

Multiscale Entanglement Renormalization Ansatz in Two Dimensions: Quantum Ising Model

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We propose a symmetric version of the multiscale entanglement renormalization ansatz in two spatial dimensions (2D) and use this ansatz to find an unknown ground state of a 2D quantum system. Results in the simple 2D quantum Ising model on the 8×8 square lattice are found to be very accurate even with the smallest nontrivial truncation parameter.

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Over the past decade, a rapid development of efficient methods for simulation of strongly correlated quantum systems took place, especially in one spatial dimension (1D). It was initiated with the, by now classic, Letter of White on the density matrix renormalization group (DMRG) algorithm [1]. Recently, the subject received new acceleration with the Letter of Vidal [2], who proposed an elegant version of the algorithm based on the idea that a state of a 1D quantum spin chain can be written as a Schmidt decomposition between any two parts of the chain. For a generic ground state, but not at a quantum critical point, the coefficients of this Schmidt decomposition decay exponentially, and the decomposition can be truncated to a finite number of terms d with an exponentially small loss of accuracy. The DMRG algorithms are equivalent to a matrix product state ansatz [3] for the ground state where each spin S is assigned $2S + 1$ matrices of size $d \times d$. Each matrix has two indices to be contracted with its two nearest neighbors in 1D. The matrix product state can be naturally generalized to two and more dimensions by replacing the matrices with higher rank tensors to accommodate more nearest neighbors [4]. These “tensor product states” [5] can also be obtained as projected entangled pair states (PEPSs) [4], the latter being a more convenient representation to prove that any quantum state can be represented accurately by a PEPS for a sufficiently large d . In 2D, unlike in 1D, exact calculation of expectation values in a PEPS is exponentially hard with increasing lattice size, but this problem can be overcome, at least for open boundary conditions, by an efficient approximate method [6] which is linear in the system size.

The ability to make efficient and accurate zero temperature simulations in 2D is of fundamental importance for our understanding of strongly correlated 2D quantum systems. It is enough to mention possible applications to high- T_c superconductors which effectively are 2D systems of strongly correlated electrons on a lattice. Their, by now classic, Hubbard model [7] has not been solved exactly despite staying in the focus of intensive research activity for several decades.

In the context of matrix product states and their generalizations, the main difficulty is that all calculations are polynomial in the truncation d , but in 2D the degree of

the polynomial is too high to go far beyond $d = 2$ or 3, which, however, may be not accurate enough. A possible solution to this problem is the multiscale entanglement renormalization ansatz (MERA) proposed in Ref. [8], where proper “renormalization” of entanglement is shown to reduce the necessary d by orders of magnitude. This economy of the truncation parameter d was demonstrated to be truly impressive in the 1D quantum Ising model, where, even at the critical point, a MERA with a modest $d = 8$ is as accurate as a matrix product state with d in the range of a few hundreds [8]. Simulations with a 1D MERA are very efficient because they are polynomial in a relatively small d [8,9].

The 1D MERA is motivated by the following real space renormalization group algorithm. Spins on a 1D lattice can be grouped into a lattice of blocks of two nearest neighbor spins. There are two possible choices of block chains A and B shifted with respect to each other by one lattice site. In a decimation step of the renormalization group, each A block is replaced by one effective block spin whose Hilbert space is truncated to its d most important states. The most important states are the eigenstates of an A block’s reduced density matrix with the highest eigenvalues. However, to keep d as small as possible but without losing much accuracy before every decimation, all pairs of nearest neighbor A blocks are partly disentangled by 2-spin unitary transformations (disentangler) acting on the 2-spin B blocks. The disentanglers are optimized to minimize the entropy of entanglement of each A block with the rest of the lattice. They remove entanglement between those pairs of nearest neighbor spins which belong to different A blocks before the A blocks are decimated. The same basic decimation step, including disentanglers, is then applied iteratively to the resulting decimated lattices of block spins. It is worth mentioning that a similar renormalization group was proposed earlier in Ref. [10] but without the disentanglers which are essential to keep d reasonably small.

