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Time evolution of an infinite projected entangled pair state: An efficient algorithm

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An infinite projected entangled pair state (iPEPS) is a tensor network ansatz to represent a quantum state on an infinite 2D lattice whose accuracy is controlled by the bond dimension D . Its real, Lindbladian, or imaginary time evolution can be split into small time steps. Every time step generates a new iPEPS with an enlarged bond dimension $D' > D$, which is approximated by an iPEPS with the original D . In P. Czarnik and J. Dziarmaga, *Phys. Rev. B* **98**, 045110 (2018), an algorithm was introduced to optimize the approximate iPEPS by maximizing directly its fidelity to the one with the enlarged bond dimension D' . In this paper, we implement a more efficient optimization employing a local estimator of the fidelity. For imaginary time evolution of a thermal state's purification, we also consider using unitary disentangling gates acting on ancillas to reduce the required D . We test the algorithm simulating Lindbladian evolution and unitary evolution after a sudden quench of transverse field h_x in the 2D quantum Ising model. Furthermore, we simulate thermal states of this model and estimate the critical temperature with good accuracy: 0.1% for $h_x = 2.5$ and 0.5% for the more challenging case of $h_x = 2.9$ close to the quantum critical point at $h_x = 3.04438(2)$.

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I. INTRODUCTION

Weakly entangled quantum states of strongly correlated systems can be efficiently represented by tensor networks [1,2]. The most popular are a 1D matrix product state (MPS) [3] and its 2D generalization: pair-entangled projected state (PEPS) [4]. An MPS provides a compact representation of ground states of gapped local Hamiltonians [1,5,6] and purifications of thermal states of local Hamiltonians [7]. It is the ansatz optimized by the density matrix renormalization group (DMRG) [8–11]. In 2D, PEPS are expected to be efficient representation of ground states of gapped local Hamiltonians [1,2] and thermal states of 2D local Hamiltonians [12,13], though in 2D the representability of area-law states by tensor networks was demonstrated to have limitations [14]. 2D tensor networks can represent fermionic systems [15–19], as was shown for both finite [20] and infinite PEPS [21,22].

Originally, PEPS was proposed as an ansatz for ground states of finite 2D systems [4,23], generalizing earlier attempts to construct trial wave-functions for specific 2D models [24]. Efficient numerical methods for infinite PEPS (iPEPS) [25–28] made it a promising new tool for strongly correlated systems. Its achievements include solution of a long-standing magnetization plateaus problem in the highly frustrated compound $\text{SrCu}_2(\text{BO}_3)_2$ [29,30] and demonstrating that the ground state of the doped 2D Hubbard model has stripe order [31]. Another example is the kagome Heisenberg antiferromagnet for which new evidence supporting gapless spin liquid was obtained [32]. This progress was made possible by new developments in iPEPS optimization [33–35], contraction [36–38], energy extrapolations [39], and universality class estimation [40–42].

These achievements encourage us to use iPEPS for a broad class of 2D states like thermal states [38,43–49], mixed states of open systems [50], or excited states [51].

Alongside iPEPS, progress was made in simulating cylinders of finite width with DMRG. They are routinely used to investigate 2D ground states [31] and recently were applied also to 2D thermal states [52,53]. Among alternative approaches are methods of direct contraction and renormalization of a 3D tensor network representing a 2D thermal density matrix [54–61] and multiscale entanglement renormalization ansatz (MERA) [62–65].

II. OUTLINE

In this paper, we implement an algorithm to simulate real, Lindbladian, and imaginary time evolution with iPEPS. The evolution operator is decomposed into small time steps using a Suzuki-Trotter decomposition [66–68]. Each time step is a product of two-site nearest-neighbor gates. It is applied to an iPEPS $|\psi\rangle$ with a bond dimension D . Every nearest-neighbor gate enlarges the dimension of the nearest-neighbor bond to which it is applied from D to $k \times D$, with $k \leq d^2$ where d is the local dimension of a lattice site. The new iPEPS represents a new state $|\psi'\rangle$. It is clear that repeated application of time steps would result in an exponential growth of the bond dimension. Therefore, after each time step it is necessary to approximate the exact new iPEPS $|\psi'\rangle$ by an approximate iPEPS—representing a state $|\psi''\rangle$ —with all bonds having the original bond dimension D . A straightforward optimization of the fidelity between the approximate $|\psi''\rangle$ and the exact $|\psi'\rangle$ is feasible [69] and, in principle, it should give the most accurate $|\psi''\rangle$, but it is not the most efficient one.

To obtain a good approximation efficiently, we consider an auxiliary iPEPS $|\tilde{\psi}''\rangle$ which is build from the same tensors as the new iPEPS $|\psi'\rangle$ except the two tensors at one of the bonds to which the nearest-neighbor gates were applied. These two exact tensors—each with the enlarged bond dimension kD along this bond—are replaced by two auxiliary tensors with the original bond dimension D . These two auxiliary tensors are optimized to maximize fidelity between the exact $|\psi'\rangle$ and the auxiliary $|\tilde{\psi}''\rangle$. Then the approximate $|\psi''\rangle$ is constructed by replacing *all* pairs of nearest-neighbor tensors by the optimal auxiliary tensors.

The optimization of the two auxiliary tensors in $|\tilde{\psi}''\rangle$ is much more efficient than optimization of an infinite number of copies of the two tensors in $|\psi''\rangle$ that is necessary to find the best $|\psi''\rangle$ straightforwardly [69]. Therefore, maximization of the fidelity between $|\psi'\rangle$ and $|\tilde{\psi}''\rangle$ (instead of $|\psi''\rangle$) is crucial for the efficiency. This local optimization is done in the exact environment of the new $|\psi'\rangle$ to give the best accuracy of the approximate $|\psi''\rangle$ while still solving a *local* variational problem.

