

Entanglement Renormalization

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We propose a real-space renormalization group (RG) transformation for quantum systems on a *D*-dimensional lattice. The transformation partially disentangles a block of sites before coarse-graining it into an effective site. Numerical simulations with the ground state of a 1D lattice at criticality show that the resulting coarse-grained sites require a Hilbert space dimension that does not grow with successive RG transformations. As a result we can address, in a quasi-exact way, tens of thousands of quantum spins with a computational effort that scales logarithmically in the system's size. The calculations unveil that ground state entanglement in extended quantum systems is organized in layers corresponding to different length scales. At a quantum critical point, each relevant length scale makes an equivalent contribution to the entanglement of a block.

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Renormalization group (RG), one of the conceptual pillars of statistical mechanics and quantum field theory, revolves around the idea of coarse-graining and rescaling transformations of an extended system [1]. These so-called RG transformations are not only a key theoretical element in the modern formulation of critical phenomena and phase transitions, but also the basis of important computational methods for many-body problems.

In the case of quantum systems defined on a lattice, Wilson's real-space RG methods [2], based on the truncation of the Hilbert space, replaced Kadanoff's spin-blocking ideas [3] with a concise mathematical formulation and an explicit prescription to implement RG transformations. But it was not until the advent of White's density matrix renormalization group (DMRG) algorithm [4] that RG methods became the undisputed numerical approach for systems on a 1D lattice. More recently, such techniques have gained renewed momentum under the influence of quantum information science. By paying due attention to entanglement, algorithms to simulate time-evolution in 1D systems [5] and to address 2D systems [6] have been put forward.

The practical value of DMRG and related methods is unquestionable. And yet, they are based on a RG transformation that notably fails to satisfy a most natural expectation, namely, to have scale invariant systems as fixed points. Instead, for such systems, the size of an effective site (as measured by the dimension of its Hilbert space) increases with each iteration of the RG transformation. This fact does not only conflict with the very spirit of RG theory, but it also has important computational implications: after a sufficiently large number of iterations, the effective sites are unaffordably large, and the numerical method is no longer viable.

In this Letter, we propose a real-space RG transformation for quantum systems on a *D*-dimensional lattice that, by *renormalizing* the amount of entanglement in the system, aims to eliminate the growth of the site's Hilbert space

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dimension along successive rescaling transformations. In particular, when applied to a scale invariant system, the transformation is expected to produce a coarse-grained system identical to the original one. Numerical tests for critical systems in D=1 spatial dimensions confirm this expectation. Our results also unveil the stratification of entanglement in extended quantum systems and open the path to a very compact description of quantum criticality.

Real-space RG and DMRG.—As originally introduced by Wilson [2], real-space RG methods truncate the local Hilbert space of a block of sites in order to reduce its degrees of freedom. Let us consider a system on a lattice \mathcal{L} in D spatial dimensions and its Hilbert space

$$\mathbb{V}_{\mathcal{L}} \equiv \bigotimes_{s \in \mathcal{L}} \mathbb{V}_{s},\tag{1}$$

where $s \in \mathcal{L}$ denotes the lattice sites and V_s has finite dimension. Let us also consider a block $\mathcal{B} \subset \mathcal{L}$ of neighboring sites, with corresponding Hilbert space

$$\mathbb{V}_{\mathcal{B}} \equiv \bigotimes_{s \in \mathcal{B}} \mathbb{V}_{s}.\tag{2}$$

In an elementary RG transformation, the lattice \mathcal{L} is mapped into a new, *effective* lattice \mathcal{L}' , where each site $s' \in \mathcal{L}'$ is obtained from a block \mathcal{B} of sites in \mathcal{L} by *coarse graining*. More specifically, the space $\mathbb{V}'_{s'}$ for site $s' \in \mathcal{L}'$ corresponds to a subspace $\mathbb{S}_{\mathcal{B}}$ of $\mathbb{V}_{\mathcal{B}}$,

$$\mathbb{V}_{\mathfrak{s}'}' \cong \mathbb{S}_{\mathcal{B}} \subseteq \mathbb{V}_{\mathcal{B}},\tag{3}$$

as characterized by an isometric tensor w, Fig (1),

$$w: \mathbb{V}'_{s'} \mapsto \mathbb{V}_{\mathcal{B}}, \qquad w^{\dagger} w = I.$$
 (4)

