Symmetric projected entangled-pair states analysis of a phase transition in coupled spin-1/2 ladders

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Infinite projected entangled-pair states (iPEPS) have been introduced to accurately describe many-body wave functions on two-dimensional lattices. In this context, two aspects are crucial: the systematic improvement of the Ansätze by the optimization of its building blocks, i.e., tensors characterized by bond dimension D, and the extrapolation scheme to reach the “thermodynamic” limit D → ∞. Recent advances in variational optimization and scaling based on correlation lengths demonstrated the ability of iPEPS to capture the spontaneous breaking of a continuous symmetry in phases such as the antiferromagnetic (Néel) phase with high fidelity, in addition to valence-bond solids which are already well described by finite-D iPEPS. In contrast, systems in the vicinity of continuous quantum phase transitions still present a challenge for iPEPS, especially when non-abelian symmetries are involved. Here, we consider the iPEPS Ansätze to describe the continuous transition between the (gapless) antiferromagnet and the (gapped) paramagnet that exists in the S = 1/2 Heisenberg model on coupled two-leg ladders. In particular, we show how accurate iPEPS results can be obtained down to a narrow interval around criticality and analyze the scaling of the order parameter in the Néel phase in a spatially anisotropic situation.

I. INTRODUCTION

One of the most challenging problem in condensed matter theory is to obtain sufficiently accurate approximations of the ground state and low-energy excitations of generic many-body Hamiltonians. For this reason, several numerical approaches have been devised in the last 30 years, including density-matrix renormalization group (DMRG) [1], dynamical mean-field theory [2], and quantum Monte Carlo (QMC) techniques [3]. Among them, the natural extensions of DMRG, such as matrix-product states [4, 5] in one dimension and projected entangled-pair states (PEPS) [6, 7] in two dimensions, represent a promising computational framework to get excellent approximations of strongly-correlated lattice models. Within this approach, the ground-state wave function is represented by means of local tensors, typically associated to the sites of the underlying lattice. These tensors have two kinds of indices: a single physical index specifying the local physical configuration (e.g., \( S^z = \pm 1/2 \)) in a spin-1/2 model and a collection of bond indices (whose number, usually, equals the coordination number of the lattice), each one having dimension \( D \). This latter quantity controls the accuracy of the Ansätze, the exact ground-state wave function being achieved for \( D \to \infty \). The bond indices on nearest-neighbor sites are contracted together, thus defining a tensor network. Furthermore, infinite systems may be considered by embedding the tensor network within a suitable environment. Such tensor networks, dubbed iPEPS, are the main focus of this work.

In the last decade, several algorithms to optimize iPEPS Ansätze have been developed and used to address challenging problems in different correlated systems, ranging from the characterization of unconventional states of matter (e.g., spin liquids in highly-frustrated spin model) to the competition between stripes and superconductivity in Hubbard or \( t-J \) models. For example, the ground state of the spin-1/2 Heisenberg model has been analysed on the kagome [8] and Shastry-Sutherland [9] lattices. Hamiltonians with an enlarged \( SU(N) \) “spin” symmetry have been also considered, to assess both magnetically ordered and disordered phases [10, 11]. In this regard, a particular attention has been devoted to the possibility to stabilize chiral spin liquids [12, 13]. As far as electronic models are concerned, the evidence in favor of stripes has been pushed for \( t-J \) [14] and Hubbard [15] models, in the vicinity of the hole doping \( \delta = 1/8 \).

By construction, the iPEPS Ansätze have been devised to describe both gapped and gapless phases, satisfying the area law [16]; however, within the optimization procedure in generic systems, gapless states are not easily obtained. Similarly, it is also not easy to correctly describe states in the vicinity of continuous quantum phase transitions. This is in a stark contrast with what happens in one spatial dimension, where tensor-network states, equipped with an appropriate scaling theory, may capture very well gapless phases and critical phenomena [17–20]. Recently, a progress in the iPEPS analysis of critical and/or gapless systems has been made thanks to two key developments. The first one is the introduction of optimization techniques, based either on diagram summations [21, 22] or the so-called automatic differentiation [23], which substantially improve the accuracy with respect to the commonly used imaginary time evolution methods. The second one is the development of finite-correlation-length scaling (FCLS) [24, 25] that allowed to leverage the well-established finite-size scaling approach to iPEPS states. In fact, the accuracy of thermodynamic estimates based on finite-\( D \) iPEPS
calculations can be considerably improved. The efficiency of these advances was recently demonstrated on a paradigmatic problem of the spin-1/2 Heisenberg $J_1 - J_2$ model on a square lattice by estimating the magnetization curve within the Néel phase, even in the vicinity of the transition to the quantum spin-liquid state [26].