This renormalization group algorithm motivates the MERA. The simplest nontrivial example of a 1D MERA is the ansatz for a periodic lattice of $N = 4$ spins:

$$T_{i_1 i_2} W_{j_1 j_2}^{i_1} W_{j_3 j_4}^{i_2} U_{k_2 k_3}^{j_2 j_3} U_{k_4 k_1}^{j_4 j_1} |k_1 k_2 k_3 k_4\rangle. \quad (1)$$

Its graphical representation is shown in Fig. 1(a). The

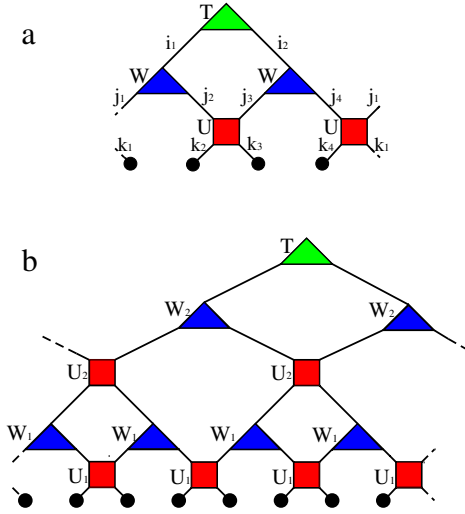


FIG. 1 (color online). In (a) the 1D MERA in Eq. (1) on a 4-site periodic lattice of spins. In (b) the 1D MERA is generalized to a periodic lattice of 8 spins.

repeated indices in Eq. (1) imply summation. The lowest layer of indices k number basis states of the 4 spins. Here the A blocks are the pairs of spins (1, 2) and (3, 4), and the B blocks are the pairs (2, 3) and (4, 1). The U 's are the disentanglers; they are unitary matrices satisfying unitarity conditions $UU^\dagger = 1$ and $U^\dagger U = 1$, or $U_{k_1 k_2}^{j_1 j_2} (U_{k_1 k_2}^{j_3 j_4})^* = \delta_{j_1 j_3} \delta_{j_2 j_4}$ and $U_{k_1 k_2}^{j_1 j_2} (U_{k_3 k_4}^{j_3 j_4})^* = \delta_{k_1 k_3} \delta_{k_2 k_4}$. The second layer of indices j numbers basis states of disentangled spins defined by, e.g., $||j_2, j_3\rangle\rangle = U_{k_2 k_3}^{j_2 j_3} |k_2, k_3\rangle$. The W 's are isometries or projectors which satisfy orthonormality relations $W_{j_1 j_2}^{i_1} (W_{j_1 j_2}^{i_2})^* = \delta_{i_1 i_2}$. Their job is to truncate the Hilbert space of the disentangled A block spins to the d most important states numbered by the upper indices $i \in \{1, \dots, d\}$: For any fixed upper index i , the matrix $W_{j_1 j_2}^i$ is the i th eigenstate of the A block reduced density matrix in the basis of states of disentangled spins $||j_1, j_2\rangle\rangle$. The eigenstates numbered by indices i become basis states $||i_1\rangle\rangle = W_{j_1 j_2}^{i_1} ||j_1, j_2\rangle\rangle$ of the effective block spin. Finally, the top tensor $T_{i_1 i_2}$, which is normalized as $T_{i_1 i_2} (T_{i_1 i_2})^* = 1$, is a quantum state in the basis $||i_1, i_2\rangle\rangle$ of the effective block spins.

In of Fig. 1(b), we show a generalization of the 4-spin ansatz in Fig. 1(a) to a periodic lattice of $N = 8$ spins. The 8 spins require one more layer of isometries and disentanglers. In general, a lattice of $N = 2^n$ spins requires $(n - 1)$ layers of isometries and disentanglers so the number of tensors that need to be stored in memory is only logarithmic in N .

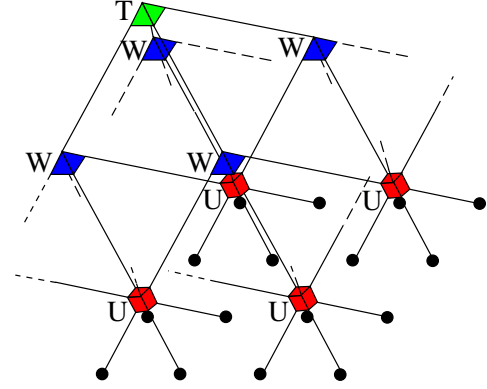


FIG. 2 (color online). The symmetric 2D MERA on a periodic 4×4 lattice. The isometries W replace 4-spin square plaquettes with one effective block spin in just one decimation step.

