LETTER

Entanglement renormalization and boundary critical phenomena

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Abstract. In this paper we study interacting quantum systems defined on a one-dimensional lattice with arbitrary boundary conditions, and employ the multiscale entanglement renormalization ansatz to study boundary critical phenomena. We show how to compute the average of any local operator as a function of the distance from the boundary as well as the deviation of the ground state energy due to the presence of the boundary. Furthermore, assuming a uniform tensor structure, we show that the multiscale entanglement renormalization ansatz implies an exact relation between bulk and boundary critical exponents known to exist for boundary critical systems.

Keywords: density matrix renormalization group calculations, other numerical approaches, entanglement in extended quantum systems (theory)

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1. Introduction

Variational approaches based on tensor networks [1] constitute a novel powerful numerical tool believed to be the key ingredient in efficiently simulating quantum many-body systems. Although a detailed understanding of their potentialities and their limitations is currently under scrutiny, there are already a number of encouraging results. Variational tensor network (VTN) methods are free of most of the problems of traditional numerical methods. Unlike quantum Monte Carlo methods, VTN ones do not suffer from the sign problem. Compared to density matrix renormalization group [2] approaches, they are more versatile and allow efficient simulation of critical correlations, long-range interactions, and two-dimensional and higher quantum systems. Indeed the density matrix renormalization group can be reformulated in terms of a particular class of tensor networks known as matrix product states [3]. VTN include also projected entangled pair states [4] that generalize matrix product states in dimensions higher than 1 and weighted graph states [5] designed for studying systems with long-range interactions.

Among the proposed VTN approaches, a very promising one is that of the so-called multiscale entanglement renormalization ansatz (MERA) [6]. MERA has been already applied successfully in the study of a number of different physically relevant systems [7,8], like quantum models on a two-dimensional lattices [9,10], interacting fermions [11], and critical systems [12]–[15], to mention but a few of the most remarkable examples. The capability of MERA to provide an accurate description of critical systems derives directly from the scale-invariant self-similarity of its tensor structure, intimately related to a real-space renormalization procedure. The structure of the MERA state is designed [6] in such a way as to reproduce scale invariance and so, for one-dimensional systems, it naturally encodes several important features of the conformal field theory (CFT) underlying the critical lattice model [13]. The critical exponents can be computed directly from the spectrum of the MERA transfer matrix [12].

Critical systems can however lack translational invariance, due to the presence of a physical boundary or to an impurity. The study of boundary critical phenomena has

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been, for many years, a very active field of research which ranges from the study of critical magnets with surfaces to quantum impurity problems (e.g. Kondo ones), or to Casimir effects (for a review of the field see for example [16]). The presence of the boundary does not spoil conformal invariance. In contrast, boundary CFTs have a very rich structure and a deep mathematical foundation (see e.g. [17]). While this started only as the study of critical two-dimensional systems in the presence of boundaries (surface critical behavior), it found applications in open-string theory (D-branes), quantum impurity problems [18], quantum out-of-equilibrium studies (quantum quenches [19]), to cite but a few. Furthermore, it attracted great attention from the mathematical community because of the recent developments of stochastic Loewner evolution [20].

In view of the connection between MERA and CFT, it is natural to wonder whether the MERA tensor network can be employed to study quantum systems with boundaries. In this work we introduce and analyze an entanglement renormalization tensor network design which takes into account the presence of a (critical) boundary, and we study its properties. This is implemented by allowing the edge spin at the boundary of the system to interact at each step with an ancillary element, describing a fictitious degree of freedom (with dimension suitable for describing the arbitrary boundary condition that we want to impose). Similarly to [12]–[14], we will focus on homogeneous configurations, where tensor elements of the same class are also identical to each other. Interestingly, this ansatz is able to capture some important properties predicted by boundary CFT. Specifically, we show that the critical exponent associated with the decay of any one-point function (as a function of the distance from the boundary) is always half of that of the bulk two-point correlation function corresponding to the same scaling operator. We also compute the boundary corrections to the ground state energy.

