

Projected entangled pair states with flexible geometry

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Projected entangled pair states (PEPS) are a class of quantum many-body states that generalize matrix product states for one-dimensional systems to higher dimensions. In recent years, PEPS have advanced understanding of strongly correlated systems, especially in two dimensions, e.g., quantum spin liquids. Typically described by tensor networks on regular lattices (e.g., square, cubic), PEPS have also been adapted for irregular graphs; however, the computational cost becomes prohibitive for dense graphs with large vertex degrees. In this paper, we present a PEPS algorithm to simulate low-energy states and dynamics defined on arbitrary, fluctuating, and densely connected graphs. We introduce a cut-off, $\kappa \in \mathbb{N}$, to constrain the vertex degree of the PEPS to a set but tunable value, which is enforced in the optimization by applying a simple edge-deletion rule, allowing the geometry of the PEPS to change and adapt dynamically to the system's correlation structure. We benchmark our flexible PEPS algorithm with simulations of classical spin glasses and quantum annealing on densely connected graphs with hundreds of spins, and also study the impact of tuning κ when simulating a uniform quantum spin model on a regular (square) lattice. Our paper opens the way to apply tensor network algorithms to arbitrary, even fluctuating, background geometries.

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Introduction. In recent decades, tensor network algorithms have become state-of-the-art numerical methods for simulating complex many-body systems [1,2]. The most famous and successful example of a tensor network is the matrix product state (MPS) [3], which has been established as a benchmark or simulating one-dimensional (1D) quantum systems. The projected entangled pair states (PEPS) method [4] extends the MPS framework to effectively simulate two-dimensional (2D) and higher-dimensional quantum systems, possibly with an arbitrary geometry [5], but incurs a significantly higher computational cost. Despite the limiting cost, PEPS have significantly advanced our understanding of strongly correlated quantum systems, in particular those with topological order [6,7], including quantum spin liquids [8].

PEPS are usually applied to approximate low-energy states or dynamics of Hamiltonians that are the sum of local operators that act only on a few neighboring sites. One constructs the PEPS tensor network according to a graph $\mathcal{P}$, the “correlation geometry”, that best reflects the (assumed) correlation structure of the target state. For Hamiltonians that are the sum of only two-site interactions, such as the Ising model, one can consider the Hamiltonian geometry $\mathcal{G}$, namely, the graph whose nodes and edges correspond to the sites and the interaction terms, respectively. Typically, $\mathcal{P}$ is chosen

to match the Hamiltonian geometry $\mathcal{G}$. In this case, when $\mathcal{P} = \mathcal{G}$, the computational cost of the PEPS roughly scales as $\approx \chi^K$, where χ is the PEPS bond dimension (namely, the maximum size of a bond index) and K is the maximum vertex degree in $\mathcal{G}$, which quickly becomes prohibitive for large K corresponding to densely connected Hamiltonians. The choice $\mathcal{P} = \mathcal{G}$ seems reasonable for translation-invariant Hamiltonians defined on regular lattices, in which case all the terms of the Hamiltonian are comparable. However, for Hamiltonians defined on irregular graphs or those with disorder—for example, classical and quantum spin glasses [9–11], which are also relevant for combinatorial optimization problems [12], Sachdev-Ye-Kitaev models [13,14], and quantum chemistry models (see, e.g., [15,16])—the correlation geometry of the target state could significantly deviate from the Hamiltonian geometry. Even for certain translation-invariant models on regular lattices in higher dimensions ($d \geq 4$), where mean-field techniques become more accurate, or models on locally tree-like lattices [17], PEPS based on a sparse $\mathcal{P}$, reflecting small correlations, may already be effective. However, guessing an effective PEPS geometry is generally a difficult task, and presents a key challenge for PEPS methods based on a fixed geometry. Additionally, we know of many situations where there is no underlying lattice at all, e.g., when simulating a quantum circuit, or for the case of a dynamical system with fluctuating background geometry.

While attaching a PEPS to a predefined lattice can be useful, this is also a stringent constraint. For one, long-range gates (Fig. 1) can only be applied by employing a sequence of swaps to bring the sites in question next to each other