Furthermore, to make the best use of the limited D , in the case of imaginary time evolution of a thermal state purification, we test applying disentangling unitary nearest-neighbor gates (disentangers) to the ancillas at the same sites as the evolution nearest-neighbor gates. The disentangers act on the ancilla indices and are optimized to minimize the necessary bond dimension D . This technique was used before for 1D MPS simulations [70,71]. Here for the first time it is implemented for 2D iPEPS where the bond dimension D is a much more limited resource.

In the same case of thermal states, we also test an even more efficient optimization scheme. It is equivalent to the full update scheme that was used before in imaginary time evolution of a pure state toward a ground state [25,33]. In this scheme the original $|\psi\rangle$ —with the smaller original D on all bonds—is used as an environment for the optimized auxiliary tensors. We benchmark this approximation for thermal states of the 2D quantum Ising model and find that it yields similar results as the ones obtained with the exact environment of $|\psi'\rangle$.

A challenging application of the algorithm is real-time evolution after a sudden quench of a parameter in a Hamiltonian. The quench excites entangled pairs of quasiparticles with opposite quasimomenta that run away from each other and make the entropy of entanglement grow asymptotically linearly in time. Therefore, a tensor network is doomed to fail after a certain finite evolution time. Nevertheless, for 1D systems MPS proved to be a useful tool to simulate time evolution after sudden quenches, see, e.g., Ref. [72]. In this paper, we simulate a sudden quench of the transverse field in the quantum Ising model to demonstrate that the same can be attempted with an iPEPS in 2D. This opens prospects for simulation of many-body localization in 2D [73] for which excitations remain localized and the entanglement growth is slow.

The growth of the entanglement can also be slowed down, or even halted, by coupling to local Markovian environment [50,74]. We provide a proof of principle simulation of Lindbladian evolution for the 2D transverse field quantum Ising model subject to dissipation [50].

Last but not least, imaginary time evolution generating thermal states of a quantum Hamiltonian can be simulated efficiently. Both the thermal states of local Hamiltonians and iPEPS representations of thermal density operators obey the area law for mutual information making an iPEPS a promising ansatz for thermal states [12]. In this paper, we simulate thermal states of the 2D quantum Ising model in the vicinity of the second-order phase transition. We add small symmetry breaking bias field h_z to smooth the evolution across the critical point. The smoothed evolution can be simulated accurately with modest computational resources. By extrapolation to $h_z = 0$, we obtain accurate estimates of the critical temperature even when the transverse field h_x is close to the quantum critical point.

The paper is organized as follows. In Sec. III, we present an algorithm for the most general case of the time evolution of thermal state's purification with disentangers. In Sec. IV, we provide benchmark results for the 2D quantum Ising model. In Sec. IV A, we present results for real-time evolution after a global quench. Section IV B presents results for evolution with Markovian master equation, while Secs. IV C and IV D present results for thermal states. In Secs. IV E and IV F, we benchmark the algorithm with disentangers and the full-update algorithm, respectively. In Sec. IV G, we compare the algorithm for thermal states with a simple update algorithm. We conclude in Sec. V. Furthermore, in Appendices A and B we provide technical details of the algorithm and the benchmark simulations.

III. EXACT-ENVIRONMENT FULL UPDATE WITH DISENTANGERS

Here we introduce the algorithm in the most general case of simulation of thermal state purification by imaginary time evolution. We call the general algorithm an exact-environment (ee) full update (FU) with disentangers (d) or eeFUd for short. Later we also consider simplified versions of the algorithm, in particular a version without disentangers (eeFU) and a version corresponding to the standard full update of iPEPS tensors [21,25] (FU), which is commonly used for ground-state optimization. The algorithm for real-time evolution of a pure state is obtained by ignoring ancillas alongside with the disentangers applied to the ancillas.

Our presentation of the general eeFUd algorithm is tailored for the quantum Ising model on an infinite square lattice that is going to be its testing ground in this paper:

$$H = - \sum_{\langle j,j' \rangle} Z_j Z_{j'} - \sum_j (h_x X_j + h_z Z_j). \quad (1)$$

Here X, Z are the Pauli operators. At zero longitudinal field $h_z = 0$ and zero temperature the model has a ferromagnetic phase with nonzero spontaneous magnetization $\langle Z \rangle$ for small enough transverse field h_x . The quantum critical point is $h_x = 3.04438(2) \equiv h_0$ [75]. For $h_x < h_0$, the model has a second-order phase transition at finite temperature belonging to the 2D classical Ising universality class. For $h_x = 0$, it becomes the 2D classical Ising model with $T_c = 2/\ln(1 + \sqrt{2}) \approx 2.269$.

FIG. 1. In (a), an elementary rank-6 tensor A of a purification is shown. The top (orange) index numbers ancilla states $a = 0, 1$, the bottom (red) index numbers spins states $s = 0, 1$, the four (black) bond indices have a bond dimension D . In (b), an iPEPS representation of the purification. Here pairs of elementary tensors at nearest-neighbor sites are contracted through their connecting bond indices. The dotted lines connect with the rest of the infinite lattice. We obtain the iPEPS representation of a pure state by reducing the dimension of ancilla indices to 1 or, equivalently, erasing the ancilla lines altogether.