The paper is organized as follows. In section 2 we introduce the tensor network and its main properties. In section 3 we discuss how the expectation values of the local observable can be computed. Assuming a uniform tensor structure, in the thermodynamic limit, these expectation values decay as a power law. We relate the associated critical exponents with those of the corresponding two-point correlations in the bulk. In section 4 we discuss the boundary corrections to the ground state energy. The conclusions of our work are summarized in section 5.

2. The tensor network

Consider a 1D lattice of \( N = 2^{n+2} \) spins (sites), of a given local dimension \( d \), with open boundary conditions. A generic pure state of such system can be expressed as

\[
|\psi^{(n)}\rangle = \sum_{\ell_1,\ldots,\ell_N=1}^{d} T_{\ell_1,\ldots,\ell_N} |\xi_{\ell_1}\cdots\xi_{\ell_N}\rangle,
\]

with \( \{|\xi_i\rangle\}_i \) a canonical basis for the single qudit and \( T \) a type-\( (0_N) \) tensor. Following the prescriptions of the MERA structure [6], we assume a formal decomposition of \( T \) which is schematically sketched in figure 1. Here we use the standard graphical convention (see e.g. [6]) for which each node of the graph represents a tensor (the emerging legs of the node being its indices), while a link connecting any two nodes represents the contraction of the corresponding indices. The yellow element at the top of the figure represents a
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Figure 1. Left panel—the entanglement renormalization network representation for $N = 32$ sites. For the bulk, the MERA structure consists of isometries and disentanglers. The boundary is represented by an additional ancillary system indicated by the gray stripe. Right panel—the alternative insertion of the boundary obtained by applying the ancilla interaction tensors (magenta crescent moons) at the same level as the disentanglers instead of the renormalizers, as is done in the left panel.

type-$\binom{0}{6}$ tensor $C$ of elements $C_{\alpha,\ell_1,\ell_2,\ldots,\ell_4,d'}$, that we can call the hat tensor. The green triangles represent instead the same $d \times d^2$ renormalizer tensor $\lambda$ of type $\binom{1}{2}$ of elements $\lambda^u_{\ell_1,\ell_2}$, and the blue circular elements represent the same $d^2 \times d^2$ disentangler tensor $\chi$ of type $\binom{2}{2}$ of elements $\chi^{u_1,u_2}_{\ell_1,\ell_2}$.

At the boundary, we introduce extra tensors that couple the sites at the border with an ancillary degree of freedom represented in figure 1 by the thick gray strip. These new elements form the lateral edges of the network and represent the boundary at each level of the MERA, i.e. at each level of the renormalization flow. As shown in the figure, each of them can be viewed as a matrix product state (yellow squares) whose bonding dimensions coincide with the coordinate space of the ancilla, which is coupled to the bulk via local coupling elements (drawn as magenta crescent moons in the figure). Via purification, we can always choose the dimension of such an ancilla to be large enough that the resulting interaction is describable with a unitary operator, that we indicate as $\alpha$, a type-$\binom{2}{2}$ tensor of elements $\alpha^{u_1,u_2}_{\ell_1,\ell_2}$. Like for the $\lambda$s and the $\chi$s, we will assume uniformity of these elements in the network (possibly allowing the ones on the left-hand side of the structure to differ from the ones on the right-hand side$^7$).