In this work, we pursue the idea of describing a continuous phase transition within the iPEPS formalism. In particular, as for the $J_1 - J_2$ model, we focus on a case where the Néel order is melted by quantum fluctuations, namely a two-dimensional system of coupled spin-1/2 Heisenberg ladders defined by

$$\mathcal{H} = J \sum_R S_R \cdot S_{R+x} + \sum_R J_R S_R \cdot S_{R+y}, \quad (1)$$

where $S_R = (S_R^x, S_R^y, S_R^z)$ is the $S = 1/2$ operator on the site $R = (x, y)$ of a square lattice, $\hat{x}$ and $\hat{y}$ are unit vectors in $x$ and $y$ direction, and $J_R = J$ or $J_R = \alpha J$, depending on the parity of $y$. By varying $\alpha$, this model interpolates between the Heisenberg model on the square lattice at $\alpha = 1$ and a system of decoupled two-leg ladders at $\alpha = 0$. In the following, we will take $J$ as the energy scale. Owing to the absence of the sign problem, this system can be studied by unbiased QMC techniques and, therefore, offers an excellent benchmark for the accuracy of iPEPS to describe a non-trivial quantum phase transition, e.g., beyond the simplest case of the Ising model in transverse field. Indeed, the Hamiltonian (1) displays a quantum critical point at $\alpha_c = 0.31407(5)$, separating a gapless antiferromagnet and a gapped paramagnet [27]. The critical exponents are compatible with the ones of the classical three-dimensional $O(3)$ Heisenberg model, as expected.

A recent iPEPS investigation of this Heisenberg model [28] highlighted the difficulties faced by the unrestricted optimizations of iPEPS tensors across the phase transition. In fact, due to the unbroken $SU(2)$ symmetry in the paramagnetic side, strong finite-$D$ effects are present, thus impeding a systematic analysis. Moreover, the optimization procedure is problematic also within the antiferromagnetic phase, where the expected $U(1)$ symmetry around the direction of the staggered magnetization is usually broken. In this work, we want to constrain the iPEPS Ansatz by imposing this $U(1)$ symmetry, thus limiting finite-$D$ effect, and optimize such symmetric tensors with the automatic differentiation [23]. In addition, we extend the FCLS analysis [24, 25] in situations with a spatial anisotropy, due to the presence of two length scales, since the correlations along the spatial $x$ and $y$ directions will be generically different in the ground state of Eq. (1). These two improvements allow us to get accurate results for the antiferromagnetic order parameter up to the critical point, as confirmed by a direct comparison with QMC calculations. Finally, we included an external staggered magnetic field in the Hamiltonian (1), which allows us to inspect the response in the order parameter, even very close to the critical point.

II. METHODS

Here, we briefly describe the structure of the iPEPS Ansatz that is used to investigate the Hamiltonian (1). In order to account for both the antiferromagnetic order in the gapless regime and the short-range valence-bond correlations in the gapped one, we consider four rank-5 tensors $t = \{a, b, c, d\}$, each one with a physical index $s$ (with dimension 2, suitable for $S = 1/2$ degrees of freedom) and four auxiliary indices $u, l, d, r$ (with dimension $D$). These tensors are arranged in a $2 \times 2$ unit cell to tile the square lattice:

