Quantum critical phase with infinite projected entangled paired states

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A classification of SU(2)-invariant Projected Entangled Pair States (PEPS) on the square lattice, based on a unique site tensor, has been recently introduced by Mambrini et al. [1]. It is not clear whether such SU(2)-invariant PEPS can either i) exhibit long-range magnetic order (like in the Néel phase) or ii) describe a genuine quantum critical point (QCP) or quantum critical phase (QCPh) separating two ordered phases. Here, we identify a specific family of SU(2)-invariant PEPS of the classification which provides excellent variational energies for the $J_1 - J_2$ frustrated Heisenberg model, especially at $J_2 = 0.5$, corresponding to the approximate location of the QCP or QCPh separating the Néel phase from a dimerized phase. The PEPS are build from virtual states belonging to the $\frac{1}{2} \otimes N \oplus 0$ SU(2)-representation, i.e. with $N$ “colors” of virtual spin-$\frac{1}{2}$. Using a full update infinite-PEPS approach directly in the thermodynamic limit, based on the Corner Transfer Matrix renormalization algorithm supplemented by a Conjugate Gradient optimization scheme, we provide evidence of i) the absence of magnetic order and of ii) diverging correlation lengths (i.e. showing no sign of saturation with increasing environment dimension) in both the singlet and triplet channels, when the number of colors $N \geq 3$. We argue that such a PEPS gives a qualitative description of the QCP or QCPh of the $J_1 - J_2$ model.

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I. INTRODUCTION

Low-dimensional quantum magnets offer a rich zoo of phases breaking a discrete (like point group or lattice) or a continuous (like spin rotation) symmetry. Often, such phases are separated by Quantum Critical Points (QCP), as described within the usual Ginsburg-Landau (GL) framework. Interestingly, it has been proposed that some QCP may not be described by the GL paradigm [2, 3]. A celebrated quantum spin model is the frustrated spin-$\frac{1}{2}$ Heisenberg model on the two-dimensional (2D) square lattice involving competition between nearest neighbor (NN) and next-nearest neighbor (NNN) antiferromagnetic (AF) couplings, $J_1$ and $J_2$ respectively. Setting $J_1 = 1$, $J_2$ controls the amount of frustration which is maximum (classically) at $J_2 = 0.5$. Large-scale Quantum Monte Carlo (QMC) simulations [4–6] has shown that the ground state (GS) of the unfrustrated ($J_2 = 0$) Heisenberg model exhibits long range (LR) AF order.

In the thermodynamic limit, the (global) spin-rotational SU(2) symmetry is spontaneously broken and the GS acquires a finite local staggered magnetization. When $J_2$ is turned on, the order parameter is gradually suppressed and a quantum phase transition to a Quantum Disordered (QD) phase [7–10] – such as a dimer [11–14] or a plaquette [15, 16] Valence Bond Crystal (VBC) – takes place (see Fig. 1). It was also argued that magnetic frustration could stabilize spin liquids (with no symmetry breaking), such as the Resonating Valence Bond (RVB) states [17] showing algebraic (short range) VBC correlations on the square (Kagome) lattice [18–21].

Recently, tremendous progress have been made in tensor network techniques [23–27], aiming to go beyond Density Matrix Renormalization Group (DMRG) methods [28] in 2D. More specifically, Projected Entangled Pair States (PEPS) [29] are variational ansätze constructed from a few local tensors, located on $M$ non-equivalent sites, and characterized by (i) one bond carrying the physical degrees of freedom (of dimension 2 for spin-$\frac{1}{2}$ systems) and (ii) $z$ “virtual” bonds ($z$ is the lattice coordination number, $z = 4$ for the square lattice) of arbitrary dimension $D$ as shown in Fig. 2(a). Interestingly, any local (gauge) or global (physical) symmetry can be implemented in PEPS [1, 30–37]. Also, a simple bulk-edge (holographic) correspondence provides...
II. SYMMETRIC PEPS ANSÄTZE