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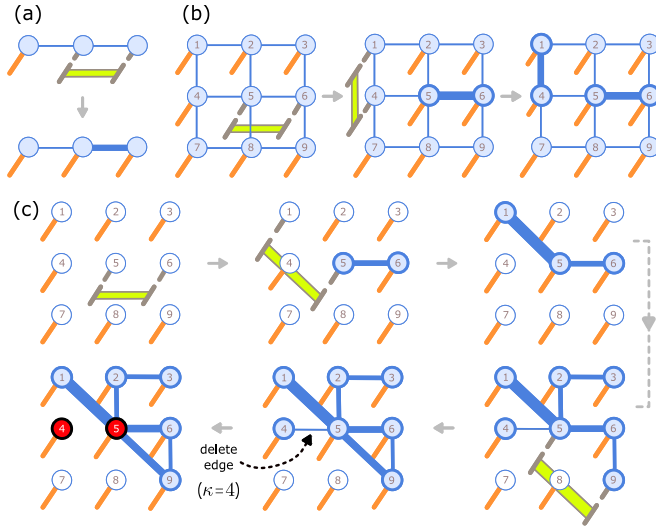


FIG. 1. (a) An MPS update after absorbing a two-site gate. (b) Absorbing two-site gates into the standard *fixed* PEPS updates the bonds but not the tensor network geometry. (c) A sequence of two-site gates corresponding to an irregular Hamiltonian applied on the flexible PEPS. Absorbing each gate adds an edge to the PEPS. After a few updates, tensor no. 5 acquires $5 > \kappa = 4$ edges, triggering an edge-deletion and updating tensors 4 and 5. The deleted bond is selected according to bond entanglement entropy score (= edge thickness).

before applying the gate, which can become very expensive. In general, it would be more beneficial to let the geometry (distance between sites) fluctuate and adapt dynamically, as the algorithm flows, to the entanglement structure that is natural to the system.

In this paper, we materialize the above intuition by proposing a PEPS algorithm based on a *flexible* geometry for simulating models defined on irregular and densely connected graphs with large K , even comparable to the system size. In order to control the exponentially scaling cost $\approx \chi^K$, we introduce a new PEPS cutoff $\kappa \in \mathbb{N} \ll K$. At any step in the optimization, we enforce that the maximum number of bond indices of the PEPS tensors remains $\leq \kappa$, but otherwise allow the PEPS geometry change and adapt to the (generally unknown) target correlation geometry, see Fig. 1. Starting, for instance, with a product state, a PEPS variational optimization or time-evolution proceeds by adding new edges (and correlations) to the tensor network. Whenever a tensor violates the κ -cutoff, we *delete* a bond index from that tensor, chosen according to a bond entanglement score. We propose a simple edge-deletion rule, which can be incorporated with standard PEPS optimization algorithms based on simple [18], cluster, or full update schemes [19,20], briefly reviewed in the Supplemental Material (SM) [21]. We demonstrate that simple updates supplemented with edge deletion already gives remarkably accurate results across several benchmarking simulations of irregular and densely connected models with hundreds of spins, up to approximately 1200 spins. (See final discussion for why simple update might be effective for the setting of this paper.)

Setup. Consider a many-body system made of L sites, described by a tensor product Hilbert space $\mathbb{V} \cong \bigotimes_{i=1}^L \mathbb{V}_i$ and a local Hamiltonian $H : \mathbb{V} \rightarrow \mathbb{V}$, which we assume is the sum of only two-site Hermitian operators $H = \sum_{ij} h_{ij}$, where h_{ij} acts nontrivially only on sites i and j , not necessarily neighbors, and as the identity on remaining sites. The total Hamiltonian H defines a graph $\mathcal{G}$ whose nodes correspond to lattice sites and sites i, j are connected with an edge only if an interaction term h_{ij} appears in the Hamiltonian.

Aims. Our goal here is to approximate the low-energy states and real-time dynamics of the system using PEPS-based time evolution methods [22]. Specifically, we would like to approximate the state $|\Psi\rangle \equiv e^{-\tau H} |\Psi_0\rangle$ (up to normalization), where the initial state $|\Psi_0\rangle$ is a product state or a simple PEPS with a small bond dimension. Here, τ is either real, in which case $|\Psi\rangle$ is a low-energy state (e.g., the ground state) resulting from an imaginary time evolution, or purely imaginary, $\tau = iT$, which corresponds to a real-time evolution for time T . Using Suzuki-Trotter decomposition, we approximate the time-evolution operator $e^{-\tau H}$ as a circuit comprised of two-site gates $g_{ij} \equiv e^{-\delta\tau h_{ij}}$, $e^{-\tau H} \approx \prod_{ij} g_{ij}$, connected according to $\mathcal{G}$ and sliced into N time steps $\delta\tau = \tau/N$. The Suzuki-Trotter decomposition is *exact* if all the two-site terms commute but otherwise incurs an error that scales polynomially with $\delta\tau$. In order to minimize the Suzuki-Trotter error, we partition each trotter step (a single time-slice) into G “layers”, $\{\mathcal{G}_k\}_{k=1}^G$, such that each layer $\mathcal{G}_k$ contains only nonintersecting (thus, commuting) gates [23]. Thus, we obtain the circuit, $e^{-\delta\tau H} \approx \prod_{k=1}^G (\bigotimes_{(i,j) \in \mathcal{G}_k} g_{ij})$.