As is customary with MERA-like configurations, to enforce efficient evaluation of local observables and correlation functions, the various elements of the network are assumed to obey specific contraction rules (a detailed analysis of the efficiency requirements for MERA can be found in [6,8,14]). In particular the renormalizers and the disentanglers obey isometric and unitary constraints respectively, i.e.

$$
\sum_{k_1,k_2} \lambda^{u}_{k_1,k_2} \bar{\lambda}^{k_1,k_2}_{\ell} = \delta^u_{\ell}, \quad \sum_{k_1,k_2} \chi^{u_1,u_2}_{k_1,k_2} \bar{\chi}^{k_1,k_2}_{\ell_1,\ell_2} = \delta^{u_1}_{\ell_1} \delta^{u_2}_{\ell_2},
$$

where $\delta^u_{\ell}$ is the Kronecker delta, while $\bar{\lambda}^{u_1,u_2}_{\ell} \equiv (\lambda^{\ell}_{u_1,u_2})^*$ and $\bar{\chi}^{u_1,u_2}_{\ell_1,\ell_2} \equiv (\chi^{\ell_1,\ell_2}_{u_1,u_2})^*$ are the adjoint counterparts of the $\lambda$ and $\chi$ tensors respectively, obtained by exchanging their

$^7$ Notice that allowing the boundary elements to change along the renormalization flow corresponds to introducing a boundary condition changing operator [17] in the language of CFT.
lower and upper indices and taking the complex conjugate. Similar conditions are imposed also for the edge tensors

$$\sum_{k_1, k_2} \alpha_{u_1, u_2}^{k_1, k_2} \delta_{\ell_1}^{u_1} \delta_{\ell_2}^{u_2} = \delta_{\ell_1}^{u_1} \delta_{\ell_2}^{u_2}. \tag{3}$$

These rules are graphically represented in figure 2. Finally, to ensure proper state normalization, the tensor $C$ is assumed to satisfy the identity

$$\sum_{a, k_1, \ldots, k_4, a'} C_{a, k_1, \ldots, k_4, a'} \bar{C}_{a, k_1, \ldots, k_4, a'} = 1. \tag{3}$$

It is worth noticing that, by simply rearranging the various tensorial components, an entanglement renormalization configuration which differs from the one given in figure 1 can be obtained. In fact, the ancilla interaction tensors $\alpha$ (the magenta crescents) can be applied at the same level as the disentanglers, instead of the renormalizers (see figure 1 right panel). Despite their different appearance, it can be shown that these two structures are formally equivalent to each other. This can be verified by grouping together the edge–ancilla interaction with the nearest linked element belonging to the lower half-level. Now, by just performing a polar decomposition [21], we obtain a structure of the opposite type (although the very first spin of the chain is now taken out the system and put into the ancilla, while the second one becomes the edge spin). Having acknowledged this equivalence, in the rest of the paper we will work with the structure of the left panel of figure 1.

3. Local averages in the presence of a boundary

In the presence of the boundary, the average of any local observable depends on the distance from the boundary itself. For a one-dimensional critical system, the case that we consider here, the space dependence will be a power law characterized by a set of critical exponents. In this section we show how to compute local averages and how to extract these exponents.

Consider a family $\mathcal{F} \equiv \{ |\psi^{(n)}\rangle; n = 2, 3, \ldots \}$ of states $|\psi^{(n)}\rangle$ of increasing size, described using homogeneous networks of the form shown in figure 1, each sharing the same structural elements (renormalizer, disentangler, edge–ancilla interaction, hat). For such a family we want to calculate the expectation value of a general observable acting on a small group of neighboring sites located at a given distance from the closest edge of
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Figure 3. Sketch of the CPT maps (a) $D_L$ and (b) $D_R$: the contracted tensor picture represents their Kraus decomposition. The shaded red boxes represent the input degree of freedom on which the maps act. The output degree of freedom is instead represented by the emerging legs of the graphs.

the system, say the left one. For instance, in the case of a three-site observable $\Theta_\ell$ acting on the sites $\ell, \ell+1$, and $\ell+2$ we have

$$\langle \Theta_\ell \rangle^{(n)} \equiv \langle \psi^{(n)} | \Theta_\ell | \psi^{(n)} \rangle = \text{Tr}[\Theta_\ell \rho_{\ell+1,\ell+2}^{(n)}], \quad (4)$$

where the site indices are counted starting from the leftmost spin as the first one, and $\rho_{\ell+1,\ell+2}^{(n)}$ is the reduced density matrix of $|\psi^{(n)}\rangle$ associated with the selected spins.