We wish here to consider transitionally invariant fully symmetric PEPS in order to (i) reduce the number of independent variational parameters and (ii) provide a good description of the critical point (or phase) where both SU(2) and lattice symmetries are preserved. For this purpose, we shall use the elegant classification of SU(2)-invariant PEPS tensors on the square lattice [1] according to (i) their virtual degrees of freedom and (ii) how they transform w.r.t the (lattice) point group symmetries (see Fig. 2(a)). For simplicity, we shall a priori restrict ourselves to tensors fully invariant under all operations of the $C_{4v}$ point group (i.e. belonging to the so-called $A_1$ IRREP). The tensors are further classified according to their virtual space $V$ given by a direct sum of SU(2)
IRREPs or “spins”, i.e. $V = \bigoplus_a s_a$. We restrict hereafter to bond dimension $D \leq 7$. Among all the possible cases listed in Table I we focus on the most interesting ones carrying low virtual spins defined by $V = \frac{1}{2} \oplus 0$ ($D = 3$), $V = \frac{1}{2} \oplus 0 \oplus 0$ ($D = 4$), $V = 1 \oplus \frac{1}{2}$ ($D = 5$), $V = \frac{1}{2} \oplus \frac{1}{2} \oplus \frac{1}{2} \oplus 0$ ($D = 5$), $V = \frac{1}{2} \oplus \frac{1}{2} \oplus 1$ ($D = 6$), $V = \frac{1}{2} \oplus 0 \oplus 0 \oplus 1$ ($D = 6$), $V = \frac{1}{2} \oplus \frac{1}{2} \oplus \frac{1}{2} \oplus 0$ ($D = 7$), spanned by a small number $D$ of independent tensors, $D = 2, 8, 4, 10, 30$ respectively, given in the Supplementary Materials of Ref. 1 (except for $D = 7$ given in the Supplementary Materials of this paper [78]). Note that a $\pi$-rotation of the spin basis is assumed on the sites of one of the two sublattices of the square lattice. In this basis, a genuine $q = q_{AF} \equiv (\pi, \pi)$ (spontaneous) magnetic order translates into a uniform $q = 0$ (spontaneous) magnetization. Subsequently, the generator of $SU(2)$ become invariant only up to translations that map the sublattices to themselves (i.e. shifts over two sites).

The iPEPS method combined with full tensor optimization – We shall now focus on the $J_1 - J_2$ spin-$\frac{1}{2}$ Heisenberg model with NN and NNN antiferromagnetic coupling $J_1$ and $J_2$, respectively, which we have studied at $J_2 = 0$ in the absence of frustration and, for strong frustration, at $J_2 = 0.5$ and $J_2 = 0.55$. Our first goal is to optimize the variational energy within each $D$-dimensional
class of SU(2)-invariant PEPS i.e finding the optimum linear superposition of the $D$ independent tensors of each class. Since the number of variational parameters remains small (maximum of $D = 30$ for $D = 7$) we have used a "brute force" CG optimization as e.g. given in Numerical Recipes [79]. However, this requires an efficient iPEPS computation of the variational energy for any set of variational parameters to "feed" the CG routine. This is performed constructing a self-consistent environment around an active $2 \times 2$ cluster (see Fig. 2(b)) using an iterative CTMRG algorithm [47, 49, 50] optimized for spatially symmetric tensors. Indeed, we have introduced simple modifications: (i) we use a unique CTM $C$ tensor (side tensor $T$) which is the same for all corners (edges) and (ii) the basic Singular Value Decomposition (SVD) in each CTMRG step to construct the environment is replaced by a (more stable) ED, the CTM being here a symmetric matrix. The largest environment dimension we could handle was $\chi = 400$ and $\chi = 294$ for $D = 5$ and $D = 7$, respectively, for which up to 350 or 400 iterations became necessary to converge the environment. Note that the initial $C$ ($T$) tensor is obtained from the $\mathbb{Z}$ tensor of Fig. 2(b) by summing over all external $l$ and $u$ (a) indices.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.png}
\caption{(Color online) (a) iPEPS variational energies of the $J_1 - J_2$ model at $J_2 = 0.5$, versus the inverse of the environment dimension $\chi$. Full (open) symbols correspond to fully optimized (fixed) tensor ansätze (see text). $\chi \rightarrow \infty$ linear extrapolations are performed using only the last data points. (b) Behavior of the $\chi \rightarrow \infty$ extrapolated energies vs the inverse of the bond dimension $D$. $D = 9$ PEPS [56] and DMRG [66] extrapolated energies are shown for comparison (see also Table II).}
\end{figure}