$$\text{iPEPS}(a, b, c, d) = \text{peps-torch}. \quad (2)$$

Observables are obtained by computing effective environments within the corner-transfer matrix method, generalized for extended unit cells [14]. The gapped phase retains all the symmetries of the Hamiltonian and, in particular it has the full $SU(2)$ spin symmetry; by contrast, the gapless phase breaks the spin-rotational symmetry, leading to a finite collinear magnetization and a residual $U(1)$ symmetry about it. Therefore, we impose an explicit $U(1)$ spin symmetry on the tensors. This can be achieved by associating integer “charges” to the two physical spin-1/2 components and the $D$ virtual degrees of freedom (on each of the bond indices) [28]. To preserve point-group symmetries of the underlying lattice, a straightforward choice is to take the same charges on all the bond indices that are equivalent under the symmetries (e.g., the $C_{4v}$ symmetry used in Ref. [28] led to such choice). Here, we do not want to impose any symmetry within the $2 \times 2$ unit cell, which allows the possibility that different charges are defined on different indices. Thus, each of the four tensors will possess a set of charges $(a_0, \ldots, a_{D-1})$ with $a_0 = a, b, c, d$ and $j = u, l, d, r$. Instead, the same charges $(u_0, \ldots, u_{D-1})$ for the physical indices are taken for all tensors. Therefore, the $U(1)$ symmetry is realized by enforcing a selection rule for the non-zero elements of the tensors $t_{\alpha \beta \gamma \delta \epsilon}^{u_l d r}$:

$$u^a + \gamma^a u^\gamma + u^\gamma \gamma^d + \gamma^d \gamma^r = N, \quad (3)$$

where, without loss of generality, we chose the case with $N = 0$ to work with invariant tensors.

The definition of these charges allows us to improve the numerical efficiency, since tensors may arranged in blocks with definite values of them, allowing a block-sparse representation. For a detailed treatment of tensor networks with $U(1)$ symmetry and linear algebra with block-sparse tensors, see Ref. [29]. Importantly, once the blocks are defined, the gradient optimization changes the tensors elements without mixing different blocks. The implementation of linear tensor algebra for abelian-symmetric tensors is provided by open-source library YAST [30] and the iPEPS algorithms built on top of it are available in the peps-torch library [31].

From a practical point of view, one possibility to identifying $U(1)$ charges (for the best variational states) is to perform imaginary-time evolution at different values of $\alpha$ by using a two-site simple-update scheme [32] starting from product states with $U(1)$ symmetry. Remarkably, this approach
does not lead to substantial improvements (in terms of physical quantities, as energy or magnetization) with respect to the charges obtained from the unrestricted optimizations of single-site iPEPS Ansätze with the $C_{4v}$ lattice symmetry in the Heisenberg model with $\alpha = 1$ [26], see Appendix A.

III. RESULTS

Let us now show the results obtained within the optimization of the iPEPS Ansätze. In order to perform a careful comparison with QMC calculations (which are numerically exact, since the spin model does not suffer from the sign problem), we apply the stochastic series expansion method [33] and perform extrapolations by decreasing the temperature (to reach ground-state properties) and increasing the size of the cluster (to reach the thermodynamic limit). Most of the QMC calculations were done on $L \times L$ lattices with periodic boundary conditions, at temperature $T = 1/(2L)$, by using the ALPS libraries [34, 35].

A. Phase diagram

In Fig. 1, we report the energy per site $e$ and the staggered magnetization $m^2$ (averaged over the $2 \times 2$ unit cell), for different values of $\alpha$ across the quantum critical point. The outcome shows that, for small bond dimension, i.e., $D \leq 3$, the accuracy is quite poor in both the antiferromagnetic and paramagnetic phases. However, once the bond dimension becomes large enough to capture the entanglement structure of the ground state, the tensor network provides an excellent variational description, not only in the paramagnetic phase, but also within the magnetically ordered phase. The accuracy of the ground-state energy is exemplified by showing the relative error with respect to the value $e_{QMC}$, obtained within the QMC approach (extrapolated in the thermodynamic limit). Indeed, the quantity $\Delta e/e_{QMC}$, with $\Delta e = |e - e_{QMC}|$ is vanishing within the statistical errors, see Fig. 1. Most importantly, the magnetization curves for finite values of the bond dimension $D$ follow the QMC data faithfully in the bulk of each phase, still overestimating the order parameter close to the critical point. We would like to mention that the present QMC results allow us to locate the critical point at $\alpha_c = 0.314(1)$, which is slightly different from the previous estimate $\alpha_c = 0.31407(5)$ [27] (see Appendix B).