We assume a uniform MERA structure. This assumption may seem an oversimplification for a system which is not translationally invariant, but it turns out that it naturally accounts for the underlying (boundary) conformal invariance. From the locality requirements imposed in figure 2, it is straightforward to verify that for all $1 \leq \ell \leq 2^{n+1} - 2$ and $n \geq 1$, the following recursion rules apply:

$$\rho_{2\ell,2\ell+1,2\ell+2}^{(n)} = D_L \left( \rho_{\ell+1,\ell+2}^{(n-1)} \right), \quad \rho_{2\ell+1,2\ell+2,2\ell+3}^{(n)} = D_R \left( \rho_{\ell+1,\ell+2}^{(n-1)} \right), \quad (5)$$

where $\rho_{\ell+1,\ell+2}^{(n-1)}$ and $\rho_{\ell+1,\ell+2}^{(n-1)}$ are three-site reduced density matrices of $|\psi^{(n-1)}\rangle \in \mathcal{F}$. In these expressions, $D_L$ and $D_R$ are completely positive trace preserving (CPT) maps that depend only on the bulk elements of the network (indeed they coincide with the $D_L$ and $D_R$ maps of an ordinary homogeneous MERA with the same $\lambda$ and $\chi$ [12]) and whose formal expressions are graphically depicted in figure 3. By means of the renormalization procedure implied by equation (5), at each application of the map the site over which the average is performed approaches the boundary in an exponential fashion. Correspondingly the network depth decreases linearly. In very close proximity to the boundary one has to define further level-recursive operations:

$$\rho_{1,2,3}^{(n)} = K_L \left( \rho_{1,2,3}^{(n-1)} \right), \quad (6)$$

8 The three-site observable is the simplest configuration that we can consider since the three-site causal cone is the smallest stable case for a MERA-like bulk [6].

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where $A$ refers to the degree of freedom belonging to the ancillary system, and $\mathcal{K}_L$ is again a CPT map, sketched in figure 4 (left). Moreover, $\rho_{A,1,2}^{(n)}$ is obtained via

$$\rho_{A,1,2}^{(n)} = \mathcal{B}_L\left(\rho_{A,1,2}^{(n-1)}\right),$$

(7)

where $\mathcal{B}_L$ is the CPT map represented in figure 4 (right). By analogy with $\mathcal{B}_L$ and $\mathcal{K}_L$, we define the CPT maps at the right boundary from the mirror images of figure 4 and we call them $\mathcal{B}_R$ and $\mathcal{K}_R$ respectively.

Because of the stability of the $(A,1,2)$ causal cone [6,8,14], approaching the thermodynamical limit we can determine the reduced density matrix in proximity to the boundary by calculating the fixed point of $\mathcal{B}_L$. This is unique provided that the CPT map is mixing [12,22], i.e.

$$\lim_{n \to \infty} \rho_{A,1,2}^{(n)} = \rho_{A,1,2}^f = \mathcal{B}_L\left(\rho_{A,1,2}^f\right).$$

(8)

We can now use this argument to obtain the expectation value in equation (4) for infinite volume. The resulting expression becomes particularly simple when $D_L = D_R = D$. In this case, indicating the integer part of $\log_2 \ell$ with $\lfloor \log_2 \ell \rfloor$, we have

$$\langle \Theta_\ell \rangle^{(\infty)} = \text{Tr} \left[ \Theta D^{\lfloor \log_2 \ell \rfloor} \circ \mathcal{K}_L(\rho_{A,1,2}^f) \right],$$

(9)

where ‘$\circ$’ stands for super-operator composition and where $D^\tau$ describes $\tau$ reiterated applications of the map $D$.

