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We show how to construct fully symmetric states without topological order on a honeycomb lattice for $S = 1/2$ spins using the language of projected entangled pair states (PEPS). An explicit example is given for the virtual bond dimension $D = 4$. Four distinct classes differing by lattice quantum numbers are found by applying the systematic classification scheme introduced by two of the authors [S. Jiang and Y. Ran, Phys. Rev. B 92, 104414 (2015)]. Lack of topological degeneracy or other conventional forms of symmetry breaking in the proposed wave functions are checked by numerical calculations of the entanglement entropy and various correlation functions. Exponential decay of all correlation functions measured are strongly indicative of the energy gap for the putative parent Hamiltonian of the state. Our work provides the first explicit realization of a featureless quantum state for spin-1/2 particles on a honeycomb lattice.

I. INTRODUCTION

A modern theme of much interest in condensed matter systems is the classification of possible phases of quantum matter in low dimensions. First noted in the context of quantum Hall physics, it has become clear that different quantum phases are labeled often by their topological characters rather than by broken symmetries as in the conventional Ginzburg-Landau paradig[1]. How to define such quantum orders and classify states accordingly in a precise way has intrigued theorists for several decades.

A powerful guide in the classification effort is the "no-go" theorem such as the celebrated Lieb-Schultz-Mattis theorem in one dimension[2] and its higher-dimensional generalizations due, for instance, to Oshikawa[3] and Hastings[4], stating that lattice spin models having a half-integer spin per unit cell must remain gapless, or if gapped, would either break conventional symmetries or turn into a topological state with fractionalized excitations. Powerful as they are, though, integer spin systems are not covered by these theorems. In one dimension we have some well-established results for integer-spin chains, e.g. $S = 1$ Haldane spin chain, saying that the ground state can be both gapped and featureless.

Turning to two dimensions, search for an analogous featureless phase not addressed by the no-go theorem can best proceed by an explicit identification of the $S = 1$ state on a Bravais lattice[5], or the $S = 1/2$ state on a honeycomb lattice with an even number of sites per unit cell[5–7]. One such construction was given recently with the $S = 1$ model on a square lattice[5], while attempts to construct featureless states for $S = 1/2$ spins on a honeycomb lattice has met only with partial success so far[5–7]. In this paper, we provide an explicit construction of the spin-1/2 wave function on a honeycomb lattice that preserves the full set of lattice symmetries plus time-reversal and SU(2) spin rotation, in addition to being devoid of topological order. Lacking both symmetry breaking and topological order, such states do not permit a straightforward field-theoretic description[5]. We instead use the recently developed classification scheme of the tensor network wave functions[8–15], in particular the one proposed by two of the authors[8], to identify all possible spin-1/2 featureless tensor network states on the honeycomb lattice for a given bond dimension of the tensor network. Intensive numerical check carried out by the authors confirm that the proposed featureless state is most likely devoid of any conventional order, and has the topological entanglement entropy[16,17] of zero.

All correlation functions measured for the proposed wave function exhibit exponential decay which, according to conventional wisdom, is characteristic of a gapped quantum ground state. In the tensor network approach, however, the parent Hamiltonian having the proposed tensor network wave function as the ground state is either unknown, or very complicated when constructed explicitly[18–20]. It is still fair to say that the spin-1/2 featureless wave function we present is a close approximation to the gapped ground state of some parent spin Hamiltonian on the honeycomb lattice.

The rest of the paper is organized in the following way. In Sec. II, we lay out the classification scheme, first worked out in Ref. 8 and adapted to the case of honeycomb lattice here. Lattice quantum numbers that help characterize different classes of symmetric tensor network wave functions are computed. Finally, an explicit construction of the fully symmetric wave function is made for one particular class. In Sec. III, extensive numerical calculations are carried out to investigate properties of the proposed wave function, with the conclusion that this is indeed the spin-1/2 featureless state we seek on the honeycomb lattice. Final thoughts and summary are given in Sec. IV.

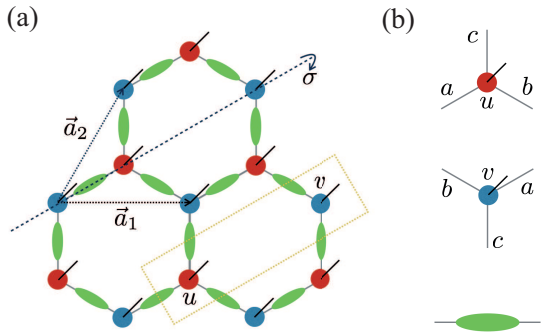

FIG. 1. (Color online) (a) Graphical representation of the tensor network state on a honeycomb lattice. (b) u- and v-site tensors are comprised of three virtual legs labeled a, b, c and one physical leg shown as an upward black line. Green ellipses in (a) represent the bond tensor that connect the virtual spins from the two ends. Bravais unit vectors are chosen as $\mathbf{a}_1 = \hat{x}$ and $\mathbf{a}_2 = (\hat{x} + \sqrt{3}\hat{y})/2$. A yellow box represents the unit cell.

II. SPIN-1/2 SYMMETRIC PEPS ON HONEYCOMB LATTICE

A. Classification scheme

The honeycomb lattice we work on and various notations for site and bond labels are shown schematically in Fig. 1(a). The method of choice for constructing featureless states is the projected entanglement pair states, or PEPS, pioneered in Ref. 21 and reviewed in Ref. 22. To construct a honeycomb PEPS, we associate every site/bond of the honeycomb lattice with a site/bond tensor. A site tensor is formed by one physical leg which supports physical spin-1/2 degrees of freedom, and three virtual legs, each with D degrees of freedom called the bond dimension. The bond tensor is formed by two virtual legs forming a nearest-neighbor bond as shown in Fig. 1(a) as a green ellipse. Each leg of the bond tensor has the degree of freedom D matching that of the site virtual leg. The physical wave function is obtained by contracting all connected virtual legs of site tensors and bond tensors.

In constructing a fully symmetric and topologically trivial state with spin-1/2 per site on a honeycomb lattice, we rely on the recently developed classification algorithm of quantum phases in terms of PEPS proposed by two of the present authors in Ref. 8. Let us briefly review the procedure here, delegating full details of the classification work on the honeycomb lattice to the Appendix A.

As shown in the yellow dashed box of Fig. 1, we label the two lattice sites in each unit cell with the sublattice index $s = u, v$. Around each lattice site we introduce three indices $i = a, b, c$ for the three bond directions. Unit cells are labeled as $x\vec{a}_1 + y\vec{a}_2$ in terms of the two Bravais unit vectors $\vec{a}_1 = \hat{x}$ and $\vec{a}_2 = \frac{1}{2}(\hat{x} + \sqrt{3}\hat{y})$. We are then able to specify all sites and virtual legs of the honeycomb lattice using the four labels, (x, y, s, i).

The lattice symmetry of the two-dimensional honeycomb lattice is generated by the following operations

$$\begin{aligned}
T_1&: (x, y, s, i) \to (x+1, y, s, i),\\
T_2&: (x, y, s, i) \to (x, y+1, s, i),\\
\sigma&: (x, y, s, a) \to (y, x, s, a),\\
&\quad (x, y, s, b/c) \to (y, x, s, c/b),\\
C_6&: (x, y, u, i) \to (-y, x+y-1, v, C_6(i)),\\
&\quad (x, y, v, i) \to (-y, x+y+1, u, C_6(i)).
\end{aligned} \tag{1}$$

In obvious notations, T_1 and T_2 are the lattice translations along the $\vec{a}_1$ and $\vec{a}_2$ directions, respectively. Reflection about the σ-axis in Fig. 1 is indicated by σ. Finally, there is the C_6 rotation about the center of one hexagon at the origin. The C_6 symmetry operation on the bond index i is defined as $C_6(a) = c, C_6(b) = a, C_6(c) = b$. We further impose the symmetry under time-reversal operation $\mathcal{T}$, as well as the spin rotation $R_{\theta\vec{n}}$, about an axis $\vec{n}$ by an angle θ, of the physical spin-1/2's.

The symmetry group of the honeycomb lattice is defined by the following algebraic relations among its generators:

$$\begin{aligned}
T_2^{-1}T_1^{-1}T_2T_1 &= \mathrm{e},\\
C_6^{-1}T_2^{-1}C_6T_1 &= \mathrm{e},\\
C_6^{-1}T_2^{-1}T_1C_6T_2 &= \mathrm{e},\\
\sigma^{-1}T_1^{-1}\sigma T_2 &= \mathrm{e},\\
\sigma^{-1}T_2^{-1}\sigma T_1 &= \mathrm{e},\\
\sigma^{-1}C_6\sigma C_6 &= \mathrm{e},\\
C_6^6 = \sigma^2 = \mathcal{T}^2 &= \mathrm{e},\\
g^{-1}\mathcal{T}^{-1}g\mathcal{T} &= \mathrm{e}, \quad (g = T_{1,2}, C_6, \sigma),\\
g^{-1}R_{\theta\vec{n}}^{-1}gR_{\theta\vec{n}} &= \mathrm{e}, \quad (g = T_{1,2}, C_6, \sigma, \mathcal{T}),
\end{aligned} \tag{2}$$

where e stands for the identity element in the symmetry group.

Due to the existence of an enlarged Hilbert space by virtual legs, the mapping from site/bond tensors to physical wave functions are many-to-one. Namely, a wave function which is globally symmetry-preserving can have its constituent site/bond tensors "gauge-transformed", by acting with an arbitrary invertible matrix $V(s, i)$ on a virtual leg i of the site tensor at s and simultaneously with its inverse matrix $V^{-1}(s, i)$ on the corresponding leg of the bond tensor. There may also exist special gauge transformations that leave every site/bond tensor invariant, up to a U(1) phase factor. Those transformations form a group, named the invariant gauge group (IGG), which governs the low energy gauge dynamics of the tensor network state as shown in Refs. 19 and 20.

With such gauge structure of the PEPS wave function in mind, let us consider various symmetry operations on PEPS. According to the general remarks above, invariance of the physical wave function $|\psi\rangle$ (up to a U(1) phase) under a specific symmetry operation g implies the following general transformation rules for the site and bond tensors:

$$T^s = \Theta_g W_g (g \circ T^s)$$
$$T^b = W_g (g \circ T^b). \quad (3)$$

Here, it is assumed that the PEPS wave function is injective.[20] We label the site tensor at s as T^s, and the bond tensor over the bond b as T^b. W_g is a leg-dependent gauge transformation acting on virtual legs of tensors. Here $g\circ$ can be spin rotation, time reversal or any lattice symmetry operation on a *physical* Hilbert space. Symmetry implementation is *projective* in the sense that the operation on the physical indices by g can be "compensated for" by the gauge operations W_g on virtual indices and the U(1) phase factor Θ_g. The site-dependent phase factor Θ_g also allows us to capture the symmetry quantum numbers of the state $|\psi\rangle$ [8].

Following the framework developed in Ref. 8, symmetry group operations pertinent to the particular lattice geometry can be cast as a set of algebraic equations as discussed in the Appendix B. By solving them, one obtains highly constrained forms of all the gauge transformation matrices W_g and Θ_g associated with the physical symmetric operation g. We should mention that IGG will in general enter these algebraic equations, influencing the outcome of the solutions for W_g and Θ_g. In keeping with the spirit of the present paper, which is the search for featureless states in the case of the spin-1/2 honeycomb lattice, we set IGG to be trivial, i.e. as an identity element.

Details of the classification procedure for symmetric PEPS with trivial IGG and how to solve for the W_g's and Θ_g's are found in the Appendix B. We should emphasize that the final expression of the tensors for the featureless state are quite transparent and can be understood without the full knowledge of the classification scheme. In the end, we obtain

$$\begin{aligned}
&W_{T_1}(s,i) = W_{T_2}(s,i) = \mathbb{I},\\
&W_{C_6}(u,a/b) = W_{C_6}(v,i) = \mathbb{I}, \quad W_{C_6}(u,c) = \chi_{C_6},\\
&W_\sigma(u,a) = W_\sigma, \quad W_\sigma(u,b/c) = \chi_{C_6} W_\sigma,\\
&W_\sigma(v,a) = \chi_{C_6}\,\chi_{\sigma C_6}\, W_\sigma, \quad W_\sigma(v,b/c) = W_\sigma,\\
&W_{\mathcal{T}}(s,i) = W_{\mathcal{T}} = \bigoplus_{k=1}^{M} (\mathbb{I}_{d_k} \otimes \mathrm{e}^{\mathrm{i}\pi S^y_k}),\\
&W_{\theta\vec{n}}(s,i) = W_{\theta\vec{n}} = \bigoplus_{k=1}^{M} (\mathbb{I}_{d_k} \otimes \mathrm{e}^{\mathrm{i}\theta\vec{n}\cdot\vec{S}_k}),\\
&\Theta_{T_1}(s) = \Theta_{T_2}(s) = 1, \quad \Theta_{C_6}(u) = \chi_{C_6}, \quad \Theta_{C_6}(v) = 1,\\
&\Theta_\sigma(u) = 1, \quad \Theta_\sigma(v) = \chi_{C_6}\chi_{\sigma C_6}, \quad \Theta_{\mathcal{T}} = 1. \quad (4)
\end{aligned}$$

Each virtual leg has the Hilbert space consisting of M different species of spins, each labeled as $\vec{S}_k$, $1 \le k \le M$. For each spin $\vec{S}_k$ one further introduces the "flavor" degeneracy of d_k, for a total virtual Hilbert space dimension

$(\chi_{C_6}, \chi_{\sigma C_6})$	$(+1,+1)$	$(+1,-1)$	$(-1,+1)$	$(-1,-1)$
C_6	$+1$	$+1$	-1	-1
σ	$+1$	-1	-1	$+1$

TABLE I. Lattice quantum numbers $(\chi_{C_6}, \chi_{\sigma C_6})$ for C_6 and σ operations for four different classes of featureless states. Sign of the wave function $|\psi\rangle$ changes by the amount shown in the second and third rows under the C_6 and σ operations, respectively, for each state characterized by the pair of quantum numbers $(\chi_{C_6}, \chi_{\sigma C_6})$ in the first row.

$$D = \sum_{k=1}^{M} d_k (2S_k + 1). \quad (5)$$

To have trivial IGG, we are required to assign only half-integer spins at the virtual legs (see Appendix B for why). We further have

$$W_\sigma = \bigoplus_{k=1}^{M} \left(\widetilde{W}^k_\sigma \otimes \mathbb{I}_{2S_k+1} \right), \quad (6)$$

where $\widetilde{W}^k_\sigma$ is a d_k-dimensional real matrix satisfying $(\widetilde{W}^k_\sigma)^2 = \mathbb{I}_{d_k}$. Notice that all W_g's in Eq. (4) are translationally invariant (independent of s).

B. Probing lattice quantum numbers

In this section, we discuss how to probe the lattice quantum numbers for a given symmetry PEPS. The lattice quantum number is an eigenvalue of lattice symmetry operator, i.e.

$$R|\psi\rangle = |\tilde{\psi}\rangle = r|\psi\rangle, \quad (7)$$

where r is the lattice quantum number of lattice symmetry operator R.

Global on-site unitary symmetry operation on a finite size PEPS is defined as [8]

$$\begin{aligned}
R|\psi\rangle = \textstyle\sum_{\{k_s\}} \mathrm{tTr}\left[(T^s_1)^{k_1} \cdots (T^s_{N_s})^{k_N}\, T^b_1 \cdots T^b_{N_b} \right]\\
\times U_R \otimes U_R \cdots U_R |k_1 \cdots k_N\rangle, \quad (8)
\end{aligned}$$

where U_R is the representation of R on Hilbert space of physical leg, and N_s (N_b) is the number of site (bond). Local actions of U_R gives a new site and bond tensors

$$\begin{aligned}
(\widetilde{T}^s)^i = (R \circ T^s)^i = \sum_j (U_R)_{ij} (T^s)^j,\\
\widetilde{T}^b = R \circ T^b = T^b, \quad (9)
\end{aligned}$$

and $\widetilde{T}$ gives a new PEPS $|\widetilde{\psi}\rangle$. We also know that for a symmetric PEPS, a site tensor should satisfy Eq. (3) and therefore

$$\widetilde{T}^s = R \circ T^s = \Theta_R^* W_R^{-1}\, T^s,$$
$$\widetilde{T}^b = R \circ T^b = W_R^{-1}\, T^b. \quad (10)$$

If all $\widetilde{T}^s$ and $\widetilde{T}^b$ are contracted to have $|\widetilde{\psi}\rangle$, all W_R^{-1}'s are canceled (since two W_R^{-1} respectively acting on site tensor and connected bond tensor are inverse each other) and only Θ_R^*'s can contributes, i.e.

$$\begin{aligned}|\widetilde{\psi}\rangle &= \sum_{\{k_s\}} \mathrm{tTr}\left[\left(\widetilde{T}^s_1\right)^{k_1}\cdots\left(\widetilde{T}^s_{N_s}\right)^{k_N}\widetilde{T}^b_1\cdots\widetilde{T}^b_{N_b}\right]|k_1\cdots k_{N_s}\rangle \\ &= \prod_{i=1}^{N_s}\Theta_R^*(i)\sum_{\{k_s\}}\mathrm{tTr}\left[\left(T^s_1\right)^{k_1}\cdots\left(T^s_{N_s}\right)^{k_N}T^b_1\cdots T^b_{N_b}\right] \\ &\quad\times|k_1\cdots k_{N_s}\rangle \\ &= \prod_{i=1}^{N_s}\Theta_R^*(i)|\psi\rangle = r|\psi\rangle. \quad (11)\end{aligned}$$

Therefore, in our construction, the lattice quantum number is as follows

$$r = \prod_{i=1}^{N_s}\Theta_R^*(i). \quad (12)$$

According to Eq. (4), possible values of Θ_R are only $+1$ and -1, and therefore PEPS constructed on the torus geometry with *even* number of unit cells would have the trivial lattice quantum number ($r = 1$) regardless of R. However, when PEPS are constructed on torus geometry with an odd number of unit cells, each PEPS belonging to four different classes can be distinguished by the lattice quantum number. Resulting lattice quantum numbers for $R = C_6$, R_π, σ are shown in Table I.

