Projected Entangled Pair States at Finite Temperature: Iterative Self-Consistent Bond Renormalization for Exact Imaginary Time Evolution

Piotr Czarnik\textsuperscript{1} and Jacek Dziarmaga\textsuperscript{1}

\textsuperscript{1}Instytut Fizyki Uniwersytetu Jagiellońskiego, ul. Lojasiewicza 11, 30-348 Kraków, Poland

(Dated: November 23, 2014)

A projected entangled pair state (PEPS) with ancillas can be evolved in imaginary time to obtain thermal states of a strongly correlated quantum system on a 2D lattice. Every application of a Suzuki-Trotter gate multiplies the PEPS bond dimension $D$ by a factor $k$. It has to be renormalized back to the original $D$. In order to preserve the accuracy of the Suzuki-Trotter (S-T) decomposition, the renormalization has in principle to take into account full environment made of the new tensors with the bond dimension $k \times D$. Here we propose a self-consistent renormalization procedure operating with the original bond dimension $D$, but without compromising the accuracy of the S-T decomposition. The iterative procedure renormalizes the bond using full environment made of renormalized tensors with the bond dimension $D$. After every renormalization, the new renormalized tensors are used to update the environment, and then the renormalization is repeated again and again until convergence.

I. INTRODUCTION

Quantum tensor networks are a competitive tool to study strongly correlated quantum systems on a lattice. Their history begins with the density matrix renormalization group (DMRG) \cite{white} - an algorithm to minimize the energy of a matrix product state (MPS) ansatz in one dimension (1D), see Ref. \cite{vidal} for a review of MPS algorithms. In the last decade, MPS was generalized to a 2D “tensor product state” widely known as a projected entangled pair state (PEPS) \cite{verstraete}. Another type of tensor network is the multiscale entanglement renormalization ansatz (MERA) \cite{sd}, and the branching MERA \cite{sd2}, that is a refined version of the real space renormalization group. Being variational methods, the quantum tensor networks do not suffer from the notorious fermionic sign problem, and thus they can be applied to strongly correlated fermions in 2D \cite{non}. A possible breakthrough in this direction is an application of the PEPS ansatz to the t-J model \cite{tj}, which is a strong coupling approximation to the celebrated Hubbard Hamiltonian of the high temperature superconductivity \cite{hubbard}. An energy of the ground state was obtained that could compete with the best variational Monte-Carlo results \cite{bqmc}.

The tensor networks also proved to be a powerful tool to study topological spin liquids (TSL). The search for realistic models gained momentum after White demonstrated the spin-liquid nature of the Kagome antiferromagnet \cite{white}. This result was obtained by a tour de force application of a quasi-1D DMRG. The DMRG investigation of TSL’s was elevated to a higher degree of sophistication in Ref. \cite{white}. Unfortunately, the MPS tensor network underlying the DMRG suffers from severe limitations in two dimensions, where it can be used for states with a very short correlation length only. In contrast, the PEPS ansatz in Fig. 1 is not restricted in this way. Its usefulness for TSL has already been demonstrated. In Ref. \cite{tj} it was shown how to represent the RVB state with the PEPS ansatz in an efficient way. In Ref. \cite{tj2} PEPS was used to classify topologically distinct ground states of the Kagome antiferromagnet. Finally, in Ref. \cite{tj3} PEPS demonstrated a TSL in the antiferromagnetic $J_1-J_2$ model.

In contrast to the ground state, finite temperature states have been explored so far mostly with the MPS \cite{mps}. In a way that can be easily generalized to 2D, the MPS is extended to finite temperature by appending each lattice site with an ancilla \cite{mps}. A thermal state is obtained by an imaginary time evolution of a pure state in the enlarged Hilbert space starting from infinite temperature. However, thermal states are of more interest in 2D, where they can undergo finite temperature phase transformations. A thermal PEPS with ancillas was considered in Ref. \cite{mps}, where finite temperature states of the 2D quantum Ising model and a spinless fermionic system were obtained. Alternative approaches to finite temperature were developed where, instead of the imaginary time evolution, a tensor network representing the partition function is directly contracted by subsequent tensor renormalizations. Another interesting alternative is based on linear optimization of local density matrices at finite $T$ \cite{mps2}.