The Jordan block decomposition [21] can then be used to simplify this expression further. Adapting the derivation for the bulk in [14] to the boundary case, we easily get

$$\langle \Theta_\ell \rangle^{(\infty)} = \sum_{\kappa} \kappa^{\lfloor \log_2 \ell \rfloor} g_{\kappa}(\lfloor \log_2 \ell \rfloor),$$

(10)

where the sum spans over the eigenvalues $\kappa$ of $D$ and $g_{\kappa}(\cdot)$ is a (finite degree) polynomial in its main argument with coefficients which depend on $\rho_{A,1,2}^f$ and $D$. Since CPT
where the summation is performed over the eigenvalues $\kappa$ entering equation (10) belong to the unit circle (i.e. $|\kappa| < 1$). Furthermore, if $\mathcal{D}$ is mixing (which is a reasonable assumption [12]), then its spectrum admits a unique eigenvector (the fixed point $\rho_f'$ of the channel) associated with $\kappa = 1$; all the remaining eigenvalues have modulus strictly smaller than 1. Under these circumstances, in the limit of large distance from the boundary, the quantity $\langle \Theta_\ell \rangle (\infty)$ converges toward its bulk limit which is obtained by computing the expectation value of $\Theta$ at the fixed point of the channel, i.e. $\langle \Theta_{\text{bulk}} \rangle (\infty) = \text{Tr}[\Theta \rho_f']$. The deviations from such limiting expression can be evaluated by keeping the largest contribution associated with the terms with $\kappa \neq 1$. This yields an exponential decay in $\log_2 \ell$ of the form

$$
\langle \Theta_\ell \rangle (\infty) = \langle \Theta_{\text{bulk}} \rangle (\infty) + \sum_{\kappa \neq 1} \kappa |\log_2 \ell| g_\kappa (|\log_2 \ell|)
= \langle \Theta_{\text{bulk}} \rangle (\infty) + \ell^{\log_2 |\kappa|} g'(\log_2 \ell),
$$

(11)

where $\kappa$ is the eigenvalue of $\mathcal{D}$ which has the largest absolute value smaller than 1 and which contributes non-trivially to equation (10), and where $g'(\log_2 \ell)$ is instead some complicated function which is dominated by a polynomial in $\log_2 \ell$. In particular, if $\Theta$ is an eigenvector of the Heisenberg adjoint of the channel $\mathcal{D}$, then equation (11) yields an exact power-law decay (without polynomial corrections), i.e.

$$
\langle \Theta_\ell \rangle (\infty) = c \kappa |\log_2 \ell| \sim c \ell^{\log_2 \kappa},
$$

(12)

where $c = \text{Tr}[\Theta \mathcal{K}_L (\rho_f'_{A,1,2})]$, and where $\kappa$ is the associated eigenvalue (notice that for such a $\Theta$ one has $\langle \Theta_{\text{bulk}} \rangle (\infty) = 0$). The above expressions show that the quantities $-\log_2 |\kappa|$ play the role of the critical exponents of the system. It is now evident that these critical exponents are half the corresponding ones for two-point correlation functions computed for the bulk, a well-known result in conformal field theory [17]. For instance, fixing the distance $\Delta \ell = 2^m$ of the two points, the bulk connected correlation function has been computed [12], and it holds that

$$
\mathcal{C}_{\Delta \ell}^{(n)} = \frac{1}{N} \sum_{\ell=1}^{N} [\langle \Theta_\ell \Theta_{\ell+\Delta \ell} \rangle (n) - \langle \Theta_\ell \rangle (n)^2 \langle \Theta_{\ell+\Delta \ell} \rangle (n)]
= \text{Tr}[\mathcal{P} (\Theta \otimes \Theta) \mathcal{P}^{\log_2 \Delta \ell} (\sigma)]
= \sum_{\xi \neq 1} \xi^{\log_2 \Delta \ell} h_\xi (\log_2 \Delta \ell),
$$