The remaining task is the explicit construction of site and bond tensors and the examination of physical properties for the state obtained from contracting the site/bond tensors. It should be cautioned that, even when the PEPS wave function is seemingly invariant under all symmetry operations, there is a chance that it actually describes a spontaneous symmetry breaking phase. To rule out these possibilities and to ensure that the constructed PEPS state is indeed a symmetric one, one should carefully measure the correlation functions for varying system sizes.

C. Explicit construction of featureless states

In order to find a featureless state, we will focus on a particular case where every virtual leg accommodates n copies of spin-1/2's, and the symmetry class where $\chi_{C_6} = \chi_{\sigma C_6} = -1$. While this is not the unique way to derive the wave function for the featureless state, the imminent goal of this paper is to show how to produce *an example* of the featureless state for honeycomb spin-1/2's, which is achievable with this particular choice of the symmetry class. One can choose the bond tensor to be the maximally entangled state $T^b = \mathbb{I}_n \otimes \mathrm{i}\sigma_2$, where $\mathbb{I}_n$ acts on the flavor space and $\mathrm{i}\sigma_2$ denotes the spin singlet formed by two virtual spin-1/2's. For the site tensor, the most general form of a spin singlet (satisfying spin-rotation symmetry) and Kramers singlet (satisfying time-reversal symmetry) tensor is given by

$$\begin{aligned}\hat{T}^s = \sum_{\alpha,\beta,\gamma}\Big(&\mathcal{C}^1_{\alpha\beta\gamma}\left(|\uparrow;\downarrow_\alpha\uparrow_\beta\downarrow_\gamma\rangle + |\downarrow;\uparrow_\alpha\downarrow_\beta\uparrow_\gamma\rangle\right) \\ &+\mathcal{C}^2_{\alpha\beta\gamma}\left(|\uparrow;\downarrow_\alpha\downarrow_\beta\uparrow_\gamma\rangle + |\downarrow;\uparrow_\alpha\uparrow_\beta\downarrow_\gamma\rangle\right) \\ &+\mathcal{C}^3_{\alpha\beta\gamma}\left(|\uparrow;\uparrow_\alpha\downarrow_\beta\downarrow_\gamma\rangle + |\downarrow;\downarrow_\alpha\uparrow_\beta\uparrow_\gamma\rangle\right)\Big). \quad (13)\end{aligned}$$

Each element of $\mathcal{C}^i$ is real to preserve the time reversal symmetry, and $\mathcal{C}^1 + \mathcal{C}^2 + \mathcal{C}^3 = 0$ due to the SU(2) spin rotation symmetry. The first spin inside the ket separated by the semicolon denotes the physical spin, the other three are virtual spins from each of the three legs for a given site, and α, β, γ label the flavor of virtual spins, with $1 \le \alpha, \beta, \gamma \le n$. For $D = 2$ (a single virtual spin-1/2 per leg), there is no PEPS solution satisfying all of lattice symmetries, hence we turn to the simplest non-trivial case with $D = 4$ (two flavors of virtual spin-1/2's, $n = 2$). Setting $\widetilde{W}_\sigma = \sigma_3$ in Eq. (6), we find that, in order to meet the condition of invariance under the C_6 and σ symmetries, only the following two independent solutions for the site tensor are possible:

$$\begin{aligned}\hat{A}^{(1)} = \mathcal{P}\Big(&2|\uparrow;\downarrow_2\uparrow_1\downarrow_2\rangle - |\uparrow;\downarrow_1\uparrow_2\downarrow_2\rangle - |\uparrow;\downarrow_1\downarrow_2\uparrow_2\rangle \\ &+2|\downarrow;\uparrow_2\downarrow_1\uparrow_2\rangle - |\downarrow;\uparrow_1\downarrow_2\uparrow_2\rangle - |\downarrow;\uparrow_1\uparrow_2\downarrow_2\rangle\Big), \\ \hat{A}^{(2)} = \mathcal{P}\Big(&|\uparrow;\downarrow_2\uparrow_1\downarrow_1\rangle - |\uparrow;\downarrow_1\uparrow_1\downarrow_2\rangle \\ &+|\downarrow;\uparrow_2\downarrow_1\uparrow_1\rangle - |\downarrow;\uparrow_1\downarrow_1\uparrow_2\rangle\Big). \quad (14)\end{aligned}$$

$\mathcal{P}$ stands for cyclic permutation of the virtual states. The general site tensor consistent with all symmetry requirements can be written as a linear combination

$$\hat{T}^s = c_1\hat{A}^{(1)} + c_2\hat{A}^{(2)}, \quad (15)$$

with arbitrary real coefficients c_1, c_2. We claim that the topologically trivial symmetric PEPS state is obtained from contracting all virtual legs of the site tensors $T^s = c_1\hat{A}^{(1)} + c_2\hat{A}^{(2)}$ and bond tensors T^b, for appropriate choices of (c_1, c_2).

There are two special cases, $c_1 = 0$ or $c_2 = 0$, for which the PEPS wave functions have the emergent U(1) IGG. For $\hat{T}^s = \hat{A}^{(1)}$ in Eq. (14), each ket state has two out of the three virtual spins with flavor index equal to 2, and one virtual spin with the flavor index 1. The state made from contracting $\hat{A}^{(1)}$ obviously preserves the flavor quantum number. A U(1) operation $U(\theta)$, defined by multiplying the (flavor index)=1 virtual spin by $e^{i\theta}$ but not the (flavor index)=2 spin, changes the site tensor by the phase $e^{i\theta}$. These gauge transformations form a U(1)

group and result in low-energy fluctuations of U(1) gauge fields, which is known to be confining at long wavelengths in two dimensions.[23] Especially, one may expect a sort of the nearest neighbor RVB with $\hat{A}^{(1)}$. The same argument shows that the state made out of $\hat{A}^{(2)}$ will likely describe the U(1) long range RVB state. However, we have found that those U(1) states are strongly dependent on the boundary condition of the tensor network state (TNS) on the finite system. For example, with a boundary condition that the virtual legs on the boundary are projected into the state $|\uparrow_1\rangle$ and $|\downarrow_1\rangle$ alternatively, the TNS made of $\hat{A}_2$ is the columnar valence bond solid state which breaks the C_6 rotation symmetry. Similarly, alternative projection of $|\uparrow_2\rangle$ and $|\downarrow_2\rangle$ into the boundary with the site tensor $T^s = \hat{A}_1$ gives a state with spontaneously broken C_6 rotation symmetry. The dependence on the boundary condition can be understood as the insertion of different number of U(1) charge, and it will be discussed later. Such U(1) invariance can be broken by choosing a suitable boundary condition such as $\alpha|\uparrow_1\rangle + \beta|\uparrow_2\rangle$ with non-zero α and β. However, since our main goal is to find a featureless state in the thermodynamic limit (independent on the boundary condition), we focus on a general site tensor made by a mixture of two basis tensors which does not have U(1) IGG itself.

In fact, we can show that the mixing of $\hat{A}_1$ and $\hat{A}_2$ states results in the long-range RVB with a particular sign definition for each singlet configuration determined by the site and bond tensors. As will be shown, our ansatz at a particular (c_1, c_2) value restores all the symmetries as the linear system size increases. Therefore, the featureless state we are proposing is a particular kind of RVB liquid state but devoid of the U(1) gauge symmetry, which sharply distinguishes our state from the well-known U(1) algebraic spin liquid states on the bipartite lattice[24,25].

III. NUMERICAL INVESTIGATION OF THE FEATURELESS WAVE FUNCTION

For convenience in numerical calculation, a unit cell was redefined so that u- and v-site tensors are directly connected within a unit cell such that $\mathbf{x}_{i,u} - \mathbf{x}_{i,v} = (\mathbf{a}_2 - 2\mathbf{a}_1)/3$ as shown in Fig. 2, where $\mathbf{x}_{i,u(v)}$ is the position vector of $u(v)$-tensor at the i-th unit cell. Expectation values of local operators $\langle\psi|O_i|\psi\rangle$ and correlators $\langle\psi|O_iO_j|\psi\rangle$ are obtained by employing the MPS-MPO compression method[26–28] to approximately contract a given tensor network wave function. Two-site variational compression is adopted[27] where the initial ansatz is given by the zip-up algorithm[29].

We proceed with the search for the featureless states with Eq. (15) for the site tensor. Choosing $c_2 = 1 - c_1$, a one-dimensional parameter space of $0 \le c_1 \le 1$ is generated and we systematically look for featureless states in this one-dimensional space. Firstly, we work out the measure of the rotation symmetry breaking

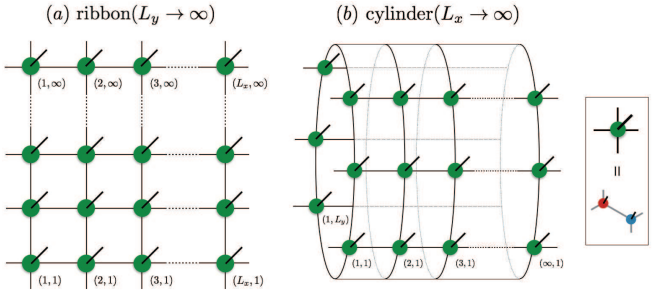

FIG. 2. (Color online) Lattice geometry used to evaluate (a) correlators and (b) entanglement entropy. A green dot denotes one unit cell, formed by u (red) and v (blue) sites of the honeycomb lattice.

$$|\langle \mathbf{S}_{i,u} \cdot \mathbf{S}_{i,v} - \mathbf{S}_{i,v} \cdot \mathbf{S}_{i+1,u} \rangle| \tag{16}$$

(difference in bond strength of two nearby bonds) as a function of $1/\log(L_x)$ for several c_2 values as shown in Fig. 3, where L_x is the number of unit cells in the $\mathbf{a}_1$-direction. The number of unit cells in the $\mathbf{a}_2$-direction, L_y, is chosen as $L_y = L_x$ in this analysis, and $c_1 + c_2 = 1$. Positions where the bond strengths $\langle \mathbf{S}_{i,u} \cdot \mathbf{S}_{i,v} \rangle$ and $\langle \mathbf{S}_{i,v} \cdot \mathbf{S}_{i+1,u} \rangle$ have been measured are close to the center of the samples. To complete the calculation one must fix the boundary conditions. For the calculations shown in Fig. 3, boundary legs are projected into the state $|\uparrow_1\rangle + |\downarrow_1\rangle$ except at $c_2 = 0$, where such boundary condition makes the whole tensor network wave function vanish. Instead we choose the boundary state $|\uparrow_2\rangle + |\downarrow_2\rangle$ to carry out the necessary calculation at $c_2 = 0$. Note that both boundary conditions we used conserve the U(1) gauge symmetry as discussed in the previous section.

As the results in Fig. 3 clearly shows, wave functions at $c_2 = 0$ and $c_2 = 1$ exhibit a finite amount of rotational symmetry breaking irrespective of the system size L_x. We take it as an indication of the symmetry-broken state at the two ends of the parameter space. For other c_2 values the degree of symmetry breaking as measured by Eq. (16) diminishes with increasing system size. The reduction is most significant for $c_2 \sim 0.1$ through $c_2 \sim 0.3$ and we take it as an indication that symmetry is restored for this range of c_2 in the thermodynamic limit. Following this reasoning we can conclude there should be at least two critical points separating the symmetric phase from the two symmetry-broken phases at $c_2 = 0$ and $c_2 = 1$, and that such phases have most likely been realized in the region $c_2 \sim 0.1$ through $c_2 \sim 0.3$. Unfortunately, pinning down the exact phase boundaries turned out to be a numerically formidable task, and goes well over the purpose of the paper which is to find an exemplary spin-1/2 featureless quantum state on the honeycomb lattice. Therefore we choose $c_2 = 0.1$ state as a candidate for the featureless state and carry out further analysis to confirm the featureless nature of the state.

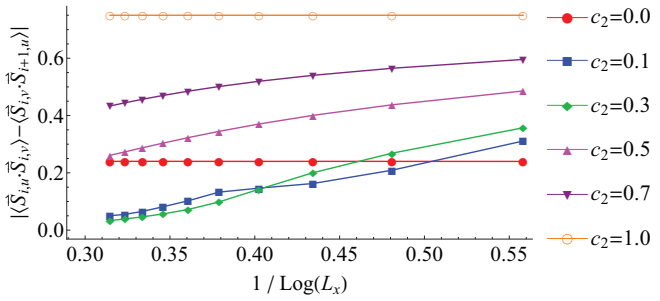

FIG. 3. (Color online) Degree of rotational symmetry breaking (quantity on the vertical axis) as a function of $1/\log(L_x)$ for several c_2 values ($c_1 + c_2 = 1$). $L_x = L_y$ is the linear size of the lattice. Rotational symmetry is broken at $c_2 = 0$ and $c_2 = 1$ as the order parameter remains almost independent of the system size L_x. Reduction of the symmetry-breaking order with the system size is indicative of the restored symmetry of the PEPS wave functions over $c_2 \sim 0.1$ through $c_2 \sim 0.3$.

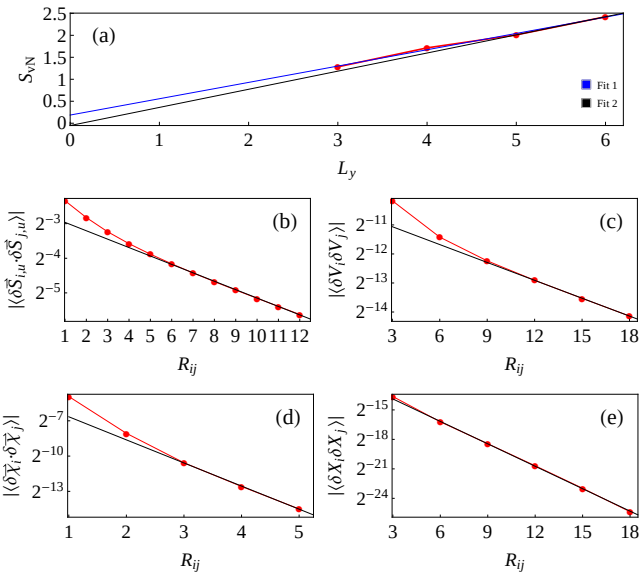

FIG. 4. (Color online) Various numerical results on the spin-1/2 PEPS made with the site tensor $\hat{T}^s = 0.9\hat{A}^{(1)} + 0.1\hat{A}^{(2)}$. (a) Entanglement entropy as a function of L_y. Two linear fits are shown, based on the numerical data at $L_y \in \{3, 4, 5, 6\}$ and $L_y \in \{5, 6\}$, respectively. (b)-(e) Plots of correlation functions ($\delta A = A - \langle A\rangle$) for (b) spin, (c) bond ($V_i = \mathbf{S}_{iu}\cdot\mathbf{S}_{iv}$), (d) vector chirality ($\boldsymbol{\chi}_i = \mathbf{S}_{iu} \times \mathbf{S}_{iv}$) and (e) scalar chirality ($X_i = \mathbf{S}_{i-1,v} \cdot \mathbf{S}_{iu} \times \mathbf{S}_{iv}$) as a function of the distance $R_{ij} = |\mathbf{x}_i - \mathbf{x}_j|/|\mathbf{a}_1|$; $\mathbf{x}_i$ is the position vector of the i-th unit cell. System size is fixed at $L_x = 37$.

For $(c_1, c_2) = (0.9, 0.1)$, topological entanglement entropy has been extracted by fitting the calculated entanglement entropy for varying system sizes. As shown in Fig. 4(a) we find the extrapolated value -0.05 consistent with the absence of topological order. To evaluate the entanglement entropy, we imposed the periodic boundary condition along the $\vec{a}_2$-direction of our ansatz wave function and employed the boundary theory of PEPS [30,31].