Here we revisit the approach of Ref. \cite{mps}, with the aim to improve its numerical efficiency. After every infinitesimal time step effected by a Suzuki-Trotter (S-T) gate, the bond dimension $D$ of a PEPS tensor is multiplied by a factor $k \geq 2$. This dimension has to be truncated/renormalized back to the original $D$ in a way that is least distortive to the new PEPS. To preserve the accuracy of the S-T decomposition, the renormalization has to take into account full environment of the renormalized bond and after the gate the environment is...
made of tensors with the enlarged bond dimension $k \times D$. The infinite environment is calculated with the help of the corner matrix renormalization [20]. It is the most time-consuming part of the time-evolution algorithm that needs to be accelerated. In this paper, we propose a self-consistent renormalization scheme that is using full environment made of renormalized tensors with the original bond dimension $D$. After every renormalization, the new renormalized tensors are used to update the environment and then the renormalization is repeated again and again until convergence. The converged renormalized tensors are accepted as the new PEPS tensors after the S-T gate. As a benchmark application, we evolve the quantum Ising model on a square lattice - both infinite and finite - across a finite-temperature second-order phase transition in a strong transverse magnetic field.

The paper is organized as follows. In Section II we introduce purifications of thermal states represented by PEPS. In Section III we remind the quantum Ising model and in Sec. IV introduce the Suzuki-Trotter decomposition in the PEPS formalism. Section V explains how the enlarged bond dimension can be truncated back to the original size $D$ with the help of an isometry. The iterative self-consistent optimization of the isometry is introduced in Section VI and translated to the language of tensor networks in Section VII that is supplemented by Appendices A and B. The benchmark results in the Ising model on an infinite lattice are presented in Section VIII and on a finite one in Sec. IX. Finally, we conclude in Section X.

II. PURIFICATION OF THERMAL STATES AS PEPS

We consider spins on an infinite square lattice with a Hamiltonian $\mathcal{H}$. Every spin has $S$ states $i = 0, ..., S - 1$ and is accompanied by an ancilla with states $a = 0, ..., S - 1$. The enlarged Hilbert space is spanned by states $\prod_s |i_s, a_s\rangle$, where the product runs over lattice sites $s$. The state of spins at infinite temperature, $\rho(\beta = 0) = \prod_s \left( \frac{1}{S} \sum_{i=0}^{S-1} |i_s\rangle \langle i_s| \right) \propto 1$, is obtained from its purification in the enlarged Hilbert space,

$$\rho(0) = \text{Tr}_{\text{ancillas}}|\psi(0)\rangle\langle \psi(0)| ,$$

where

$$|\psi(0)\rangle = \prod_s \left( \frac{1}{S} \sum_{i=0}^{S-1} |i_s\rangle \langle i_s| \right)$$

is a product of maximally entangled states of every spin with its ancilla. The state $\rho(\beta) \propto e^{-\beta \mathcal{H}}$ at finite $\beta$ is obtained from

$$|\psi(\beta)\rangle \propto e^{-\frac{1}{2} \beta \mathcal{H}} |\psi(0)\rangle \equiv U(\beta) |\psi(0)\rangle$$

after imaginary time evolution for time $\beta$ with $\frac{1}{2} \mathcal{H}$.

For an efficient simulation of the time evolution, we represent $|\psi(\beta)\rangle$ by a translationally invariant PEPS with the same tensor $A^{|a|}_{tr,\beta}(\beta)$ at every site. In the quantum Ising model that we consider in this paper, translational invariance is not broken and a unit cell encloses one lattice site. Here $i$ and $a$ are the spin and ancilla indices respectively, and $u,r,d,l = 0, ..., D - 1$ are bond indices to contract the tensor with similar tensors at the nearest neighbor sites, see Fig. 1A. The Ansatz is

$$|\psi(\beta)\rangle = \sum_{\{i_s, a_s\}} \Psi_A[\{i_s, a_s\}] \prod_s |i_s, a_s\rangle \equiv |\psi_A\rangle .$$

Here the sum runs over all pairs of indices $i_s, a_s$ at all sites $s$. The amplitude $\Psi_A$ is the tensor contraction in Fig. 1B. The initial state (2) can be represented by a tensor

$$A^{|a|}_{urdl} = \delta^{ia} \delta_{u0} \delta_{r0} \delta_{d0} \delta_{l0}$$

with the minimal bond dimension $D = 1$.