Isometry w can now be used to map a state $|\Psi\rangle \in \mathbb{V}_{\mathcal{L}}$ [typically, a ground state] into a coarse-grained state $|\Psi'\rangle \in \mathbb{V}_{\mathcal{L}'}$. A thoughtful selection of subspace $\mathbb{S}_{\mathcal{B}}$ is essential. On the one hand, its dimension m should be as small as possible because the cost of subsequent tasks, such

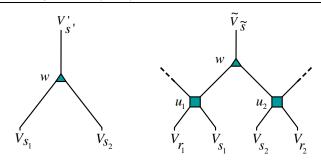


FIG. 1 (color online). Isometries and disentanglers. Left: a standard numerical RG transformation builds a coarse-grained site s', with Hilbert space dimension m, from a block of two sites s_1 and s_2 through the isometry w of Eq. (4). Right: by using the disentanglers u_1 and u_2 of Eq. (7), short-range entanglement residing near the boundary of the block is eliminated before the coarse-graining step. As a result, the coarse-grained site \tilde{s} requires a smaller Hilbert space dimension \tilde{m} , $\tilde{m} < m$.

as computing expectation values for local observables, grows polynomially with m. On the other hand, $\mathbb{S}_{\mathcal{B}}$ needs to be large enough that $|\Psi'\rangle$ retains all relevant properties of $|\Psi\rangle$. White identified the optimal choice as part of his DMRG algorithm [4]. Let $\rho^{[\mathcal{B}]}$ denote the reduced *density matrix* of $|\Psi\rangle$ on block \mathcal{B} . Then the optimal subspace is

$$\mathbb{S}_{\mathcal{B}} \equiv \langle |\rho_1\rangle, \cdots, |\rho_m\rangle \rangle, \tag{5}$$

where $|\rho_i\rangle$ are the *m* eigenvectors of $\rho^{[\mathcal{B}]}$ with largest eigenvalues p_i , and *m* is such that $\epsilon \geq 1 - \sum_{i=1}^m p_i$, with ϵ a preestablished truncation error, $\epsilon \ll 1$.

Notice that m refers to the amount of entanglement between \mathcal{B} and the rest of the lattice, $\mathcal{L} - \mathcal{B}$, as characterized by the rank of the truncated Schmidt decomposition

$$|\Psi\rangle \approx \sum_{i=1}^{m} \sqrt{p_i} |\rho_i\rangle \otimes |\sigma_i\rangle, \qquad |\sigma_i\rangle \in \mathbb{V}_{\mathcal{L}-\mathcal{B}}.$$
 (6)

In other words, the performance of DMRG-based methods depends on the amount of entanglement in $|\Psi\rangle$.

Entanglement Renormalization.—We propose a technique to reduce the amount of entanglement between the block \mathcal{B} and the rest of the lattice \mathcal{L} while still obtaining a quasiexact description of the state of the system. This is achieved by deforming, by means of a unitary transformation, the boundaries of the block \mathcal{B} before truncating its Hilbert space, see Fig. 1.