Correlation functions were measured for spin, bond, vector spin chirality, and scalar spin chirality, in order to determine the gapped nature of the state. To minimize the numerical instability caused by lower and upper boundaries of the tensor network wave function, compression is repeated until the convergence of MPS $|\Psi_n\rangle \simeq \mathcal{O}|\Psi_{n-1}\rangle$ is achieved, where $|\Psi_n\rangle$ is the nth stage MPS and $\mathcal{O}$ is the MPO.

As one can see in Fig. 4, all correlators decay exponentially in the fixed system size $L_x = 37$, and varying the distance between two operators O_i and O_j. We double-checked in Fig. 5 the exponential decays of all correlators by varying L_x and fixing the position of operators O_i and O_j to be at $L_x/3$ and $2L_x/3$, respectively. System size L_x is appropriately set to take trimerization into account those take place in bond and scalar chirality correlations. Further analysis on correlation length as a function of reduced bond dimension d has been examined to reveal the saturations of all correlation lengths eventually in large bond dimention as shown in Fig. 6. Lattice and spin rotation symmetries are numerically confirmed as well. Based on such overwhelming body of evidences, we conclude that our ansatz PEPS is a topologically trivial, fully symmetric and gapped quantum state.

We also measured the entanglement entropy for the U(1) states ($c_1 = 0$ or $c_2 = 0$). In both cases, it depends on the number of flavor 1 states and flavor 2 states we put on the boundary virtual legs. Physically, we can interpret flavor states as U(1) gauge charges. For boundary conditions with different total flavor numbers, we end up with wave functions supporting different number of electric field lines along the length of cylinder. These states are orthogonal to each other, and in general give different entanglement entropies.

IV. CONCLUSION

We have identified an exemplary state of a featureless quantum insulator on the honeycomb lattice of spin-1/2's, based on the methodical search scheme developed in Ref. 8. Four distinct classes have been identified as a result of our search. We propose a state whose physical properties are consistent with the featureless quantum state. Compared to previous works on constructing the featureless wave functions[5–7], the present method offers a much more systematic way to classify tensor network states consistent with symmetry and topological constraints. The liquid phase we constructed is intrinsically strongly interacting, as there is no way to adiabatically connect them to free electronic states. Exponentially decaying correlations are indicative of the gapped nature of the featureless state, provided an appropriate parent Hamiltonian is designed to have our state as the ground state first. These results may thus be relevant for correlated electronic materials on the honeycomb lattice. For

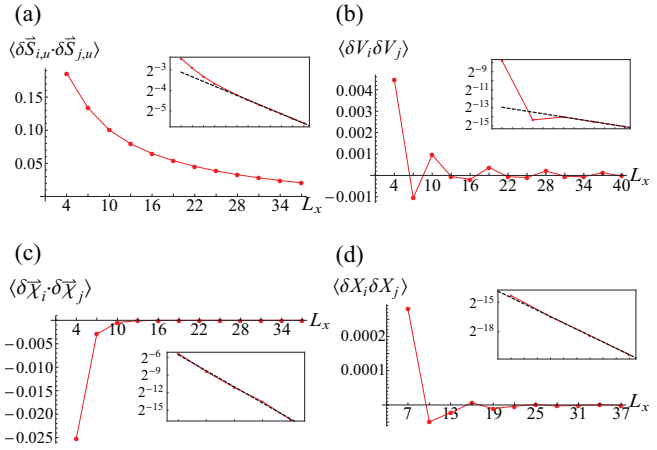

FIG. 5. (Color online) (a) Spin, (b) bond, (c) vector chirality, and (d) scalar chirality correlations as a function of the system size L_x, at the separation distance equal to $L_x/3$. Inset in each figure is a plot with logarithmic y-scale and its linear fit. Exponential decays are observed in all the correlators.

instance, evidences for a putative spin liquid ground state have been reported for $Ba_3CuSb_2O_9$ [32,33], in which the spin-1/2 Cu may form a honeycomb lattice [34].

ACKNOWLEDGMENTS

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Appendix A: Classification of projected entangled pair states on the honeycomb lattice with trivial invariant gauge group

In this section, we classify symmetric projected entangled pair states (PEPS) on the honeycomb lattice with a half-integer spin per site.

1. General symmetry considerations on PEPS

In this subsection, we lay out general symmetry transformation rules for PEPS on an infinite honeycomb lattice with a half-integer spin per site. For PEPS which are consistent with all the global symmetries discussed in the previous subsection, site tensors and bond tensors should satisfy the relations[8]

$$\begin{aligned} T^{(x,y,s)} &= \Theta_S(x,y,s)\Big(\prod_i W_S(x,y,s,i)\Big)\, S\circ T^{(x,y,s)} \\ B^{(x,y,s,i|x',y',s',i)} &= W_S^{-1}(x,y,s,i)[W_S^{-1}(x',y',s',i)]^t\, S\circ B^{(x,y,s,i|x',y',s',i)}. \end{aligned} \tag{A1}$$

Each site tensor $T^{(x,y,s)}$ resides at the unit cell (x,y) and sublattice site s, while the bond tensor $B^{(x,y,s,i|x',y',s',i')}$ is defined across the bond $(x,y,s,i|x',y',s',i')$ between adjacent sites. As is apparent from Fig. 1, a given pair of adjacent sites $(x,y,s|x',y',s')$ uniquely specifies the virtual bond indices associated with that bond. Our choice of the bond index guarantees $i=i'$ for any given bond. We denote each symmetry operation $S=T_1,T_2,C_6,\sigma,\mathcal{T},R_{\theta\vec{n}}$ on the tensors symbolically as $S\circ T^{(x,y,s)}$ and $S\circ B^{(x,y,s,i|x',y',s',i)}$, respectively. $W_S(x,y,s,i)$ is a matrix that implements the gauge transformation on the leg (x,y,s,i). Finally, $\Theta_S(x,y,s)$ is a site-dependent U(1) phase factor associated with each symmetry operation. Symmetry of the PEPS state is thus made explicit by the requirement that the site tensor $T^{(x,y,s)}$ remain invariant after applying the assumed symmetry operation on it ($S\circ T^{(x,y,s)}$), once proper re-adjustments through similarity ($W_S(x,y,s,i)$) and phase ($\Theta_S(x,y,s)$) transformations are further carried out. One can equally well view Eq. (A1) as the "definition" of the symmetric PEPS. The symmetry operation S acts projectively on the local tensors. The global wave function obtained by piecing together the site and bond tensors that transform according to Eq. (A1) will naturally meet the symmetry requirements.

At first sight it is unclear whether a given tensor $T^{(x,y,s)}$ obeys a particular symmetry constraint or not, due to the enormous gauge freedom implied by $W_S(x,y,s,i)$'s and $\Theta_S(x,y,s)$'s in the projective definition of the symmetry operation. A large body of the calculations carried out in this note is tantamount to the "gauge fixing" of the non-Abelian gauge fields $W_S(x,y,s,i)$ and the Abelian gauge fields $\Theta_S(x,y,s)$ without violating the symmetry of the physical fields $T^{(x,y,s)}$. Before we present the details of the gauge-fixing procedure there is one more requisite concept in the tensor network theory that deserves some mention. This is the concept of invariant gauge group, or IGG.

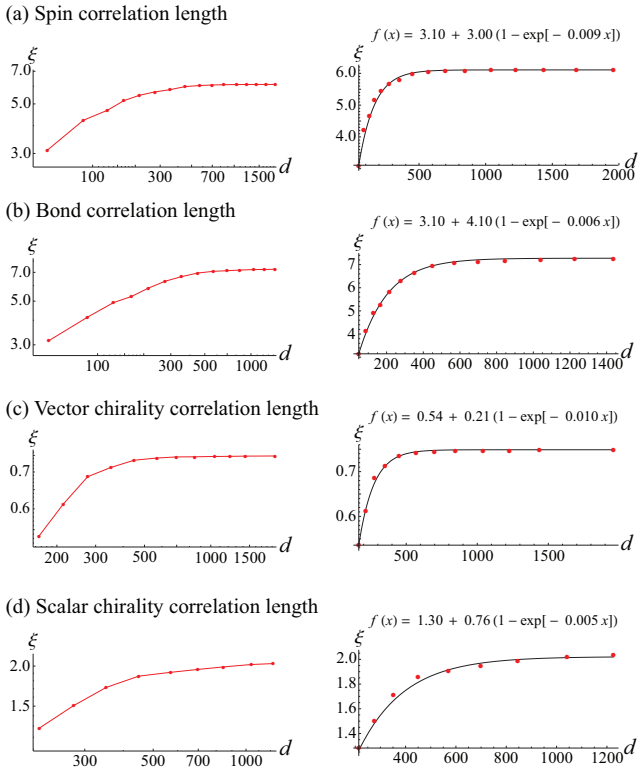

FIG. 6. (Color online) (a) Spin, (b) bond, (c) vector chirality, and (d) scalar chirality correlation length ξ as a function of bond dimension d, with log-log scale on the left panel and with fitting function $f(x)$ on the right panel. Each correlation length tends to saturate in large bond dimension.

The notion of IGG plays a central role in the classification scheme of PEPS introduced in Ref. 8, as it did in Wen's PSG classification of parton models [1,35]. In essence, one can identify a particular kind of gauge transformation matrices $W(x,y,s,i)$ such that both site and bond tensors are invariant under it - up to a phase factor. Such similarity transformation matrix and the phase factor will be denoted $\eta(x,y,s,i)$ and $\mu(x,y,s)$, respectively, then the statement of IGG becomes

$$T^{(x,y,s)} = \mu(x,y,s)\Big(\prod_i \eta(x,y,s,i)\Big)\, T^{(x,y,s,i)},$$
$$B^{(x,y,s,i|x',y',s',i)} = [\eta^{-1}(x,y,s,i)]^t [\eta^{-1}(x',y',s',i)]^t\, B^{(x,y,s,i|x',y',s',i)}. \quad \text{(A2)}$$

The IGG is said to be trivial iff we can set $\eta(x,y,s,i) = \mathbb{I}$ (μ can still be a nontrivial phase factor). Nontrivial IGG's lead to PEPS with gauge dynamics [8]. In this work, however, we are solely interested in the case of trivial IGG, e.g. IGG $= \mathbb{I}$, as the non-trivial IGG is likely to lead to topologically ordered ground states.

As will become clear, search for symmetric PEPS is tantamount to a systematic reduction of W_S's and Θ_S's for all symmetries S to a few simple forms through the gauge-fixing procedure. Once all the gauge fields are fixed, Eq. (A1) will act as constraint equations that can be solved to narrow down the possible forms of site and bond tensors. Once those gauge variables have been found, however, there is an additional U(1) phase redundancy

$$W_S(x,y,s,i) \to \varepsilon_S(x,y,s,i) W_S(x,y,s,i),$$
$$\Theta_S(x,y,s) \to \Big(\prod_i \varepsilon_S^*(x,y,s,i)\Big)\Theta_S(x,y,s), \quad \text{(A3)}$$

that also leaves Eq. (A1) invariant. It means there is an intrinsic redundancy, dubbed the ε-ambiguity in Ref. [8], associated with a given (W_S, Θ_S). The set of $\varepsilon_S(x,y,s,i)$'s also forms a group, called the χ-group [8]. The ε_S-ambiguity, along with several other ambiguities to be discussed below, will be used to our advantage to "fix" the symmetry matrix W_S associated with a particular symmetry operation S.

There is a more subtle kind of ambiguity in the definition of tensors and gauge matrices (W's) dubbed the "gauge equivalence" in Ref. 8. Let's take some $T^{(x,y,s)}$ and $W_S(x,y,s,i)$'s that already obey the symmetry conditions (A1). Although it might seem at first that one has arrived at a unique solution for the site tensor with all the proper symmetry requirements, in reality it is not the case. To show this is the case, introduce some arbitrary similarity matrix $V(x,y,s,i)$ to construct a new site tensor,

$$\begin{aligned}\overline{T}^{(x,y,s)} &= \Big(\prod_i V(x,y,s,i)\Big) T^{(x,y,s)} \\ &= \Theta_S(x,y,s)\Big(\prod_i V(x,y,s,i) W_S(x,y,s,i)\Big)\, S\circ T^{(x,y,s)},\end{aligned} \tag{A4}$$

where the second line follows from $T^{(x,y,s)}$ being the symmetric tensor. Now let's further define a new gauge matrix $\overline{W}_S(x,y,s,i)$ related to $W_S(x,y,s,i)$ through

$$\begin{aligned}\overline{\overline{W}}_S(x,y,s,i) &= V(x,y,s,i) W_S(x,y,s,i)\, S\, V^{-1}(x,y,s,i)\, S^{-1} \\ &= V(x,y,s,i) W_S(x,y,s,i) V^{-1}(S^{-1}(x,y,s,i)).\end{aligned} \tag{A5}$$

Using $\overline{W}_S(x,y,s,i)$ one can re-write (A4) as

$$\overline{T}^{(x,y,s)} = \Theta_S(x,y,s)\Big(\prod_i \overline{W}_S(x,y,s,i)\Big)\, S\circ \overline{T}^{(x,y,s)}, \tag{A6}$$

which is exactly the symmetry operator defined in Eq. (A1). In other words, any given solution $\{T^{(x,y,s)}, W_S(x,y,s,i)\}$ of the symmetry equation leads to a whole family of solutions $\{\overline{T}^{(x,y,s)}, \overline{W}_S(x,y,s,i)\}$ through the similarity matrix $V_S(x,y,s,i)$. Of course there is really only one, or a few physical solutions for the symmetric tensor and the rest are simply gauge-equivalent copies. This is the notion of gauge equivalence. Rather than being annoyed by it, one can utilize the extra freedom to choose the basis in which the gauge matrices W_S take on the simplest possible form, for instance a basis in which W_S appears as coordinate-independent. Similarly, there is gauge equivalence under the U(1) transformation of $\Theta_S(x,y,s)$,

$$\Theta_S(x,y,s) \to \overline{\Theta}_S(x,y,s) = \Phi(x,y,s)\Theta_S(x,y,s)\Phi^*(S^{-1}(x,y,s)), \tag{A7}$$

for arbitrary $\Phi(x,y,s)\in \mathrm{U}(1)$. These two transformations were respectively called V-ambiguity and Φ-ambiguity in Ref.[8].

In the next few sections we explain how each of the symmetry equations in Eq. (2) together with the various ambiguities mentioned in this subsection actually play out to fix the gauge fields W_S and Θ_S.

2. Translational symmetry consideration

First, let us consider the statement $T_2^{-1}T_1^{-1}T_2T_1 = \mathrm{e}$ regarding the translation symmetry, and ask what it implies for the site tensor $T^{(x,y,s)}$. Each symmetry operation acts projectively on the site tensor according to Eq. (A1). Applying them in sequence, we get

$$\begin{aligned}&(T_2^{-1}W_{T_2}^{-1}\Theta_{T_2}^*)(T_1^{-1}W_{T_1}^{-1}\Theta_{T_1}^*)(\Theta_{T_2}W_{T_2}T_2)(\Theta_{T_1}W_{T_1}T_1)\circ T^{(x,y,s)} = T^{(x,y,s)} \\ &\quad = \mu_{12}\,\eta_{12}\,T^{(x,y,s)} = (\mu_{12}\chi_{12}^*)(\chi_{12}\eta_{12})\,T^{(x,y,s)}.\end{aligned} \tag{A8}$$

Several simplifying notations introduced here are

$$\begin{aligned}\Theta_{T_k}W_{T_k} &\equiv \Theta_{T_k}(x,y,s)\Big(\prod_i W_{T_k}(x,y,s,i)\Big),\ (k=1,2), \\ (\mu_{12}\chi_{12}^*)(\chi_{12}\eta_{12}) &\equiv \left[\mu_{12}(x,y,s)\left(\prod_i \chi_{12}^*(x,y,s,i)\right)\right]\left[\left(\prod_i \chi_{12}(x,y,s,i)\right)\eta_{12}(x,y,s,i)\right].\end{aligned}$$

Note that $T^{(x,y,s)} = \mu_{12}\,\eta_{12}\,T^{(x,y,s)}$ in the second line of Eq. (A8) is a re-statement of IGG, which we take to be trivial and hence η_{12} and μ_{12} are set to be $\mathbb{I}$ and 1, respectively, and thus the symmetry equation for the site tensor becomes

$$(T_2^{-1}W_{T_2}^{-1}\Theta_{T_2}^*)(T_1^{-1}W_{T_1}^{-1}\Theta_{T_1}^*)(\Theta_{T_2}W_{T_2}T_2)(\Theta_{T_1}W_{T_1}T_1)\circ T^{(x,y,s)} = T^{(x,y,s)}. \tag{A9}$$

Extra U(1) phase factors $\chi_{12}(x,y,s,i)$ are introduced as well.