In Ref. [8] MERA was generalized further to 2D, and in Ref. [11] it was put in a more general unifying framework. In this Letter, we propose the alternative 2D ansatz in Fig. 2. In this symmetric ansatz, 2×2 square plaquettes are replaced by effective block spins in each decimation step. The symmetric ansatz is disentangling in a systematic way all those pairs of nearest neighbor (NN) spins which belong to different 2×2 -spin decimation blocks; see Fig. 3, where the spins on a 2D square lattice are grouped into blue and red plaquettes. We propose that in each decimation step each blue plaquette is replaced by an effective block spin whose Hilbert space is truncated to its d most important states, but before each decimation, the blue plaquettes are partly disentangled by 4-spin unitary disentanglers acting on the red plaquettes. They remove entanglement between all those pairs of NN spins which belong to different blue decimation blocks. Indeed, note that, in Fig. 3, all links joining such pairs of spins are painted red. These red links are naturally grouped into red plaquettes, and the proposed 4-spin disentanglers remove all of the unwanted “red” NN entanglement before the following decimation. It is essential here that the red plaquettes are disjoint, because thanks to this all of the unwanted red entanglement can be removed by the small 4-spin disentanglers acting on individual red plaquettes. Other decimation schemes either do not remove all of the unwanted NN entanglement between different decimation blocks, or they would require disentanglers acting on more than 4 spins.

The symmetric variant of the renormalization group motivates the MERA shown in Fig. 2 in the case of a 4×4 periodic lattice. This graph represents the quantum state

$$T_{i_1 i_2} \begin{pmatrix} W_{j_1 j_2}^{i_1} \\ W_{j_2 j_1}^{i_2} \end{pmatrix} \begin{pmatrix} W_{j_3 j_4}^{i_1} \\ W_{j_4 j_3}^{i_2} \end{pmatrix} \begin{pmatrix} U_{k_1 k_2}^{j_1 j_2} \\ U_{k_3 k_4}^{j_3 j_4} \end{pmatrix} \begin{pmatrix} U_{k_1 k_2}^{j_3 j_4} \\ U_{k_3 k_4}^{j_1 j_2} \end{pmatrix} \begin{pmatrix} k_{11} & k_{12} & k_{13} & k_{14} \\ k_{21} & k_{22} & k_{23} & k_{24} \\ k_{31} & k_{32} & k_{33} & k_{34} \\ k_{41} & k_{42} & k_{43} & k_{44} \end{pmatrix} \quad (2)$$

Here the double subscript indices numerate rows and columns of the lattice. A generalization to greater $2^n \times 2^n$ lattices is obtained by adding $(n - 2)$ layers of isometries and disentanglers.

In this Letter, we use MERA to find the ground state of the spin- $\frac{1}{2}$ transverse quantum Ising model

$$H = -g \sum_i X_i - \sum_{\langle i,j \rangle} Z_i Z_j \quad (3)$$

on 2×2 , 4×4 , and 8×8 periodic square lattices. Here X and Z are Pauli matrices. T and all layers of different W and U were optimized to minimize total energy. Provided that the minimization preserves all constraints on T , W , and U (respectively: normalization, orthonormality, and unitarity), there is no need to obtain W^i 's as leading eigenstates of reduced density matrices and to construct U 's as disentanglers that minimize the entropy of those matrices. The W 's and U 's that minimize the energy are at the same time good candidates for, respectively, the leading eigenstates and optimal disentanglers.

In most calculations, we used $d = 2$ in all tensors, i.e., the minimal nontrivial value of the truncation parameter, except for the 8×8 lattice, where it was necessary to increase the parameter to $d = 3$ but only in the top tensor T near the critical $g = 3.04$. For any g , the initial state for the minimization was the Schrödinger cat state $|\uparrow\uparrow\uparrow \dots\rangle + |\downarrow\downarrow\downarrow \dots\rangle$, which is the ground state when $g \rightarrow 0$. This state translates into trivial disentanglers $U = 1$, the top T having only two nonzero elements $T_{1111} = T_{2222} = 1/\sqrt{2}$, and all W 's being nonzero only when $W_{1111}^1 = W_{2222}^2 = 1$. As we were looking for the ground state, we assumed that all tensors T , W , and U are real. The tensor T and each tensor W^i are quantum states on a 2×2 square plaquette. Each tensor T or W^i has four lower indices with each index numbering d states of its corresponding spin. We assume that T is symmetric under all exchanges of lower indices