A. Purification of thermal states

The structure of the algorithm is the most general in case of imaginary time evolution generating thermal states. Their purifications are pure states in an enlarged Hilbert space of physical spins and virtual ancillas. Every spin with states $s = 0, 1$ is accompanied by an ancilla with states $a = 0, 1$. The space is spanned by states $\prod_j |s_j, a_j\rangle$, where j numbers lattice sites. The Gibbs operator at an inverse temperature β is obtained from its purification $|\psi(\beta)\rangle$ by tracing out the ancillas:

$$\rho(\beta) \propto e^{-\beta H} = \text{Tr}_a |\psi(\beta)\rangle \langle \psi(\beta)|. \quad (2)$$

At $\beta = 0$, we choose the purification as a product over lattice sites,

$$|\psi(0)\rangle = \prod_j \sum_{s=0,1} |s_j, s_j\rangle, \quad (3)$$

to initialize its imaginary time evolution

$$|\psi(\beta)\rangle = G(\beta) e^{-\frac{1}{2}\beta H} |\psi(0)\rangle = G(\beta) U(-i\beta/2) |\psi(0)\rangle. \quad (4)$$

Here the evolution operator $U(\tau) \equiv e^{-i\tau H}$ acts in the Hilbert space of spins and $G(\beta)$ is an arbitrary unitary gauge transformation acting on ancillas. With the initial state Eq. (3), Eq. (2) becomes

$$\rho(\beta) \propto U(-i\beta/2) U^\dagger(-i\beta/2) \quad (5)$$

with the gauge transformation canceled out.

Just like a pure state of spins, the purification can be represented by an iPEPS, see Fig. 1. In the following, we use the gauge freedom to minimize its bond dimension D . Therefore, $G(\beta)$ will often be referred to as a disentangler.

B. Suzuki-Trotter decomposition

In the second-order Suzuki-Trotter decomposition [66–68], the evolution operator is split into a product of small time

steps, $U(\tau) = U(d\tau)^N$, and each small time step is approximated as

$$U(d\tau) = U_h(d\tau/2) U_{ZZ}(d\tau) U_h(d\tau/2), \quad (6)$$

where

$$U_{ZZ}(d\tau) = \prod_{\langle j, j' \rangle} e^{id\tau Z_j Z_{j'}}, \quad U_h(d\tau) = \prod_j e^{id\tau h_j} \quad (7)$$

are elementary classical gates and $h_j = h_x X_j + h_z Z_j$. The action of the local gate U_h on iPEPS is trivial: it modifies every iPEPS tensor simply by acting on its physical index with $e^{id\tau h_j}$.

C. Sublattices

To implement the gate $U_{ZZ}(d\tau)$, we divide the infinite square lattice into two sublattices A and B, with two different PEPS tensors at each sublattice, see Fig. 2(a). On the A-B checkerboard, the gate becomes a product of four commuting nearest-neighbor gates:

$$U_{ZZ}(d\tau) = U_0^x(d\tau) U_1^x(d\tau) U_0^y(d\tau) U_1^y(d\tau). \quad (8)$$

Here x (y) is the horizontal (vertical) direction spanned by $\vec{e}_x$ ($\vec{e}_y$),

$$U_s^x(d\tau) = \prod_{mn} e^{id\tau Z_{2m+s-1,n} Z_{2m+s,n}}, \quad (9)$$

$$U_s^y(d\tau) = \prod_{mn} e^{id\tau Z_{m,2n+s-1} Z_{m,2n+s}}, \quad (10)$$

and $Z_{m,n}$ is an operator at site $m\vec{e}_x + n\vec{e}_y$. For the sake of definiteness, in the following we focus on $U_0^x(d\tau)$. The other nearest-neighbor gates are implemented analogously.

D. Nearest-neighbor gate

To facilitate application of $U_0^x(d\tau)$ to iPEPS, first of all we use a singular value decomposition to rewrite a two-site term $e^{id\tau Z_j Z_{j'}}$ acting on a nearest-neighbor bond as a contraction of two smaller tensors acting on each site:

$$e^{id\tau Z_j Z_{j'}} = \sum_{\mu=0,1} z_{j,\mu} z_{j',\mu}. \quad (11)$$

Here μ is a bond index with a bond dimension 2 and $z_{j,\mu} \equiv \sqrt{\Lambda_\mu} (Z_j)^\mu$, where $\Lambda_0 = \cos d\tau$ and $\Lambda_1 = i \sin d\tau$.

Consequently, when the global gate $U_0^x(d\tau)$ is applied to the checkerboard iPEPS $|\psi\rangle$ with tensors A and B in Fig. 2(a), then every pair of tensors A and B at nearest-neighbor sites $(2m-1)\vec{e}_x + n\vec{e}_y$ and $2m\vec{e}_x + n\vec{e}_y$ is applied with the SVD-decomposed nearest-neighbor-gate, see Fig. 2(b). At the same time, its ancilla indices are applied with a nearest-neighbor disentangling gauge transformation g . The result is an exact purification $|\psi'\rangle = \tilde{g} U_0^x(d\tau) |\psi\rangle$, where $\tilde{g}$ is a tensor product of all g 's applied to all the considered nearest-neighbor bonds. When tensors A and B are contracted with their respective z 's, they become, respectively, A' and B' connected by an index with a doubled bond dimension $2D$, see Fig. 2(c). Finally, $|\psi'\rangle$ is approximated by a new iPEPS $|\psi''\rangle$ with the original bond dimension D at every bond, see Fig. 2(d). Its tensors A'' and B'' are optimized together with the disentangler g to maximize fidelity between the exact $|\psi'\rangle$ and the approximate $|\psi''\rangle$.