Flexible PEPS algorithm. We now describe our new PEPS algorithm to approximate the trotterized time evolution from state $|\Psi_0\rangle$ towards $|\Psi\rangle$. At any step in the evolution, the instantaneous state is approximated as a PEPS $|\mathcal{P}_t\rangle \in \mathbb{V}$ whose geometry $\mathcal{P}_t$ is now allowed to change along the time evolution such that $|\Psi_0\rangle = |\mathcal{P}_0\rangle$ and $|\Psi\rangle \approx |\mathcal{P}_N\rangle$. We choose $|\Psi_0\rangle = |\mathcal{P}_0\rangle$ to be a product state, corresponding to an edgeless graph $\mathcal{P}_0$. The initial evolution proceeds by adding bonds to the PEPS. Specifically, gate g_{ij} creates entanglement between sites i and j , captured by creating a bond between tensors located at those sites. The PEPS at time t consists of a set of tensors $\{\Gamma_t^{[i]}\}_{i=1}^L$ and diagonal matrices $\{\lambda_t^{[i,j]}\}_{i,j}$, attached to the nodes i and edges $[i, j]$ of the graph $\mathcal{P}_t$, respectively, and represents a state $|\mathcal{P}_t\rangle \in \mathbb{V}$, which can be recovered by contracting all the PEPS tensors. The basic optimization step consists of updating the PEPS tensor network after applying a single two-site gate. In this paper, we apply the *simple update* scheme (see the Supplemental Material [21]) absorbing the gate locally into the PEPS and ignoring the rest of the system, which already gave accurate results across a range of benchmarking simulations. As the gates are applied, the PEPS becomes increasingly more connected, thus, escalating the computational cost of the updates, rapidly becoming prohibitive for densely connected Hamiltonians. In order to control this cost, we now enforce a vertex constraint, namely, no PEPS tensor is allowed to have more than $\kappa \in \mathbb{N}$ bond indices at any time in the evolution. If after applying a gate a tensor violates this constraint, we proceed to remove a bond index from that tensor. In order to reduce the impact on expectation values of local observables acting at that site, we propose to remove the bond with minimal *bond entanglement entropy* (BEE) $\mathcal{E}_{i,j} \equiv -\sum_m \lambda_m^{[i,j]} \log_2(\lambda_m^{[i,j]})$, where $\lambda_m^{[i,j]}$ are

the entries of the diagonal bond matrix $\lambda^{[i,j]}$ [24]. In order to delete index a between nodes x and y , we truncate the bond matrix $\lambda^{[x,y]}$ keeping only the *largest* singular value and the corresponding left and right singular vectors, which are then absorbed into the vertex tensors $\Gamma^{[x]}$, $\Gamma^{[y]}$ as

$$\Gamma_{\dots, a, \dots}^{[x]} \rightarrow (\lambda_{\max}^{[x,y]})^{1/2} \Gamma_{\dots, a=1, \dots}^{[x]}, \quad (1)$$

$$\Gamma_{\dots, a, \dots}^{[y]} \rightarrow (\lambda_{\max}^{[x,y]})^{1/2} \Gamma_{\dots, a=1, \dots}^{[y]}. \quad (2)$$

We assume here that the singular values are sorted in descending order along the diagonal of $\lambda^{[x,y]}$, i.e., $a = 1$ corresponds to the largest singular value. Slicing and scaling tensors, Eqs. (1) and (2), incurs minimal computational cost, and the overall cost of the flexible PEPS algorithm is still dominated by the cost of the PEPS updates, roughly scaling as $\approx \chi^k$ (compared to $\approx \chi^K$ for a fixed PEPS).

Although heuristic, we found that the BEE is a meaningful edge-deletion score. First, as we demonstrate later, our edge-deletion rule has an intuitive impact when applied to *uniform* models on *regular* lattices, in particular, we demonstrate that BEE can be used to locate critical points in such models with reasonable accuracy (see the SM [21]). Second, for several densely connected Hamiltonians, we observed that the *bond spectrum* $S_i \equiv \{\mathcal{E}_{i,j}\}_j$ of site i —namely, sorted BEE values of all the bonds at i —decays exponentially with the vertex degree, thus, the impact of the BEE-based truncation is potentially controllable.