(13)

where the summation is performed over the eigenvalues $\xi$ of the CPT map $\mathcal{P} = \frac{1}{2} (\mathcal{D}_L \otimes \mathcal{D}_L + \mathcal{D}_R \otimes \mathcal{D}_R)$, and where $h_\xi (\cdot)$ is a polynomial function of its argument (in this expression, $\sigma$ stands for a traceless operator while finally $N = 2^{n+2}$ is the size of the associated homogeneous MERA with periodic boundary conditions). The result then follows on noticing that by construction $\mathcal{P} = \mathcal{D} \otimes \mathcal{D}$, so the $\xi$ can be expressed as products $\kappa \kappa'$ of the eigenvalues of $\mathcal{D}$. In particular if as in equation (12), $\Theta$ is an eigenvector the Heisenberg adjoint of $\mathcal{D}$, we have that $\Theta \otimes \Theta$ is an eigenvector of the adjoint of $\mathcal{P}$ at the eigenvalue $\xi = \kappa^2$ and, thus,

$$
\mathcal{C}_{\Delta \ell}^{(n)} = c' \kappa^{2 \log_2 \Delta \ell} = c' (\Delta \ell)^{2 \log_2 \kappa},
$$

(14)

which proves the claim (here $c' = \text{Tr}[\Theta \otimes \Theta] \sigma$).

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In a similar fashion one can also compute $m$-point correlation functions. The expressions become however very cumbersome. In the appendix we sketch this calculation in two important cases where simple limiting expressions can be recovered.

4. Corrections to the ground state energy due to the presence of boundaries

In the presence of a boundary, the average of the extensive observables (the ground state energy for example) does contain a bulk and a boundary contribution. In this section, we investigate the total ground state energy for a local Hamiltonian (with interactions among sites at maximum distance $\nu$) of the form

$$ H = \sum_{j=1}^{L-\nu+1} H_{j-j+\nu}, \quad (15) $$

where $\nu$ is the number of sites involved in the model interaction $H$. While this problem is easily solved in a level-recursive manner for a MERA structure (in which periodic boundary conditions hold), when explicit conditions over a defined boundary are involved things become slightly more complicated.

Suppose, for simplicity, that the interaction is again a $\nu=3$-body operator. Notice that under this assumption equation (15) can be used to describe also first-neighboring coupling Hamiltonians (in principle one should also include a term of the form $H^{(3)}_{1,2,3} = \alpha H^{(2)}_{1,2} \otimes \mathbb{1}_{3} + (1-\alpha) \mathbb{1}_{1} \otimes H^{(2)}_{2,3}$; this term however does not modify the scaling laws and can be omitted from the calculation). If we are to evaluate the energy density we have

$$ \frac{\langle H \rangle}{L-\nu+1} = \text{Tr}[H \bar{\rho}^{(n)}_3], \quad (16) $$

where

$$ \bar{\rho}^{(n)}_3 \equiv \frac{1}{2n+2} \sum_{j=1}^{2n} \rho^{(n)}_{j,j+1,j+2}. $$

We need to build a recursive function which relates this average density matrix to the one belonging to the previous tensor level $\bar{\rho}^{(n-1)}_3$. Of course, the boundaries will play some role too in this relation:

$$ \bar{\rho}^{(n)}_3 = \frac{1}{2n+2} \left[ \mathcal{K}_L \left( \rho^{(n-1)}_{A,1,2} \right) + \mathcal{K}_R \left( \rho^{(n-1)}_{2n+1-1,2n+1,A'} \right) \right] + \left( 1 - \frac{1}{2n+1} \right) \mathcal{D} \left( \bar{\rho}^{(n-1)}_3 \right) \quad (17) $$

(here $\mathcal{D}$ is the average of $\mathcal{D}_L$ and $\mathcal{D}_R$). This equation shows the contributions of both bulk and edge terms; nevertheless, when we approach the thermodynamical limit $n \to \infty$, the contribution of the first two terms vanishes in every norm, because any density matrix has trace norm bounded by 1 and CPT maps are contractive.