III. TRANSVERSE FIELD QUANTUM ISING MODEL ON A SQUARE LATTICE

We proceed with

$$\mathcal{H} = - \sum_{(s,s')} Z_s Z_{s'} - h \sum_s X_s \equiv \mathcal{H}_{ZZ} + \mathcal{H}_X .$$

Here $Z, X$ are Pauli matrices. The model has a ferromagnetic phase with a non-zero spontaneous magnetization $\langle Z \rangle$ for small $h$ and large $\beta$. At $h = 0$ the critical point is $\beta_0 = -\ln(\sqrt{2} - 1)/2 = 0.441$, and at zero temperature the quantum critical point is $b_0 = 3.044$, see Ref. [21].

IV. SUZUKI-TROTTER DECOMPOSITION

We define $U_{ZZ}(\Delta \beta) \equiv e^{-\frac{1}{4} \mathcal{H}_{ZZ} \Delta \beta}$ and $U_{X}(\Delta \beta) \equiv e^{-\frac{1}{4} \mathcal{H}_X \Delta \beta}$ for the interaction and the transverse field re-
spectively. In the second-order Suzuki-Trotter decomposition a small time step is a product
\[ U(d\beta) = U_X(d\beta/2)U_Z(d\beta)U_X(d\beta/2) + \mathcal{O}(d\beta^3). \] (7)

The action of \( U_X(d\beta) \) on PEPS replaces \( A_{\text{trbl}} \) with
\[ A'_{\text{trbl}} + \tanh(h \, d\beta/2) \sum_j X^{ij} A_{\text{trbl}}^{ja}, \] (8)
of the same bond dimension \( D \). The action of \( U_Z(d\beta) \) maps \( A \) to a new tensor
\[ B_{2l+s_l,2r+s_r,2b+s_b,2l+s_l} = \sum_{j=0,1} [Z^s \tanh^s(d\beta/2)]^{ij} A_{\text{trbl}}^{ja} \] (9)
\[ (-1)^{is} \tanh^s(d\beta/2) A_{\text{trbl}}^{ia} \] (10)
see Fig. 2. Here the indices \( s_l, s_r, s_b, s_t \in \{0,1\} \), and \( s = s_l + s_r + s_b + s_t \). This is an exact map, but \( B \) has the bond dimension 2\( D \) instead of the original \( D \).

![Fig. 2. The action of \( U_{Z}(d\beta) \) on \( A \) (left) maps \( A \) to a new tensor \( B \) (right) in Eq. (11) with the bond dimension 2\( D \) instead of the original \( D \).](image)

V. TENSOR RENORMALIZATION

The bond dimension has to be truncated back to \( D \) in a way least distortive to the exact new PEPS \( \psi_B \). This renormalization can be done with an isometry \( W \) that maps from 2\( D \) back to \( D \) dimensions:
\[ \sum_{u',r',d',l'=0}^{2D-1} W_{u'}^u W_{r'}^r W_{d'}^d W_{l'}^l B_{u'r'd'l'}^{ia} = A_{ardl}^{ia}, \] (12)
see Fig. 3. Here \( A \) is a candidate for a new tensor after the infinitesimal time step with bond indices \( u, r, d, l = 0, ..., D-1 \). The isometry is a variational parameter and the renormalized new PEPS \( \psi_A \) is a function of this parameter. \( W \) should maximize a figure of merit like e.g. a fidelity
\[ F = \langle \psi_A | \psi_B \rangle \] (13)

between the exact \( |\psi_B\rangle \) and the renormalized \( |\psi_A\rangle \).

From the point of view of numerical efficiency the fidelity has a disadvantage that it involves tensor \( B \) with the doubled bond dimension. Since the exact \( B \) is a reference for the optimized \( A \), it may appear impossible to eliminate without a crude approximation. In the following, we optimize \( A \) avoiding this overhead, but without compromising the accuracy of the second-order Suzuki-Trotter decomposition.