Let us specialize, for simplicity, to a 1D lattice and to a block \mathcal{B} made of just two contiguous sites s_1 and s_2 . Let r_1 and r_2 be the two sites immediately to the left and to the right of \mathcal{B} . Then, we consider unitary transformations u_1 and u_2 , the *disentanglers*, acting on the pairs of sites r_1s_1 and s_2r_2 ,

$$u_1: \mathbb{V}_{r_1} \otimes \mathbb{V}_{s_1} \to \mathbb{V}_{r_1} \otimes \mathbb{V}_{s_1}, \qquad u_1^{\dagger} u_1 = u_1 u_1^{\dagger} = I,$$

$$u_2: \mathbb{V}_{s_2} \otimes \mathbb{V}_{r_2} \to \mathbb{V}_{s_2} \otimes \mathbb{V}_{r_2}, \qquad u_2^{\dagger} u_2 = u_2 u_2^{\dagger} = I.$$

$$(7)$$

Properly chosen disentanglers reduce the short-range en-

tanglement between the block \mathcal{B} and its immediate neighborhood [7]. The original state $\rho^{[\mathcal{B}]}$ of block \mathcal{B} ,

$$\rho^{[\mathcal{B}]} = \operatorname{tr}_{r_1 r_2} [\rho^{[r_1 s_1 s_2 r_2]}], \tag{8}$$

is now replaced with a partially disentangled state $\tilde{\rho}^{[\mathcal{B}]}$,

$$\tilde{\rho}^{\,[\mathcal{B}]} = \mathrm{tr}_{r_1 r_2} [(u_1 \otimes u_2) \rho^{[r_1 s_1 s_2 r_2]} (u_1 \otimes u_2)^{\dagger}], \qquad (9)$$

which has a smaller effective rank \tilde{m} , $\tilde{m} < m$. Our RG transformation consists of two steps: (i) First we decrease or *renormalize* the amount of entanglement between block \mathcal{B} and the rest of \mathcal{L} . This is achieved with disentanglers that act locally around the boundary of \mathcal{B} [8]. The block does not become completely disentangled because only entanglement localized near its boundaries can be removed. (ii) Then, as in Wilson's proposal, we *truncate* the Hilbert space of block \mathcal{B} , and we do so following White's idea to target the support of the block's density matrix. But instead of keeping the support of the original $\rho^{[\mathcal{B}]}$, we retain the (smaller) support of the partially disentangled density matrix $\tilde{\rho}^{[\mathcal{B}]}$.

The above steps, characterized by unitary and isometric tensors u and w, produce an alternative coarse-grained lattice $\tilde{\mathcal{L}}$ and a coarse-grained state $|\tilde{\Psi}\rangle \in \mathbb{V}_{\tilde{\mathcal{L}}}$ that contains less entanglement than $|\Psi'\rangle \in \mathbb{V}_{\mathcal{L}'}$. Importantly, the expectation value $\langle \Psi|o|\Psi\rangle = \mathrm{tr}[o\rho^{[\mathcal{R}]}]$, where o is an observable defined on a small set of sites $\mathcal{R} \subset \mathcal{L}$, can be efficiently computed from just $|\tilde{\Psi}\rangle$, u, w, and o. There are two ways: (i) as described in [9], $\rho^{[\mathcal{R}]}$ can be computed from $\tilde{\rho}^{[\tilde{\mathcal{R}}]} \equiv \mathrm{tr}_{\tilde{\mathcal{L}}-\tilde{\mathcal{R}}} |\tilde{\Psi}\rangle\langle\tilde{\Psi}|$, where $\tilde{\mathcal{R}}$ is the set of sites of $\tilde{\mathcal{L}}$ causally connected to \mathcal{R} through u and w; (ii) alternatively, we can use u and w to lift o from \mathcal{L} to $\tilde{\mathcal{L}}$, producing \tilde{o} , and exploit that $\langle \Psi|o|\Psi\rangle = \langle \tilde{\Psi}|\tilde{o}|\tilde{\Psi}\rangle$.

The lifting from \mathcal{L} to $\tilde{\mathcal{L}}$ of operators generates, by iteration, a well-defined RG flow in the space of Hamiltonians [8,10] such that, in the 1D case, an interaction term $H^{(3)}$ acting on at most three consecutive sites of \mathcal{L} is mapped into an interaction term $\tilde{H}^{(3)}$ acting also on at most three consecutive sites in $\tilde{\mathcal{L}}$ [analogous rules apply in D>1 spatial dimensions]. Thus, in spite of the fact that disentanglers deform the original tensor product structure of $\mathbb{V}_{\mathcal{L}}$, the above rescaling transformation preserves *locality*, in that it maps local theories into local theories.