B. Finite-correlation-length scaling

Obtaining accurate and reliable estimates of the observables (e.g., the energy per site or the staggered magnetization) within iPEPS Ansätze represents an important issue that has been addressed since their definition. Recently, an interesting step forward has been obtained for magnetic states that break a continuous symmetry (e.g., the antiferromagnetic one in the Heisenberg model). In this case, the presence of gapless modes induces a diverging correlation length. When working on finite clusters, as in standard QMC approaches, this fact translates into well-defined size-scaling laws of the physical quantities [36, 37]. Instead, within iPEPS, we directly work in the thermodynamic limit (that is mimicked by the embedding procedure) and, therefore, it is not possible to straightforwardly apply the same scaling laws; still, the correlation length $\xi$ is finite for any finite value of the bond dimension $D$ and diverges with $D \to \infty$. As a result, it has been suggested [24, 25] that the FCLS analysis can be defined in terms of $\xi$ instead of the cluster size as

$$e(\xi) = e_0 + \frac{a}{\xi^3} + O\left(\frac{1}{\xi^4}\right),$$

$$m^2(\xi) = m_0^2 + \frac{b}{\xi} + O\left(\frac{1}{\xi^2}\right),$$

where $a$ and $b$ are suitable constants. The system we are interested in, i.e., the Heisenberg model on coupled two-leg ladders, presents a complication, as it breaks the $\pi/2$-rotational symmetry for $\alpha \neq 1$, leading to two distinct length scales.

FIG. 1. Energy per site (upper panel) and staggered magnetization (lower panel) for optimized iPEPS with $U(1)$ symmetry and $2 \times 2$ unit cell. The results for $D = 3, \ldots, 6$ are reported, as well as the ones obtained with the FCLS extrapolation, see text. In addition, QMC results are also shown for the thermodynamic extrapolation. The inset in the upper panel shows the relative error of the iPEPS energies (with FCLS extrapolations) with respect to the QMC ones (with thermodynamic extrapolations).

The inset in the upper panel gives a sketch of the super-exchanges in Hamiltonian (1), where intra-ladder $J$ (inter-ladder $\alpha J$) couplings are denoted by black solid (gray dashed) lines.
Within finite-$D$ iPEPS calculations, we have access to both of them by looking at the spectrum of the transfer matrices along $x$ (i.e., within ladders) and $y$ (i.e., across ladders). Thus, we obtain two correlation lengths ($\xi_x$ and $\xi_y$) and perform FCLS independently for both of them. The extrapolated values $e_0$ and $m^2$ are independent of choice of the correlation length direction, while the parameters $a$ and $b$ depend on the choice. It must be emphasized that these FCLS relations are expected to be valid exclusively for a Goldstone phase with a spontaneously broken continuous symmetry, where the correlation length diverges with increasing $D$. Instead, within the paramagnetic gapped phase, $\xi$ remains finite in the thermodynamic limit, thus implying that Eqs. (4) and (5) cannot be applied. The impossibility to fit the numerical data for a given $\alpha$ within this scheme is then taken as the evidence that the state is not gapless (antiferromagnetic). At the quantum critical point, we still expect Eq. (4) to hold, while the order parameter scaling is replaced with a quantum critical form $m(\xi) \approx \xi^{-\Delta_m}$, with $\Delta_m$, the scaling dimension of the order parameter at the critical point [24].

The results for the energy per site $e$ are reported for selected values of $\alpha$ in Fig. 2. Within the magnetically ordered phase (but also close to the quantum critical point), the extrapolations of the FCLS analysis using either $\xi_x$ or $\xi_y$ give consistent values, providing an internal verification of the approach. Most importantly, the staggered magnetization $m^2$ can be also extracted for infinite correlation length, see Fig. 3. The extrapolated results are in very good agreement with QMC estimates, up to values of the inter-ladder couplings that are very close to the critical point. Beyond the critical point, the system develops a gap and thus the FCLS fails to provide the correct scaling, where correlation lengths remain finite. Nevertheless, within the paramagnetic regime, finite-$D$ iPEPS calculations are able to recover accurate results. Indeed, for $\alpha \lesssim 0.28$, a vanishing magnetization is already obtained with $D = 5$. However, upon approaching criticality, i.e., at $\alpha = 0.3$, finite-$D$ iPEPS retain a small residual magnetization (at least up to $D = 6$). In fact, close to the critical point, the correlation length far surpasses the values of $\xi_x$ and $\xi_y$ that our finite-$D$ iPEPS can support. Hence, the FCLS analysis can be used to improve the estimates of the energy. Still, some important deviations in the scaling laws are clearly visible, see Fig. 3. Finally, let us remark that the iPEPS optimization in the narrow region near criticality is technically difficult due to presence of instabilities (see Appendix C).