![Fig. 3. The action of the isometry \( W \) on the exact new tensor \( B \), compare Eq. (12). The isometry truncates the bond dimension from 2\( D \) back to the original \( D \).](image)

VI. SELF-CONSISTENT ISOMETRY OPTIMIZATION

Suppose that we want to optimize an isometry on just one bond in \( |\psi_A\rangle \), but with isometries on all other bonds fixed as \( W \). This optimization could be done with the fidelity \( F \) in Eq. (13) as a figure of merit, but with the numerical overhead of using tensor \( B \) that we want to avoid. However, when \( W \) is already close enough to the optimal one, then \( F \) will not be distorted much if we replace \( |\psi_B\rangle \) by \( |\psi_A\rangle \) with \( W \) on all bonds. In fact, when \( D \) is large enough and \( W \) is optimal, then there will be no distortion at all. This observation motivates a more efficient figure of merit for the single bond:
\[ \tilde{F}[\tilde{W}] = \langle \tilde{\psi}_A | \psi_B \rangle. \] (14)

Here \( \tilde{\psi}_A \) is a PEPS with a variational \( \tilde{W} \) on the optimized bond and fixed \( W \) on all other bonds.

Once the optimal \( \tilde{W} \) on the single bond is found, it becomes a new \( W \) and is applied at all other bonds as well, and then the optimization of the single bond is repeated again. This optimization loop is iterated until \( W \) converges to a self-consistent fixed point. Once converged, the \( A \) in Eq. (12) with the converged \( W \) is accepted as the new tensor \( A \) after the infinitesimal time step.

In the next Section, we translate this algorithm to the language of tensor networks.
VII. TENSOR NETWORKS FOR SELF-CONSISTENT OPTIMIZATION

To begin with, a tensor network representing the norm $\langle \psi_A | \psi_A \rangle$ is obtained in two steps: first $A$ is contracted with its conjugate to make a transfer tensor $a$, see Fig. 4A, and then the transfer tensors are contracted as in Fig. 4B. This infinite contraction can be done approximately with the help of the corner matrix renormalization [20], see Appendix A.

However, what we actually need to optimize the isometry $\tilde{W}$ on a single bond is a PEPS $|\psi'_A \rangle$, where all bonds are renormalized with the current $W$ except for the tensors on the single bond whose bond indices along this bond are left unrenormalized. Its fidelity $\langle \psi'_A | \psi_A \rangle$, shown in Fig. 5B, is a contraction of transfer tensors $a$ except for the single bond, where the two $a$’s are replaced by $b$’s introduced in Fig. 5A. Finally, in contrast to Fig. 5B, in Fig. 5C we refrain from contracting the unrenormalized bond indices. The result is a “bond environment matrix” $E$ whose trace equals the fidelity in Fig. 5B, $\text{Tr} E = \langle \psi'_A | \psi_A \rangle$.

The indices of $E$ are in fact unrenormalized indices of tensor $B$. When they are renormalized by the variational isometry $W$, then the environment becomes

$$E_{kl}^{\text{ren}} = \sum_{m,n=0}^{2D-1} \tilde{W}_k^m \tilde{W}_l^n E_{mn}$$

such that $\text{Tr} E^{\text{ren}} = \tilde{F}[\tilde{W}]$ is the fidelity for the single bond in Eq. (14). Since this figure of merit depends only on the symmetric part of $E$, the isometry is optimal when $W_k$’s are the eigenvectors of the symmetric part with the $D$ largest eigenvalues.

$W$ is optimized iteratively. In every iteration a new bond environment $E$ is calculated with a current isometry $W$, see Appendix A and then used to obtain a new isometry $W$. The iterations are repeated until convergence of the $D$ leading eigenvalues of $E$. Once converged, the $A$ in Eq. (12) is accepted as a new PEPS tensor after the infinitesimal time step.

VIII. BENCHMARK RESULTS

In order to evolve PEPS across the symmetry breaking phase transition we add to the Hamiltonian a tiny longitudinal bias $H_Z = -\delta \sum_s Z_s$ to smooth out the transition at a finite $\beta_c(h)$. We present results for the transverse field $h = \frac{2}{3} h_c$ that is large enough to introduce substantial quantum fluctuations and significantly increase $\beta_c$ above the Onsager’s $\beta_0$. 