In the same way as DMRG is related to matrix product states (MPS) [11], the above RG transformation is naturally associated to a new ansatz for quantum many-body states on a D dimensional lattice. The multiscale entanglement renormalization ansatz (MERA) consists of a network of isometric tensors (namely the isometries u and disentanglers w corresponding to successive iterations of the RG transformation) locally connected in D+1 dimensions. The extra direction τ , related to the RG flow, grows only as the logarithm of the lattice dimensions, see Fig. 2. Several properties of the MERA together with its connection to quantum circuits are described in [9].

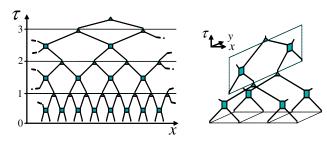


FIG. 2 (color online). Left: MERA for a 1D lattice with periodic boundary conditions. Notice the fractal nature of the tensor network. Translational symmetry and scale invariance can be naturally incorporated, substantially reducing the computational complexity of the numerical simulations. Right: building block of a MERA for a 2D lattice. Disentanglers and isometries address one of the *x* and *y* spatial directions at a time.

Example.—Figures 3 and 4 study the ground state of the 1D quantum Ising model with transverse magnetic field,

$$H = \sum_{\langle s_1, s_2 \rangle} \sigma_{s_1}^x \otimes \sigma_{s_2}^x + h \sum_s \sigma_s^z, \tag{10}$$

for an infinite lattice [12]. The *entanglement entropy* between a block \mathcal{B} of L adjacent spins and the rest of the lattice, defined in terms of the eigenvalues $\{p_i\}$ of $\rho^{[\mathcal{B}]}$ as

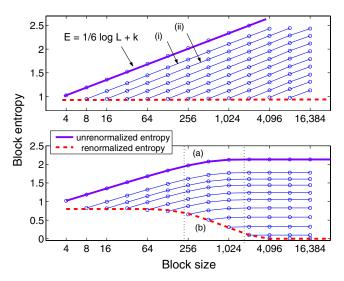


FIG. 3 (color online). Scaling of the entropy of entanglement in 1D quantum Ising model with transverse magnetic field. Up: in a critical lattice $[h=1\ \text{in}\ \text{Eq.}\ (10)]$, the unrenormalized entanglement of the block scales with the block size L according to Eq. (11). Instead, the renormalized entanglement remains constant under successive RG transformations, as a clear manifestation of scale invariance. Line (i) corresponds to using disentanglers only in the first RG transformation. Line (ii) corresponds to using disentanglers only in the first and second RG transformation. Down: in a noncritical lattice $[h=1.001\ \text{in}\ \text{Eq.}\ (10)]$, the unrenormalized entanglement scales roughly as in the critical case until it saturates (a) for block sizes comparable to the correlation length. Beyond that length scale, the renormalized entanglement vanishes (b) and the system becomes effectively unentangled.

 $S(\mathcal{B}) \equiv -\sum_{i} p_i \log_2 p_i$, scales at criticality (h = 1) with the block size L as [14]

$$S_L \approx \frac{1}{6} \log_2 L. \tag{11}$$

On the other hand, off criticality $S(\mathcal{B})$ grows monotonically with L until it reaches a saturation value for a block size comparable to the correlation length in the system. Figure 3 shows the effect of disentanglers on the entanglement entropy of a block. Most notably, the renormalized entanglement of a block in the critical case is reduced to a small value that is constant throughout the RG flow. Correspondingly, as Fig. 4 shows, the Hilbert space dimension \tilde{m} of a block of size $L = 2^{\tau}$ can be kept constant as we increase τ , allowing in principle for an arbitrary number of iterations of the RG transformation. Our calculations, involving the reduced density matrix of up to $L = 2^{14} = 16$. 384 spins, have been conducted with Hilbert spaces of dimension $\tilde{m}=8$, while keeping the truncation error ϵ at each step fixed below 5×10^{-7} . We estimate that without disentanglers, an equivalent error ϵ requires a Hilbert space of $m \approx 500-1000$ dimensions for the largest spin blocks. This exemplifies the computational advantages of using disentanglers.