C. The effect of a staggered magnetic field

In the previous section, we focused on estimating observables of the ground state of the $SU(2)$-symmetric Hamiltonian (1). Here, we explicitly break this symmetry to investigate the phase transition with a complementary nonsymmetric approach [24, 38, 39]. In particular, we follow the approach of Refs. [24, 39], which recently used tensor networks to compute running exponents in critical quantum systems.

To explicitly break the $SU(2)$, we supplement the Hamil-

![FIG. 2. FCLS extrapolations for the energy $e$, by using both horizontal ($\xi_x$, full symbols and lines) and vertical ($\xi_y$, empty symbols and dashed lines) correlation lengths, for a few values of the inter-ladder couplings $\alpha$. The symbols correspond to iPEPS with $D = 3$ (diamonds), $D = 4$ (squares), $D = 5$ (triangles), and $D = 6$ (pentagons). The colors follow the $\alpha$ color scheme of Fig. 3.](image1)

![FIG. 3. FCLS extrapolations for staggered magnetization $m^2$, by using both vertical ($\xi_y$, left part) and horizontal ($\xi_x$, right part) correlation lengths for $0.29 \leq \alpha \leq 1$. The symbols correspond to iPEPS with $D = 3$ (diamonds), $D = 4$ (squares), $D = 5$ (triangles), and $D = 6$ (pentagons); thermodynamic extrapolations from QMC data are also reported (stars).](image2)
tonian (1) with an external staggered field $h$, which directly couples to the order parameter:

$$\mathcal{H}_h = \mathcal{H} - h \sum_R (-1)^{x+y} S_R^z,$$

where $R = (x, y)$. Then, for any $h \neq 0$, the ground state has a finite correlation length and develops a finite staggered magnetization $m = m(h, \alpha)$ in response to the staggered field $h$. The response for $h \to 0^+$ is different within magnetically ordered or disordered phases. In both cases, the magnetization is an analytic function of $h$, with two distinct regimes:

$$m(\alpha, h) = a(\alpha) h + O(h^2) \quad \text{for } \alpha < \alpha_c, \ h \to 0^+, \quad (7)$$

$$m(\alpha, h) = m(\alpha, 0) + O(h) \quad \text{for } \alpha > \alpha_c, \ h \to 0^+, \quad (8)$$

where $a(\alpha)$ is a suitable constant. By contrast, at criticality (i.e., for $\alpha = \alpha_c$), the magnetization is not analytic and the response follows a power-law behavior:

$$m(\alpha_c, h) \propto h^{1/\delta}, \quad \text{for } h \to 0^+, \quad (9)$$

where $\delta$ is a critical exponent, which only depends on the universality class of the phase transition. The best estimate of $\delta$ (within the expected universality class of the classical three-dimensional $O(3)$ Heisenberg model) is $1/\delta = 0.20916$ [40].

To probe the system’s response at fixed $\alpha$, we define the logarithmic derivative

$$[1/\delta](\alpha, h) = \frac{\partial \log m(\alpha, h)}{\partial \log h}, \quad (10)$$

which is usually referred to as running exponent. For each value of $h$, we optimize the $U(1)$-symmetric iPEPS Ansatz and compute the average staggered magnetization $m(\alpha, h)$. Then, we estimate the logarithmic derivative by using finite differences. The QMC results are based on a direct improved estimator for the running exponent, see Ref. [39]. The outcomes are shown in Fig. 4, where the running exponent and the correlation length $\xi_c$ of iPEPS are reported for the three different regimes (with $D = 2, \ldots, 6$).