Energetics – Variational energies (per site) in each class of tensors are shown in Fig. 3(a) for $J_2 = 0.5$, as a function of the inverse of the environment dimension $\chi$. A rapid comparison between the different classes (for intermediate $\chi$) reveals that, for identical bond dimension $D$, the classes $V = \frac{1}{2} \otimes N \oplus 0$ with $N = 1, 2$ and 3 (of bond dimensions $D = 3, 5$ and 7, respectively) give the best results. Hence, hereafter we shall focus on this PEPS family defined in terms of $N$ “colors” of spin-$\frac{1}{2}$. Note that the case $N = 1$ was studied previously in Ref. [69]. Tensors are fully optimized up to a maximum bond dimension $\chi_{\text{opt}}$, e.g. for $D = 5$, $\chi_{\text{opt}} = 4D^2 = 100$ and, for $D = 7$, $\chi_{\text{opt}} = 2D^2 = 98$. Then, using environment dimensions $\chi > \chi_{\text{opt}}$ together with the fixed optimized tensor obtained at $\chi = \chi_{\text{opt}}$, one gets true upper bounds of the variational energy. In contrast, for $D = 3$, $\chi_{\text{opt}} = 12D^2 = 108$ already gives the absolute best tensor with enough accuracy. Generically, we found that the energy always decreases with increasing $\chi$ and, at large enough $\chi$, linear fits can be performed in $1/\chi$ to provide $\chi \rightarrow \infty$ extrapolations, also upper bounds of the ($D$-dependent) variational energies. Note that our $D = 7$ extrapolation $-0.4954$ lies within only 0.2% of the extrapolated value $-0.4958$ obtained using cluster update finite size $D = 9$ PEPS [56]. We have plotted our $\langle 1/D \rangle$ results as a function of $1/D$ in Fig. 3(b) showing perfect consistency with the above-mentioned $D = 9$ result together with the DMRG extrapolation $-0.4968$ of Ref. 66. This agreement is remarkable considering the fact that we use only a unique tensor parametrized by a small number of coefficients. Good variational energies have also been found for the simple NN Heisenberg model ($J_2 = 0$) as well as for larger frustration $J_2 = 0.55$ as shown in Appendix A. Our results are summarized in Table II and compared to the best estimates, from Quantum Monte Carlo at $J_2 = 0, 5, 6$ and from DMRG [66], VMC [70] and finite-size PEPS [56] at $J_2 = 0.5$ and $J_2 = 0.55$. We note however that our variational energies for $J_2 = 0$ and $J_2 = 0.55$ are slightly less accurate as for $J_2 = 0.5$. In fact, we believe $J_{2c}$ is close to 0.5 and we argue below that our (optimized) PEPS is capable of picking up the critical nature of the QCP or QCPh. For $J_2 = 0.55$ translation symmetry breaking is likely to occur spontaneously, which is not captured by our homogeneous ansatz. The ansatz does not either sustain magnetic LR order, that may explain its lower accuracy at $J_2 = 0$.

### III. CORRELATION FUNCTIONS

Once the PEPS $|\Psi_0\rangle = |\Psi(D, \chi_{\text{opt}})\rangle$ has been optimized using the largest possible environment dimension $\chi = \chi_{\text{opt}}(D)$, various correlation functions can be computed (e.g. along the $e_x$ horizontal direction), like (i) the spin-spin correlations,

$$C_s(d) = \langle S_i \cdot S_{i+d_e} \rangle_0,$$

(ii) the (connected) longitudinal dimer-dimer correlations,

$$C_{dL}^{(1)}(d) = \langle D_{i}^{x} D_{i+d_e}^{x} \rangle_0 - \langle D_{i}^{x} \rangle_0 \langle D_{i+d_e}^{x} \rangle_0.$$
| J  | 0   | 0.5 | 0.55 |
|----|-----|-----|------|
| QMC | -0.66944 |     |      |
| DMRG | -0.4968 | -0.4863 |      |
| VMC | -0.4970(5) | -0.4870(5) |      |
| D = 9 PEPS  | -0.4958(3) | -0.4857(2) |      |
| D = 7 iPEPS  | -0.6677 | -0.4950 | -0.4830 |