FIG. 2. In (a), an infinite square lattice is divided into two sublattices with tensors A (brighter green) and B (green). In (b), SVD decomposition of the nearest-neighbor gate in Eq. (11) is applied to spin indices of every considered nearest-neighbor pair of tensors A and B . At the same time, a disentangler g is applied to their ancilla indices. The result is an exact purification $|\psi'\rangle$. In (c), the tensors A and B can be conveniently fused with their respective pair of z tensors becoming new tensors A' and B' with a doubled bond dimension $2D$. In (d), the algorithm optimizes g together with new tensors A'' and B'' —that have the original bond dimension D —so that an approximate new iPEPS $|\psi''\rangle$ made of A'' and B'' has a maximal fidelity to the exact $|\psi'\rangle$.

E. Bond fidelity

The optimization aims at maximizing the global fidelity:

$$F = \frac{\langle \psi'' | \psi' \rangle \langle \psi' | \psi'' \rangle}{\langle \psi'' | \psi'' \rangle}. \quad (12)$$

A direct maximization of F is feasible [69] but not the most efficient approach.

To introduce a more efficient algorithm, we define an auxiliary state $|\tilde{\psi}''\rangle$, where the diagram in Fig. 2(c) is replaced by Fig. 2(d), not at all the considered bonds but only at one.

FIG. 3. In (a), tensor A' is contracted with its complex conjugate into a transfer tensor t_A . In (b), tensor B' is contracted with its complex conjugate into a transfer tensor t_B . In (c), the tensor environment for the bond $A'' - B''$. The environment is a rank-6 tensor, each index has dimension D^2 .

In other words, at all the bonds the tensor network $|\tilde{\psi}''\rangle$ is the same as the exact $|\psi'\rangle$ except at one particular bond.

The efficient algorithm maximizes local bond fidelity,

$$\tilde{F} = \frac{\langle \tilde{\psi}'' | \psi' \rangle \langle \psi' | \tilde{\psi}'' \rangle}{\langle \tilde{\psi}'' | \tilde{\psi}'' \rangle}, \quad (13)$$

with respect to A'' , B'' , and g . Once converged, A'' and B'' are placed at all sites in the new iPEPS $|\psi''\rangle$. This global placement of the locally optimized tensors is an approximation when compared to the global optimization in Ref. [69].

However, as the optimized bond in Eq. (13) is surrounded by the exact environment of $|\psi'\rangle$, then—for D large enough to cause negligible truncation errors—the approximation should not compromise the accuracy in a significant way.

The rank-6 bond environment in Fig. 3(c) is obtained approximately with the corner transfer matrix renormalization group (CTMRG) [28,76–78]. It is an approximate numerical method with a refinement parameter: an environmental bond dimension χ . All following results were checked for convergence with increasing χ . Considering numerical cost, CTMRG is the bottleneck of the algorithm.

The unitary disentanglers accelerate the convergence with D at no extra leading cost in the bottleneck CTMRG, because in all overlaps in Eq. (13) the disentanglers in bra and ket layers cancel out ($g^\dagger = 1$) on all bonds except the optimized one.

Therefore, the key to the efficiency is that in all the overlaps in Eq. (13) the tensor environment for the optimized bond is

the same, see Fig. 3(c), and depends neither on the optimized tensors A'' and B'' nor the disentangler g . It is, therefore, calculated only once.

F. Optimization loop

Tensors A'' and B'' and the disentangler g are optimized iteratively in a loop until $\tilde{F}$ is maximized. Up to normalization, the best $|\tilde{\psi}''\rangle$ that maximizes $\tilde{F}$ also minimizes the norm

$$|||\tilde{\psi}''\rangle - |\psi'\rangle||^2 = \langle\tilde{\psi}''|\tilde{\psi}''\rangle - \langle\tilde{\psi}''|\psi'\rangle - \langle\psi'|\tilde{\psi}''\rangle + \langle\psi'|\psi'\rangle. \quad (14)$$

For fixed A'' and B'' , the norm is linear in g . Therefore, when we define a tensor environment for g ,

$$E(g) = \frac{\partial\langle\psi'|\tilde{\psi}''\rangle}{\partial g^*}, \quad (15)$$

see Fig. 4(c), the norm is minimized by $g = uv^\dagger$, where the unitary u and v come from a singular value decomposition $E(g) = u\lambda v^\dagger$.

For fixed $B''(A'')$ and g , the norm Eq. (14) is quadratic in $A''(B'')$. Therefore, when we define metric tensors and gradients:

$$G_A = \frac{\partial^2\langle\tilde{\psi}''|\tilde{\psi}''\rangle}{\partial(A'')^*\partial(A'')}, \quad V_A = \frac{\partial\langle\tilde{\psi}''|\psi'\rangle}{\partial(A'')^*}, \quad (16)$$

$$G_B = \frac{\partial^2\langle\tilde{\psi}''|\tilde{\psi}''\rangle}{\partial(B'')^*\partial(B'')}, \quad V_B = \frac{\partial\langle\tilde{\psi}''|\psi'\rangle}{\partial(B'')^*}, \quad (17)$$

see Figs. 4(a) and 4(b), the quadratic form is minimized by $A'' = G_A^{-1}V_A$ ($B'' = G_B^{-1}V_B$), where in practice the inverse means a pseudoinverse.

The optimizations are repeated in a loop,

$$\dots \rightarrow g \rightarrow A'' \rightarrow B'' \rightarrow \dots, \quad (18)$$

until a self-consistency is achieved and $\tilde{F}$ is converged.

Finally, to reduce the numerical cost of the algorithm in actual calculations, we do not work with the full tensors A'' and B'' , but with smaller reduced tensors A''_{red} and B''_{red} described in Appendix A.