FIG. 4. In A, tensor $A$ is contracted with its conjugate through their spin and ancilla indices. The contraction is a transfer tensor $a$. In B, a contraction of the transfer tensors is the norm $\langle \psi_A | \psi_A \rangle$ of the PEPS with tensor $A$.

FIG. 5. In A, a transfer tensor $b$ on a site where one of the bond indices is left unrenormalized by the isometry. In B, the fidelity $\langle \psi'_A | \psi_A \rangle$ between the renormalized PEPS $|\psi_A \rangle$ and the PEPS $|\psi'_A \rangle$ with the unrenormalized bond. In C, same as in B, but with the unrenormalized bond index left uncontracted. This network is the bond environment matrix $E$. 

FIG. 5B. In A, a transfer tensor $b$ on a site where one of the bond indices is left unrenormalized by the isometry. In B, the fidelity $\langle \psi'_A | \psi_A \rangle$ between the renormalized PEPS $|\psi_A \rangle$ and the PEPS $|\psi'_A \rangle$ with the unrenormalized bond. In C, same as in B, but with the unrenormalized bond index left uncontracted. This network is the bond environment matrix $E$.
Figure 6 shows the order parameter \( \langle Z \rangle \) as a function of \( \beta \) for \( \delta = 10^{-6} \). The slope \( d\langle Z \rangle/d\beta \) is the steepest at \( \beta_c = 0.589 = 1.33\beta_0 \). This local observable requires \( D \geq 6 \) and a relatively small environmental bond dimension, \( M \geq 12 \), to converge. Long range correlations are more demanding on \( M \), as demonstrated by the ferromagnetic correlator in Fig. 7. For \( \delta = 10^{-6} \) we need \( M \geq 20 \) to converge a finite correlation length, \( \xi \approx 224 \). It is finite thanks to the bias: \( \delta = 0 \) would make both \( \xi \) and \( M \) diverge making accurate evolution across \( \beta_c \) impossible.

![Image](image-url)

FIG. 6. The ferromagnetic magnetization \( \langle Z \rangle \) as a function of \( \beta \) for the transverse field \( h = \frac{3}{2}h_0 \) and the longitudinal bias \( \delta = 10^{-6} \). This magnetization and other local observables are converged for \( D \geq 6 \) and \( M \geq 12 \). Here we show results for \( M = 16 \).

![Image](image-url)

FIG. 7. The ferromagnetic correlator, \( C_{zz}(R) = \langle Z_{(x+h,y)}Z_{(x,y)} \rangle - \langle Z \rangle^2 \), for the transverse field \( h = \frac{3}{2}h_c \), the longitudinal bias \( h_Z = 10^{-6} \), at the critical \( \beta_c = 0.589 \). The correlator is converged for \( M \geq 24 \) and \( D \geq 6 \). Here we show \( D = 6 \). In A, a logarithmic plot emphasizing exponential tails for large \( R \): \( C_{zz}(R) \sim e^{-R/\xi} \). The correlation length increases with \( M \) until it converges at \( \xi = 224 \) which is finite thanks to the finite bias. In B, a log-log plot emphasizing a power law decay for intermediate \( R \), \( C_{zz}(R) \sim R^{-\eta} \). The best fit is \( \eta = 0.28 \) - close to \( \eta = \frac{1}{4} \) in the Ising’s class.

IX. FINITE LATTICE

On a finite \( N \times N \) lattice the self-consistent algorithm is basically the same as on the infinite one except that contraction of finite networks, like the one in Fig. 8 can be done with matrix product states [22] instead of corner matrix renormalization. A finite lattice is also less symmetric than the infinite one, hence different bonds and their environments \( E \) are not equivalent. One has to sweep across the lattice optimizing each bond separately - modulo residual symmetries - and repeat the sweeps until convergence of all bonds.

![Image](image-url)

FIG. 8. One of the bond environments on a 5 \( \times \) 5 lattice.

Figure 9 shows a ferromagnetic correlator along a diagonal of an 11 \( \times \) 11 lattice. The finite lattice size itself is enough to smooth the transition, hence there is no need for the longitudinal bias here, \( \delta = 0 \).