Discussion.—The above numerical exploration suggests an appealing picture, also confirmed by subsequent calculations involving other 1D and 2D quantum models [10]. Entanglement in the ground state of the quantum spin chain is organized in layers corresponding to different length scales in the system. The entanglement of a given length

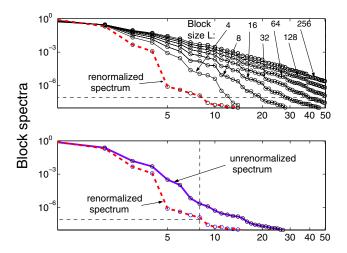


FIG. 4 (color online). Spectrum of the reduced density matrix of a spin block. Up: as the size L of the spin increases, the number m of eigenvalues $\{p_i\}$ required to achieve a given accuracy ϵ , see Eq. (5), also increases. In particular, m grows roughly exponentially in the number $\tau = \log_2 L$ of RG transformations. The spectrum resulting from applying disentanglers leads to a significantly smaller \tilde{m} invariant along successive RG transformations. Down: spectrum of the reduced density matrix of 2^{τ} spins immediately before and after using the disentanglers at the τ^{th} coarse-graining step. These spectra are essentially independent of the value of $\tau = 1, \cdots, 14$.

scale can be modified by means of a disentangler that acts on a region as large as that length scale. We detect two situations: (i) Off criticality, the entanglement between a block of sites \mathcal{B} and the rest of the lattice \mathcal{L} consists roughly of contributions from layers of length scale not greater than the correlation length in the system. Therefore, after a sufficiently large number of RG transformations with disentanglers, the effective ground state becomes a product state, that is, completely disentangled. (ii) At criticality, instead, the entanglement between \mathcal{B} and the rest of \mathcal{L} receives equivalent contributions from all length scales (smaller than the size of \mathcal{B})—see [9] for a justification of the logarithmic scaling of Eq. (11). In this case, by applying disentanglers, we obtain a coarse-grained lattice identical to the original one, including an effective Hamiltonian identical (up to a proportionality constant) to the original one [10]. In either case, a fixed point of the RG transformation is attained after a sufficient number of iterations. Noncritical theories collapse into the trivial fixed point (a product state) while critical theories correspond to a nontrivial fixed point (an entangled state expected to depend on the universality class of critical theory). We conjecture that this picture, fully consistent with known facts of RG [1], holds also for quantum lattices in D > 1 spatial dimensions. Interestingly, a third type of fixed point is possible, in the case of a ground state with either long-range order or topological order [15].

In summary, we have presented a quasiexact real-space RG transformation that, when tested in 1D systems, produces effective sites of bounded dimension and has (scale invariant) critical systems as its nontrivial fixed points. The key feature of our approach is a local deformation of the tensor product structure of the Hilbert space of the lattice, that identifies and factorizes out those local degrees of freedom that are uncorrelated from the rest. This deformation is such that local operators are mapped into local operators, so that relevant expectation values for the original system can be efficiently computed from the coarse-grained system.

We conclude with two remarks. First, a scale invariant critical ground state leads to disentanglers u and isometries w that are the same at each iteration of the RG transformation. A single pair (u, w), depending on $O(\tilde{m}^4)$ parameters, is thus seen to specify the ground state, leading to an extremely compact characterization that deserves further study. Second, renormalization group techniques are extensively used also in classical problems, where the

MERA can efficiently represent partition functions of lattice systems, extending the scope of this work beyond the study quantum systems.

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