(\gamma)$, RG transformations eventually bring the system to the attractive point $\gamma = 1$, $x = 0$ which represents the ferromagnetic phase. While starting from $\gamma > 0$, $x < x_c(\gamma)$, it is brought to another fixed point at $\gamma = 0$, $x = \infty$, corresponding to the paramagnetic phase. On the critical line $x = x_c(\gamma)$, there is a critical fixed point $0 < \gamma = \gamma_c \leq 1$. The physical critical fixed point is $\gamma_c = 1$, $x_c = 1$. In table 1, we list the critical field for $\gamma \simeq 0$ and 1, critical fixed point and some of the critical exponents obtained from 321D scheme. To show the effect of the disentangler, we also list the corresponding results from 321II scheme, which is identical to 321D except that it does not have disentangler, for comparison. One can easily see that adding the disentangler greatly improves the accuracy of the phase boundary and the critical exponents. For example, without the disentangler, the critical field for the Ising model is $x_c(1) = 1.291$ from 321I scheme while with disentangler it is 1.081. Moreover, these two schemes give different critical fixed points. For 321II schemes, it is $\gamma_c = 1$, $x_c = 1.291$ which is in consistence with the results from standard RSRG and DMRG schemes. However, with disentangler the critical fixed point becomes $\gamma_c = 0.801$, $x_c = 1.071$ for 321D scheme, clearly deviates from that of 321I scheme. Comparing to the 321II scheme, with the 321D scheme, one gets more accurate critical magnetic field $x_c$, which is a relevant parameter, but less accurate critical anisotropy $\gamma_c$, which is an irrelevant parameter in the AXY model. The difference in the positions of the critical fixed point is a result purely from the disentangler. It further reveals the role of the disentangler in MERA scheme. Namely, the disentangler changes the position of the critical fixed point so that the critical system has smaller SRE and can be better represented by small truncation dimension.

The number of the look-ahead steps also affects the accuracy. Generally speaking, larger $\tau$ leads to more accurate results but also larger computational costs. The optimal choice of $\tau$ can be understood from RG and MERA point of view. The wave function obtained here is a variational one in the product state form. For a system that is not close to the critical regime, a few RG transformations should bring the system to the attractive fixed points such as the paramagnetic or ferromagnetic states, whose ground states are the simple product states. Therefore for a system away from critical regime, one can use the wave function in the form of eq. (2) with small $\tau$ to represent the ground state accurately. Further increasing $\tau$ should only have small effect since the disentanglers and isometries on the top layers would be identical to each other as the system flows to the trivial fixed points. When the system is close to the critical point, one needs more RG transformations, hence larger $\tau$, to bring the system to the product state. Exactly at the critical points, one needs infinite $\tau$ to represent the ground state faithfully using the product state form. In this case, the disentanglers and isometries on the lowest layers are different from each other since the irrelevant terms are different at different RG stages. As one goes up to the higher layer, these irrelevant terms eventually vanish and the system is brought to the critical fixed point. After that, the disentanglers and isometries will be the same for different layers due to the scale invariance. In practice, one can choose a few “free” layers with different disentanglers and isometries, then put scale-invariant layers on top of the “free” layers. This scale-invariant MERA scheme was used to study the properties of various critical systems [6]. It was believed that the scale-invariant MERA can only be applied to the critical system. However, we argue that since it can be seen as an approximation of MERA with infinite look-ahead steps, one can expect that the scale-invariant MERA can represent the system faithfully in the vicinity of the fixed points no matter they are critical or noncritical.

The results with different look-ahead steps are listed in table 1. At first glance, it seems that different look-ahead steps do not lead to any significant difference in phase boundary and critical exponents. Product state MERA and scale-invariant MERA also only give a slight
Table 1: Phase boundary and critical exponents under different MERA schemes. The scheme is denoted by $n\pi z Z$, where $n$ is the block size, $\tau$ is the look-ahead step, $x$ can be 1 for the simple product state or $\infty$ for scale-invariant scheme, and $Z$ is “D” or “I” for schemes with or without disentangler, respectively. The additional “(4)” in the last column means that the results are obtained with 4 states retained.

|       | Exact | 321D | 321I | 32$\times$D | 521D | 521I | 32$\times$D(4) |
|-------|-------|------|------|-------------|------|------|--------------|
| $x_c(0)$ | 1     | 1    | 1    | 1           | 1    | 1    | 1            |
| $x_c(1)$ | 1     | 1.081| 1.291| 1.092       | 1.110| 1.233| 1.001        |
| $\gamma_c$ | 1    | 0.801| 1    | 0.803       | 0.835| 1    |              |
| $x_c(\gamma_c)$ | 1    | 1.071| 1.291| 1.081       | 1.097| 1.233|              |
| $\nu$   | 1     | 0.977| 0.864| 0.976       | 0.936| 0.878| 1.112        |
| $z$     | 1     | 1.037| 1.288| 1.036       | 1.039| 1.239| 1.033        |
| $\beta$ | 0.125 | 0.194| 0.261| 0.194       | 0.211| 0.211| 0.131        |