Various translation operations appearing in the above equation can be implemented directly once we realize that, for instance,

$$T_2^{-1}W_{T_2}^{-1}(x,y,s,i) = T_2^{-1}W_{T_2}^{-1}(x,y,s,i)T_2T_2^{-1} = W_{T_2}^{-1}(x,y+1,s,i)T_2^{-1}, \tag{A10}$$

in the first bracket, and

$$T_2^{-1}(T_1^{-1}W_{T_1}^{-1}(x,y,s,i)) = (T_1T_2)^{-1}W_{T_1}(x,y,s,i)T_1T_2(T_1T_2)^{-1} = W_{T_1}(x+1,y+1,s,i)(T_1T_2)^{-1}, \tag{A11}$$

in the second bracket and so on. Carrying out all the translation operations in Eq. (A8) gives

$$\begin{aligned}&\Theta_{T_2}^*(x,y+1,s)\Theta_{T_1}^*(x+1,y+1,s)\Theta_{T_2}(x+1,y+1,s)\Theta_{T_1}(x+1,y,s)\times\\&\left(\prod_i W_{T_2}^{-1}(x,y+1,s,i)W_{T_1}^{-1}(x+1,y+1,s,i)W_{T_2}(x+1,y+1,s,i)W_{T_1}(x+1,y,s,i)\right)T^{(x,y,s)}\\&\qquad = T^{(x,y,s)}.\end{aligned} \tag{A12}$$

The condition for this equation to hold is[8]

$$\begin{aligned}&W_{T_2}^{-1}(x,y{+}1,s,i)W_{T_1}^{-1}(x{+}1,y{+}1,s,i)W_{T_2}(x{+}1,y{+}1,s,i)W_{T_1}(x{+}1,y,s,i){=}\chi_{12}(x,y,s,i),\\&\Theta_{T_2}^*(x,y{+}1,s)\Theta_{T_1}^*(x{+}1,y{+}1,s)\Theta_{T_2}(x{+}1,y{+}1,s)\Theta_{T_1}(x{+}1,y,s){=}\left(\prod_i\chi_{12}^*(x,y,s,i)\right).\end{aligned} \tag{A13}$$

In other words, realizing the translational symmetry of the site tensor projectively amounts to finding a set of $W_{T_{1,2}}$ matrices and $\Theta_{T_{1,2}}$ phases that satisfy the two equations above.

Thus far, $\chi_{12}(x,y,s,i)$ appear to be arbitrary phase factors. Recall, however, that there is an ε_{T_i}-ambiguity in the definition of W_{T_i}'s and Θ_{T_i}'s,

$$\begin{aligned}W_{T_i}(x,y,s,i) &\to \varepsilon_{T_i}(x,y,s,i)W_{T_i}(x,y,s,i),\\ \Theta_{T_i}(x,y,s) &\to \Theta_{T_i}(x,y,s)\left(\prod_i \varepsilon_{T_i}^*(x,y,s,i)\right),\end{aligned}$$

which can be interpreted as transformation rules for χ_{12}:

$$\chi_{12}(x,y,s,i) \to \varepsilon_{T_2}^*(x,y{+}1,s,i)\varepsilon_{T_1}^*(x{+}1,y{+}1,s,i)\varepsilon_{T_2}(x{+}1,y{+}1,s,i)\varepsilon_{T_1}(x{+}1,y,s,i)\chi_{12}(x,y,s,i).$$

Utilizing this freedom in choosing $\varepsilon_{T_{1(2)}}(x,y,s,i)$ one can fix $\chi_{12}(x,y,s,i) = 1$! In other words, the W's and Θ's associated with the translational invariance obey the relations

$$\begin{aligned}&W_{T_2}^{-1}(x,y{+}1,s,i)W_{T_1}^{-1}(x{+}1,y{+}1,s,i)W_{T_2}(x{+}1,y{+}1,s,i)W_{T_1}(x{+}1,y,s,i){=}1,\\&\Theta_{T_2}^*(x,y{+}1,s)\Theta_{T_1}^*(x{+}1,y{+}1,s)\Theta_{T_2}(x{+}1,y{+}1,s)\Theta_{T_1}(x{+}1,y,s){=}1.\end{aligned} \tag{A14}$$

In the next step we prove that $W_{T_2}(x,y,s,i)$ and $\Theta_{T_2}(x,y,s,i)$ can be "fixed" to the identity $\mathbb{I}$ and 1, by judiciously invoking V- and Φ-ambiguities, respectively. Due to the ambiguities we can first transform W_{T_2}'s and Θ_{T_2}'s as

$$W_{T_2}(x,y,s,i) \to \overline{W}_{T_2}(x,y,s,i) = V(x,y,s,i)W_{T_2}(x,y,s,i)V^{-1}(x,y-1,s,i),$$
$$\Theta_{T_2}(x,y,s) \to \overline{\Theta}_{T_2}(x,y,s) = \Phi(x,y,s)\Theta_{T_2}(x,y,s)\Phi^*(x,y-1,s). \tag{A15}$$

From the first line it is clear that if we imposed the recursive relation

$$V(x,y-1,s,i) = V(x,y,s,i)W_{T_2}(x,y,s,i)$$

for the V-matrices, one could transform all $\overline{W}_{T_2}$'s to be the identity. Likewise one can set $\Theta_{T_2}(x,y,s,i) = 1, \forall (x,y,s,i)$ with the choice $\Phi(x,y-1,s) = \Phi(x,y,s)\Theta_{T_2}(x,y,s)$. In summary, both gauge fields W_{T_2} and Θ_{T_2} associated with the translation symmetry $S = T_2$ can be chosen as identities through the gauge-fixing procedure outlined so far.

It was mentioned earlier that once the gauge field are fixed, Eq. (A1) can be used to constrain the form of the site tensor as well. Indeed, now that $W_{T_2} = \mathbb{I}$ and $\Theta_{T_2} = 1$ irrespective of the coordinates, Eq. (A1) reduces to an extremely simple form

$$T_2 \circ T^{(x,y,s)} = T^{(x,y+1,s)} = T^{(x,y,s)} \tag{A16}$$

implying the y-independence of the site tensor: $T^{(x,y,s)} = T^{(x,0,s)}$. The local site tensors have become y-independent in this particular gauge choice.

Now that W_{T_2} is fixed to $\mathbb{I}$, we want to also restrict the V-matrix to be independent of the y-coordinate, $V(x,y,s,i) = V(x,s,i)$, so that further application of the V-ambiguity

$$W_{T_2} \to V(x,y,s,i)W_{T_2}V^{-1}(x,y-1,s,i) \tag{A17}$$

will not alter the choice $W_{T_2} = \mathbb{I}$. Since ε_{T_2} can vary W_{T_2} up to arbitrary phase, we fix $\varepsilon_{T_2} = 1$ such that $W_{T_2} = \mathbb{I}$ is completely fixed regardless of remaining V- and ε- ambiguigies. A similar reasoning gives remaining $\Phi(x,y,s) = \Phi(x,0,s)$.

Next we turn to the prospect of fixing the gauge fields associated with another translational symmetry $S = T_1$. First insert $W_{T_2}(x,y,s,i) = \mathbb{I}$ and $\Theta_{T_2}(x,y,s) = 1$ into Eq. (A13) to find

$$W_{T_1}(x+1,y+1,s,i) = W_{T_1}(x+1,y,s,i) = W_{T_1}(x+1,s,i),$$
$$\Theta_{T_1}(x+1,y+1,s) = \Theta_{T_1}(x+1,y,s) = \Theta_{T_1}(x+1,s). \tag{A18}$$

It turns out both W_{T_1} and Θ_{T_1} are y-independent. Utilizing the y-independent V-matrix Φ-phase we can implement the transformation

$$W_{T_1}(x,s,i) \to V(x,s,i)W_{T_1}(x,s,i)V^{-1}(x-1,s,i),$$
$$\Theta_{T_1}(x,s) \to \Phi(x,s)\Theta_{T_1}(x,s)\Phi^*(x-1,s). \tag{A19}$$

Clearly one can choose $V(x,s,i)$ and $\Phi(x,s)$ such that $W_{T_1}(x,y,s,i)$ and $\Theta_{T_1}(x,y,s)$ are both coordinate-independent and equal to unity. This is the central conclusion of this subsection, that both gauge fields W_{T_i} and Θ_{T_i} $(i = 1,2)$ associated with the translation symmetries $S = T_1, T_2$ can be fixed to the most trivial form everywhere - a simple identity. Referring to Eq. (A1), it follows readily that the site tensors must also be site-independent:

$$T^{(x,y,s)} = T^{(0,0,s)} = T^{(s)}. \tag{A20}$$

Again, we fix $\varepsilon_{T_1}(x,y,s,i) = 1$ to leave $W_{T_1}(x,y,s,i) = \mathbb{I}$. To leave $W_{T_{1,2}} = \mathbb{I}$ and $\Theta_{1,2} = 1$ invariant, the V-matrix and the Φ-phase must be sublattice-independent,

$$V(x,y,s,i) = V(s,i), \quad \Phi(x,y,s) = \Phi(s). \tag{A21}$$

We will adopt these conditions in all subsequent considerations of V- and Φ-ambiguities.

3. Rotational symmetry consideration

Now let us consider the C_6 rotation symmetry. Following from the two group relations

$$\begin{aligned} C_6^{-1}T_2^{-1}C_6T_1 &= \mathrm{e}, \\ C_6^{-1}T_2^{-1}T_1C_6T_2 &= \mathrm{e}, \end{aligned} \tag{A22}$$

we have

$$\begin{aligned} (C_6^{-1}W_{C_6}^{-1}\Theta_{C_6}^*)(T_2^{-1}W_{T_2}^{-1}\Theta_{T_2}^*)(\Theta_{C_6}W_{C_6}C_6)(\Theta_{T_1}W_{T_1}T_1)\circ T^{(x,y,s)} &= T^{(x,y,s)}, \\ (C_6^{-1}W_{C_6}^{-1}\Theta_{C_6}^*)(T_2^{-1}W_{T_2}^{-1}\Theta_{T_2}^*)(\Theta_{T_1}W_{T_1}T_1)(\Theta_{C_6}W_{C_6}C_6)(\Theta_{T_2}W_{T_2}T_2)\circ T^{(x,y,s)} &= T^{(x,y,s)}. \end{aligned} \tag{A23}$$

Manipulations similar to those carried out for translaional symmetries give

$$\begin{aligned} &\Theta_{C_6}^*(C_6(x,y,s))\Theta_{T_2}^*(T_2C_6(x,y,s))\Theta_{C_6}(T_2C_6(x,y,s))\Theta_{T_1}(C_6^{-1}T_2C_6(x,y,s)) \\ &W_{C_6}^{-1}(C_6(x,y,s,i))W_{T_2}^{-1}(T_2C_6(x,y,s,i))W_{C_6}(T_2C_6(x,y,s,i))W_{T_1}(C_6^{-1}T_2C_6(x,y,s,i))\ T^{(x,y,s)} \\ &\quad = T^{(x,y,s)}, \end{aligned} \tag{A24}$$

and

$$\begin{aligned} &\Theta_{C_6}^*(C_6(x,y,s))\Theta_{T_2}^*(T_2C_6(x,y,s))\Theta_{T_1}(T_2C_6(x,y,s))\Theta_{C_6}(T_1^{-1}T_2C_6(x,y,s)) \\ &\Theta_{T_2}(C_6^{-1}T_1^{-1}T_2C_6(x,y,s))W_{C_6}^{-1}(C_6(x,y,s,i))W_{T_2}^{-1}(T_2C_6(x,y,s,i)) \\ &W_{T_1}(T_2C_6(x,y,s,i))W_{C_6}(T_1^{-1}T_2C_6(x,y,s,i))W_{T_2}(C_6^{-1}T_1^{-1}T_2C_6(x,y,s,i))\ T^{(x,y,s)} \\ &\quad = T^{(x,y,s)}. \end{aligned} \tag{A25}$$

The product of phase factors and the product of W-matrices separately obey the equations

$$\begin{aligned} &W_{C_6}^{-1}(C_6(x,y,s,i))W_{T_2}^{-1}(T_2C_6(x,y,s,i))W_{C_6}(T_2C_6(x,y,s,i))W_{T_1}(C_6^{-1}T_2C_6(x,y,s,i)) \\ &\qquad = \chi_{T_1C_6}(x,y,s,i), \\ &W_{C_6}^{-1}(C_6(x,y,s,i))W_{T_2}^{-1}(T_2C_6(x,y,s,i))W_{T_1}(T_2C_6(x,y,s,i))\times \\ &\quad W_{C_6}(T_1^{-1}T_2C_6(x,y,s,i))W_{T_2}(C_6^{-1}T_1^{-1}T_2C_6(x,y,s,i)) = \chi_{T_2C_6}(x,y,s,i), \end{aligned} \tag{A26}$$

and

$$\begin{aligned} &\Theta_{C_6}^*(C_6(x,y,s))\Theta_{T_2}^*(T_2C_6(x,y,s))\Theta_{C_6}(T_2C_6(x,y,s))\Theta_{T_1}(C_6^{-1}T_2C_6(x,y,s)) \\ &\qquad = \left(\prod_i \chi_{T_1C_6}^*(x,y,s,i)\right), \\ &\Theta_{C_6}^*(C_6(x,y,s))\Theta_{T_2}^*(T_2C_6(x,y,s))\Theta_{T_1}(T_2C_6(x,y,s))\times \\ &\quad \Theta_{C_6}(T_1^{-1}T_2C_6(x,y,s))\Theta_{T_2}(C_6^{-1}T_1^{-1}T_2C_6(x,y,s)) = \left(\prod_i \chi_{T_2C_6}^*(x,y,s,i)\right). \end{aligned} \tag{A27}$$

Up to this point we have deliberately not employed the the facts $W_{T_{1,2}} = \mathbb{I}$, $\Theta_{T_{1,2}} = 1$ proven in the previous subsection. When we use these, Eqs. (A26) and (A27) simplify to

$$\begin{aligned} W_{C_6}^{-1}(C_6(x,y,s,i))W_{C_6}(T_2C_6(x,y,s,i)) &= \chi_{T_1C_6}(x,y,s,i), \\ W_{C_6}^{-1}(C_6(x,y,s,i))W_{C_6}(T_1^{-1}T_2C_6(x,y,s,i)) &= \chi_{T_2C_6}(x,y,s,i), \end{aligned} \tag{A28}$$

and

$$\Theta^*_{C_6}(C_6(x,y,s))\Theta_{C_6}(T_2C_6(x,y,s)) = \left(\prod_i \chi^*_{T_1C_6}(x,y,s,i)\right),$$
$$\Theta^*_{C_6}(C_6(x,y,s))\Theta_{C_6}(T_1^{-1}T_2C_6(x,y,s)) = \left(\prod_i \chi^*_{T_2C_6}(x,y,s,i)\right). \tag{A29}$$

We introduce the ε_{C_6}-ambiguity into Eq. (A28) such that $\chi_{T_1C_6}$ and $\chi_{T_2C_6}$ transform to

$$\chi_{T_1C_6}(x,y,s,i) \to \varepsilon^*_{C_6}(C_6(x,y,s,i))\varepsilon_{C_6}(T_2C_6(x,y,s,i))\chi_{T_1C_6}(x,y,s,i),$$
$$\chi_{T_2C_6}(x,y,s,i) \to \varepsilon^*_{C_6}(C_6(x,y,s,i))\varepsilon_{C_6}(T_1^{-1}T_2C_6(x,y,s,i))\chi_{T_2C_6}(x,y,s,i). \tag{A30}$$

Utilizing such freedom one can set $\chi_{T_1C_6}(x,y,s,i) = 1$ and hence deduce

$$W_{C_6}(x,y,s,i) = W_{C_6}(x,y+1,s,i) = W_{C_6}(x,0,s,i) \tag{A31}$$

from Eq. (A28). The remaining ε_{C_6} ambiguity must satisfy

$$\varepsilon(x,y,s,i)W_{C_6}(x,y,s,i) = \varepsilon(x,0,s,i)W_{C_6}(x,0,s,i),$$

leading to $\varepsilon(x,y,s,i) = \varepsilon(x,y,0,i)$, and therefore one can only set $\chi_{T_2C_6}(x,0,s,i) = 1$. With $\chi_{T_2C_6}(x,0,s,i) = 1$, Eq. (A28) reads

$$W_{C_6}(x,0,s,i) = W_{C_6}(x-1,1,s,i) = W_{C_6}(x-1,0,s,i) = W_{C_6}(0,0,s,i).$$

It follows that W_{C_6} (and hence the remaining ε_{C_6}-ambiguity) is only sublattice- and leg-dependent. Such property of W_{C_6} in turn allows us to have $\chi_{T_2C_6}(x,y,s,i) = 1$ for $\forall(x,y,s,i)$ from Eq. (A28). For similar reasons Θ_{C_6} can be shown to have dependence on the sublattice label s only. Overall,

$$W_{C_6}(x,y,s,i) = W_{C_6}(s,i), \quad \Theta_{C_6}(x,y,s) = \Theta_{C_6}(s), \quad \varepsilon_{C_6}(x,y,s,i) = \varepsilon_{C_6}(s,i). \tag{A32}$$

W_{C_6} and Θ_{C_6} satisfy another set of equations due to the group relation $(C_6)^6 = \mathrm{e}$, which read

$$W_{C_6}(x,y,s,i)W_{C_6}(C_6^{-1}(x,y,s,i))\cdots W_{C_6}(C_6^{-5}(x,y,s,i)) = \chi_{C_6}(x,y,s,i),$$
$$\Theta_{C_6}(x,y,s)\Theta_{C_6}(C_6^{-1}(x,y,s))\cdots\Theta_{C_6}(C_6^{-5}(x,y,s)) = \left(\prod_i \chi^*_{C_6}(x,y,s,i)\right). \tag{A33}$$

Invoking the (x,y)-independence of the W_{C_6} derived in Eq. (A32), the first line in Eq. (A33) becomes

$$W_{C_6}(u,a)W_{C_6}(v,b)W_{C_6}(u,c)W_{C_6}(v,a)W_{C_6}(u,b)W_{C_6}(v,c) = \chi_{C_6}(u,a). \tag{A34}$$

Lack of dependence on (x,y) on the left side of the equation forces the same independence on the right side as well. There are five other relations like this from cyclic permutations of the (s,i) label.