G. Full update imaginary time evolution

As explained before, the environmental CTMRG procedure is the numerical bottleneck. In the presented general eeFUD algorithm, the environment is the exact $|\psi'\rangle$ with the enlarged bond dimension $2D$ (or kD in general) on the considered bonds. It is a natural question if the $|\psi'\rangle$ -environment could be replaced by a more efficient $|\psi\rangle$ -environment with D on all bonds. This would reduce the algorithm to its simplified FUD version.

At first glance, the answer is no. As $|\psi\rangle$ differs from the exact $|\psi'\rangle$ by an error linear in $d\beta$, then also the environment differs from the exact one by an error linear in $d\beta$. In a simple model of error propagation—assuming that the environment error causes an error of $|\psi''\rangle$ proportional to the error of the environment, i.e., linear in $d\beta$ and that an error of the final state is a sum of errors at all intermediate steps—the error of the final state does not depend on $d\beta$ and, therefore, it cannot be eliminated by decreasing $d\beta$.

FIG. 4. In all panels, each of the six indices of the environment in Fig. 3(c) was split into a ket (upper) and a bra (lower) index, each of dimension D . In (a), metric tensor G_A . In (b), gradient V_A . In (c), tensor environment for the disentangler $E(g)$.

However, below in Sec. IV F we present numerical evidence that—at least for evolution across a thermal critical point that is smoothed by a tiny symmetry-breaking bias—the approximate environment makes negligible difference to the results. We demonstrate also that results extrapolated to the zero bias limit are mutually consistent.

H. Real-time evolution

In addition to missing ancilla lines and disentanglers, one more simplification occurs in case of real-time evolution of pure states. As the nearest-neighbor gates are unitary, they cancel out in the overlaps in Eq. (13) at all bonds except the

FIG. 5. Transverse magnetization $\langle X \rangle$ (left column) and relative energy error per site $\Delta E/E_0$ (right column) after a sudden quench from a ground state in a limit of $h_x \rightarrow \infty$, with all spins pointing along x , down to a finite $h_x = 2h_0$ (top row), $h_x = h_0$ (middle row), and $h_x = h_0/10$ (bottom row). With increasing bond dimension $D = 2, \dots, 8$ the magnetization appears converged for increasingly long times. The relative energy error is defined as $\Delta E/E_0$, where $E_0 = -h_x$ is the initial energy at $t = 0^+$ right after the quench and $\Delta E = E(t) - E_0$ is the energy error. The energy conservation shows improvement with increasing D .

optimized one with A'' and B'' . Consequently, in Figs. 3(a) and 3(b), the tensors A' and B' can be substituted by A and B . All indices of the transfer tensors, t_A and t_B , have the same dimension D^2 speeding up the bottleneck CTMRG procedure. Therefore, for real-time evolution, the eeFU algorithm simplifies to the FU algorithm.

IV. RESULTS

A. Real-time evolution after quench

We begin with simulations of a real-time evolution in the Ising model Eq. (1) without the bias field, $h_z = 0$. A sudden quench is considered from a limit of $h_x \rightarrow \infty$ down to $h_x = 2h_0$ within the same paramagnetic phase, $h_x = h_0$ at the quantum critical point, and $h_x = h_0/10$ deep in the ferromagnetic phase. The initial state is the ground state with all spins pointing along x and full transverse magnetization $\langle X \rangle = 1$. Figure 5 shows the magnetization $\langle X \rangle$ and relative energy error per site E after the sudden quench at $t = 0$ for different bond dimensions. With increasing D , the overall energy conservation improves and the transverse magnetization appears converged for longer times.

The simulations converge the fastest for $h_x = h_0/10$. This transverse field is close to $h_x = 0$ when the Hamiltonian becomes classical and $D = 2$ is enough to represent the evolution exactly. More physically, at $h_x = 0$ quasiparticles have a flat dispersion relation, hence they are not able to propagate and spread entanglement. The opposite case is the critical $h_x = h_0$ when the quasiparticles are gapless, hence they are excited in large numbers and propagate quickly. Here the convergence with increasing D is slower.

FIG. 6. Time evolution of the longitudinal magnetization $\langle Z \rangle$ with the Markovian master Eq. (19) initialized with all spins pointing down: $\langle Z \rangle = -1$. Different colors correspond to different bond dimensions. With increasing D the curves appear converged over an increasing range of evolution time.

B. Markovian master equation

After vectorization of a density matrix ρ , the real-time algorithm can be easily adapted to evolve a Markovian master equation [50,79]. The vectorized ρ_{vec} is represented by an iPEPS that is isomorphic to an iPEPO representing the density matrix operator ρ .

We test the algorithm for the Lindblad master Eq. [50]:

$$\dot{\rho} = -i[H, \rho] + \sum_j \left(L_j \rho L_j^\dagger - \frac{1}{2} \{L_j^\dagger L_j, \rho\} \right). \quad (19)$$

Here the Hamiltonian is again the quantum Ising model on an infinite square lattice,

$$H = \frac{V}{4} \sum_{\langle j, j' \rangle} Z_j Z_{j'} + \frac{h_x}{2} \sum_j X_j, \quad (20)$$

and $L_j = \sqrt{\gamma}(X_j - iY_j)/2$ is a spin-lowering operator.

We set the dissipation rate $\gamma = 1$ and, as in Ref. [50], consider the interaction strength $V = 5\gamma$. We choose $h_x = 2\gamma$ and an initial state with all spins polarized down: $\langle Z_j \rangle = -1$. Figure 6 shows the longitudinal magnetization $\langle Z \rangle$ in function of time. With increasing D , the magnetization plots appear to converge over an increasing range of time.

C. Thermal states with the eeFU algorithm

In this subsection, we analyze results obtained by the imaginary time evolution of a thermal state purification with the eeFU algorithm. Here we neither use disentanglers nor the cheaper environment computed using $|\psi\rangle$, that we postpone to Secs. IV E and IV F, respectively. The eeFU results presented here will serve as a benchmark for the other methods.