![Image](image-url)

FIG. 9. Ferromagnetic correlator \( \langle Z_{3,3}Z_{9,9} \rangle \) between sites \( (3,3) \) and \( (9,9) \) on a diagonal of an 11 \( \times \) 11 lattice as a function of \( \beta \). Here the transverse field \( g = \frac{3}{4}g_c \), the longitudinal bias \( \delta = 0 \), and a bond dimension in the matrix product state is \( M_{\text{MPS}} = 16 \). The correlator is converged for bond dimension \( D \geq 5 \) and \( M_{\text{MPS}} \geq 16 \).

X. CONCLUSION

We presented an iterative self-consistent renormalization of the PEPS bond dimension after a Suzuki-Trotter gate. The procedure takes into account full environment made of self-consistently renormalized tensors to preserve the accuracy of the Suzuki-Trotter decomposition. The protocol brings us closer to a numerically exact imaginary time evolution that can be used to obtain thermal states of strongly correlated systems.
ACKNOWLEDGMENTS

This work was supported by the Polish National Science Center (NCN) under Project DEC-2013/09/B/ST3/01603.

[1] S. R. White, Phys. Rev. Lett. 69, 2863 (1992).
[2] U. Schollwöck, Annals of Physics 326, 96 (2011).
[3] F. Verstraete and J. I. Cirac, cond-mat/0407066; V. Murg, F. Verstraete, and J. I. Cirac, Phys. Rev. A 75, 033605 (2007); G. Sierra and M. A. Martin-Delgado, arXiv:cond-mat/011170; T. Nishino and K. Okunishi, J. Phys. Soc. Jpn. 69, 3966 (1999); Y. Nishio, N. Maeshima, A. Gendiar, and T. Nishino, cond-mat/0401115; J. Jordan, R. Orús, G. Vidal, F. Verstraete, and J. I. Cirac, Phys. Rev. Lett. 101, 250602 (2008); Z.-C. Gu, M. Levin, and X.-G. Wen, Phys. Rev. B 78, 205116 (2008); H. C. Jiang, Z. Y. Weng, and T. Xiang, Phys. Rev. Lett. 101, 090603 (2008); Z. Y. Xie, H. C. Jiang, Q. N. Chen, Z. Y. Weng, and T. Xiang, Phys. Rev. Lett. 103, 160601 (2009); P.-C. Chen, C.-Y. Lai, and M.-F. Yang, J. Stat. Mech.: Theory Exp. (2009) P10001; R. Orús and G. Vidal, Phys. Rev. B 80, 094403 (2009).
[4] G. Vidal, Phys. Rev. Lett. 92, 224005 (2004); G. Vidal, Phys. Rev. Lett. 101, 110501 (2008); L. Cincio, J. Dziarmaga, and M. M. Rams, Phys. Rev. Lett. 100, 240603 (2008); G. Evenbly and G. Vidal, Phys. Rev. Lett. 102, 180406 (2009); G. Evenbly and G. Vidal, Phys. Rev. B 79, 144108 (2009).
[5] G. Evenbly and G. Vidal, Phys. Rev. Lett. 112, 240502 (2014); Phys. Rev. B 89, 235113 (2014).
[6] T. Barthel, C. Pineda, and J. Eisert Phys. Rev. A 80, 042333 (2009); P. Corboz and G. Vidal, Phys. Rev. B 80, 165129 (2009); P. Corboz, G. Evenbly, F. Verstraete, and G. Vidal, Phys. Rev. A 81, 010303(R) (2010); C. V. Kraus, N. Schuch, F. Verstraete, and J. I. Cirac, Phys. Rev. A 81, 052338 (2010); C. Pineda, T. Barthel, and J. Eisert, Phys. Rev. A 81, 050303(R) (2010); Z.-C. Gu, F. Verstraete, and X.-G. Wen, arXiv:1004.2563 (2010).