It is our assumption, throughout the construction of the PEPS wave function, that the bond tensor B remains invariant under the multiplication by the χ-group element. As a result, the two χ-group elements multiplied on either side of a bond tensor must be conjugate, e.g.

$$\varepsilon(v,a) = \varepsilon^*(u,a), \quad \varepsilon(v,b) = \varepsilon^*(u,b), \quad \varepsilon(v,c) = \varepsilon^*(u,c). \tag{A35}$$

Using this result and applying the ε_{C_6}-ambiguity to transform $W_{C_6}(s,i) \to \varepsilon_{C_6}(s,i)W_{C_6}(s,i)$ in Eq. (A34) gives a factor

$$|\varepsilon_{C_6}(u,a)|^2|\varepsilon_{C_6}(u,b)|^2|\varepsilon_{C_6}(u,c)|^2 = 1 \tag{A36}$$

multiplying the left hand side. Recall that in certain cases like Eq. (A30) we were able to fix χ factor by utilizing the ε-ambiguity. In the case of ε_{C_6}-ambiguity, as we can see, χ_{C_6} cannot be fixed in this way.

Earlier construction of the V-ambiguity matrix in regard to two translational symmetries forced us to work with only those V's that are independent of the unit cell coordinates (x, y), but still dependent on internal labels (s, i) [see Eq. (A21)]. One can use what's left in the degrees of freedom in $V(s, i)$ to help fix $W_{C_6}(s, i)$, for instance, as follows:

$$\begin{aligned}
&W_{C_6}(u,a) \to V^{-1}(u,a)W_{C_6}(u,a)V^{-1}(C_6^{-1}(u,a)) = \mathbb{I},\\
&W_{C_6}(u,b) \to V^{-1}(u,b)W_{C_6}(u,b)V^{-1}(C_6^{-1}(u,b)) = \mathbb{I},\\
&W_{C_6}(u,c) \to V^{-1}(u,c)W_{C_6}(u,c)V^{-1}(C_6^{-1}(u,c)) = \chi_{C_6}(s,i) = \chi_{C_6},\\
&W_{C_6}(v,i) \to V^{-1}(v,i)W_{C_6}(v,i)V^{-1}(C_6^{-1}(v,i)) = \mathbb{I}\ (i = a,b,c).
\end{aligned} \tag{A37}$$

In short, we can fix the W_{C_6} matrices as

$$W_{C_6}(u,a) = W_{C_6}(u,b) = W_{C_6}(v,a) = W_{C_6}(v,b) = W_{C_6}(v,c) = \mathbb{I}, W_{C_6}(u,c) = \chi_{C_6}\mathbb{I}. \tag{A38}$$

In the process of fixing W_{C_6} we are also making use of the property $\chi_{C_6}(s, i) = \chi_{C_6}$. Finally, fixing all the W_{C_6} matrices as proportional to the identity also restricts one's choice of the V-matrix to be independent of (s, i) labels,

$$V(s,i) = V. \tag{A39}$$

From the invariance of the bond tensor under the χ-group operation one must have $\chi_{C_6}(\bar{s}, i) = \chi^*_{C_6}(s, i)$, where $\bar{s}$ is the opposite sublattice of s. Since $\chi_{C_6}(s, i) = \chi_{C_6}$ was shown to be independent of (s, i), we conclude that $\chi_{C_6} = \chi^*_{C_6}$, which is true iff

$$\chi_{C_6} = \pm 1. \tag{A40}$$

Moving to the Θ_{C_6}-fixing, the second line of Eq. (A33), using the (x, y)-independence of Θ_{C_6}, becomes

$$[\Theta_{C_6}(u)\Theta_{C_6}(v)]^3 = \chi_{C_6}. \tag{A41}$$

Under the remaining phase ambiguity $\Phi(s)$ [Eq. (A21)], we have

$$\begin{aligned}
\Theta_{C_6}(u) &\to \Phi(u)\Theta_{C_6}(u)\Phi^*(v),\\
\Theta_{C_6}(v) &\to \Phi(v)\Theta_{C_6}(v)\Phi^*(u),
\end{aligned}$$

which can be used to fix $\Theta_{C_6}(v) = 1$. Then, Eq. (A42) becomes

$$[\Theta_{C_6}(u)]^3 = \chi_{C_6}. \tag{A42}$$

For later convenience, we also calculate the symmetry transformation rule associated with the π-rotation symmetry $R_\pi \equiv C_6^3$:

$$\begin{aligned}
\Theta_{R_\pi}W_{R_\pi}R_\pi &\equiv (\Theta_{C_6}W_{C_6}C_6)(\Theta_{C_6}W_{C_6}C_6)(\Theta_{C_6}W_{C_6}C_6)\\
&= \Theta_{C_6}(s)\Theta_{C_6}(C_6^{-1}(s))\Theta_{C_6}(C_6^{-2}(s))\ W_{C_6}(s,i)W_{C_6}(C_6^{-1}(s,i))W_{C_6}(C_6^{-2}(s,i))\ R_\pi.
\end{aligned} \tag{A43}$$

We see that W_{R_π} and Θ_{R_π} can be defined as

$$\begin{aligned}
W_{R_\pi}(s,i) &= W_{C_6}(s,i)W_{C_6}(C_6^{-1}(s,i))W_{C_6}(C_6^{-2}(s,i)),\\
\Theta_{R_\pi}(s) &= \Theta_{C_6}(s)\Theta_{C_6}(C_6^{-1}(s))\Theta_{C_6}(C_6^{-2}(s)).
\end{aligned} \tag{A44}$$

In the gauge chosen before [Eq. (A37)], one can determine W_{R_π} and Θ_{R_π} using Eq. (A44) as follows

$$\begin{aligned}
&W_{R_\pi}(u, a/c) = \chi_{C_6}, \quad W_{R_\pi}(u,b) = 1,\\
&W_{R_\pi}(v, a/c) = 1, \quad W_{R_\pi}(v,b) = \chi_{C_6},\\
&\Theta_{R_\pi}(u) = 1, \quad \Theta_{R_\pi}(v) = \chi_{C_6}.
\end{aligned}$$

4. Reflection symmetry consideration

Now, let us add reflection. One can do similar algebraic calculations as Eqs. (A24) and (A25) for the group relations $\sigma^{-1}T_1^{-1}\sigma T_2 = \mathrm{e}$ and $\sigma^{-1}T_2^{-1}\sigma T_1 = \mathrm{e}$ to find the corresponding algebraic equations

$$\begin{aligned} &W_\sigma^{-1}(\sigma(x,y,s,i))W_\sigma(T_2\sigma(x,y,s,i)) = \chi_{\sigma T_1}(x,y,s,i),\\ &W_\sigma^{-1}(\sigma(x,y,s,i))W_\sigma(T_1\sigma(x,y,s,i)) = \chi_{\sigma T_2}(x,y,s,i), \end{aligned} \tag{A45}$$

and

$$\begin{aligned} &\Theta_\sigma^*(\sigma(x,y,s))\Theta_\sigma(T_2\sigma(x,y,s)) = \Big(\textstyle\prod_i \chi^*_{\sigma T_1}(x,y,s,i)\Big),\\ &\Theta_\sigma^*(\sigma(x,y,s))\Theta_\sigma(T_1\sigma(x,y,s)) = \Big(\textstyle\prod_i \chi^*_{\sigma T_2}(x,y,s,i)\Big). \end{aligned} \tag{A46}$$

The gauge $W_{T_{1,2}}(x,y,s,i) = \mathbb{I}$ was used. Invoking the ε_σ-ambiguity we can set $\chi_{\sigma T_1}(x,y,s,i) = 1$. The remaining ε_σ-ambiguity should satisfy

$$\varepsilon^*_\sigma(x,y,s,i)\varepsilon_\sigma(x,y+1,s,i) = 1 \quad \longrightarrow \quad \varepsilon_\sigma(x,y,s,i) = \varepsilon_\sigma(x,0,s,i),$$

and therefore, one can fix $\chi_{\sigma T_2}(x,0,s,i) = 1$. Then, using Eq. (A45), one can arrive at

$$W_\sigma(x,y,s,i) = W_\sigma(x,0,s,i) = W_\sigma(0,0,s,i) \equiv W_\sigma(s,i), \tag{A47}$$

and similarly for Θ_σ

$$\Theta_\sigma(x,y,s) = \Theta_\sigma(s). \tag{A48}$$

In order to preserve the site independence of W_σ and Θ_σ, the remaining ε_σ-ambiguity must also be site-independent, i.e. $\varepsilon_\sigma(x,y,s,i) = \varepsilon_\sigma(s,i)$.

Next, the equation corresponding to $\sigma^2 = \mathrm{e}$ reads

$$\begin{aligned} &W_\sigma(s,i)W(\sigma^{-1}(s,i)) = \chi_\sigma(s,i),\\ &\Theta_\sigma(s,i)\Theta(\sigma^{-1}(s,i)) = \prod_i \chi^*_\sigma(s,i), \end{aligned} \tag{A49}$$

and therefore

$$\begin{aligned} &[W_\sigma(s,a)]^2 = \chi_\sigma(s,a),\\ &W_\sigma(s,b)W_\sigma(s,c) = \chi_\sigma(s,b) = \chi_\sigma(s,c). \end{aligned} \tag{A50}$$

Under ε_σ transformation, we have

$$\begin{aligned} &\chi_\sigma(s,a) \to \varepsilon^2_\sigma(s,a)\chi_\sigma(s,a),\\ &\chi_\sigma(s,b) \to \varepsilon_\sigma(s,b)\varepsilon_\sigma(s,c)\chi_\sigma(s,b). \end{aligned}$$

So, we can set $\chi_\sigma(s,i) = 1$ resulting in

$$\begin{aligned} &[W_\sigma(s,a)]^2 = 1,\\ &W_\sigma(s,b)W_\sigma(s,c) = 1. \end{aligned} \tag{A51}$$

The remaining ε_σ-ambiguity satisfies

$$1 = [\varepsilon_\sigma(s,a)]^2 = \varepsilon_\sigma(s,b)\varepsilon_\sigma(s,c). \tag{A52}$$

For the group relation $\sigma^{-1}C_6\sigma C_6 = \mathrm{e}$, the corresponding equation is

$$W_\sigma^{-1}(\sigma(s,i))W_{C_6}(\sigma(s,i))W_\sigma(C_6^{-1}\sigma(s,i))W_{C_6}(C_6(s,i)) = \chi_{\sigma C_6}(s,i).$$

Namely, we have

$$\begin{aligned} &W_\sigma(u,a)W_\sigma(v,b) = \chi_{\sigma C_6}(u,a) = \chi_{\sigma C_6}(v,b),\\ &W_\sigma(u,b)W_\sigma(v,a) = \chi_{C_6}\chi_{\sigma C_6}(u,b) = \chi_{C_6}\chi_{\sigma C_6}(v,a),\\ &W_\sigma(u,c)W_\sigma(v,c) = \chi_{\sigma C_6}(u,c) = \chi_{\sigma C_6}(v,c). \end{aligned} \tag{A53}$$

Since χ's are bond-dependent phases, we have $\chi_{\sigma C_6}(u,i)\chi_{\sigma C_6}(v,i) = \chi_{\sigma C_6}(u,i)\chi^*_{\sigma C_6}(u,i) = 1$ which leads

$$\chi_{\sigma C_6}(u,a)\chi_{\sigma C_6}(u,b) = 1,$$
$$\chi_{\sigma C_6}(u,c) = \pm 1.$$

Using remaining ε_σ transformation in Eq. (A52), we are able to set

$$\chi_{\sigma C_6}(u,a) \to \varepsilon_\sigma(u,a)\chi_{\sigma C_6}(u,a)\varepsilon_\sigma(v,b) = \varepsilon_\sigma(u,a)\chi_{\sigma C_6}(u,a)\varepsilon^*_\sigma(u,b) = 1,$$
$$\chi_{\sigma C_6}(v,b) \to \varepsilon_\sigma(u,a)\chi_{\sigma C_6}(v,b)\varepsilon_\sigma(v,b) = \varepsilon^*_\sigma(v,a)\chi_{\sigma C_6}(v,b)\varepsilon_\sigma(v,b) = 1.$$

Then, the remaining ε_σ-ambiguity should satisfy

$$\varepsilon_\sigma(u,a)\varepsilon^*_\sigma(u,b) = 1 = \varepsilon_\sigma(v,a)\varepsilon^*_\sigma(v,b), \quad \varepsilon_\sigma(u,a) = \pm 1,$$

and hence $\varepsilon_\sigma(s,i) = \varepsilon_\sigma = \pm 1$. Now, we can solve Eqs. (A50) and (A53) as

$$W_\sigma(u,a) = W_\sigma, \quad W_\sigma(u,b) = \chi_{\sigma C_6} W_\sigma, \quad W_\sigma(u,c) = \chi_{\sigma C_6} W_\sigma,$$
$$W_\sigma(v,a) = \chi_{C_6}\chi_{\sigma C_6} W_\sigma, \quad W_\sigma(v,b) = W_\sigma, \quad W_\sigma(v,c) = W_\sigma.$$

where $\chi_{\sigma C_6} \equiv \chi_{\sigma C_6}(u,c) = \pm 1$ and $W^2_\sigma = \mathbb{I}$.

It should be cautioned that this is not a complete specification of the gauge matrix W_σ associated with reflection symmetry yet. A more accurate determination of W_σ will be carried out after we considered the spin rotation symmetry in a later subsection.

For the phase factor, the equation reads

$$[\Theta_\sigma(s)]^2 = 1,$$
$$\Theta_\sigma(u)\Theta_{C_6}(u)\Theta_\sigma(v)\Theta_{C_6}(v) = \chi_{\sigma C_6}.$$

Remember we have $[\Theta_{C_6}(u)]^3 = \chi_{C_6}$ as well as $\Theta_{C_6}(v) = 1$. Inserting back to above equations, we conclude

$$\Theta_{C_6}(u) = \chi_{C_6},$$
$$\Theta_\sigma(u) = \Theta_\sigma,$$
$$\Theta_\sigma(v) = \chi_{C_6}\chi_{\sigma C_6}\Theta_\sigma,$$

where $\Theta_\sigma = \pm 1$. By using $\varepsilon_\sigma = \pm 1$ ambiguity, we can set $\Theta_\sigma = 1$.