In the gapped phase (for $\alpha = 0.2$), the magnetization is linear in $h$ (linear response) and, therefore, the running exponent saturates at 1 for $h \to 0$, as also obtained numerically from both QMC and iPEPS data (with $D \geq 4$). The iPEPS correlation length saturates for $h \lesssim 0.005$, with small finite-$D$ corrections. Indeed, in the gapped phase, even finite-$D$ iPEPS provide precise description of the system as the area law is upheld, which is supported by a direct comparison between iPEPS (with $D \geq 4$) and QMC (for $L \geq 32$). The $D = 3$ iPEPS cannot faithfully capture gapped phase at $\alpha = 0.2$, since it retains finite $m$ and thus responds more akin to the Néel phase.

Within the magnetically ordered phase (for $\alpha = 0.4$), the magnetization saturates to a finite value and the running exponent goes to zero for $h \to 0$. Indeed, the logarithmic derivative $[1/\delta](\alpha, h)$ has a non-monotonic behavior, with a broad peak at intermediate values of the staggered field $h$. This feature is correctly captured by iPEPS. QMC calculations also reproduce the broad peak, even though at small values of $h$ a huge upturn is present due to size effects; therefore, for

FIG. 4. $U(1)$-symmetric iPEPS with $D = 3, \ldots, 6$ in the presence of external staggered field $h$. Upper panels: Running exponent as a function of $h$ for the gapped phase with $\alpha = 0.2$ (left), at criticality $\alpha = 0.31407$ (middle), and in the Néel phase $\alpha = 0.4$ (right). The value of the critical exponent $1/\delta$ is reported at the critical point. QMC results are also reported for comparison, with faded colors marking the data affected by finite lattice size. Bottom panels: horizontal correlation length $\xi_c$ as a function of $h$. 

large enough system size $L$, the two methods converge to the same curve for sufficiently large values of the staggered field $h$. Here, it seems as though QMC simulations provide an upper bound of the thermodynamic limit, while iPES provides a lower bound of it. Still the presence of the broad peak is robust and appears in the region of $h$ where both $D \geq 5$ iPES and $L \geq 32$ QMC data are in excellent agreement.

At the critical point $\alpha = \alpha_c$, the running exponent is expected to converge towards $1/\delta = 0.20916$, as mentioned before. The available iPES and QMC calculations (for $D \leq 6$ and $L \leq 128$, respectively) are still somewhat away from the saturation regime, however the numerical data monotonously increase, without the broad peak in the magnetically ordered phase. While the validity of the QMC results is limited by the finite size $L$, for iPES it is limited by the finite correlation length induced by the bond dimension $D$. Within iPES, as the field $h$ is decreased, the correlation lengths initially grow, but then flatten out (with large finite-$D$ corrections), in contrast to the expected diverging behavior of the gapless regime. From the direct comparison between QMC and iPES data, we can estimate that the iPES response for $D = 6$ gives a faithful estimation of the exact result down to $h \approx 10^{-2}$. Then, for smaller fields, the running exponent data for iPES and large-$L$ QMC simulations start to deviate as iPES becomes increasingly biased by the induced finite correlation length.