[7] J. Hubbard, Proc. Roy. Soc. (London), Ser. A 276, 238 (1963); P. W. Anderson, Science 235, 1196 (1987).
[8] P. Corboz, R. Orús, B. Bauer, and G. Vidal, Phys. Rev. B 81, 165104 (2010); P. Corboz, S. R. White, G. Vidal, and M. Troyer, Phys. Rev. B 84, 041108 (2011); P. Corboz, T. M. Rice, M. Troyer, Phys. Rev. Lett. 113, 040402 (2014).
[9] D. A. Ivanov, Phys. Rev. B 70, 104503 (2004); W.-J. Hu, F. Becca, S. Sorella, Phys. Rev. B 85, 081110(R) (2012).
[10] S. Yan, D. A. Huse, and S. R. White, Science 332, 1173 (2011).
[11] L. Cincio and G. Vidal, Phys. Rev. Lett. 110, 067208 (2013).
[12] D. Poilblanc, N. Schuch, D. Pérez-García, and J. I. Cirac, Phys. Rev. B 86, 014404 (2012).
[13] D. Poilblanc, N. Schuch, Phys. Rev. B 87, 140407(R) (2013).
[14] L. Wang, D. Poilblanc, Z.-C. Gu, X.-G. Wen, and F. Verstraete, Phys. Rev. Lett. 111, 037202 (2013).
[15] F. Verstraete, J. J. García-Ripoll, and J. I. Cirac, Phys. Rev. Lett. 93, 207204 (2004); M. Zwolak and G. Vidal, Phys. Rev. Lett. 93, 207205 (2004); A.E. Feiguin and S.R. White, Phys. Rev. B 72, 220401 (2005).
[16] S. R. White, arXiv:0902.4475; E.M. Stoudenmire and Steven R. White, New J. Phys. 12, 055026 (2010); I. Pizorn, V. Eisler, S. Andergassen, and M. Troyer, New J. Phys. 16, 073007 (2014).
[17] P. Czarnik, L. Cincio, and J. Dziarmaga, Phys. Rev. B 86, 245101 (2012); P. Czarnik and J. Dziarmaga, Phys. Rev. B 90, 035144 (2014).
[18] Z. Y. Xie, H. C. Jiang, Q. N. Chen, Z. Y. Weng, T. Xiang, Phys.Rev.Lett. 103, 160601 (2009); H.H. Zhao, Z.Y. Xie, Q.N. Chen, Z.C. Wei, J.W. Cai, T. Xiang, Phys. Rev. B 81, 174411 (2010); W. Li, S.-J. Ran, S.-G. Gong, Y. Zhao, B. Xi, F. Ye, and G. Su, Phys. Rev. Lett. 106, 127202 (2011); Z. Y. Xie, J. Chen, M. P. Qin, J. W. Zhu, L. P. Yang, and T. Xiang, Phys. Rev. B 86, 045139 (2012); Shi-Ju Ran, Wei Li, Bin Xi, Zhe Zhang and Gang Su, Phys. Rev. B 86, 134429 (2012); S.-J. Ran, B. Xi, T. Liu, and G. Su, Phys. Rev. B 88, 064407 (2013); A. Denbleyker, Y. Liu, Y. Meurice, M. P. Qin, T. Xiang, Z. Y. Xie, J. F. Yu, H. Zou, Phys. Rev. D 89, 016008 (2014).
[19] L. Poulin and M. B. Hastings, Phys. Rev. Lett. 106, 080403 (2011); A. J. Ferris and D. Poulin, Phys. Rev. B 87, 205126 (2013).
[20] R. J. Baxter, J. Math. Phys. 9, 650 (1968); J. Stat. Phys. 19, 461 (1978); T. Nishino and K. Okunishi, J. Phys. Soc. Jpn. 65, 891 (1996); R. Orús and G. Vidal, Phys. Rev. B 80, 094403 (2009); R. Orús, Phys. Rev. B 85, 205117 (2012); R. Orús, Ann. of Phys. 349, 117 (2014); Ho N. Phien, I. P.McCulloch, G. Vidal, arXiv:1411.0391.
[21] H. Rieger, N. Kawashima, Europ. Phys. J. B 9, 233 (1999); H.W.J. Blote and Y. Deng, Phys. Rev. E 66, 066110 (2002).
[22] F. Verstraete, J.I. Cirac, V. Murg, Adv. Phys. 57, 143 (2008).