5. Time reversal symmetry consideration

In this subsection, we consider the time reversal symmetry. Since the time reversal symmetry commute with all lattice symmetries $g^{-1}\mathcal{T}^{-1}g\mathcal{T} = \mathrm{e}$, where $g = T_{1,2}, C_6, \sigma$, we have

$$\begin{aligned}
&(g^{-1}W_g^{-1}\Theta^*_g)(\mathcal{T}^{-1}W_\mathcal{T}^{-1}\Theta^*_\mathcal{T})(\Theta_g W_g g)(\Theta_\mathcal{T} W_\mathcal{T}\mathcal{T}) \circ T^{(x,y,s)} \\
&\quad = \Theta^*_g(g(x,y,s))\Theta_\mathcal{T}(g(x,y,s))\Theta^*_g(g(x,y,s))\Theta^*_\mathcal{T}(x,y,s) \times \\
&\qquad W_g^{-1}(g(x,y,s,i))[W_\mathcal{T}^{-1}(g(x,y,s,i))]^* W^*_g(g(x,y,s,i))W^*_\mathcal{T}(x,y,s,i) \circ T^{(x,y,s)} = T^{(x,y,s)},
\end{aligned}$$

and therefore

$$W_g^{-1}(g(x,y,s,i))[W_\mathcal{T}^{-1}(g(x,y,s,i))]^* W^*_g(g(x,y,s,i))W^*_\mathcal{T}(x,y,s,i) = \chi_{g\mathcal{T}}(x,y,s,i), \tag{A54}$$
$$\Theta^*_g(g(x,y,s))\Theta_\mathcal{T}(g(x,y,s))\Theta^*_g(g(x,y,s))\Theta^*_\mathcal{T}(x,y,s) = \prod_i \chi^*_{g\mathcal{T}}(x,y,s,i). \tag{A55}$$

Recall that under the $\varepsilon_\mathcal{T}$-ambiguity, $\chi_{g\mathcal{T}}$ transforms as

$$\chi_{g\mathcal{T}}(x,y,s,i) \to \varepsilon_\mathcal{T}(g(x,y,s,i))\chi_{g\mathcal{T}}(x,y,s,i)\varepsilon^*_\mathcal{T}(x,y,s,i).$$

For $g = T_{1,2}$, one can use such $\varepsilon_\mathcal{T}$-ambiguity to set $\chi_{T_{1,2}\mathcal{T}}(x,y,s,i) = 1$, and the residual $\varepsilon_\mathcal{T}$ should become coordinate-independent: $\varepsilon_\mathcal{T}(x,y,s,i) = \varepsilon_\mathcal{T}(s,i)$. Therefore, in the gauge chosen previously, i.e. $W_{T_{1,2}}(x,y,s,i) = \mathbb{I}$, Eq. (A54) gives us the coordinate independence

$$W_{\mathcal{T}}(x,y,s,i) = W_{\mathcal{T}}(s,i), \quad \Theta_{\mathcal{T}}(x,y,s) = \Theta_{\mathcal{T}}(s).$$

For the C_6 symmetry,

$$W_{C_6}^{-1}(C_6(s,i))[W_{\mathcal{T}}^{-1}(C_6(s,i))]^* W_{C_6}^*(C_6(s,i)) W_{\mathcal{T}}^*(s,i) = \chi_{C_6\mathcal{T}}(s,i), \tag{A56}$$

one can use the remaining $\varepsilon_{\mathcal{T}}$ ambiguity to fix $\chi_{C_6\mathcal{T}}(s,i) = 1$. The remaining $\varepsilon_{\mathcal{T}}$-ambiguity should satisfy $\varepsilon_{\mathcal{T}}(C_6(s,i))\varepsilon_{\mathcal{T}}^*(s,i) = 1$, or $\varepsilon_{\mathcal{T}}(C_6(s,i)) = \varepsilon_{\mathcal{T}}(s,i)$. For this to hold, one must have $\varepsilon_{\mathcal{T}}(s,i) = \varepsilon_{\mathcal{T}} = \pm 1$. Inserting Eq. (A37) into Eq. (A56), one obtains the invariance of $W_{\mathcal{T}}$ under the C_6 rotation, $W_{\mathcal{T}}(C_6(s,i)) = W_{\mathcal{T}}(s,i)$, which leads to the coordinate independence

$$W_{\mathcal{T}}(s,i) = W_{\mathcal{T}}. \tag{A57}$$

A similar reasoning also gives coordinate-independent phase factor $\Theta_{\mathcal{T}}(s) = \Theta_{\mathcal{T}}$.

As for the reflection symmetry $g = \sigma$, the corresponding symmetry condition $g^{-1}\mathcal{T}g\mathcal{T} = e$ implies

$$W_\sigma^{-1}(s,i)[W_{\mathcal{T}}^{-1}]^* W_\sigma^*(\sigma(s,i)) W_{\mathcal{T}}^* = W_\sigma^{-1}[W_{\mathcal{T}}^{-1}]^* W_\sigma^* W_{\mathcal{T}}^* = \chi_{\sigma\mathcal{T}}, \tag{A58}$$

which shows $\chi_{\sigma\mathcal{T}}(s,i) = \chi_{\sigma\mathcal{T}}$ is independent of the sublattice and virtual leg labels. Combined with the general property of the χ-group $\chi(\bar{s},i) = \chi^*(s,i)$, we also find $\chi_{\sigma\mathcal{T}}(s,i) = \chi_{\sigma\mathcal{T}}(\bar{s},i) = \chi_{\sigma\mathcal{T}}^*(s,i)$, or $\chi_{\sigma\mathcal{T}} = \pm 1$. Furthermore, application of Eq. (A55) to the reflection symmetry gives

$$\Theta_\sigma^* \Theta_{\mathcal{T}} \Theta_\sigma^* \Theta_{\mathcal{T}}^* = \prod_i \chi_{\sigma\mathcal{T}} = (\chi_{\sigma\mathcal{T}})^3 = 1.$$

The only self-conjugate U(1) phase factors are $\chi_{\sigma\mathcal{T}} = 1$. Under the overall Φ-ambiguity, $\Theta_{\mathcal{T}}$ transforms as $\Theta_{\mathcal{T}} \to \Phi\Theta_{\mathcal{T}}\Phi$. Thus, we can always set $\Theta_{\mathcal{T}} = 1$.

Now we come to the group relation $\mathcal{T}^2 = \mathrm{e}$, which gives

$$\begin{aligned} T^{(x,y,s,i)} &= \Theta_{\mathcal{T}} \left(\prod_i W_{\mathcal{T}}\right) \mathcal{T} \Theta_{\mathcal{T}} \left(\prod_j W_{\mathcal{T}}\right) \mathcal{T} \circ T^{(x,y,s,i)} \\ &= \Theta_{\mathcal{T}} \Theta_{\mathcal{T}}^* \left(\prod_i W_{\mathcal{T}} W_{\mathcal{T}}^*\right) \mathcal{T}^2 \circ T^{(x,y,s,i)}. \end{aligned} \tag{A59}$$

Since $\Theta_{\mathcal{T}}\Theta_{\mathcal{T}}^* = 1$, and the action of $\mathcal{T}^2$ on the site tensor gives $-T^{(x,y,s,i)}$ due to our assumption that physical spin degrees of freedom are half-integers, the above equation is equivalent to having $T^{(x,y,s)} = -\left(\prod_i W_{\mathcal{T}} W_{\mathcal{T}}^*\right) T^{(x,y,s,i)}$, or

$$W_{\mathcal{T}} W_{\mathcal{T}}^* = \chi_{\mathcal{T}} = -1, \tag{A60}$$

for each leg of the honeycomb lattice. We conclude, as a consequence, that virtual legs only support Kramers doublets[8].

6. Spin rotation symmetry consideration

Let us add spin rotation symmetry. Since SU(2) group has no non-trivial projective symmetry and nontrivial 1D representation, one can always set χ's, η's and $\Theta_{\theta\vec{n}}$ to be trivial ones[8].

The on-site spin rotation symmetry operator $U_{\theta\vec{n}}$ commutes with all other symmetries. Namely, we have

$$g^{-1} U_{\theta\vec{n}}^{-1} g U_{\theta\vec{n}} = \mathrm{e}$$

where $g = T_{1,2}, C_6, \sigma, \mathcal{T}$. Symmetry group equations give

$$W_g^{-1}(g(x,y,s,i))W_{\theta\vec{n}}^{-1}(g(x,y,s,i))W_g(g(x,y,s,i))W_{\theta\vec{n}}(x,y,s,i)=\mathbb{I},\quad (g=T_{1,2},C_6,\sigma)$$
$$[W_{\mathcal{T}}^{-1}(x,y,s,i)]^*[W_{\theta\vec{n}}^{-1}(x,y,s,i)]^*[W_{\mathcal{T}}(x,y,s,i)]^*W_{\theta\vec{n}}(x,y,s,i)=\mathbb{I}. \tag{A61}$$

Then, similar to the time reversal case, by solving the corresponding equations for $g=T_{1,2},C_6$, one can find that $W_{\theta\vec{n}}(x,y,s,i)$ acts identically on all virtual legs: $W_{\theta\vec{n}}(x,y,s,i)=W_{\theta\vec{n}}$. For $g=\sigma,\mathcal{T}$, one obtains

$$W_\sigma^{-1}W_{\theta\vec{n}}^{-1}W_\sigma W_{\theta\vec{n}}=\mathbb{I},$$
$$(W_{\mathcal{T}}^{-1})^*(W_{\theta\vec{n}}^{-1})^*W_{\mathcal{T}}^*W_{\theta\vec{n}}=\mathbb{I}. \tag{A62}$$

From the equation $U_{\theta=2\pi}=\mathrm{e}$, we have $W_{2\pi\vec{n}}=\chi_{\theta=2\pi}$. Since we only consider systems with a half-integer spin per site satisfying $U_{\theta=2\pi}\circ T^{(x,y,s)}=-T^{(x,y,s)}$, a symmetric PEPS should satisfy $[W_{2\pi\vec{n}}]^3U_{\theta=2\pi}\circ T^{(x,y,s)}=T^{(x,y,s)}$ and hence $[W_{2\pi\vec{n}}]^3=(\chi_{\theta=2\pi})^3=-1$. Thus, we once again conclude $W_{2\pi\vec{n}}=\chi_{\theta=2\pi}=-1$, namely, virtual legs can only accommodate half-integer spins.

Using the remaining overall V-ambiguity, $W_{\theta\vec{n}}\to VW_{\theta\vec{n}}V^{-1}$, we can set $W_{\theta\vec{n}}$ as

$$W_{\theta\vec{n}}=\bigoplus_{k=1}^{M}(\mathrm{I}_{d_k}\otimes \mathrm{e}^{\mathrm{i}\theta\vec{n}\cdot\vec{S}_k}), \tag{A63}$$

that is, $W_{\theta\vec{n}}$ acts trivially in the flavor space and as a unitary rotation on the virtual spins. Here each $\vec{S}_k$ represents a half-integer spin of size S_k, and I_{d_k} implies there are d_k copies of the spin $\vec{S}_k$. We get the total dimension of the Hilbert space for a virtual leg as $D=\sum_{k=1}^{M}d_k(2S_k+1)$. Any remaining V-ambiguity must leave this form of $W_{\theta\vec{n}}$ invariant, or

$$V\left[\bigoplus_{k=1}^{M}(\mathbb{I}_{d_k}\otimes \mathrm{e}^{\mathrm{i}\theta\vec{n}\cdot\vec{S}_k})\right]V^{-1}=\bigoplus_{k=1}^{M}(\mathbb{I}_{d_k}\otimes \mathrm{e}^{\mathrm{i}\theta\vec{n}\cdot\vec{S}_k}), \tag{A64}$$

and therefore must be of the form

$$V=\bigoplus_{k=1}^{M}(\widetilde{V}_k\otimes\mathbb{I}_{2S_k+1}),$$

where $\widetilde{V}_k$ is an arbitrary d_k-dimensional invertible matrix. Apart from the freedom in choosing the dimensionality d_k and the size of the spin S_k, the form of the gauge matrix $W_{\theta\vec{n}}$ is completely fixed by Eq. (A63).

We return to the consideration of the general form of W_σ. Recall that we left off at $W_\sigma^2=\mathbb{I}$ in the earlier discussion of the reflection symmetry. As W_σ must satisfy the first line of Eq. (A62), and given the $W_{\theta\vec{n}}$ form shown in Eq. (A64), it will have to take on the form

$$W_\sigma=\bigoplus_{k=1}^{M}(\widetilde{W}_\sigma^k\otimes\mathbb{I}_{2S_k+1}), \tag{A65}$$

where $(\widetilde{W}_\sigma^k)^2=\mathbb{I}$ to satisfy $W_\sigma^2=\mathbb{I}$. Since the time reversal operation reverses the spin direction, the most general form of $W_{\mathcal{T}}$ satisfying Eq. (A62) with Eq. (A64) is also constrained,

$$W_{\mathcal{T}}=\bigoplus_{k=1}^{M}(\widetilde{W}_{\mathcal{T}}^k\otimes\mathrm{e}^{\mathrm{i}\pi S_k^y}), \tag{A66}$$

where $\widetilde{W}_{\mathcal{T}}^k$ is a d_k-dimensional invertible matrix. One can use the remaining V-ambiguity to fix $\widetilde{W}_{\mathcal{T}}^k$, $\widetilde{W}_{\mathcal{T}}^k\to\widetilde{V}_k\widetilde{W}_{\mathcal{T}}^k[\widetilde{V}_k^{-1}]^*=\mathbb{I}_{d_k}$, such that

$$W_{\mathcal{T}} = \bigoplus_{k=1}^{M} (\mathbb{I}_{d_k} \otimes \mathrm{e}^{\mathrm{i}\pi S_k^y}), \tag{A67}$$

and the remaining V-ambiguity satisfies $\widetilde{V}_k \, \widetilde{V}_k^* = \mathbb{I}_{d_k}$. Plugging Eqs. (A65) and (A67) into Eq. (A58), one obtains

$$\widetilde{W}_\sigma^k = (\widetilde{W}_\sigma^k)^*. \tag{A68}$$

7. Summary

The results obtained in previous subsections are summarized below. For all the symmetries S considered in this work, the associated gauge transformations and phase factors are unit-cell-independent:

$$W_S(x, y, s, i) = W_S(s, i), \quad \Theta_S(x, y, s) = \Theta_S(s).$$

Further symmetry consideration then identified the structure of each gauge matrix W_S to be

$$\begin{aligned}
&W_{T_1}(s,i) = W_{T_2}(s,i) = \mathbb{I};\\
&W_{C_6}(u, a/b) = W_{C_6}(v, a/b/c) = \mathbb{I}, \quad W_{C_6}(u, c) = \chi_{C_6};\\
&W_{R_\pi}(u, a/c) = \chi_{C_6}, \quad W_{R_\pi}(u, b) = 1, \quad W_{R_\pi}(v, a/c) = 1, \quad W_{R_\pi}(v, b) = \chi_{C_6};\\
&W_\sigma(u, a) = W_\sigma, \quad W_\sigma(u, b/c) = \chi_{\sigma C_6} W_\sigma, \quad W_\sigma(v, a) = \chi_{C_6} \cdot \chi_{\sigma C_6} W_\sigma, \quad W_\sigma(v, b/c) = W_\sigma;\\
&W_{\mathcal{T}}(s,i) = W_{\mathcal{T}} = \bigoplus_{k=1}^{M} (I_{d_k} \otimes \mathrm{e}^{\mathrm{i}\pi S_k^y});\\
&W_{\theta\vec{n}}(s,i) = W_{\theta\vec{n}} = \bigoplus_{k=1}^{M} (I_{d_k} \otimes \mathrm{e}^{\mathrm{i}\theta\vec{n}\cdot\vec{S}_k}).
\end{aligned} \tag{A69}$$

Finally, $W_\sigma = \bigoplus_{k=1}^{M} (\widetilde{W}_\sigma^k \otimes \mathbb{I}_{2S_k+1})$, where $\widetilde{W}_\sigma^k$ is a d_k-dimensional matrix with real entries satisfying $(\widetilde{W}_\sigma^k)^2 = \mathbb{I}_{d_k}$. The associated phase factors are

$$\begin{aligned}
&\Theta_{T_1}(s) = \Theta_{T_2}(s) = 1;\\
&\Theta_{C_6}(u) = \chi_{C_6}, \quad \Theta_{C_6}(v) = 1;\\
&\Theta_{R_\pi}(u) = 1, \quad \Theta_{R_\pi}(v) = \chi_{C_6};\\
&\Theta_\sigma(u) = 1, \quad \Theta_\sigma(v) = \chi_{C_6} \cdot \chi_{\sigma C_6};\\
&\Theta_{\mathcal{T}} = 1.
\end{aligned} \tag{A70}$$

Appendix B: Solving the Hilbert space constraints for PEPS

In this section, we solve the constraints imposed on the Hilbert space of tensors by the symmetry transformation rules worked out thus far. We first identify the Hilbert space structure for a single leg, then subsequently fix the bond and site tensors.

1. Hilbert space structure for a single leg

We are focusing on systems with a physical spin-$\frac{1}{2}$ Kramers doublet per site. In other words, every physical leg is isomorphic to a two-dimensional Hilbert space $\mathbb{V}_{\frac{1}{2}}$ supporting a spin-$\frac{1}{2}$ Kramers doublet.

There are two kinds of virtual legs, one extending out from site tensors, and the other from bond tensors. The two virtual spaces, or virtual legs, are connected to each other in the sense of tensor contraction and are called dual

spaces[8]. In the previous section we identified the tensor structures of $W_\sigma, W_\mathcal{T}$, and $W_{\theta\vec{n}}$. Based on that, we see that site virtual leg is isomorphic to a space $\mathbb{V}$ that can be decomposed as

$$\mathbb{V} \cong \bigoplus_{k=1}^{M} (\mathbb{D}_{S_k} \otimes \mathbb{V}_{S_k}). \tag{B1}$$

$\mathbb{V}_{S_k}$ is the Hilbert space for the SU(2) spin-S_k and $\mathbb{D}_{S_k}$ is a d_k-dimensional space that labels the "flavor degeneracy" for each spin-S_k. The basis that spans the space $\mathbb{V}$ can be labeled as

$$|S_k, t_\alpha, m_\beta\rangle = |S_k, t_\alpha\rangle \otimes |S_k, m_\beta\rangle \tag{B2}$$

where $|S_k, t_\alpha\rangle \in \mathbb{D}_{S_k}$ labels the basis in the flavor space, while $|S_k, m_\beta\rangle \in \mathbb{V}_{S_i}$ labels an eigenstate of $\vec{S}^2 = S_k(S_k+1)$ and S^z.