This means that the extensive influence of the boundary upon the lattice grows more slowly than the size of the system, a physically sound and known property. To quantitatively describe such behavior, we compute the (total) energy associated with the block of the first $2^\tau-1$ spins near a boundary, say the left one. In our notation this corresponds to

$$ E^{(n)}_{1,2^\tau-1} = \left\langle \sum_{j=1}^{2^\tau-1} H_{j\ldots j+2} \right\rangle = \text{Tr} \left[ H_3 \sum_{j=1}^{2^\tau-1} \rho^{(n)}_{j,j+1,j+2} \right]. \quad (18) $$
Exploiting the usual formalism of level-growing CPT maps, we can rewrite the sum in (18) as
\[
\sum_{j=1}^{2\tau-1} \rho_{j,j+1,j+2}^{(n)} = \sum_{p=0}^{\tau-1} 2^p D^p \circ K_L \circ B_L^{\tau-p-1} \left( \rho_{A,1,2}^{(n-\tau)} \right).
\] (19)

Now, we can successfully approach the thermodynamical limit while keeping \(\tau\) fixed. Recalling that \(\rho_{A,1,2}^f\) is the fixed point of \(B_L\), we obtain
\[
E_{1...2\tau-1}^{(th)} = \text{Tr} \left[ H_3 \cdot \sum_{p=0}^{\tau-1} 2^p D^p \circ K_L \left( \rho_{1,2}^f \right) \right].
\] (20)

As expected, the result diverges for \(\tau \to \infty\) since the series is made of terms growing in trace norm. To explicitly estimate how this quantity deviates from its corresponding value in the bulk as \(\tau\) grows we evaluate the following quantity:
\[
\Delta E_{1...2\tau-1}^{(th)} = - (2^\tau - 1) \text{Tr} \left[ H_3 \rho_3^f \right] + \text{Tr} \left[ H_3 \sum_{p=0}^{\tau-1} 2^p D^p \circ K_L \left( \rho_{1,2}^f \right) \right]
= \text{Tr} \left[ H_3 \sum_{p=0}^{\tau-1} 2^p D^p \left\{ K_L \left( \rho_{A,1,2}^f \right) - \rho_3^f \right\} \right].
\] (21)

Notice that in this case the map \(D\) applies to a traceless operator; therefore if we decompose the argument in a basis of generalized eigenvectors for \(D\), it must have null component over the unique state of eigenvalue 1. As a result the boundary contribution to the ground state energy has the form
\[
\Delta E_{1...\infty}^{(th)} = \sum_{\kappa_D \neq 1} \sum_{p=0}^{\infty} (2\kappa_D)^p g_{\kappa_D}(p),
\] (22)

where \(g(\cdot)\) is a polynomial in its main argument. Looking at equation (22), we notice that the inner sum diverges for any eigenvalue \(\kappa_D\) of \(D\) greater than or equal to 1/2, unless the \(g\) are identically zero for such values of \(\kappa_D\). In general this will happen when \(\rho_3^f - K_L(\rho_{A,1,2}^f)\) has null component over any generalized eigenspace whose \(\kappa_D \geq 1/2\).

Interestingly, the capability of such a deviation to diverge is another manifestation that the MERA states of figure 1 are critical: indeed only the integral of a power-law function can diverge, while for an exponentially decaying correlation function the integral of the corresponding action is always finite.

5. Conclusions

In this paper we exploited the properties of MERA to describe boundary critical phenomena. We considered the case of a one-dimensional critical system with a boundary. To this end we modified the local structure of the MERA at the boundary to account for more flexibility in its description.

Besides showing how to compute local observables, we achieved two main results. First of all we showed, as predicted by boundary conformal field theory, that the critical exponent associated with the decay of the one-point function (as a function of the

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distance from the boundary) is always half of that of the bulk two-point correlation function corresponding to the same scaling operator. Secondly we computed the boundary corrections to the ground state energy and determined its scaling behavior. As in the bulk case, and also in the presence of the boundary, most of the critical properties are determined solely by the eigenvalues of the MERA transfer matrix.

