Lieb-Schultz-Mattis theorem and its generalizations from the perspective of the symmetry-protected topological phase

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We ask whether a local Hamiltonian with a featureless (fully gapped and nondegenerate) ground state could exist in certain quantum spin systems. We address this question by mapping the vicinity of certain quantum critical point (or gapless phase) of the d-dimensional spin system under study to the boundary of a $(d+1)$-dimensional bulk state, and the lattice symmetry of the spin system acts as an onsite symmetry in the field theory that describes both the selected critical point of the spin system and the corresponding boundary state of the $(d+1)$-dimensional bulk. If the symmetry action of the field theory is nonanomalous, i.e., the corresponding bulk state is a trivial state instead of a bosonic symmetry-protected topological (SPT) state, then a featureless ground state of the spin system is allowed; if the corresponding bulk state is indeed a nontrivial SPT state, then it likely excludes the existence of a featureless ground state of the spin system. From this perspective, we identify the spin systems with SU(N) and SO(N) symmetries on one-, two-, and three-dimensional lattices that permit a featureless ground state. We also verify our conclusions by other methods, including an explicit construction of these featureless spin states.

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I. INTRODUCTION

The Lieb-Schultz-Mattis (LSM) theorem [1], and its higher-dimensional generalizations [2,3], state that if a quantum spin system defined on a lattice has odd number of spin-$\frac{1}{2}$ per unit cell, then any local spin Hamiltonian which preserves the spin and translation symmetry cannot have a featureless (gapped and nondegenerate) ground state. This implies that any symmetry-allowed Hamiltonian on the spin Hilbert space defined above can only have the following possible scenarios: (i) its ground state spontaneously breaks either the spin symmetry or the lattice symmetry, hence leads to degenerate ground states and possible gapless Goldstone modes; (ii) it has gapped and degenerate ground states without breaking any symmetry, i.e., its ground state develops a topological order (the second possibility can only happen in two- and higher-dimensional systems); (iii) its ground state has algebraic (power-law) correlation function of physical quantities, and the spectrum is again gapless [this scenario happens most often in one-dimensional (1D) spin systems, while still possible in higher dimensions].

On the other hand, there are lattice spin systems for which one can very easily construct a local Hamiltonian with a featureless ground state that preserves all the symmetry. One class of such states are called the Affleck-Kennedy-Lieb-Tasaki (AKLT) states [4], which can be constructed for an integer spin chain in 1D, the spin-2 antiferromagnet on the square lattice, and the spin-$\frac{3}{2}$ antiferromagnet on the honeycomb lattice, etc. Of course, these systems violate the crucial "odd number of spin-$\frac{1}{2}$ per unit cell" assumption of the LSM theorem.

However, there are also some spin systems in the "middle ground" where the answers are not so clear. These systems do not meet the key assumption of the LSM theorems, while a simple analog of the AKLT state mentioned above does not obviously exist. For example, the honeycomb lattice has two sites per unit cell, thus a spin-$\frac{1}{2}$ system on the honeycomb lattice has even number of spin-$\frac{1}{2}$ per unit cell, and hence there is no LSM theorem to exclude a featureless ground state. But, it has been a long-standing problem whether a featureless spin-$\frac{1}{2}$ state exists or not on the honeycomb lattice. Another example is the spin-1 antiferromagnet on the square lattice. Depending on the Hamiltonian, possible states of this system include the Néel state which spontaneously breaks the spin symmetry, and a nematic type of valence bond solid state which breaks the lattice rotation symmetry, etc. But, the existence of a featureless state is not obvious. However, recent progresses indicate that featureless states do exist in these two "middle ground" examples mentioned above [5–7], with a more sophisticated construction compared with the AKLT state.

Another seemingly very different subject is the symmetry-protected topological (SPT) state [8,9], which is a generalization of topological insulators. By definition, the ground state of the $(d+1)$-dimensional bulk of a SPT phase must be gapped and nondegenerate, while its d-dimensional boundary state must be either gapless or degenerate, as long as certain symmetries are preserved. In the last few years, the classification of bosonic SPT states with onsite internal symmetries has been well understood [8–17]. The d-dimensional boundary of a $(d+1)$-dimensional SPT state, just like those d-dimensional spin systems where the LSM theorem applies, cannot be trivially gapped. The key difference between these two systems is that the former is (usually) protected by an onsite symmetry, while the latter is protected by the spin and lattice symmetries together. However, the fact that neither system permits a featureless state suggests that we can potentially formulate both systems in a similar way. The connection to three-dimensional

(3D) bulk SPT states has been exploited in order to understand the fractional excitations of two-dimensional (2D) topological orders with both spin and lattice symmetries [18].

Since we are comparing two d-dimensional systems with very different ultraviolet regularizations, their analog can only be made precise when both systems are tuned close to a point where a low-energy field theory description becomes available. For example, the relation between the gapless spin chain and the anomaly of a Z_2 global symmetry (the onsite interpretation of the translation symmetry) was made in Ref. [19]. Thus, for our purpose, when we analyze a d-dimensional spin system, we will first tune it to a critical point described by a field theory, then interpret the lattice symmetry as an onsite symmetry, and interpret the d-dimensional field theory as the boundary state of a $(d+1)$-dimensional bulk. If the corresponding $(d+1)$-dimensional bulk is a trivial state instead of a nontrivial SPT state, then a featureless spin state must exist not too far from that critical point in the phase diagram; if the corresponding bulk is indeed a nontrivial SPT state, then it highly suggests that a featureless spin ground state does not exist.

However, the latter statement may not be necessarily true: If around that selected critical point of the spin system the field theory is formally equivalent to a SPT boundary state, it only rules out the featureless spin state at the vicinity of that critical point. But, in principle, a featureless state could be far away from the critical point in the phase diagram, and hence beyond the reach of the field theory.