Similarly, every bond-originating virtual leg is isomorphic to the dual space of $\mathbb{V}$, labeled $\bar{\mathbb{V}}$, which can be decomposed as

$$\bar{\mathbb{V}} \cong \bigoplus_{k=1}^{M} (\bar{\mathbb{D}}_{S_k} \otimes \bar{\mathbb{V}}_{S_k}) \tag{B3}$$

with the basis $\langle S_k, t_\alpha, m_\beta| = \langle S_k, t_\alpha| \otimes \langle S_k, m_\beta|$.

2. Constraints on bond tensors

Having established the Hilbert space structure of a single virtual leg, we are able to construct the Hilbert space of a bond tensor $\mathbb{V}_B$ as the tensor product, $\mathbb{V}_B \cong \bar{\mathbb{V}} \otimes \bar{\mathbb{V}}$. According to Eq. (B3), $\mathbb{V}_B$ can be decomposed as

$$\begin{aligned} \mathbb{V}_B \cong & \bigoplus_{i,j} ((\bar{\mathbb{D}}_{S_i} \otimes \bar{\mathbb{D}}_{S_j}) \otimes (\bar{\mathbb{V}}_{S_i} \otimes \bar{\mathbb{V}}_{S_j})) \\ \cong & \bigoplus_{i,j,k} ((\bar{\mathbb{D}}_{S_i} \otimes \bar{\mathbb{D}}_{S_j}) \otimes (\bar{\mathbb{V}}^{S_k}_{S_i S_j} \otimes \bar{\mathbb{V}}_{S_k})) \end{aligned}$$

where $\bar{\mathbb{V}}^{S_k}_{S_i S_j}$ is the "fusion space" denoting different ways to fuse spins S_i and S_j to form a spin S_k. According to the representation theory of SU(2), $\bar{\mathbb{V}}^{S_k}_{S_i S_j}$ is isomorphic to $\mathbb{C}$ if $|S_i - S_j| \le S_k \le S_i + S_j$ and zero otherwise.

We require the bond tensor to be a spin singlet, so the bond Hilbert space is restricted to the $S = 0$ space

$$\mathbb{V}_B^{S=0} \cong \bigoplus_{i=1}^{M} ((\bar{\mathbb{D}}_{S_i} \otimes \bar{\mathbb{D}}_{S_i}) \otimes (\bar{\mathbb{V}}^{S=0}_{S_i S_i} \otimes \bar{\mathbb{V}}_{S=0})),$$

where we used the fact that $\bar{\mathbb{V}}^{S=0}_{S_i S_j}$ vanishes unless $S_i = S_j$ and $S_k = 0$. The bond state $\hat{B}_b$ (labeled with a carat) can be decomposed as

$$\hat{B}_b = \sum_{k;\alpha_1,\alpha_2;\beta_1,\beta_2} \langle S_k, t_{\alpha_1}, m_{\alpha_2}| \otimes \langle S_k, t_{\beta_1}, m_{\beta_2}| (\widetilde{B}_b^{S_k})_{\alpha_1\beta_1} (K_{S_k})_{\alpha_2\beta_2},$$

where $\alpha_1, \beta_1 = 1, \cdots, d_k$, $\alpha_2, \beta_2 = 1, \cdots, 2S_k + 1$, and $\widetilde{B}_b^{S_k}$ is some d_k-dimensional matrix. K_{S_k} is a $(2S_k+1)$-dimensional Clebsch-Gordan (CG) matrix ensuring the "spin singlet state",

$$(K_S)_{\alpha\beta} = \langle S, m_\alpha, S, m_\beta | S_{\text{tot}} = 0, m_{\text{tot}} = 0\rangle = (-1)^{S-m_\alpha} \delta_{m_\alpha, -m_\beta}, \tag{B4}$$

$m_\alpha = -S + \alpha - 1$. K_S is antisymmetric for half-integer S. Since the bond state is also a Kramers singlet, we require $\widetilde{B}_b^{S_k}$ to be a real matrix in order to preserve the time reversal symmetry. Instead of the bond state $\hat{B}_b$ itself, we work with its matrix form B_b in the following:

$$B_b = \bigoplus_{k=1}^{M} (\widetilde{B}_b^{S_k} \otimes K_{S_k}). \tag{B5}$$

Now, let us consider various constraints on B_b from lattice symmetry. For translation symmetry, the associated gauge transformation $W_{T_{1,2}} = \mathbb{I}$ is trivial and thus $B_b = T_{1,2} \circ B_b$. In other words, all bond tensors ought to be translationally invariant. We are therefore left with three independent bond tensors within a unit cell, which can be labeled as $B_{(u,a|v,a)}$, $B_{(u,b|v,b)}$ and $B_{(u,c|v,c)}$. Under the π-rotation symmetry we have

$$\begin{aligned} B_{(u,i|v,i)} &= W_{R_\pi}^{-1}(u,i)[W_{R_\pi}^{-1}(v,i)]^{\mathrm{t}} R_\pi \circ B_{(u,i|v,i)} \\ &= W_{R_\pi}^{-1}(u,i)[W_{R_\pi}^{-1}(v,i)]^{\mathrm{t}} B_{(v,i|u,i)} = \chi_{C_6}[B_{(u,i|v,i)}]^{\mathrm{t}}. \end{aligned} \tag{B6}$$

According to Eq. (B5) and the fact that K_{S_k} is antisymmetric in our case, we conclude that one of the following must hold:

- $\chi_{C_6} = 1$, $\widetilde{B}_b^{S_k} = -(\widetilde{B}_b^{S_k})^{\mathrm{t}}$. Namely, $\widetilde{B}_b^{S_k}$ is a real antisymmetric matrix.
- $\chi_{C_6} = -1$, $\widetilde{B}_b^{S_k} = (\widetilde{B}_b^{S_k})^{\mathrm{t}}$. Namely, $\widetilde{B}_b^{S_k}$ is a real symmetric matrix.

From C_6-rotation symmetry one obtains the following additional constraints:

$$\begin{aligned} B_{(u,a|v,a)} &= W_{C_6}^{-1}(u,a)[W_{C_6}^{-1}(v,a)]^{\mathrm{t}} C_6 \circ B_{(u,a|v,a)} = B_{(v,b|u,b)}, \\ B_{(u,b|v,b)} &= W_{C_6}^{-1}(u,b)[W_{C_6}^{-1}(v,b)]^{\mathrm{t}} C_6 \circ B_{(u,b|v,b)} = B_{(v,c|u,c)}, \\ B_{(u,a|v,a)} &= W_{C_6}^{-1}(u,c)[W_{C_6}^{-1}(v,c)]^{\mathrm{t}} C_6 \circ B_{(u,c|v,c)} = B_{(v,a|u,a)}. \end{aligned} \tag{B7}$$

Combined with Eq. (B6), we conclude

$$B_{(u,a|v,a)} = \chi_{C_6}\, B_{(u,b|v,b)} = B_{(u,c|v,c)}.$$

Thus, once we fix a single bond tensor, say $B_{(u,a|v,a)}$, all other bond tensors are uniquely determined.

We can impose an extra constraint for reflection symmetry operator $W_\sigma = \bigoplus_{k=1}^{M} (\widetilde{W}_\sigma^k \otimes \mathbb{I}_{2S_k+1})$. To see where this comes from, we write the reflection symmetry relation [Eq. (A1)] for the bond tensor $B_{(u,a|v,a)}$,

$$B_{(u,a|v,a)} = W_\sigma^{-1}(u,a)[W_\sigma^{-1}(v,a)]^{\mathrm{t}} \sigma \circ B_{(u,a|v,a)} = \chi_{C_6} \cdot \chi_{\sigma C_6} W_\sigma\, B_{(u,a|v,a)}\, [W_\sigma]^{\mathrm{t}}.$$

Inserting Eq. (B5) in the above equation, we conclude

$$\widetilde{B}_b^{S_k} = \chi_{C_6} \cdot \chi_{\sigma C_6} \widetilde{W}_\sigma^{S_k}\, \widetilde{B}_b^{S_k}\, [\widetilde{W}_\sigma^{S_k}]^{\mathrm{t}}. \tag{B8}$$

3. Constraints on site tensors

Similar to bond tensors, the Hilbert space of a site tensor has the following tensor product structure:

$$\begin{aligned} \mathbb{V}_T &\cong \mathbb{V}_{S_0} \otimes \mathbb{V} \otimes \mathbb{V} \otimes \mathbb{V} \\ &\cong \bigoplus_{i_a, i_b, i_c} (\mathbb{D}_{S_{i_a} S_{i_b} S_{i_c}} \otimes \mathbb{V}_{S_0} \otimes \mathbb{V}_{S_{i_a}} \otimes \mathbb{V}_{S_{i_b}} \otimes \mathbb{V}_{S_{i_c}}) \\ &\cong \bigoplus_{i_a, i_b, i_c, k} (\mathbb{D}_{S_{i_a} S_{i_b} S_{i_c}} \otimes \mathbb{V}_{S_0 S_{i_a} S_{i_b} S_{i_c}}^{S_k} \otimes \mathbb{V}_{S_k}), \end{aligned}$$

where $\mathbb{D}_{S_{i_a} S_{i_b} S_{i_c}} \equiv \mathbb{D}_{S_{i_a}} \otimes \mathbb{D}_{S_{i_b}} \otimes \mathbb{D}_{S_{i_c}}$ labels the product flavor space associated with half-integer spins $S_{i_a}, S_{i_b}, S_{i_c}$ on three virtual legs. The basis of $\mathbb{D}_{S_{i_a} S_{i_b} S_{i_c}}$ is labeled as $|S_{i_a}, t_\alpha\rangle \otimes |S_{i_b}, t_\beta\rangle \otimes |S_{i_c}, t_\gamma\rangle$. The physical spin space $\mathbb{V}_{S_0}$ has the spin S_0.

$V^{S_k}_{S_0 S_{i_a} S_{i_b} S_{i_c}}$ is the fusion space, which denotes different ways to fuse the four spins $S_0, S_{i_a}, S_{i_b}, S_{i_c}$ to form a spin S_k. The fusion process can be broken down to three successive steps, fusing two spins at each step as (i) $(S_0, S_{i\alpha}) \to S_\alpha$, (ii) $(S_\alpha, S_{i_b}) \to S_\beta$, (iii) $(S_\beta, S_{i_c}) \to S_k$. One can write the overall fusion space accordingly as

$$\mathbb{V}^{S_k}_{S_0 S_{i_a} S_{i_b} S_{i_c}} \cong \bigoplus_{\alpha,\beta} \mathbb{V}^{S_k}_{S_\beta S_{i_c}} \otimes \mathbb{V}^{S_\beta}_{S_\alpha S_{i_b}} \otimes \mathbb{V}^{S_\alpha}_{S_0 S_{i_a}}. \tag{B9}$$

We are only considering site tensors that are SU(2) singlets, which means the Hilbert space $\mathbb{V}_T$ can be restricted to the $S = 0$ sector,

$$\mathbb{V}^{S=0}_T \cong \bigoplus_{i_a, i_b, i_c} (\mathbb{D}_{S_{i_a} S_{i_b} S_{i_c}} \otimes \mathbb{V}^{S=0}_{S_0 S_{i_a} S_{i_b} S_{i_c}} \otimes \mathbb{V}_{S=0}).$$

Basis states spanning the space $\mathbb{V}^{S=0}_{S_0 S_{i_a} S_{i_b} S_{i_c}} \otimes \mathbb{V}_{S=0}$ can be expressed as

$$\hat{K}^l_{S_0 S_{i_a} S_{i_b} S_{i_c}} \equiv \sum_{j,\alpha,\beta,\gamma} (K^l_{S_0 S_{i_a} S_{i_b} S_{i_c}})^j_{\alpha\beta\gamma} |S_0, m_j\rangle \otimes |S_{i_a}, m_\alpha\rangle \otimes |S_{i_b}, m_\beta\rangle \otimes |S_{i_c}, m_\gamma\rangle. \tag{B10}$$

The coefficient matrix $\hat{K}^l_{S_0 S_{i_a} S_{i_b} S_{i_c}}$ mix the original basis states $|S_0, m_j\rangle \otimes |S_{i_a}, m_\alpha\rangle \otimes |S_{i_b}, m_\beta\rangle \otimes |S_{i_c}, m_\gamma\rangle$ to produce mutually orthogonal singlet states labeled by different l.

Earlier it was shown that the symmetric site tensor can be chosen to have no spatial dependence: $T^{(x,y,s)} = T^{(s)}$ where $s = u, v$ is the sublattice index. For each s, one can decompose the site tensor $T^{(s)}$ as

$$T^{(s)} = \bigoplus_{i_a, i_b, i_c, l} (\widetilde{T}^l_{S_{i_a} S_{i_b} S_{i_c}} \otimes K^l_{S_0 S_{i_a} S_{i_b} S_{i_c}}), \tag{B11}$$

where the state $\sum_{\alpha,\beta,\gamma} (\widetilde{T}^l_{S_{i_a} S_{i_b} S_{i_c}})_{\alpha\beta\gamma} |S_{i_a}, t_\alpha\rangle \otimes |S_{i_b}, t_\beta\rangle \otimes |S_{i_c}, t_\gamma\rangle$ lives in the flavor space $\mathbb{D}_{S_{i_a} S_{i_b} S_{i_c}}$.

Now, let us consider lattice symmetries. The two independent tensors, $T^{(u)}$ and $T^{(v)}$, are related by π-rotation symmetry:

$$T^{(u)} = \Theta_{R_\pi} W_{R_\pi} R_\pi \circ T^u = (\chi_{C_6})^2 T^{(v)} = T^{(v)}. \tag{B12}$$

In the gauge we have chosen, all site tensors are identical.

From C_6 rotation symmetry, we obtain the following constraints

$$\begin{aligned} (T^{(u)})^j_{\alpha\beta\gamma} &= (T^{(v)})^j_{\beta\gamma\alpha}, \\ (T^{(v)})^j_{\alpha\beta\gamma} &= (T^{(u)})^j_{\beta\gamma\alpha}, \end{aligned} \tag{B13}$$

implying invariance of the site tensor under the simultaneous cyclic permutation of the virtual spin and flavor indices (α, β, γ) living on legs (a, b, c) and the sublattice index (u, v). Since $T^{(u)} = T^{(v)}$ from the earlier argument, we conclude $T^{(u)}$ is invariant under the even permutation of virtual leg indices:

$$(T^{(u)})^j_{\alpha\beta\gamma} = (T^{(u)})^j_{\beta\gamma\alpha} = (T^{(u)})^j_{\gamma\alpha\beta}. \tag{B14}$$

For the reflection symmetry σ, we have the following constraint

$$\begin{aligned} (T^{(u)})^j_{\alpha\beta\gamma} &= \sum_{\alpha',\beta',\gamma'} \Theta_\sigma(u) [W_\sigma(u,a)]_{\alpha\alpha'} [W_\sigma(u,b)]_{\beta\beta'} [W_\sigma(u,c)]_{\gamma\gamma'} (T^{(u)})^j_{\alpha'\gamma'\beta'} \\ &= \sum_{\alpha',\beta',\gamma'} (W_\sigma)_{\alpha\alpha'} (W_\sigma)_{\beta\beta'} (W_\sigma)_{\gamma\gamma'} (T^{(u)})^j_{\alpha'\gamma'\beta'}. \end{aligned} \tag{B15}$$

Finally, in order to have a time-reversal-invariant site tensor, we require $\widetilde{T}^l_{S_{i_a} S_{i_b} S_{i_c}}$ to be matrices with only real entries.

4. Explicit constructions

In constructing the bond and site tensors explicitly, we must begin by specifying the exact dimensionality d_k and the spin size S_k for the bond Hilbert space. We choose $S_k = 1/2$ only, excluding higher spin sizes such as $S_k = 3/2$ for simplicity of calculation, for the dimension of the virtual leg equal to $D = n \times 2$ for n copies of spin-1/2's.

For the spin-$\frac{1}{2}$ case, we get the Clebsh-Gordon matrix $K_{1/2} = \mathrm{i}\sigma_2$ from Eq. (B4), and then, for a single bond tensor, Eq. (B5) is simplified as

$$B_b = \widetilde{B}_b \otimes \mathrm{i}\sigma_2. \tag{B16}$$

As the discussion following Eq. (B6) shows, there are two choices of $\widetilde{B}_b$ depending on the sign of χ_{C_6}:

- $\chi_{C_6} = 1$, $\widetilde{B}_b = \mathbb{I}_{n/2} \otimes \mathrm{i}\sigma_2$. The flavor space dimension n is even.
- $\chi_{C_6} = -1$, $\widetilde{B}_b = \mathrm{Diag}(\pm 1, \pm 1, \dots)$. It is diagonal matrix of arbitrary dimension, with entries either +1 or -1.