Fig. 4: (Color online) $\partial^2 E / \partial h^2$, which is proportional to the susceptibility, as a function of magnetic field for $\gamma = 1$ obtained from different schemes: (a) solid (black) curve, 321D; dashed (red) curve, 331D; dash-dotted (blue) curve, 32$\times$D; dotted (green) curve, 33$\times$D. (b) Dotted (green) curve, 33$\times$D; dashed (red) curve, 34$\times$D; dash-dotted (blue) curve, 52$\times$D; solid (black) curve, 53$\times$D. The arrows mark the critical fields obtained from RG flow. Note that the scales of these two panels are different and the (green) dotted curves in the figure correspond to the same data from 33$\times$D scheme.

We now turn to the accuracy of RG for different block size. In table 1 we list the critical fields and critical exponents obtained from different block sizes. It is known that the accuracy of the traditional RSRG can be improved by increasing the block size [13,15,20,21]. This fact is justified by the results without disentangler. As shown in the table, $x_c(1)$ is improved from 1.291 of the 3-site block scheme to 1.233 of the 5-site block scheme. But with the disentangler, increasing the block size leads to slightly worse results, at least when the block size is small. Both the phase boundary and the critical exponents are getting a bit worse off when the block size increases from 3 to 5 and further to 7. However, as one can see from fig. 4(b), like increasing the look-ahead step, increasing the block size also improves the consistency of the overall calculations. The 52$\times$D and 53$\times$D schemes produce the susceptibility peaks similar to that from 33$\times$D and 34$\times$D schemes, respectively. From this aspect, the increasing of the block size does improve the overall accuracy in some sense. Following the logics of ref. [21], without the disentangler, the accuracies of the critical field and the critical exponents increase asymptotically as the inverse of the block size or logarithm of the block size. Since the results obtained from MERA with disentangler are always better than that without disentangler, it is expected that the accuracy on the phase boundary and critical exponents can be improved by increasing the block size when the block is large enough. However, increasing block size to improve the accuracy of the phase boundary and critical exponents is not a good strategy due to the following two reasons. One is the non-monotonic dependence of the accuracy on the block size and the formidable calculational cost of MERA scheme with larger block sizes. The other reason is that, as the block size increases, the disentangler becomes close to identity and the difference between the results with and without disentangler gradually diminishes. This trend is seen by comparing the results from 321D, 321I, 521D and 521I schemes listed in table 1. In practice, using small block size but larger truncation dimension is a more
feasible approach for one-dimensional systems with short-range interactions. The optimal scheme for this kind of systems is ternary MERA, but the other block sizes are also acceptable when desired.

We now turn to RG with more than 2 states retained on each coarse-grained site. Theoretically, when one keeps $2^l$ states, one can treat the coarse-grained site as a multi-site composed of $l$ sites and write down the corresponding renormalized Hamiltonian [13,22]. However, the MERA RG transformation make the renormalized Hamiltonian very complicated even with only 4 states retained. Besides the next-nearest neighbor two-body interaction resulted from the normal RSRG process, MERA also introduces additional irrelevant two-body terms such as $(S_i^z - S_{i+1}^z)$ and $S_i^z S_{i+1}^z$, three-body terms like $S_i^z S_{i+1}^z S_{i+2}^z$ and four-body terms such as $S_i^z S_{i+1}^z S_{i+2}^z S_{i+3}^z$. Tracking the RG flow for AXY becomes a tedious task even for the 4-state case. A simpler way to draw the phase boundary is to look at the susceptibility, whose peak position consists with the phase boundary when the look-ahead step is large enough. The critical field for $\gamma = 1$ and the corresponding critical exponents are calculated and listed in table 1 for $\gamma = 4$. One sees that using a larger truncate dimension indeed greatly increases the accuracy of phase boundary and the critical exponents as it should be. One can obtain much more accurate critical exponents by using even larger truncation dimension [6].

In conclusion, we study the RG flow of one-dimensional AXY model and obtain the phase boundary and the corresponding critical exponents using different MERA schemes with the different block sizes, look-ahead steps, and truncation dimensions. It is understood that the disentangler reduces the short-range entanglement by changing the system to a new system of the same universality class but with smaller short-range entanglement. Especially for AXY model, it is shown analytically that the optimized disentangler reduces the entanglement by rotating the system in the parameter space spanned by the anisotropy and the magnetic field. We further study how the block size, look-ahead step and truncation dimension affect the accuracy. It is shown that increasing the block size and look-ahead step improves the overall calculation consistency. A larger truncation dimension leads to much more accurate results in the phase diagram and critical exponents.

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