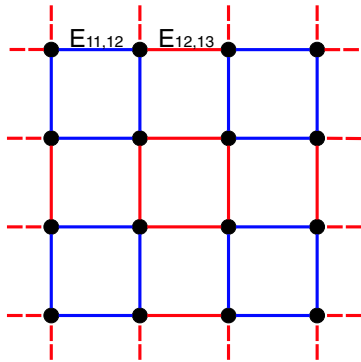


FIG. 3 (color online). The symmetric decimation in 2D: Each blue 4-spin square plaquette is replaced by a block spin whose Hilbert space is truncated to its d most important states, but before this decimation a unitary 4-spin disentangler is applied to each red plaquette. The disentanglers remove unwanted entanglement between all those (red) nearest neighbor pairs of spins which belong to different (blue) decimation blocks.

that correspond to symmetry transformations of the 2×2 plaquette. As each W^i is an eigenstate of a reduced density matrix, it must be either symmetric or antisymmetric under each of these symmetry transformations. In all considered cases, we found that the lowest energy is obtained when all W^i 's are assumed symmetric under all transformations. In this symmetric subspace, it is convenient to parametrize the tensors as (here $d = 2$)

$$T_{abcd} \simeq \sum_{\alpha=1}^6 t_{\alpha} v_{abcd}^{\alpha}, \quad W_{abcd}^i \simeq \sum_{\alpha=1}^6 w_{\alpha}^i v_{abcd}^{\alpha}, \quad (4)$$

$$U = \exp\left(i \sum_{\alpha=1}^{21} q^{\alpha} A_{\alpha}\right),$$

where \simeq means equality up to normalization. Here $v_{abcd}^{\alpha} = \langle abcd | v^{\alpha} \rangle$, where the states

$$\begin{aligned} |v^1\rangle &= |0000\rangle, & |v^2\rangle &= |1111\rangle, \\ |v^3\rangle &= (|0110\rangle + |1001\rangle)/\sqrt{2}, \\ |v^4\rangle &= (|1000\rangle + |0100\rangle + |0010\rangle + |0001\rangle)/2, \\ |v^5\rangle &= (|0111\rangle + |1011\rangle + |1101\rangle + |1110\rangle)/2, \\ |v^6\rangle &= (|1100\rangle + |0011\rangle + |0101\rangle + |1010\rangle)/2 \end{aligned} \quad (5)$$

are a basis of symmetric states on the 2×2 plaquette. A_{α} 's are imaginary 4-spin Hermitian operators invariant under the symmetries of the 2×2 plaquette:

$$\begin{aligned} A_1 &\simeq Y_1 + Y_2 + Y_3 + Y_4, \\ A_2 &\simeq X_1 Y_2 + Y_1 X_2 + X_2 Y_4 + Y_2 X_4 + X_3 Y_4 \\ &\quad + Y_3 X_4 + X_3 Y_1 + Y_3 X_1, \dots, \\ A_{21} &\simeq Y_1 Y_2 Y_4 + Y_2 Y_4 Y_3 + Y_4 Y_3 Y_1 + Y_3 Y_1 Y_2. \end{aligned} \quad (6)$$

Each A_{α} is a symmetrized sum of tensor products of Pauli matrices with each term in the sum including an odd number of Y 's. They are normalized so that $\text{Tr} A_{\alpha}^{\dagger} A_{\beta} = \delta_{\alpha\beta}$.

The minimized energy is a sum of all bond energies $E_{i,j} = \langle -\frac{1}{4}gX_i - \frac{1}{4}gX_j - Z_i Z_j \rangle$. However, thanks to the assumed symmetry of the tensors, only some of them need to be calculated. For example, on the 4×4 lattice in Fig. 3, one needs to evaluate only two bond energies: $E_{11,12}$ and $E_{12,13}$. By symmetry, all other bond energies are equal to either $E_{11,12}$ or $E_{12,13}$, and the total energy is $\langle H \rangle = 16E_{11,12} + 16E_{12,13}$. In a similar way, the 8×8 square lattice has 6 and, in general, an $N \times N$ square lattice has $\frac{N^2}{16} + \frac{N}{4}$ independent bond energies. The total number of bonds is $2N^2$, so for a large N we save a factor of 32 simply by using the assumed tensor symmetries. Thus, for a large N , the cost of calculating energy is proportional to the lattice size times the cost of calculating any bond energy $E_{i,j}$ which is logarithmic in N and polynomial in d . Here the proof follows similar lines as in Ref. [8]. Indices are contracted along causal cones whose horizontal cross sec-