Note that we have chosen the bond tensor to be a maximally entangled state by gauge transformation.

Let us consider the site tensor. According to the representation of SU(2), for four spin-$\frac{1}{2}$'s on a single site tensor (one physical leg plus three virtual legs), we have

$$\mathbb{V}^0_{\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}} \cong \left(\mathbb{V}^0_{\frac{1}{2}\frac{1}{2}} \otimes \mathbb{V}^{\frac{1}{2}}_{\frac{1}{2}0} \otimes \mathbb{V}^0_{\frac{1}{2}\frac{1}{2}}\right) \oplus \left(\mathbb{V}^0_{\frac{1}{2}\frac{1}{2}} \otimes \mathbb{V}^{\frac{1}{2}}_{\frac{1}{2}1} \otimes \mathbb{V}^1_{\frac{1}{2}\frac{1}{2}}\right). \tag{B17}$$

For each of the two ways to generate the total spin zero we have the K-tensor in Eq. (B10) given as

$$\begin{aligned}(K_1)^j_{\alpha\beta\gamma} &= (\mathrm{i}\sigma_2)_{j\alpha}(\mathrm{i}\sigma_2)_{\beta\gamma},\\ (K_2)^j_{\alpha\beta\gamma} &= \sum_{\mu\nu}(\mathrm{i}\sigma)_{j\nu} C^{\frac{1}{2},m_\nu}_{\frac{1}{2},m_\alpha;1,m_\mu} C^{1,m_\mu}_{\frac{1}{2},m_\beta;\frac{1}{2},m_\gamma}.\end{aligned} \tag{B18}$$

Here, $m_i = -S - 1 + i$ is the S^z quantum number, and $C^{J,m_J}_{S_1,m_1;S_2,m_2} \doteq \langle S_1 m_1 S_2 m_2 | J m_J\rangle$ denotes the CG coefficient.

By introducing basis $|\uparrow\rangle$, $|\downarrow\rangle$ for spin-$\frac{1}{2}$, the two orthogonal basis for $\mathbb{V}^0_{\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}} \otimes \mathbb{V}_0$ read

$$\begin{aligned}\hat{K}_1 &= |\uparrow\rangle \otimes (|\downarrow\uparrow\downarrow\rangle - |\downarrow\downarrow\uparrow\rangle) - |\downarrow\rangle \otimes (|\uparrow\uparrow\downarrow\rangle - |\uparrow\downarrow\uparrow\rangle),\\ \hat{K}_2 &= |\uparrow\rangle \otimes (2|\uparrow\downarrow\downarrow\rangle - |\downarrow\uparrow\downarrow\rangle - |\downarrow\downarrow\uparrow\rangle) + |\downarrow\rangle \otimes (2|\downarrow\uparrow\uparrow\rangle - |\uparrow\uparrow\downarrow\rangle - |\uparrow\downarrow\uparrow\rangle).\end{aligned}$$

The first spin is physical, the second, third, fourth spins are virtual at the legs a, b, c, respectively.

According to the above discussion, the site tensor T^s can be decomposed as

$$T^s = \left(\widetilde{T}_1 \otimes K_1\right) \oplus \left(\widetilde{T}_2 \otimes K_2\right),$$

where we have $\widetilde{T}_{1,2}$ denote quantum states in the flavor space $\mathbb{D}_{\frac{1}{2}\frac{1}{2}\frac{1}{2}}$. Remember $\widetilde{T}_{1,2}$ is real since the site tensor is a Kramers singlet. Further, we require the site tensor satisfies Eq. (B14).

For a virtual leg with dimension $D = n \times 2$, we introduce a set of basis $|\uparrow_\alpha\rangle$, $|\downarrow_\alpha\rangle$, where $\alpha = 1, \dots, n$ labels the extra degeneracy. Thus, the site state can be expressed as

$$\begin{aligned}\hat{T}^s &= A_1 \otimes \hat{K}_1 + A_2 \otimes \hat{K}_2\\ &= \sum_{\alpha,\beta,\gamma} \Big\{ (A_1)_{\alpha\beta\gamma} \Big[|\uparrow\rangle \otimes \big(|\downarrow_\alpha\uparrow_\beta\downarrow_\gamma\rangle - |\downarrow_\alpha\downarrow_\beta\uparrow_\gamma\rangle\big) - |\downarrow\rangle \otimes \big(|\uparrow_\alpha\uparrow_\beta\downarrow_\gamma\rangle - |\uparrow_\alpha\downarrow_\beta\uparrow_\gamma\rangle\big)\Big]\\ &\qquad + (A_2)_{\alpha\beta\gamma} \Big[|\uparrow\rangle \otimes \big(2|\uparrow_\alpha\downarrow_\beta\downarrow_\gamma\rangle - |\downarrow_\alpha\uparrow_\beta\downarrow_\gamma\rangle - |\downarrow_\alpha\downarrow_\beta\uparrow_\gamma\rangle\big)\\ &\qquad + |\downarrow\rangle \otimes \big(2|\downarrow_\alpha\uparrow_\beta\uparrow_\gamma\rangle - |\uparrow_\alpha\uparrow_\beta\downarrow_\gamma\rangle - |\uparrow_\alpha\downarrow_\beta\uparrow_\gamma\rangle\big)\Big]\Big\}.\end{aligned}$$

The Greek indices α, β, γ run over the flavor degeneracy 1 through n. We can simplify the above equation as

$$\begin{aligned}\hat{T}^s = \sum_{\alpha,\beta,\gamma} \Big\{ &\big(A_1 - A_2\big)_{\alpha\beta\gamma}\big(|\uparrow\rangle \otimes |\downarrow_\alpha\uparrow_\beta\downarrow_\gamma\rangle + |\downarrow\rangle \otimes |\uparrow_\alpha\downarrow_\beta\uparrow_\gamma\rangle\big) \\ &- \big(A_1 + A_2\big)_{\alpha\beta\gamma}\big(|\uparrow\rangle \otimes |\downarrow_\alpha\downarrow_\beta\uparrow_\gamma\rangle + |\downarrow\rangle \otimes |\uparrow_\alpha\uparrow_\beta\downarrow_\gamma\rangle\big) \\ &+ 2\big(A_2\big)_{\alpha\beta\gamma}\big(|\uparrow\rangle \otimes |\uparrow_\alpha\downarrow_\beta\downarrow_\gamma\rangle + |\downarrow\rangle \otimes |\downarrow_\alpha\uparrow_\beta\uparrow_\gamma\rangle\big)\Big\}.\end{aligned}$$

Further, according to Eq. (B14), cyclic permutation of the virtual spins results in the identical tensor, which in turn imposes the conditions on $A_{1,2}$ as

$$\big(A_1 - A_2\big)_{\alpha\beta\gamma} = -\big(A_1 + A_2\big)_{\gamma\alpha\beta} = 2\big(A_2\big)_{\beta\gamma\alpha} \equiv \mathcal{C}_{\alpha\beta\gamma}, \tag{B19}$$

for any values of α, β and γ. For the $n = 1$ (no flavor degeneracy) case, solving Eq. (B19) with $\alpha = \beta = \gamma = 1$ automatically gives $A_{1,2} = 0$. Namely, one cannot write a fully symmetric wavefunction with trivial IGG on honeycomb lattice with $D = 2$ ($n = 1$) PEPS.

For $n = 2$ ($D = 4$), one can choose $W_\sigma = \sigma^3$ and easily solve the above equation imposing the constraint by reflection [Eq. (B15)]. Thus, one can find the following 2 independent solutions

$$\begin{aligned}\hat{A}^{(1)} &= \mathcal{P}\Big(2|\uparrow;\downarrow_2\uparrow_1\downarrow_2\rangle - |\uparrow;\downarrow_1\uparrow_2\downarrow_2\rangle - |\uparrow;\downarrow_1\downarrow_2\uparrow_2\rangle + 2|\downarrow;\uparrow_2\downarrow_1\uparrow_2\rangle - |\downarrow;\uparrow_1\downarrow_2\uparrow_2\rangle - |\downarrow;\uparrow_1\uparrow_2\downarrow_2\rangle\Big), \\ \hat{A}^{(2)} &= \mathcal{P}\Big(|\uparrow;\downarrow_2\uparrow_1\downarrow_1\rangle - |\uparrow;\downarrow_1\uparrow_1\downarrow_2\rangle + |\downarrow;\uparrow_2\downarrow_1\uparrow_1\rangle - |\downarrow;\uparrow_1\downarrow_1\uparrow_2\rangle\Big),\end{aligned} \tag{B20}$$

where $\mathcal{P}$ stands for cyclic permutation of the virtual spins. Here, we use the $\hat{A}$ for the expression of the state that includes the spin basis.

The linear combination $\hat{T}^s = c_1\hat{A}^{(1)} + c_2\hat{A}^{(2)}$ with arbitrary real coefficients c_λ is the most general fully symmetric spin liquid states within our classification scheme. The states thus constructed are generically topologically trivial since the trivial IGG was used in classifying possible spin liquid states. However, there are two special cases, namely $c_1 = 0$ or $c_2 = 0$. In those cases, the PEPS wavefunctions actually have emergent $U(1)$ IGG. To identify the nontrivial IGG, let us consider the case where $\hat{T}^s = \hat{A}^{(1)}$. The site tensor share the feature that all its components are formed by two flavor 2 spins and a single flavor 1 spin. We define the action on virtual legs $U(\theta)$ as multiplying $\mathrm{e}^{\mathrm{i}\theta}$ on flavor 2 spins while keeping spins with flavor 1 untouched. Then, it is straightforward to check that the whole PEPS is invariant (up to a U(1) phase) under the gauge transformation which act $U(\theta)$ on all virtual legs of tensors on site u, $U(-\theta)$ on virtual legs of tensors on site v, and $U^{-1}(\theta)$ or $U^{-1}(-\theta)$ on virtual legs of bond tensors for any θ. The above obervation also holds for $\hat{T}^s = \hat{A}^{(2)}$ once we define $U(\theta)$ as acting $\mathrm{e}^{\mathrm{i}\theta}$ on spins with flavor 1 and leaving flavor 2 spins untouched. These kind of gauge transformations form a U(1) group. In other words, the wavefunctions considered above describe U(1) spin liquids, which will generally be confined in the long wavelength in two dimenstions [23], and lead to spontaneous symmetry breaking phases. Therefore, one should choose c_i to be nonzero to avoid nontrivial IGG.

Appendix C: Symmetric fermionic PEPS on honeycomb lattice

In this section, we will construct a symmetric wavefunction for a half-filled spinless femion system defined on honeycomb lattice using fermionic PEPS.

Let us consider the maximally entangled virtual (auxiliary) fermionic bond state

$$|\mathrm{bond}\rangle = (\alpha_u^\dagger + \alpha_v^\dagger)|0\rangle_{aux} = |10\rangle_{aux} + |01\rangle_{aux},$$

where $\alpha_u^\dagger$ and $\alpha_v^\dagger$ are the creation operators of auxiliary fermions for the bond between the sublattice sites u and v, acting on the vacuum $|0\rangle_{aux}$ of the auxiliary fermion. The input state is obtained by covering all the bonds of honeycomb lattice with the above bond state, $|\mathrm{input}\rangle \equiv \prod_{\in \mathrm{all\,bonds}} |\mathrm{bond}\rangle$ as depicted by green ellipses in Fig. 1 (a). To obtain a physical quantum state one acts with a projector, $Q = \prod_i Q_{iu}Q_{iv}$ [36,37] defined here as

$$\begin{aligned}Q_{iu} &= \mathcal{U}^{f_i}_{a_i b_i c_i}(c_{iu}^\dagger)^{f_i}|0\rangle_p\langle 0|_{aux}(\alpha_{iu})^{a_i}(\beta_{iu})^{b_i}(\gamma_{iu})^{c_i}, \\ Q_{iv} &= \mathcal{V}^{f_i'}_{l_i m_i n_i}(c_{iv}^\dagger)^{f_i'}|0\rangle_p\langle 0|_{aux}(\alpha_{iv})^{l_i}(\beta_{iv})^{m_i}(\gamma_{iv})^{n_i},\end{aligned} \tag{C1}$$

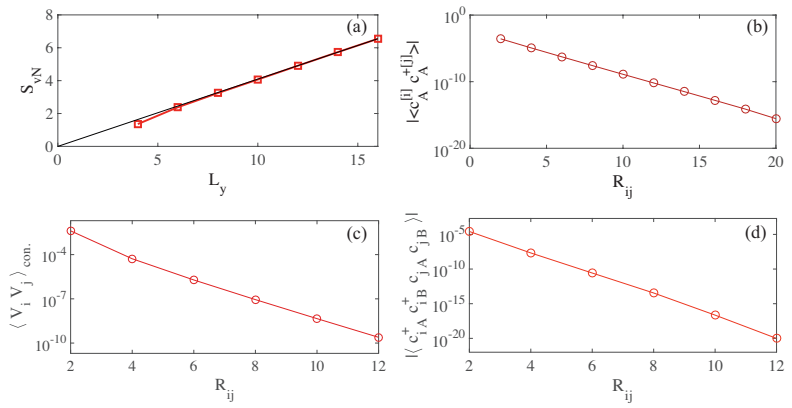

FIG. C1. (Color online) Results for fermionic PEPS with the projector defined in Eq. (C2). Plots of (a) entanglement entropy, (b) equal time Green's function, (c) bond correlation ($V_i = c^\dagger_{iu}c_{iv}$), and (d) pairing correlation as a function of the distance $R_{ij} = |\mathbf{x}_i - \mathbf{x}_j|/|\mathbf{a}_1|$, where $\mathbf{x}_i$ is the position vector of i-th unit cell.

where $c^\dagger_{is}$ is the creation operator of the physical fermion on the sublattice-s in the i-th unit cell, and $|0\rangle_p$ is the vacuum of the physical fermion. Virtual fermion operators $\alpha_{is}, \beta_{is}, \gamma_{is}$ act respectively on the a, b, c bonds around the site $s = u, v$ shown in Fig. 1(b). Summation over the fermion occupation numbers 0 and 1 are assumed for the indices $a_i, b_i, c_i, l_i, m_i, n_i, f_i, f'_i$. The resulting quantum state is $|\psi\rangle = Q|\text{input}\rangle$.

The choice of the projectors are dictated by the requirement to get a fully symmetric and half-filled quantum state. We choose to project singly (doubly) occupied three-leg virtual fermion state ($a_i + b_i + c_i = 1(2)$) in Eq. (C1)) into an empty (singly occupied) physical fermion state ($f_i = 0(1)$) in Eq. (C1)). Further considering the lattice symmetry we propose the following ansatz

$$\begin{aligned} Q_{is} = &|0\rangle_p\langle 0|_{aux}\,(\alpha_{is} + \beta_{is} + \gamma_{is}) \\ &+ c^\dagger_{is}|0\rangle_p\langle 0|_{aux}\,(\beta_{is}\alpha_{is} + \gamma_{is}\beta_{is} + \alpha_{is}\gamma_{is})\,. \end{aligned} \tag{C2}$$

Working with the tensor network of fermionic PEPS requires more careful consideration than its bosonic counterpart due to the introduction of fermionic swap gates to account for the anti-commuting property of fermions[38,39].

The entanglement entropy of our fermionic PEPS ansatz was obtained using the same sample geometry and the contraction technique as in the earlier bosonic PEPS calculation, imposing a similar threshold for numerical errors. As shown in Fig. C1 (a), $S_{\text{TEE}} = 0.008$ was extracted by fitting the entanglement entropy data, in nice agreement with the topologically trivial nature of the ansatz state. In order to measure the expectation values of operators, we employ the same method and algorithm with the same threshold for numerical error to contract the fermionic PEPS as before in the bosonic case.

Equal-time Green's function $\langle c_{iu}c^\dagger_{ju}\rangle$, the bond correlation function $\langle V_iV_j\rangle - \langle V_i\rangle\langle V_j\rangle$ ($V_i = c^\dagger_{iu}c_{iv}$), and the pair correlation function $\langle c^\dagger_{iu}c^\dagger_{iv}c_{ju}c_{jv}\rangle$ are calculated, assuming the open geometry with zigzag edges along the horizontal directions and armchair edge along the vertical directions. Virtual vacuum states are imposed along the whole boundary. All the correlations are rotationally symmetry and exponentially decaying as shown in Fig. C1 (b)-(d), confirming the existence of the energy gap. By measuring the occupation, we confirmed that the ansatz is half-filled: $\langle c^\dagger_{is}c_{is}\rangle = 1/2$. Therefore, we conclude our ansatz is a fully symmetric, topologically trivial, gapped and half-filled fermionic quantum state without charge density order and superconducting order.

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