IV. CONCLUSIONS AND OUTLOOK

The analysis of quantum phase transitions by variational methods relies on a few aspects: first, a flexible Ansatz for the ground-state wave function, allowing a description of different kinds of phases by tuning its parameters; second, a practical optimization scheme of such parameters to get the best approximate ground state; finally, a way to analyze the results, possibly extrapolating to the thermodynamic limit. Here, we have shown that symmetric tensor networks, when implemented with a variational optimization, allow for accurate description of the transition between a gapped paramagnet and gapless Néel antiferromagnet, thus overcoming the issues arising within the imaginary-time evolution approach that has been emphasized in a recent work [28]. The selection of the correct symmetry structure for tensors by the choice of their charges is crucial, as they determine the physical properties of the wave function. Most importantly, once the tensors have been variationally optimized, our simulations show that the physical observables, such as the energy or the order parameter, are robust to small variations of these charges. Although the region close to the critical point remains a challenge, it is in principle tractable by increasing the bond dimension $D$. Already with data up to $D = 6$ and FCSL scaling, we could locate the critical point with an accuracy of about 5%, demonstrating the applicability of this analysis even in the case of two different length scales $\xi_x$ and $\xi_y$. Finally, inspired by the recent works of Refs. [24, 39], we have included an external staggered field $h$ in the Hamiltonian and compared the iPES results with the ones obtained by QMC. Away from the critical point $\alpha > \alpha_c$ (i.e., within the Néel phase) the running exponent $1/\delta(\alpha, h)$ shows a broad peak at finite field $h$, indicative of magnetic order [39]. The robustness of the peak can be established by locating the inflection point in the growing iPES correlation length as the external field $h$ is decreased. Peaks at fields larger than inflection point represent genuine features of the system, while finite-$D$ effects may generate spurious peaks at fields smaller than the inflection point. Our findings corroborate the fact that the analysis of the running exponent is a useful diagnosis within the antiferromagnetic regime, away from the critical point. This proof of concept analysis shows the potential of the method put forward in Ref. [39] for future application of iPES, e.g., on questions of the stability of quantum spin liquids.

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Appendix A: Comparison among $U(1)$ classes

First of all, we discuss the preparation of the initial $U(1)$-symmetric states for the optimization by imaginary-time evolution. We consider two scenarios of evolution by starting from simple $U(1)$-symmetric product states: a classical Néel antiferromagnet (NEEL) and a product state of singlets placed on the rungs of ladders (VBS). The imaginary-time evolutions were performed by using two-site simple update (SU) with the second-order Trotter approximation. To track the convergence of SU, we evaluate energy using corner-transfer matrix environments, with modest environment dimension $\chi \approx D^2$. Starting with the time step $\delta \tau = 0.02$, the state is evolved until an energy increase is observed, in which case the SU step is not performed and the time step is halved $\delta \tau \to \delta \tau / 2$. The evolution ends once the time step becomes smaller than $\delta \tau = 10^{-8}$.

The $U(1)$-structure of the evolved NEEL and VBS states show slight variations in charges $\vec{e}_j^\alpha$. Moreover, depending on bond dimension $D$ and $\alpha$, the charges do not necessarily respect spatial symmetries of the model (1). For example, at $D = 5$ and $6$ the charges on left ($j = l$) and right ($j = r$) bonds of tensors come out different. Then, we perform a further optimization of the NEEL and VBS states by using gradient descent and compare the resulting physical observables with the ones obtained from optimal states with identical charges $\vec{e}_j^\alpha$ for all bonds $j$, here denoted as U1B class. The results for the energy per site $\epsilon$ and the local magnetization $m$ are shown in Fig. 5. The data for $D = 3$ show that optimized VBS states have substantially worse energies than NEEL and U1B states. Instead, for $D > 3$, all these states have very similar energies, differences being at most of order $2 \times 10^{-4}$. The order parameter displays a similar behavior. A minor exception is represented by the $D = 4$ VBS case, which displays slight breaking of translation symmetry along $y$-axis even in the $\alpha = 1$ limit. In particular, the nearest-neighbor spin-spin correlations show staggered pattern with $\langle \vec{S}_{x,y} \cdot \vec{S}_{x,y+1} \rangle - \langle \vec{S}_{x,y+1} \cdot \vec{S}_{x,y+2} \rangle \approx 3 \times 10^{-4}$. Overall, the SU-evolved states provide reasonable accurate initial states for the variational optimization of $U(1)$-symmetric iPEPS. Irrespective of the differences in the $U(1)$ charges, the final variational minima for different classes give quantitatively the similar physical picture.

Appendix B: Size scaling analysis of the transition by the QMC technique

Here, we provide some standard details on locating the transition point $\alpha_c$ from QMC simulations. To estimate $\alpha_c$, we have computed the spin stiffness $\rho_s$, defined using the winding number:

$$\rho_s = \frac{T}{2} \left\langle \sum_i (W_i^x)^2 + (W_i^y)^2 \right\rangle$$  \hspace{1cm} (B1)

where $i$ runs over loops in the space-time SSE configurations and the brackets denote the Monte Carlo average.