Appendix A: Corner matrix renormalization

An infinite tensor network, like the one on the left of Fig. 10 cannot be contracted exactly. Fortunately, what we need in general is not this number, but an environment for a few tensors of interest. For instance, in Fig. 10, we want an environment for the transfer tensor $a$ in the center. The environment is a tensor that remains after removing the central tensor from the infinite network. From the point of view of the central tensor, its environment can be substituted with an effective environment, made of finite corner matrices $C$ and top tensors $T$, that appears to the central tensor the same as the exact envi-
environment as much as possible. The environmental tensors are contracted with each other by indices of dimension $M$. Increasing $M$ makes the effective environment more accurate, and for a finite correlation length the environment is expected to converge at a finite $M$.

For the sake of simplicity, here in the Ising model, we assume that tensors $A, B, a$ are isotropic in their four bond indices. Consequently, $C$ is symmetric and top is symmetric in its environmental indices.

Finite tensors $C$ and $T$ represent infinite sectors of the network on the left of Fig. 10. The tensors are converged by iterating the corner matrix renormalization in Fig. 11. In every renormalization step, the corner matrix is enlarged with one tensor $a$ and two $T$'s. This operation represents the top-left corner sector in Fig. 10 absorbing one more layer of tensors $a$. Once the environment is converged, it can be used to calculate efficiently either observables or the bond environment $E$, see Fig. 12. Initialization of the iterative corner renormalization is discussed in Appendix B.

![Fig. 10](image1.png)

**Fig. 10.** On the left, the norm $\langle \psi_A | \psi_A \rangle$ in Fig. 4B. This infinite contraction cannot be done exactly, hence it is approximated by the finite network on the right. Corner matrices $C$ and top tensors $T$ effectively represent corresponding infinite sectors of the network on the left separated by the dashed blue lines. Their (red) environmental bonds have dimension $M$. The environmental tensors $C$ and $T$ should be such that, to the transfer tensor $a$ in the center, its environment on the right appears the same as its exact environment on the left as much as possible. They are obtained by iterating the corner matrix renormalization in Fig. 11 until convergence.

**Appendix B: Gauge accelerator for corner matrix renormalization**

The iterative procedure in Fig. 11 converging the environmental tensors is the most time-consuming part of the algorithm. It is accelerated by using in the environment the renormalized tensor $A$ instead of the full tensor $B$, but at the price of repeating the self-consistent iterative update of $A$ (or equivalently $W$). Before every update of $A$, the environment has to be converged with current $A$. Once $A$ is updated, the environment has to be converged again with the updated $A$, and so forth until convergence of $A$. Fortunately, the convergence of the environment can be accelerated with a good choice of initial tensors $C_0$ and $T_0$. When $A$ is already close to convergence and it is changed little by its update, then the previous tensors $C$ and $T$, converged before the latest update of $A$, can be reused as the initial tensors. Moreover, they can be improved even further at negligible cost.

The update changes tensor $A$ by updating the isometry from an old $W$ to a new $W'$. As explained in Fig. 13A, the bottom index of tensor $T$ is actually a fusion of two bond indices of two tensors $A$, and these bond indices are in fact bond indices of tensors $B$ renormalized by the old isometry $W$. We would like to replace this old $W$ with the new $W'$ but, since $W$ is not invertible, this cannot be done exactly. However, as explained in Figs. 13B and C, we can apply an orthogonal (gauge) transformation to the bottom index of $T$ that is as close to the exact replacement $W \rightarrow W'$ as possible. The transformed $T_0$ is a better starting point than the $T$ converged before the update of $W$.
FIG. 13. In (A), the bottom index of tensor $T$ effectively comes out from tensor $a$, see Figs. 10 and 11. It is a fusion of two bond indices, each of dimension $D$, coming out from two tensors $A$, see Fig. 4A. Each bond index of tensor $A$ is actually a bond index of tensor $B$ renormalized by isometry $W$, see Fig. 3. In (B), an overlap between old isometry $W$ and new $W'$ is a $D \times D$ matrix. It can be subject to a singular value decomposition, $W'W^T = U\lambda V^T$, with singular values $\lambda$. In (C), an orthogonal matrix $UV^T$ is applied to each bottom index of the old tensor $T$. It is a gauge transformation that provides a better starting point $T_0$ for the iterative procedure in Fig. 11 converging the environmental tensors.