We generate thermal states for transverse fields $h_x = 2.5$ and $h_x = 2.9$. Quantum Monte Carlo T_c estimates for these fields are $T_c = 1.2737(6)$ and $T_c = 0.6085(8)$, respectively [80]. Both differ significantly from Onsager's $T_c \approx 2.269$ at $h_x = 0$ demonstrating that for these fields quantum

FIG. 7. Thermal states obtained by imaginary time eeFU evolution of a purification. In (a) and (b), the longitudinal magnetization $m = \langle Z \rangle$ as a function of the inverse temperature β for longitudinal symmetry breaking bias field $h_z = 0.01$ and two different values of the transverse field $h_x = 2.5$ (a) and $h_x = 2.9$ (b). With increasing D , the magnetization plots appear to converge. The $D = 5$ magnetization plot appears to be already converged. The convergence is slower for the larger transverse field $h_x = 2.9$ for which quantum fluctuations are stronger. In (c), we show m for smaller $h_z = 3 \times 10^{-4}$ and $h_x = 2.9$. Smaller h_z makes simulations more demanding, but again the $D = 5$ magnetization plot appears to be converged.

fluctuations are strong. Particularly challenging is the case of $h_x = 2.9$ which is close to the quantum critical point at $h_x = 3.04438(2)$, see Ref. [75].

We observe that close to the critical point, characterized by infinite correlation length, CTMRG convergence is very slow. Due to nonanalytic β -dependence, the results are also very sensitive to the time-step $d\beta$. Therefore, converging results

FIG. 8. A comparison of the eeFU with variational tensor network renormalization (VTNR) [38,46,47] for $h_x = 2.9$ and $h_z = 0.01$. Both methods converge to each other with increasing D . The convergence is faster for the eeFU algorithm.

near the critical point would be very expensive. To reduce these problems, we introduce a small longitudinal bias field h_z which takes the state away from the critical one.

In Fig. 7, we show convergence with D of the magnetization $m(\beta) = \langle Z(\beta) \rangle$ obtained with $0.0003 \leq h_z \leq 0.01$. In Fig. 8, we compare the m obtained by the eeFU method with that from the variational tensor network renormalization (VTNR) for $h_x = 2.9$ and $h_z = 0.01$ [38,46,47]. We see that both methods converge to each other, though the eeFU approach converges faster.

D. Estimation of critical temperatures

To estimate the critical temperature T_c of the second-order phase transition, we assume that the order parameter m , that is converged in D , can be obtained for a symmetry-breaking field h_z that is small enough to fall into the scaling regime. This assumption leads to scaling ansatzes for m and its derivative m' [81] with respect to $t = (T - T_c)/T_c$:

$$m \sim h_z^{1/\delta} f(th_z^{-1/\tilde{\beta}\delta}), \quad (21)$$

$$m' \sim h_z^{(\tilde{\beta}-1)/\tilde{\beta}\delta} g(th_z^{-1/\tilde{\beta}\delta}). \quad (22)$$

Here f and g are nonuniversal scaling functions and δ and $\tilde{\beta}$ are critical exponents of the phase transition. We use here $\tilde{\beta}$ instead of conventional β to distinguish it from the inverse temperature β . For finite h_z the derivative m' has a peak at temperature $T^* > T_c$. Therefore, from Eq. (22) follows scaling of T^* :

$$T^* - T_c \sim h_z^{1/\tilde{\beta}\delta}. \quad (23)$$

We use this scaling to estimate T_c and $1/\tilde{\beta}\delta$.

For $h_x = 2.5$, using $0.0005 \leq h_z \leq 0.01$ and $D = 5$ we obtain $T_c = 1.2745(7)$ and $1/\tilde{\beta}\delta = 0.549(4)$, see Fig. 9. We find that the results are converged in the Suzuki-Trotter step $d\beta$ and the environmental bond dimension χ for $d\beta = 0.002$ and $\chi = 25$, respectively. The fitted T_c agrees with the QMC

FIG. 9. In (a), $m'(T)$ for $h_x = 2.5$ and $D = 5$. The blue dashed line shows the QMC T_c . In (b), T_c is estimated by fitting the scaling Eq. (23) of m' peaks $T^*(h_z)$. Here we use $0.0005 \leq h_z \leq 0.01$ and $D = 5$. We obtain $T_c = 1.2745(7)$ and $1/\tilde{\beta}\delta = 0.549(4)$. The obtained T_c agrees with the QMC $T_c = 1.2737(6)$ [80], while obtained $1/\tilde{\beta}\delta$ is close to the exact value $1/\tilde{\beta}\delta = 8/15 \approx 0.533$ (it differs from the exact value by 3%).

estimate $T_c = 1.2737(6)$ [80] and $1/\tilde{\beta}\delta$ is within 3% of the exact value $8/15$.

For $h_x = 2.9$, quantum fluctuations are stronger making the estimation more challenging. Using $0.0005 \leq h_z \leq 0.01$ and $D = 5$ we obtain $T_c = 0.6055(10)$ and $1/\tilde{\beta}\delta = 0.563(4)$, see Fig. 10. These estimates are within 0.5% and 6%, respectively, of the QMC's $T_c = 0.6085(8)$ [80] and the exact $1/\tilde{\beta}\delta = 8/15$. We find that results are converged in the Suzuki-Trotter step and the environmental bond dimension for $d\beta = 0.005$ and $\chi = 25$, respectively.