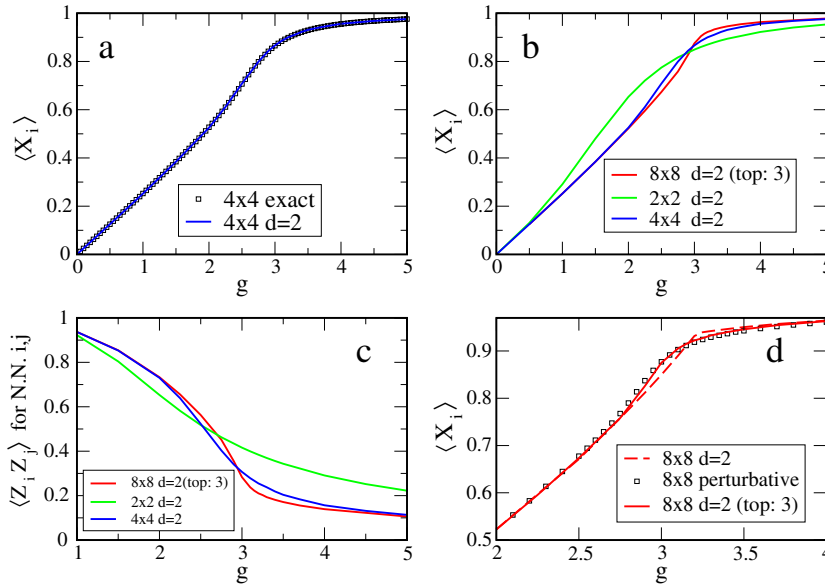


FIG. 4 (color online). In (a), we compare transversal magnetization $\langle X \rangle$ on the 4×4 lattice obtained from MERA and exact diagonalization. In (b) and (c), the transversal magnetization and nearest neighbor ferromagnetic correlator obtained from MERA are shown for different lattice sizes. In (d), we compare transversal magnetization on the 8×8 lattice when $d = 2$ in all tensors and when it is increased to $d = 3$ in the top tensor with the perturbative results from Ref. [12].

tion is 3×3 (or 4×4) spins when cut above (or below) a layer of isometries W . To avoid the intermediate 4×4 stage, we do not apply all isometries first and then all disentanglers, but we apply some isometries earlier than others, gradually including disentanglers; i.e., we pass through a series of intermediate nonhorizontal cross sections never exceeding 11 spins.

Energy was minimized with respect to the variational parameters $\{t_\alpha, w_\alpha^i, q^\alpha\}$ in Eq. (4) using different standard minimization routines, but the best performance was achieved with the simplest steepest descent method with gradients of the energy estimated from finite differences. Our calculations demonstrate that the energy of MERA can be minimized in a fairly straightforward manner.

In Fig. 4, we summarize our results for 2×2 , 4×4 , and 8×8 periodic square lattices. Of special interest are Figs. 4(a) and 4(d), where we compare transversal magnetization obtained from MERA with exact results on the 4×4 lattice and perturbative results on the 8×8 lattice. On the 4×4 lattice, $d = 2$ was accurate enough, but on the 8×8 lattice, d in the top tensor had to be increased to $d = 3$. This was necessary because with increasing lattice size the Ising model develops a critical point at $g = 3.04$ —this tendency can be seen in Figs. 4(b) and 4(c).

In conclusion, we proposed and tested a symmetric version of MERA in 2D. By using the smallest nontrivial truncation parameter $d = 2$ in most tensors and fairly straightforward optimization methods, we obtained surprisingly accurate numerical results for the ground state of the 2D quantum Ising model. This is, we think, an encouraging result, but, as the Ising model that we consider is relatively simple, it remains to be seen how well MERA can deal with more complicated models.

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Note added.—When this Letter was in the final stage of preparation, the e-print [13] appeared, where a similar symmetric ansatz was proposed.

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