FIG. 5. Left panels: energy per site obtained optimizing NEEL and VBS states with respect to the one obtained within the U1B class, i.e., $\delta \epsilon = |\epsilon(\text{NEEL}) - \epsilon(\text{U1B})|$ (circles) and $\delta \epsilon = |\epsilon(\text{VBS}) - \epsilon(\text{U1B})|$ (squares) for different values of the bond dimension $D$. Right panels: magnetization $m$ obtained from NEEL, VBS, and U1B states. Observables are evaluated at finite $\chi$, i.e., $\chi = 71$ for $D = 3$, $\chi = 64$ for $D = 4$, $\chi = 50$ for $D = 5$ and $\chi = 72$.

The results for different system sizes $L_x \times L_y$ are shown in Fig 6. At criticality, the scaled spin stiffness $L_x \rho_s$ is constant (taking the dynamical exponent $z = 1$ at the transition), thus allowing to estimate the location of the transition at $\alpha_c = 0.31467(1)$. Note that the Binder cumulant crossing also leads to a similar critical value (data not shown). In addition, we have also checked that data collapse of $\rho_s$ and magnetization are compatible with known exponents $\nu = 0.707$ and $\beta = 0.3689$.

Appendix C: Instability in optimization

The optimization of the iPEPS wave function is performed by using the steepest-descent algorithm, implemented with the line search method (i.e., by using a step length that is adapted along the optimization procedure) [41]. In the proximity of the critical point, performing the line search is crucial to ob-
tain stable variational optimizations, especially for the cases with $D = 5$ and 6. In Fig. 7 (upper panel), we show typical cases done without line search, such that unstable regimes, with an erratic behavior of the energy, are obtained. The same kind of problem appears in simulations with or without the $U(1)$ symmetry.

When performing the optimization, we always work at constant environment bond dimension $\chi_{opt}$. The states obtained in the erratic regime can show energies $e(\chi_{opt})$, which are lower than the reference QMC results. This is possible because the iPEPS thermodynamic estimate of energy, for which the variational principle holds, is obtained only in the limit of $\chi \to \infty$. When the line search is employed, it suppresses the erratic regime as the energy is not allowed to increase in course of optimization. In this case, we assess the severity of this instability by comparing the lowest energies that are realized in the vicinity of $\chi_{opt}$ with the energy obtained from the $\chi \to \infty$ limit. The results for $D = 3, \ldots, 6$ and $0.2 \leq \alpha \leq 0.4$ are shown in Fig. 7 (lower panel). This behavior resembles the overtraining, often encountered in the optimization of artificial neural networks, since the variational optimization of iPEPS does not directly optimize the thermodynamic estimate of energy $e(\chi \to \infty)$, but only its finite-$\chi$ approximation. In the previous study of the $J_1 - J_2$ model (using highly-constrained single-site iPEPS Ansatz [26]), $e(\chi)$ was a monotonically decreasing function already from modest values of $\chi$. Here, we instead observe that $e(\chi)$ attains shallow spurious minima, with depth at most $O(10^{-5})$, compared to corresponding $e(\chi \to \infty)$ thermodynamic estimates.

FIG. 6. QMC results for the scaling analysis of the spin stiffness $\rho_s$ as a function of $\alpha$ for system with $L_x = L_y$ (upper panel) and $L_x = 2L_y$ (lower panel). The temperature has been chosen as $T = 1/(2L_x)$ to ensure convergence to the ground-state properties. The vertical black line and shaded area indicate $\alpha_c = 0.31475(10)$ estimate and its uncertainty.

FIG. 7. Upper panel: example of optimizations without line search at $\alpha = 0.28$ (with $D = 5$ and $\chi = 75$) both with and without explicit $U(1)$ symmetry. Optimizations are initialized from the $\alpha = 0.3$. The red line shows the comparison with QMC extrapolation. Lower panel: difference between thermodynamic estimate of the energy ($\chi \to \infty$ limit) and its minimal value for fixed environment dimension $\chi$ for optimized $U(1)$ symmetric states. The optimizations were done for $D = 3, 4, 5,$ and $6$ at $\chi_{opt} = 54, 64, 100, \text{and } 108$, respectively. In all cases, the line search was employed.