Results. We now demonstrate that our flexible PEPS algorithm based on simple updates + simple measurements (see the SM [21]), works reasonably well for simulations of (1) classical Ising spin glasses, (2) disordered quantum annealing, and (3) the uniform 2D quantum Ising model.

(1) *Classical spin glasses.* We applied the flexible PEPS algorithm to find the ground of a classical Ising spin glass defined on a graph $\mathcal{G}$, $H_{\text{Ising-SG}} \equiv \sum_i h_i Z_i + \sum_{ij} J_{ij} Z_i Z_j + C$, where i, j enumerate the vertices of $\mathcal{G}$, each vertex corresponds to a site described by $\mathbb{C}^2$, $Z_i = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, and C is a constant. All the eigenstates of $H_{\text{Ising-SG}}$ are product states, since $H_{\text{Ising-SG}}$ is already diagonal in the Z basis on each site. Finding the ground product state of this model is equivalent to solving a generally NP-hard [25] quadratic unconstrained binary optimization (QUBO) problem, corresponding to minimizing the cost function $F = \sum_{ij} x_i Q_{ij} x_j$, where $x_i \in [0, 1]$ is a (classical) binary variable, and Q is the quadratic cost matrix. The classical Ising spin glass $H_{\text{Ising-SG}}$ maps to a QUBO by identifying $h_i = (Q_{ii} + \sum_j Q_{ij}/2)$, $J_{ij} = Q_{ij}$, and $C = \sum_{ij} (Q_{ii}/2 + Q_{ij}/4)$. The binary string $x_0, x_1, \dots, x_L$ that minimizes F corresponds to the ground state $|\psi_G\rangle = |x_0\rangle \otimes |x_1\rangle \dots \otimes |x_L\rangle$ of $H_{\text{Ising-SG}}$.

We approximated $|\psi_G\rangle$ using the flexible PEPS by simulating trotterized imaginary-time evolution starting from the state $|+\rangle = \bigotimes_i (\frac{1}{\sqrt{2}}|0\rangle_i + \frac{1}{\sqrt{2}}|1\rangle_i)$. The PEPS was optimized by combining simple updates with the BEE edge-deletion rule. The algorithm often converged to an entangled state with a small bond dimension ($=2$ or 3), which we expected to have a large overlap with the ground product state. We sampled 100 product states from the converged PEPS by adapting (see the SM [21]) the perfect sampling algorithm for the MPS [26,27] and chose the sampled state with the lowest energy as the solution.

We approximated the ground state of $H_{\text{Ising-SG}}$ for several values of h_i and J_{ij} . We chose eight random models (by randomly sampling h_i and J_{ij}), labeled as R1–R8, consisting between 80 and 128 spins and nine models from the QPLIB database [28], Q1–Q9, consisting between 561 and 1225 spins, see the SM [21] for details; models Q1–Q9 are not very dense (vertex degree ≤ 4) but are known to be hard. Figure 2 (bottom) shows the error of the ground-state energy relative to the solution obtained using the Gurobi software (applied to the QUBO formulation of these models), see also the SM [21]. We found that the flexible PEPS exactly matches the energy for all the randomly generated models and incurs only up to 1% error for the QPLIB models. Remarkably, our simple method was also able to find a *better* solution for some of the QPLIB models when the Gurobi optimization time was limited to 300 seconds, comparable to the time taken by the PEPS algorithm. These results demonstrate the potential of the flexible PEPS for solving hard combinatorial optimization problems.

(2) *Simulated quantum annealing.* Next, we applied the flexible PEPS algorithm to simulate *quantum annealing*, specifically, to approximate the real-time dynamics of the time-dependent Hamiltonian $H_{\text{SQA}}(\lambda_\tau) = \lambda_\tau H_{\text{Ising-SG}} - (1 - \lambda_\tau) \sum_i X_i$, $X_i = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, and $0 \leq \tau \leq 1$ is varied adiabatically between $\lambda_0 = 1$ and $\lambda_1 = 0$. We again chose the initial state $|+\rangle$, which here is the ground state of the initial Hamiltonian $H_{\text{SQA}}(0) = \sum_i X_i$. When λ_τ is varied adiabatically, the time-evolved state $|\psi_\tau\rangle \equiv e^{i\delta\tau H_{\text{SQA}}(\lambda_\tau)} |\psi\rangle$ remains close to the ground state of the instantaneous Hamiltonian $H_{\text{SQA}}(\lambda_\tau)$ throughout the evolution, thus converging at $\lambda = 1$ to the ground state of the classical Ising model $H_{\text{Ising-SG}}$ (equivalently, to the solution of the corresponding QUBO). As opposed to the classical imaginary time-evolution discussed previously, here the evolution is driven by a quantum Hamiltonian, which introduces a trotter error, which we mitigated by choosing a small trotter step. We used the annealing schedule plotted in the SM [21], a rescaled version of the schedule of the D-wave physical annealer. The results are shown in Fig. 2 (top, left/right). We found that the algorithm performed poorly for randomly generated problems giving up to 75% error, but performed better for the structured QPLIB problems giving $\approx 8\%$ error. We believe that this poor performance is caused by breaking of adiabaticity, which diverges the time-evolved state from the instantaneous ground state. As an attempt to course-correct, we also simulated a *hybrid annealing*, which incorporates intermittent *imaginary-time* evolution driven by the instantaneous Hamiltonian to steer the state back towards the instantaneous ground state. This approach gave much more accurate results, shown in Fig. 2 (bottom), giving up to 4% error for the randomly generated problems and up to 1% error for QPLIB problems, comparable with classical imaginary time-evolution, but remarkably beating Gurobi on more problems.