E. Thermal states with the eeFud algorithm

Next we test the eeFud algorithm with disentanglers, comparing it to the eeFU algorithm without the disentanglers for the more challenging $h_x = 2.9$. We compare the magnetization and T_c , $1/\tilde{\beta}\delta$ obtained by the scaling Eq. (23), see Fig. 11 and Table I. We see that for $D = 4$ results obtained with disentanglers are closer to convergence in D than those without disentanglers. For $D = 4$ the T_c and $1/\tilde{\beta}\delta$ estimated with disentanglers are an order of magnitude more accurate than those without disentanglers. For $D = 5$, which is large

FIG. 10. In (a), $m'(T)$ for $h_x = 2.9$ and $D = 5$. The blue dashed line shows the QMC T_c . In (b) T_c and $1/\tilde{\beta}\delta$ are estimated by fitting the scaling Eq. (23) of m' peaks $T^*(h_z)$. Here we use $0.0005 \leq h_z \leq 0.01$ and $D = 5$ obtaining $T_c = 0.6055(10)$ and $1/\tilde{\beta}\delta = 0.563(4)$.

enough to obtain good accuracy also without disentanglers, both methods give similar results.

We conclude that it is possible to improve accuracy by using the disentanglers. The better accuracy with disentanglers comes at a price of more iterations of the optimization loop Eq. (18) and larger reduced tensors, see Appendix A. The cost of an iteration of the optimization loop is subleading as compared to the cost of the CTMRG.

F. Thermal states with the FU algorithm

We compare results obtained by the more efficient FU algorithm with the approximate environment and the eeFU with the exact environment. Figure 12 shows that both algorithms give very similar magnetization plots. The estimates of T_c and $1/\tilde{\beta}\delta$ listed in Table II are also the same within their error bars which are also similar. We conclude that quality of the results is the same for both algorithms.

G. Thermal states with simple update (SU) algorithm

One can consider simplifying and accelerating the algorithm even further by replacing the full update (FU) of the PEPS tensors with the simple update (SU) [26]. The SU truncates the enlarged bond dimension kD by means of a singular value decomposition of the pair of PEPS tensors.

FIG. 11. In (a) and (b), we show the longitudinal magnetization $m = \langle Z \rangle$ in function of the inverse temperature β obtained with (eeFud) and without (eeFU) the disentanglers for the transverse field $h_x = 2.9$. In (a) results for the longitudinal symmetry breaking field $h_z = 0.01$. In (b) results for more demanding $h_z = 5 \times 10^{-4}$. In both cases the $D = 4$ results with the disentanglers are much closer to the converged $D = 5 - 6$ results. We see also that the $D = 5$ results with the disentanglers are equivalent to the $D = 5 - 6$ results obtained without them. In (c) T_c and $1/\tilde{\beta}\delta$ estimation by the scaling Eq. (23) for $0.0005 \leq h_z \leq 0.01$ and $D = 4, 5$. The results corroborate the conclusions drawn from (a) and (b). Numerical values of the fitted T_c and $1/\tilde{\beta}\delta$ are listed in Table I.

Therefore, it ignores long range correlations in the environment of the truncated bond. The SU allows for larger D because the bottleneck CTMRG procedure is needed only to compute observables in the final state. Recently, thermal state

TABLE I. Comparison of T_c and $1/\tilde{\beta}\delta$ obtained in Fig. 11(c) for $h_x = 2.9$ using $0.0005 \leq h_z \leq 0.01$ with the eeFU and eeFud algorithms. For $D = 4$, the disentanglers improve accuracy by one order of magnitude. For $D = 5$, both methods give the same accuracy. In order to enable direct comparison of the time evolution with and without the disentanglers we use here the same reduced tensors for both methods, see Appendix A. The usage of the larger reduced tensors accounts for a small discrepancy between the $D = 5$ eeFU result without the disentangler shown here and the eeFU result in Fig. 10 that was obtained with smaller reduced tensors.

Method	D	T_c	$1/\tilde{\beta}\delta$
eeFU	4	0.38(2)	0.37(3)
eeFud	4	0.582(2)	0.539(5)
eeFU	5	0.6100(7)	0.571(3)
eeFud	5	0.6099(8)	0.569(3)
QMC [80]	-	0.6085(8)	-
exact	-	-	$8/15 \approx 0.533$

simulation by the SU—using time evolution of the density operator—was proposed in Ref. [82].

Here we compare the SU with the FU scheme. Our SU algorithm is a straightforward generalization of the ground state algorithm [21] to a purification of a thermal state. In Fig. 13, we compare thermal states generated by both algorithms for $h_x = 2.9$ and $h_z = 5 \times 10^{-4}$. With increasing D the SU magnetization moves slowly toward the converged $D = 5, 6$ FU magnetization but even for $D = 14$ it is still far from it. In Table III, we compare estimates of T_c and $1/\tilde{\beta}\delta$ obtained for $h_x = 2.9$ by the peak scaling Eq. (23) with $0.0005 \leq h_z \leq 0.01$. Even for the largest $D = 12$, the SU estimates are much worse than the FU estimates for $D = 5$. Given that already for $D = 12$ SU requires more time than FU for $D = 5$, we conclude that the FU algorithm by far outperforms the SU algorithm, at least in the present example.

FIG. 12. A comparison of thermal states obtained by the FU and the eeFU algorithms. Here $h_x = 2.9$ and $h_z = 3 \times 10^{-4}$. Both algorithms give similar results.

TABLE II. Comparison of T_c and $1/\tilde{\beta}\delta$ obtained for $h_x = 2.5$ and $h_x = 2.9$ by the FU and the eeFU algorithms. We use here the peak scaling Eq. (23) for $0.0005 \leq h_z \leq 0.01$. Both algorithms have similar accuracy.