**TABLE II.** Comparison between our $D = 7$ iPEPS results ($\chi \rightarrow \infty$ extrapolations) and the best estimates in the literature, for $J_2 = 0$, $J_2 = 0.5$ and $J_2 = 0.55$ : $J_2 = 0$ results are obtained by QMC [5, 6]. At finite $J_2$, we quote energies obtained by extrapolations to the thermodynamic limit using DMRG [66], VMC [70] and finite-size $D = 9$ PEPS [56]. Note that the $D = 7$ iPEPS energies are only upper bounds of the true variational energies (see text).

and (iii) the (connected) transverse dimer-dimer correlations,

$$C_d^{(T)}(d) = \langle D_{i}^{u} D_{i+de_{x}}^{u} \rangle - \langle D_{i}^{u} \rangle \langle D_{i+de_{x}}^{u} \rangle,$$

where dimer operators $D_{i}^{u} = S_{i} S_{i+e_{x}}$, and $D_{i}^{d} = S_{i} S_{i+e_{y}}$ are oriented either along the $e_{x}$ (horizontal) or $e_{y}$ (vertical) directions, respectively, and the expectation values are taken in the optimized $|\Psi_{opt}\rangle$ PEPS.

The calculations of correlators are accomplished using the set-up shown in Fig. 4(a-c). Appropriate transfer matrices are used so that one can construct arbitrarily long strips. Here the site tensor is fixed to its optimized output using $\chi = \chi_{opt}(D)$ (hereafter we use $\chi_{opt} = 49$ for $D = 7$) while the environment dimension $\chi > \chi_{opt}(D)$ can be then further increased to reach convergence, which is easily achieved for short distance $r$. A comparison between the results obtained with the two ansätze $V = 2 \oplus 2 \oplus 0$ (a) and $V = 2 \oplus 1 \oplus 2 \oplus 0$ (b) is shown in Fig. 5 for $J_2 = 0.5$. Although a fast decay of the dimer-dimer correlations is seen in both cases, the behavior of the (staggered) spin-spin correlations is qualitatively different : for $D = 7$ [$C_s(r)$] seems to approach a finite value while, for $D = 5$ (or $D = 3$ as well), it steadily decays to zero. This signals the emergence, for $D \geq 7$, of a finite staggered magnetization as defined by $m_{stag}(\chi) = \sqrt{\lim_{r \rightarrow \infty} |C_s(r)|}$. We note however that, strictly speaking, for finite $\chi$ the above limit should vanish since the correlations are cut-off above some correlation length $\xi_{\chi}(\chi)$ (see below). In other words, the strip of Fig. 4(a) is, crudely speaking, similar to a quasi-1D physical strip (ladder) of effective width $L_{eff}(\chi)$ [80], which can not sustain long-range magnetic order from Mermin-Wagner theorem (MWT) [81]. However, MWT may not, strictly speaking, apply to a transfer operator as for a true Hamiltonian. In addition, for $D = 7$ the SU(2) symmetry is spontaneously broken : small deviations from a perfectly SU(2)-symmetric environment act as a small symmetry-breaking (AF) "field" and the local spin operator acquires a finite value $\langle S_{i}^{z} \rangle = \cos(q_{AF} \cdot 1) m_{stag}$ oscillating at the antiferromagnetic wave vector $q_{AF}$. As shown in Appendix B, $m_{stag}(\chi)$ vanishes in the $\chi \rightarrow \infty$ limit, physically corresponding to the limit of an infinitely wide strip $L_{eff} \rightarrow \infty$. This implies that the infinite 2D system recovers the full SU(2) spin symmetry encoded in the tensor ansatz. We have seen similar behaviors also for $J_2 = 0$ and $J_2 = 0.55$ as well (see Appendix B).

Interestingly, the scaling of $m_{stag}$ to zero may depend slightly of the initial CTM of the CTMRG procedure to converge the environment. In contrast, for $D = 3$ and $D = 5$ the system remains spin isotropic even for finite $\chi$, the spin correlators $\langle S_{i}^{x} S_{j}^{y} \rangle$ being independent on $\alpha = x, y, z$, as checked explicitly. This signals a qualitative change of behavior when $N \geq 3$ which we identify in the next section.