A remarkable feature of treating boundary critical phenomena with MERAs is that it is enough to consider a uniform tensor network. This is the result of the scale invariance of the underlying tensor network which holds also in the presence of boundaries. In addition to the practical advantage in the numerical simulations, this observation further clarifies the properties of the MERA. It is worth noticing that such a property (that is the basis of the effectiveness of a bounded MERA) is physically equivalent to the fact that, in boundary critical phenomena, the operator content of the bulk is not influenced by the boundary [16], suggesting that maybe the connection between MERA and general renormalization group theory is deeper than what is nowadays understood.

One-dimensional systems display the peculiar feature that the boundary can be critical only when also the bulk is. This is not the case in higher dimensions [16], where we can have a critical boundary in a gapped system, resulting in a richer scenario for the boundary–bulk phase diagram. This richness will be reflected in the possibility of having different compositions of tensor structure. In this paper we considered a matrix product state (at the border) connected to a MERA. It is easy to imagine that, for describing critical surfaces in a non-critical bulk, different compositions of tensor networks are required.

During the writing of this work a paper by Evenbly et al appeared in the archive discussing boundary critical phenomena and using MERA; see [23].

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Appendix: Two-point functions in proximity to the boundary

In this appendix we sketch how to compute two-point correlation functions. There is no single general formula in this case. Using our formalism of maps and tensor contractions, one has to consider different cases in accordance with where the causal cones of the selected sites intercept each other and/or intercept the boundary. Let us assume calculation of \(\langle \Theta_{\ell_1} \Theta_{\ell_2} \rangle^{(\infty)}\) (for simplicity we choose \(\Theta\) to be a three-body primary field, i.e. an eigenoperator of the Heisenberg adjoint of the \(D\) map). Let \(n_1 = \lfloor \log_2 \ell_1 \rfloor\), \(n_2 = \lfloor \log_2 \ell_2 \rfloor\), and without loss of generality \(\ell_2 \geq \ell_1\). Consider the two limiting cases:

- \(n_2 > n_1\): this is the case where one of the two points is nearer to the edge compared to the other point. When this condition holds, the causal cone of \(\ell_1\) intercepts the boundary before connecting with the causal cone of \(\ell_2\).

\[
\langle \Theta_{\ell_1} \Theta_{\ell_2} \rangle^{(\infty)} = \text{Tr} \left[ (\Theta \otimes \Theta) D^{n_1-2} \otimes D^{n_2-3}(\tilde{\rho}_1) \right],
\]

(A.1)
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where $\tilde{\rho}_1$ is some six-body density matrix with a non-scaling dependence on $\ell_1$ and $\ell_2$. The scaling behavior of the previous quantity is then

$$\langle \Theta_{\ell_1} \Theta_{\ell_2} \rangle^{(\infty)} \sim c_e (\ell_1 \ell_2)^{\log_2 \kappa},$$

(A.2)

where $\kappa$ is the one-point critical exponent for $\Theta$, as in equation (12).

• $n_2 = n_1$: in this case the two points are next to each other, and the boundary is far away; this means that the causal cones intercept each other before connecting to the edge of the system:

$$\langle \Theta_{\ell_1} \Theta_{\ell_2} \rangle^{(\infty)} = \text{Tr} \left[ (\Theta \otimes \Theta)(D \otimes D)^{[\log_2(\ell_2 - \ell_1)]} (\tilde{\rho}_2) \right],$$

(A.3)

In this case the scaling behavior resembles the one shown for the bulk (14)

$$\langle \Theta_{\ell_1} \Theta_{\ell_2} \rangle^{(\infty)} \sim c_b (\ell_1 - \ell_2)^{2 \log_2 \kappa}.$$

(A.4)

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