Method	h_x	D	T_c	$1/\tilde{\beta}\delta$
eeFU	2.5	5	1.2745(7)	0.549(4)
FU	2.5	5	1.2746(6)	0.549(3)
QMC [80]	2.5	-	1.2737(6)	-
eeFU	2.9	5	0.6055(10)	0.563(4)
FU	2.9	5	0.6061(19)	0.564(7)
QMC [80]	2.9	-	0.6085(8)	-
exact	-	-	-	$8/15 \approx 0.533$

V. CONCLUSION

We tested efficient algorithms to simulate real, Lindbladian, and imaginary time evolution with infinite PEPS. The key to the efficiency is local optimization of iPEPS tensors. In the case of imaginary time evolution of a thermal purification, the accuracy can be improved by disentanglers applied to ancillas that reduce the necessary bond dimension. The efficiency can be enhanced further by reusing the tensor environment from the previous gate. This simplification reduces the algorithm to the full update scheme. We presented numerical evidence that this simplification does not affect the accuracy. However, further simplification to the simple update scheme is a step too far, at least for determining critical data in presence of strong quantum fluctuations. In such case, the accuracy to determine the critical temperature deteriorates dramatically, when using the simple update.

A proof of principle demonstration was provided for unitary real-time evolution after a sudden quench of the Hamiltonian, Lindbladian evolution with a Markovian master equation, and imaginary time evolution generating thermal states. In the last case, we used temperature dependence of the order parameter for different strengths of the small symmetry-

FIG. 13. A comparison of thermal states obtained by the full update (FU) algorithm and the simple update (SU) evolution of a thermal state purification for $h_x = 2.9$ and $h_z = 5 \times 10^{-4}$. With increasing D , the SU magnetization moves slowly toward the converged FU magnetization ($D = 5, 6$) but even for the largest $D = 14$ it is still far from it.

TABLE III. Comparison of simple update (SU) and FU estimates of T_c and $1/\tilde{\beta}\delta$ obtained by the peak scaling Eq. (23). Here $h_x = 2.9$ and we use $0.0005 \leq h_z \leq 0.01$ to perform the scaling. The $D = 6 - 12$ SU results have much worse quality than $D = 5$ FU results. Given that already for $D = 12$ it takes longer to obtain the poor quality SU results than the good quality FU results with $D = 5$, we conclude that the FU far outperforms the SU scheme.

Method	D	T_c	$1/\tilde{\beta}\delta$
SU	6	0.867(2)	1.04(7)
SU	8	0.788(2)	1.06(5)
SU	10	0.741(3)	1.00(5)
SU	12	0.704(11)	0.85(11)
FU	5	0.6061(19)	0.564(7)
QMC [80]	-	0.6085(8)	-
exact	-	-	$8/15 \approx 0.533$

breaking bias field to estimate critical temperature by extrapolation to the limit of vanishing bias field. We obtained a good accuracy of the critical temperature in the 2D quantum Ising model: 0.1% for the transverse field $h_x = 2.5$ and 0.5% for the more challenging $h_x = 2.9$ that is close to the quantum critical point at $h_x = 3.0444$.

FIG. 14. Tensors A and B are decomposed into isometries Q_A and Q_B and smaller reduced tensors A_{red} and B_{red} . A similar decomposition, with the same Q_A and Q_B , applies to the pairs A', B' and A'', B'' . We show two versions of reduced tensors. The larger ones are intended for simulations with disentanglers while the smaller ones, which leave ancilla indices with the isometries, for simulations without the disentanglers.

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APPENDIX A: REDUCED TENSORS

For the sake of clarity, in the main body of the paper the algorithms were presented with full tensors A and B . In our actual numerical calculations, however, we optimize reduced tensors, see Fig. 14. The full tensor A (B) is a contraction of an isometry Q_A (Q_B) with a reduced tensor A_{red} (B_{red}). It is obtained with the help of QR decomposition,

$$A = Q_A A_{\text{red}}, \quad (\text{A1})$$

where Q_A is an isometry and A_{red} is an upper triangular matrix. For spin 1/2 and with disentangler, A_{red} has $16D^2$ elements instead of $4D^4$ elements of the full tensor A . In the case without the disentanglers, one can also use the smaller reduced tensors with just $4D^2$ elements.

In the local optimization procedure, isometries Q_A and Q_B are held constant:

$$A' = Q_A A'_{\text{red}}, \quad A'' = Q_A A''_{\text{red}}, \quad (\text{A2})$$

$$B' = Q_B B'_{\text{red}}, \quad B'' = Q_B B''_{\text{red}}. \quad (\text{A3})$$

Rather than full tensors A'' and B'' , only A''_{red} and B''_{red} are subject to optimization in the loop Eq. (18). We note that the reduced tensors are commonly used in ground-state iPEPS simulations, see, e.g., Ref. [21].

For $D > 2$, using the reduced tensors we decrease cost of the tensor optimization Eq. (18). The larger reduced tensors are necessary for simulations with the disentanglers. Our numerical tests suggest that the smaller ones are better for simulations without disentanglers as they provide the same accuracy as the larger ones while reducing the cost of the optimization loop. However, in Sec. IV E we use the larger reduced tensors both with and without disentanglers to make the comparison more reliable.

APPENDIX B: NUMERICAL DETAILS

As a criterion of CTMRG convergence, we use change of the reduced tensors two-site environment. We demand relative change of its two-norm per iteration smaller than 10^{-10} . The time cost of obtaining full update T_c and $1/\beta\delta$ estimates for $h_x = 2.9$ and $D = 5$ shown in Table II was five to six days, using a 14 core, 2.20 GHz, Intel Xeon Gold 5120 processor.

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