**Diverging correlation lengths** – The results described above give some hints that, when $D = 7$, the spin-spin correlations become algebraic at long distance. However, for finite bond dimension $\chi$, the strips of Fig. 4(a-c) can seen as effective 1D systems. Then, finite correlation lengths $\xi_{D}(\chi)$ naturally emerge as the inverse of the gaps of finite-dimensional $D_{eff}^{2} \times D_{eff}^{2}$ transfer matrices, where $D_{eff} = D_{\chi}$ (Fig. 4(a,b)) or $D_{eff} = D_{\chi}^{x}$ (Fig. 4(c)) is the effective dimensions of the associated 1D MPS. Using empirical findings for the correlation length $\xi_{1D}$ in critical 1D systems [73–75], $\xi_{1D}(D) \sim D^{\kappa}$, one then expects that $\xi_{D}(\chi) \sim (D_{eff})^{\kappa}$, $\kappa > 0$, which should diverge with $\chi$ as a power law for critical PEPS. Hence, criticality (if any) is restored only in the $\chi \rightarrow \infty$ limit and finite-$\chi$ scaling is necessary to obtain informations on the QCP or QCPh. Note that, when spin rotational symmetry is (artificially) broken at finite $\chi$, it is important to consider the connected spin-spin correlator $\tilde{C}_{s}(d) = C_{s}(d) - (m_{stag})^{2}$. From straightforward fits of the long-distance correlations at $J_2 = 0.5$ (see Appendix C) we have extracted the correlation lengths $\xi_{D}(\chi)$ associated to the $\tilde{C}_{s}$, $C_{d}^{(T)}$ and $C_{d}^{(T)}$ correlation functions and results are shown in Fig. 6. For $D = 3$ or $D = 5$ we find a clear saturation of the spin-spin correlation lengths to small values while the dimer-dimer correlations lengths diverge linearly with $\chi$. Such a behavior is typical of bi-partite dimer models [82] or of the NN RVB state on the square lattice [18, 20] due to $U(1)$-gauge symmetry. In fact, the $D = 3$ PEPS can be viewed as an extended-range RVB state [69] and the $D = 5$ PEPS as an extended-range two-color RVB state. Plotting the dimer correlation lengths in Fig. 6(c,e) as a function of $\chi/D^{2}$ clearly reveals the similarities between $D = 5$ and $D = 7$. However, in the case of the spin correlations, a sudden qualitative change occurs at $D = 7$ for which we find that the spin-spin correlation length no longer saturates but increases linearly with $\chi$, as the dimer correlation lengths do (see Appendices C and D for details). No sign of saturation of the correlation lengths is observed up to the largest available environment dimensions. This suggests that the (optimized) $D = 7$ PEPS is critical in the limit $\chi \rightarrow \infty$ or, at least, can very well describe a critical state.

**Power-law exponents** – Whenever the correlation length $\xi_{D}(\chi)$ diverges (or becomes very large), one expect
FIG. 4. [Color online] One dimensional strips used to compute the spin-spin (a), the longitudinal dimer-dimer (b) and the transverse dimer-dimer (c) correlation functions. A transfer matrix is applied recursively \(d-1\) times (a,c) or \(d-2\) times (b) in the direction of the strip.

FIG. 5. [Color online] Short-distance correlation functions at \(J_2 = 0.5\) for \(V = \frac{1}{2} \oplus \frac{1}{2} \oplus 0\) (a) and \(V = \frac{1}{2} \oplus \frac{1}{2} \oplus \frac{1}{2} \oplus 0\) (b). Large environment dimensions \(\chi\) are used ensuring full convergence of the correlations at short distance \((r<10)\).

To see power-law behaviors in the correlation functions,

\[
C_s(d) \sim d^{-(1+\eta_s)},
\]

\[
C_d(d) \sim d^{-(1+\eta_d)},
\]

in the range of distance \(1<d<\xi_D\), where \(\eta_s\) and \(\eta_d\) defined e.g. in Ref. [83] are the anomalous dimensions. Note however that this scaling regime can be observed only when \(\xi_D(\chi)\) has reached a sufficiently large value.