(3) *2D uniform quantum transverse field Ising model.* We also applied the flexible PEPS to approximate the ground state of the *uniform* quantum Ising model with nearest-neighbor interactions, $H_{\text{TFIM}} = \sum_i \sum_{ij} Z_i Z_j + \lambda \sum_i X_i$, on an infinite square lattice. We approximated the ground states of this model using flexible PEPS based on simple updates and

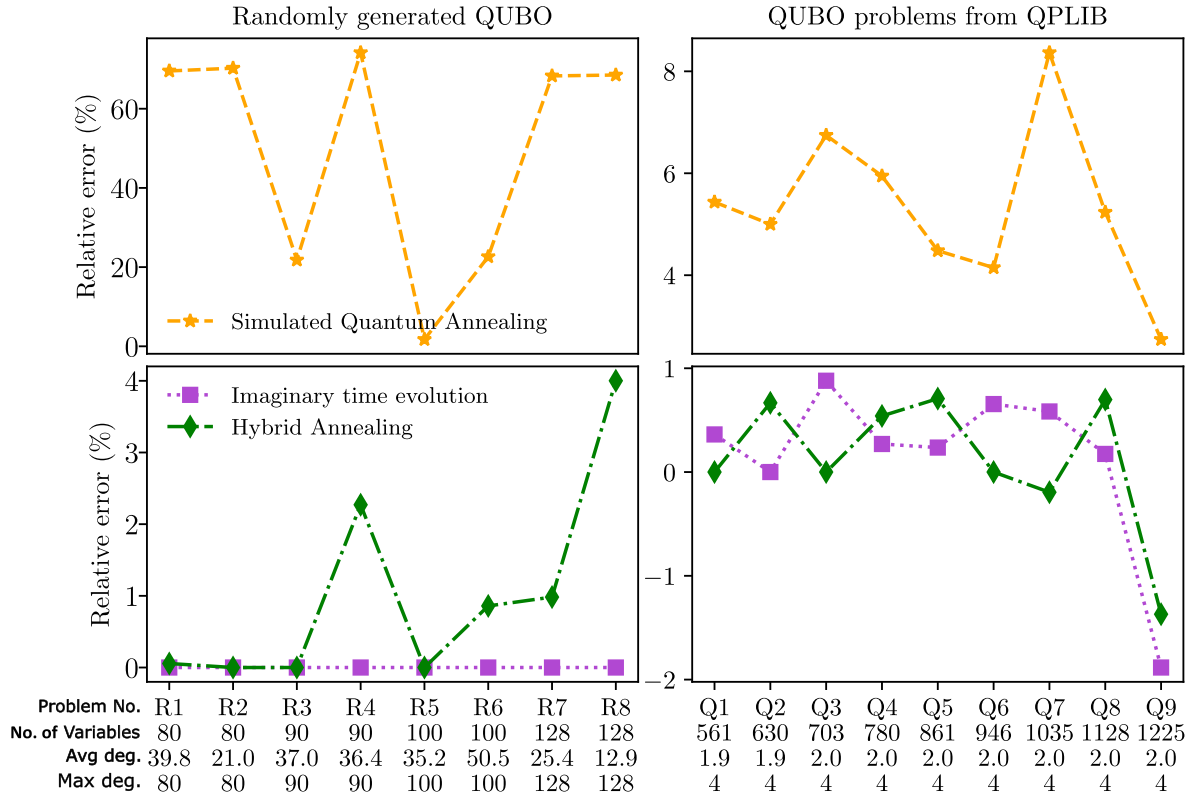


FIG. 2. Relative error (%) of the flexible PEPS algorithm vs Gurobi for QUBO problems (details listed along x axis) when using imaginary time evolution, quantum annealing, and hybrid annealing. Simulation details in the SM [21].

a 3×3 unit cell, varying $\kappa = 2, 3, 4$. Figure 3 shows the single-site magnetization averaged over the unit cell, computed using the “simple measurements” scheme (see the SM

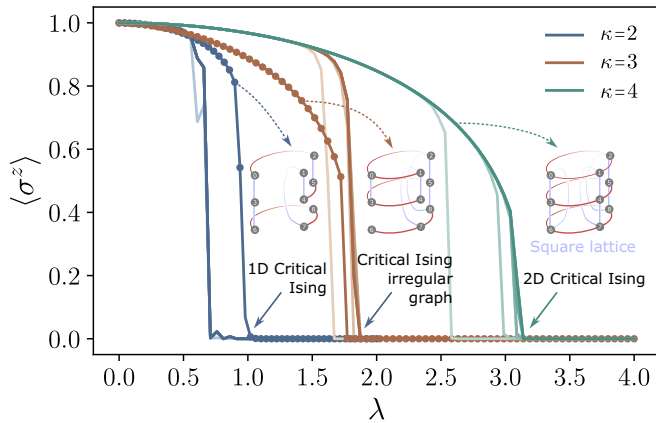


FIG. 3. Average single-site spin magnetization vs the strength of the magnetic field λ for the ground state of the uniform 2D quantum transverse field Ising model H_{TFIM} on a square lattice. Curves without markers correspond to *flexible* PEPS simulations with $\kappa = 2, 3, 4$. For each κ , the results were converged by increasing bond dimension, lighter curves correspond to smaller bond dimensions. The curves with markers correspond to *fixed* PEPS simulations of Ising models defined on the “critical” geometries shown here (see the SM [21]) that were recovered from the flexible-PEPS simulations.

[21]). We found that PEPS with $\kappa = 4$, equal to the coordination number of the square lattice, accurately locates the 2D Ising critical point around ≈ 3.1 . But, as perhaps is expected, flexible PEPS with $\kappa = 2, 3$ performed poorly in locating the critical point. However, an interesting feature emerged—the flexible PEPS curves for $\kappa = 2, 3$, nonetheless, displayed sharp transitions, at $\lambda \approx 1$ and $\lambda \approx 2$, respectively. (In fact, the average bond entanglement entropy also exhibited similar transitions, see the SM [21].) In order to understand these sharp transitions, we tracked the (dynamic) geometry of the flexible PEPS across the transitions. The “critical” geometries manifesting precisely at the transitions are depicted in Fig. 3. The critical geometry for $\kappa = 2$ is a chain with periodic boundaries, but with an optimization-determined site order, while $\kappa = 3$ corresponded to an irregular graph with average vertex degree of ≈ 2.6 . For $\kappa = 4$, we recovered the 2D square lattice at the critical point. We then simulated two different quantum Ising models I_2, I_3 defined on the critical geometries for $\kappa = 2, 3$, respectively, using the usual *fixed* PEPS, and found (solid markers in Fig. 3) that the locations of the sharp transitions, $\lambda \approx 1$ and $\lambda \approx 2$, observed in the flexible PEPS simulations coincide with the critical points of I_2, I_3 respectively. (In particular, $\lambda = 1$ is the critical point of the quantum transverse field Ising model on a spin chain I_2 .) Thus, when applying our edge-deletion rule in simulations of uniform Hamiltonians, we find a correspondence between limiting the number of PEPS bonds and truncating the corresponding Hamiltonian terms. This correspondence, which

is compatible with the intuition that all PEPS bonds must be equally prominent when $\mathcal{P} = \mathcal{G}$, suggests that our heuristic edge-deletion strategy behaves reasonably in the familiar setting of uniform models. Note that in Fig. 3, the geometry of the Flexible PEPS is changing along the solid curves, while the solid markers are for fixed PEPS based only on the critical geometries. Consequently, for any fixed κ away from the critical points the solid markers deviate from the solid curves.

Discussion and outlook. We have introduced a flexible PEPS algorithm that can adapt the underlying tensor network geometry to the correlation structure of the target state while maintaining a manageable number of bond indices, thus extending PEPS techniques to irregular and densely connected Hamiltonians (defined even on fluctuating background geometries) for hundreds of sites. We have demonstrated that a straightforward PEPS algorithm combining only simple updates with a bond entanglement entropy-based edge-deletion rule already works remarkably well for a range of problems; however, we expect a systematic improvement by upgrading to cluster or full updates. On the other hand, the fact that simple updates work reasonably well for the class of densely connected Hamiltonians considered here is surprising. The simple update PEPS scheme is an uncontrolled approximation because it neglects the environment tensors when updating PEPS during time evolution or variational optimization. While this limitation is significant, the approximation is known to work well on tree graphs or loopy graphs that are locally tree-like. However, we believe there are two further complementary scenarios where the simple update can also perform effectively when applied to simulating the ground state of densely connected, disordered Hamiltonians. We believe that some of the successful applications of the flexible PEPS, introduced here as a heuristic method, could potentially be explained by the two scenarios outlined below.