FIG. 6. [Color online] Scaling of the various correlation lengths at \(J_2 = 0.5\) vs (a) environment dimension \(\chi\) or (b)-(e) \(\chi/D^2\), for \(V = \frac{1}{2} \oplus 0\) (open squares), \(V = \frac{1}{2} \oplus \frac{1}{2} \oplus 0\) (open circles) and \(V = \frac{1}{2} \oplus \frac{1}{2} \oplus \frac{1}{2} \oplus 0\) (large dots and crosses). (a) Spin-spin correlations; (b,c) Transverse dimer-dimer correlations; (d,e) Longitudinal dimer-dimer correlations.

To obtain estimates of the exponents \(1+\eta_s\) and \(1+\eta_d\) we have plotted spin-spin and (longitudinal) dimer-dimer correlations at \(J_2 = 0.5\) in Fig. 7(a,b) using log-log scales. For \(D = 3\) \((D = 5)\) the dimer correlation length is very large (is large) for the largest \(\chi\) we can reach and, from fits of the data in the range \(1<d<100\) \((1<d<20)\),
one can easily extract the exponent $1 + \eta_d \simeq 1.25$ ($1 + \eta_d \simeq 1.5$). For $D = 7$, it is difficult to extract accurate exponents since cross-overs to exponential decays occur rapidly around $d \sim \xi_s \simeq 6$, for both the spin-spin and dimer-dimer correlations. However, the systematic trend of the data with $\chi$ in Fig. 7(a,b) suggests $\eta_s \sim 0.6$ and $\eta_d \sim 1.2$.

\[ \xi_D(\chi) \simeq f_D \chi/D^2, \]

where the prefactor $f_D$ depends weakly on $D$, the main effect of increasing the bond dimension being to rescale the environment dimension $\chi \rightarrow \chi_D = \chi/D^2$. We note nevertheless that, although our data are consistent with (6), one cannot rule out that some of the correlation lengths may saturate to a finite, although large, value.

Related $J − Q$ models can be investigated with QMC [83] and $\eta_s \simeq 0.35(2)$ and $\eta_d \simeq 0.20(2)$ have been obtained (for the $J − Q_2$ model), which seem to deviate substantially from our estimates above. However, our estimation of $\eta_s$ seems consistent with the VMC result [71] $\eta_s \sim 0.5$ obtained for the $J_1 − J_2$ Heisenberg model at $J_2 = 0.5$.

Note that the power-law exponent $1 + \eta_d$, extracted from the correlations at intermediate distances $d < \xi_D(\chi)$, seems to increase significantly with $D$. The predicted large value of the $D \rightarrow \infty$ dimer anomalous dimension might indicate that dimer correlations at the QCP or within the QCPH are significantly suppressed compared to $J − Q$ models.

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Appendix A: Scaling of the $D = 7$ variational energy vs inverse environment dimension

We report in Fig. 8(a-c) the variational energies of the $V = \frac{1}{2} \oplus \frac{1}{2} \oplus \frac{1}{2} \oplus 0$ PEPS ansatz for the $J_1 - J_2$ model at $J_2 = 0$ (unfrustrated case), $J_2 = 0.5$ and $J_2 = 0.55$. The parameters of the PEPS are optimized with an environment dimension $\chi_{\text{opt}} = D^2 = 49$, independently for each value of $J_2$. For $J_2 = 0.5$ we also carried out the optimization with $\chi_{\text{opt}} = 2D^2 = 98$, providing a slightly better energy. The environment dimension $\chi > \chi_{\text{opt}}$ is then increased, keeping the PEPS tensor fixed, and the energy is extrapolated linearly with $1/\chi$. At $J_2 = 0.5$, an excellent agreement is found with extrapolation from $D = 9$ PEPS cluster update [56]. For $J_2 = 0$ and $J_2 = 0.55$ a less good agreement is found with QMC [5, 6] and PEPS cluster update [56], respectively (see text for explanation).