(1) *Dense connectivity with strong disorder.* Strongly disordered Hamiltonians may flow to Hamiltonians acting on locally tree-like graphs under coarse-graining transformations such as the strong disorder renormalization group (SDRG) [29,30]. SDRG iteratively removes the strongest disorder bonds while renormalizing nearby Hamiltonian couplings. Characterizing Hamiltonians that exhibit such an RG flow could provide insight into how to leverage a dynamical geometry—as in the flexible PEPS—to improve tensor net-

work simulations. Additionally, it is worth investigating whether our edge-deletion procedure mirrors SDRG-like decimation, but applied to quantum states rather than Hamiltonians.

(2) *Dense connectivity with weak disorder.* In systems with dense connectivity and relatively weak disorder (i.e., a more uniform interaction), the simple update might effectively capture an emergent mean-field (low-entanglement) description owing to monogamy of entanglement.

We believe, however, that dynamic site ordering—a feature central to the flexible PEPS algorithm—is crucial for capturing the correct SDRG flow in scenario (1) or the low-entanglement structure in scenario (2). Analogous to arbitrarily permuting the sites of a chain of nearest-neighbor Bell state pairs, which introduces artificially high bipartite entanglement and complicates the state’s description, committing to a fixed site order—for instance, by choosing a particular spanning tree graph of the Hamiltonian graph—is likely to result in a superficially complicated representation of the state. Furthermore, in disordered systems, the optimal site ordering that minimizes entanglement is generally not obvious. An additional difficulty in fixing a site order this way is that densely connected graphs can have extremely large number of spanning trees (which can be counted using the Kirchhoff’s matrix tree theorem). Therefore, as demonstrated in this paper, dynamically adjusting the site ordering can potentially reduce simulation costs significantly by better aligning the PEPS representation with the underlying correlation structure of the system.

Finally, we remark that when $\kappa = 2$, the PEPS reduces to a flexible MPS with dynamic site order determined by the optimization, which already worked well for some spin glass problems (see Fig. 1 and the SM [21]). Interesting directions for future work include applications of the flexible PEPS to SYK models, assessing the potential of the flexible MPS for simulating densely connected disordered models, and understanding whether tuning κ in flexible PEPS simulation of a *generic* uniform model also locates critical points of the same model defined on various geometries.

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- [1] R. Orús, A practical introduction to tensor networks: Matrix product states and projected entangled pair states, *Ann. Phys. (NY)* **349**, 117 (2014).
 - [2] J. I. Cirac, D. Pérez-García, N. Schuch, and F. Verstraete, Matrix product states and projected entangled pair states: Concepts, symmetries, theorems, *Rev. Mod. Phys.* **93**, 045003 (2021).
 - [3] M. Fannes, B. Nachtergaele, and R. F. Werner, Finitely correlated states on quantum spin chains, *Commun. Math. Phys.* **144**, 443 (1992).
 - [4] F. Verstraete and J. I. Cirac, Renormalization algorithms for quantum-many body systems in two and higher dimensions, [arXiv:cond-mat/0407066](https://arxiv.org/abs/cond-mat/0407066).
 - [5] S. S. Jahromi and R. Orús, Universal tensor-network algorithm for any infinite lattice, *Phys. Rev. B* **99**, 195105 (2019).
 - [6] N. Schuch, D. Pérez-García, and I. Cirac, Classifying quantum phases using matrix product states and projected entangled pair states, *Phys. Rev. B* **84**, 165139 (2011).
 - [7] N. Schuch, D. Poilblanc, J. I. Cirac, and D. Pérez-García, Topological order in the projected entangled-pair states formalism: Transfer operator and boundary Hamiltonians, *Phys. Rev. Lett.* **111**, 090501 (2013).
 - [8] D. Poilblanc, N. Schuch, D. Pérez-García, and J. I. Cirac, Topological and entanglement properties of resonating valence bond wave functions, *Phys. Rev. B* **86**, 014404 (2012).

- [9] J. L. van Hemmen, Classical spin-glass model, *Phys. Rev. Lett.* **49**, 409 (1982).
- [10] K. Binder and A. P. Young, Spin glasses: Experimental facts, theoretical concepts, and open questions, *Rev. Mod. Phys.* **58**, 801 (1986).
- [11] M. Mezard, G. Parisi, and M. Virasoro, *Spin Glass Theory And Beyond: An Introduction To The Replica Method And Its Applications*, World Scientific Lecture Notes in Physics (World Scientific, Singapore, 1987).
- [12] A. Lucas, Ising formulations of many np problems, *Front. Phys.* **2**, 5 (2014).
- [13] S. Sachdev and J. Ye, Gapless spin-fluid ground state in a random quantum Heisenberg magnet, *Phys. Rev. Lett.* **70**, 3339 (1993).
- [14] A. Kitaev, A simple model of quantum holography, Talks at KITP, April 7, 2015 and May 27, 2015; available at <https://online.kitp.ucsb.edu/online/entangled15/kitaev/>.
- [15] G. K.-L. Chan, Quantum chemistry, classical heuristics, and quantum advantage, *Faraday Discuss.* **254**, 11 (2024).
- [16] S. Szalay, M. Pfeffer, V. Murg, G. Barcza, F. Verstraete, R. Schneider, and O. Legeza, Tensor product methods and entanglement optimization for *ab initio* quantum chemistry, *Int. J. Quantum Chem.* **115**, 1342 (2015),.
- [17] S. Patra, S. S. Jahromi, S. Singh, and R. Orús, Efficient tensor network simulation of IBM's largest quantum processors, *Phys. Rev. Res.* **6**, 013326 (2024).
- [18] H. C. Jiang, Z. Y. Weng, and T. Xiang, Accurate determination of tensor network state of quantum lattice models in two dimensions, *Phys. Rev. Lett.* **101**, 090603 (2008).
- [19] M. Lubasch, J. I. Cirac, and M.-C. Bañuls, Algorithms for finite projected entangled pair states, *Phys. Rev. B* **90**, 064425 (2014).
- [20] M. Lubasch, J. I. Cirac, and M.-C. Bañuls, Unifying projected entangled pair state contractions, *New J. Phys.* **16**, 033014 (2014).
- [21] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/PhysRevResearch.7.L012002> for (i) brief review of peps algorithms (simple, cluster, and full updates and computing expectation values), (ii) sampling from the flexible peps, (iii) details of the peps simulations for qubo problems, and (iv) critical peps geometries from the simulation of the uniform 2D quantum Ising model (v) flexible mps.
- [22] For concreteness, we focus on PEPS time-evolution algorithms to approximate the low-energy states and dynamics of the system, but our flexible PEPS updates can also be incorporated in PEPS-based variational algorithms.
- [23] Consider a graph with six nodes numbered 0,1,...,5, and edges: [(0,1), (1,2), (2,3), (3,4), (4,5), (0,3), (2,4), (3,5)]. We can group these edges into four layers of nonintersecting edges: Layer1 = [(0,1), (2,3), (4,5)], Layer2 = [(1,2), (3,4)], Layer3 = [(0,3), (2,4)], Layer4 = [(3,5)]. Note that for several problems studied in this paper we also tested the straightforward gate sequence (0,1),(0,2)...(1,2),(1,3)... with with a small trotter step = 0.01. Surprisingly, we obtained comparable results despite incurring an uncontrolled trotter error.
- [24] We also tried a slightly different edge-deletion strategy. If the new bond resulting from the current gate update has bond entanglement in the lowest 30% then we remove that bond. Otherwise, we remove the bond with the least bond entanglement entropy. This strategy worked better for some models.
- [25] F. Barahona, On the computational complexity of Ising spin glass models, *J. Phys. A: Math. Gen.* **15**, 3241 (1982).
- [26] E. M. Stoudenmire and S. R. White, Minimally entangled typical thermal state algorithms, *New J. Phys.* **12**, 055026 (2010).
- [27] A. J. Ferris and G. Vidal, Perfect sampling with unitary tensor networks, *Phys. Rev. B* **85**, 165146 (2012).
- [28] F. Furini, E. Traversi, P. Belotti, A. Frangioni, A. M. Gleixner, N. Gould, L. Liberti, A. Lodi, R. Misener, H. D. Mittelmann *et al.*, QPLIB: A library of quadratic programming instances, *Math. Prog. Comp.* **11**, 237 (2019).
- [29] G. Refael and E. Altman, Strong disorder renormalization group primer and the superfluid–insulator transition, *C. R. Phys.* **14**, 725 (2013).
- [30] F. Iglói and C. Monthus, Strong disorder RG approach—A short review of recent developments, *Eur. Phys. J. B* **91**, 290 (2018).