![FIG. 8. (Color online) (a) $D = 7$ iPEPS variational energies of the $J_1 - J_2$ model at $J_2 = 0$ (a), $J_2 = 0.5$ (b) and $J_2 = 0.55$, versus the inverse of the environment dimension $\chi$. Full (open) symbols correspond to fully optimized (fixed) tensor ansätze (see text). $\chi \to \infty$ linear extrapolations are performed using only the last data points. Comparisons with QMC [5, 6] and finite size $D = 9$ PEPS extrapolations (with error bars) [56] are shown.](image)

Appendix B: Scaling of the $D = 7$ staggered magnetization vs inverse environment dimension

We report in Fig. 9(a-c) the spurious staggered magnetization of the $V = \frac{1}{2} \oplus \frac{1}{2} \oplus \frac{1}{2} \oplus 0$ PEPS ansatz for the $J_1 - J_2$ model at $J_2 = 0$ (unfrustrated case), $J_2 = 0.5$ and $J_2 = 0.55$ (optimized using $\chi_{\text{opt}} = D^2 = 49$). The procedure is the same as in Appendix A and the data are plotted vs $\chi$. For all $J_2$ values, the scaling (algebraic fits) is consistent with vanishing $m_{\text{stag}}$ when $\chi \to \infty$. Full SU(2) invariance is recovered in this case.

![FIG. 9. (Color online) (a) $D = 7$ iPEPS staggered magnetization of the $J_1 - J_2$ model at $J_2 = 0$ (a), $J_2 = 0.5$ (b) and $J_2 = 0.55$, versus environment dimension $\chi$. $\chi \to \infty$ extrapolations are based on power-law fits. The exact (QMC) value of $m_{\text{stag}}$ [5, 6] at $J_2 = 0$ is shown.](image)

Appendix C: Extracting the correlation lengths $\xi_D(\chi)$ from the long distance correlations

In order to extract the correlation lengths associated to the various correlation functions $C_\lambda(d)$ ($\lambda = S, D$) defined in the paper in Eqs. (1), (2) and (3), we have computed the long-distance correlations using the transfer matrix methods sketched in Fig. 2. Due to a finite gap in the relevant transfer matrices for all finite dimensions $D$ and $\chi$, one expects an exponential decay of all correlations,

$$ C_\lambda(d) \sim C_0 \exp(-d/\xi^D(\chi)) , $$

at sufficiently large distance $d$ (typically $d > \xi^D(\chi)$). Let us summarize the procedure : First, the local tensors for $D = 3, 5$ and 7 are obtained by a full CG optimization (for $J_2 = 0.5$) using a given environment dimension $\chi_{\text{opt}} = 108, 100$ and 49, respectively. The correlations in these fixed PEPS are then computed for increasing values of the environment dimension $\chi$ in two steps : (i) For every choice of $\chi \geq \chi_{\text{opt}}$, the new converged CTM $C$ and edge tensor $T$ are computed (by the iterative renormalization scheme) and, finally, (ii) used to compute the correlation functions in the setup shown in Fig. 2(a-c). Results are displayed using semilogarithmic scales in Figs. 10(a), 11(a) and 12(a). By fitting the asymptotic linear behaviors of the data according to $\ln C_\lambda(d) = -(1/\xi) d + c_0$, one straightforwardly gets the correlation lengths $\xi$ from the slopes $-1/\xi$. 
The scaling of the correlation lengths $\xi_D$ with $\chi$ are shown in Figs. 10(b), 11(b,c) and 12(b,c). For $D = 3$ and $D = 5$, one observes a clear saturation of the spin correlation lengths $\xi_3$ and $\xi_5$ to rather small values (less than 2 lattice spacings) while the dimer correlation length scales linearly with $\chi$ suggesting that $\xi_D \to \infty$ in the limit $\chi \to \infty$, for which the calculation becomes exact. Note that the (extrapolated) spin correlation length increases with $D$ while the divergence of the dimer correlation length becomes weaker. For $D = 7$, one has to consider the connected part of the spin-spin correlation, subtracting off the contribution from the spurious staggered spin density background. The spin correlation length no longer saturates but rather increases linearly with the environment dimension $\chi$. This strongly suggests that $\xi_7$ diverges in the limit $\chi \to \infty$, that is consistent with a power-law decay of the correlation function. We believe our numerical results also support the divergence of both dimer-dimer correlation lengths, as well. Note however that, although the transverse and longitudinal dimer-dimer correlation lengths seem to match for $D = 3$ and $D = 5$, they deviate substantially for $D = 7$, which may be related to the non-vanishing of the spin-spin correlation in that case.

Appendix D: Comparison between correlation functions in the $D = 7$ PEPS

In principle, correlation lengths can also be extracted directly from the low-energy eigenvalues of the zero dimensional transfer matrix of the one-dimensional tensor network structures arising in Fig. 4. It would be the same transfer matrix for spin-spin and (longitudinal) dimer-dimer correlation function, but the difference would be how the corresponding virtual eigenvectors of these eigenvalues transform under the symmetry. In a perfectly
SU(2)-symmetric state giving rise to a SU(2)-symmetric environment (as it occurs for $D = 3$ and $D = 5$), different selection rules for the singlet (dimer) and the triplet (spin) channels lead to separate blocks of the transfer matrix and, hence, to different correlation lengths, in agreement with our findings. However, for $D = 7$ spontaneous SU(2) symmetry breaking occurs and the environment acquires some (staggered) magnetization $\mathbf{m}_{stag}$. We believe spin-rotational invariance ($U(1)$ symmetry) is still preserved around the direction of the staggered magnetization. The latter can be pointing in any (arbitrary) direction in the $(x, z)$ plane making difficult the symmetry analysis of the zero dimensional transfer matrix arising in Fig. 4. Analysis of the correlation functions given e.g. by Eqs. 1, 2 or 3 is more straightforward.

At this point, it is not clear whether the long distance spin correlation described in the text is an artifact of the symmetry breaking that i) may lead to a mixture of (diverging) singlet and (short-range) triplet correlations or ii) may lead to "Goldstone critical behavior" of the transverse spin correlation function. We give arguments below that none of the above applies and argue that the critical behavior of the spin correlation function is an intrinsic feature of the $D = 7$ PEPS spin liquid.

\begin{equation}
S_i = S_i^\parallel n + S_i^\perp ,
\end{equation}

where $n$ is a unit vector along $\mathbf{m}_{stag}$, $S_i^\parallel = \mathbf{S}_i \cdot n$ and $S_i^\perp = \mathbf{S}_i - (\mathbf{S}_i \cdot n) \mathbf{n}$. The spin correlation function can be then split into its longitudinal and transverse components as $C_s(d) = C_s^\parallel(d) + C_s^\perp(d)$ with,

\begin{align}
C_s^\parallel(d) &= \langle S_i^\parallel S_{1+d}^\parallel \rangle_0 , \\
C_s^\perp(d) &= \langle S_i^\perp S_{1+d}^\perp \rangle_0 .
\end{align}

For a true singlet wave function (for which $\mathbf{m}_{stag} = 0$), whatever the choice of the vector $n$, one gets $C_s^\perp(d) = 2C_s^\parallel(d)$. As shown in Fig. 13(a) this is also true for the $D = 7$ PEPS, at short distance only (in semi-log scale the two curves are just shifted by ln 2). At longer distance, however, the longitudinal and transverse spin correlations show different exponential decays. As shown in Fig. 13(b) the correlation length of the longitudinal correlations is much shorter than the one of the transverse correlations. However, both seem to diverge with increasing $\chi_i$ suggesting that both correlators are critical, possibly power-law, in the $\chi \to \infty$ limit. This is different from a "Goldstone mechanism" for which the longitudinal correlations remain short-range. Finally, we compare the two spin correlation lengths to the (longitudinal) dimer correlation length. Fig. 13(b) shows that none of the three (diverging) correlation length match, suggesting that the (supposedly) critical behavior of the spin-spin correlation is not induced by the critical behavior of the dimer correlation and is an intrinsic property of the $D = 7$ PEPS.

\begin{figure}[h]
\centering
\includegraphics[width=0.7\textwidth]{fig13.png}
\caption{(Color online) (a) Longitudinal and transverse spin correlations versus distance in the SU(2)-symmetry broken $D = 7$ PEPS, for several values of $\chi$ (semi-log scale). Tensors are the same as in Fig. 10. (b) Correlation lengths extracted from linear fits of the large-distance behaviors are shown versus $\chi$ and compared to the (longitudinal) dimer correlations. Note that, eventually, beyond some large cross-over length scale (which increases with $\chi$), the decay of the longitudinal correlation function is governed by the asymptotic (larger) correlation length of the transverse correlation function.}
\end{figure}

For this purpose, we decompose the local spin operator into its longitudinal and transverse spin components,