In Secs. II–V, we will discuss SU(N) and SO(N) systems on a 1D chain, 2D square lattice, 2D honeycomb lattice, and 3D cubic lattice, respectively, by mapping them to the boundary of 2D, 3D, and 4D bulk states. We will identify those spin systems that permit a featureless ground state. For all of these spin systems, we can explicitly construct a featureless tensor product state that is an analog of the AKLT state. Some examples of these featureless states will be discussed in Sec. VI. In Sec. VI we will also verify our conclusions by making connection with a previous study on LSM theorem based on lattice homotopy class [20].

II. 1D SPIN CHAIN

A. SU(2) spin-$\frac{1}{2}$ chain

In this section we first discuss one-dimensional spin chains with SU(2) symmetry. The low-energy physics of the Heisenberg antiferromagnetic spin-$\frac{1}{2}$ chain with a SU(2) spin symmetry can be captured by the following nonlinear sigma model in (1 + 1)D with a Wess-Zumino-Witten (WZW) term at level 1 [21]:

$$\mathcal{S} = \int dx\, d\tau\, \frac{1}{g}(\partial_\mu \vec{n})^2 + \frac{2\pi i}{\Omega_3}\int_0^1 du\, \epsilon_{abcd} n^a \partial_\tau n^b \partial_x n^c \partial_u n^d, \tag{1}$$

where $\vec{n}$ is a four-component vector with unit length, and Ω_3 is the volume of S^3 with unit radius. The physical meaning of $\vec{n}$ is that (n_1,n_2,n_3) is the three-component Néel order parameter, while $n_4 \sim \phi$ is the valence bond solid (VBS) order parameter. If there is a SO(4) rotation symmetry of the four-component vector $\vec{n}$, the coupling constant g will flow to a fixed point, which corresponds to the $SU(2)_1$ conformal field

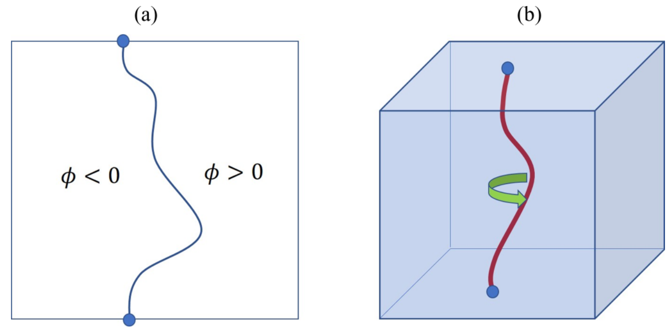

FIG. 1. (a) The decorated domain-wall construction of the 2D SPT state whose boundary is analogous to a SU($2N$) spin chain with a LSM theorem. A 1D SPT state with PSU($2N$) symmetry is decorated to each domain wall, and the domain wall terminates at the boundary with a dangling projective representation of the PSU($2N$) SPT state. (b) The decorated vortex line construction of the 3D SPT state whose boundary is analogous to a 2D spin system either on the square or honeycomb lattice. Again, we decorate each vortex line with a 1D SPT state. But, when the 2D boundary is mapped to the square and honeycomb lattice spin systems, the vortex line in the bulk has a Z_4 and Z_3 conservation, which must be compatible with the classification of the 1D SPT state decorated on each vortex line in order to guarantee a nontrivial 3D SPT.

theory [22,23]. The SO(4) symmetry becomes an emergent symmetry of the spin-$\frac{1}{2}$ Heisenberg chain in the infrared: the Néel and VBS order parameters both have the same scaling dimension $[\vec{n}] = \frac{1}{2}$. The key symmetry of the system is the spin SU(2) symmetry, and the translation symmetry. (n_1,n_2,n_3) transforms as a vector under spin SU(2), and $n_4 \sim \phi$ is a SU(2) singlet; and under translation by one lattice constant, $T_x : \vec{n} \to -\vec{n}$. The physical meaning of Eq. (1) is the intertwinement between the Néel and VBS order parameters: the domain wall of the VBS order parameter carries a spin-$\frac{1}{2}$.

The field theory Eq. (1) also describes the boundary of a 2D bosonic SPT state with SO(3)$\times Z_2$ symmetry [24,25], where Z_2 acts as $\vec{n} \to -\vec{n}$. This SPT state can be understood as the decorated domain-wall construction [26]: we decorate every Z_2 symmetry-breaking domain wall in the 2D bulk with a Haldane phase with SO(3) symmetry [Fig. 1(a)], then proliferate the Z_2 domain walls to restore the Z_2 symmetry. The so-constructed phase in the bulk is the desired SO(3)$\times Z_2$ SPT phase. And at the 1D boundary of the system, there is a spin-$\frac{1}{2}$ degree of freedom localized at every Z_2 domain wall, which is also the boundary state of the Haldane phase decorated at each Z_2 domain wall in the bulk. This is consistent with the physics of the spin-$\frac{1}{2}$ chain.

This simple example demonstrates that the lattice translation symmetry, once interpreted as an onsite symmetry in a field theory, is equivalent to an "anomalous" symmetry of the boundary of a higher-dimensional SPT state. And by definition the boundary of a SPT state cannot be trivially gapped without degeneracy, which is consistent with the LSM theorem of the spin-$\frac{1}{2}$ chain [1]. The method of identifying the translation symmetry of a 1D system as a Z_2 onsite symmetry was also used in Ref. [19], and a symmetry-protected critical phase and renormalization group (RG) flow were identified.

Here, we stress that the 1D SPT phase decorated at a Z_2 domain wall must have a Z_2 classification as long as the symmetry G of the 1D SPT phase commutes with the Z_2, i.e., two of the 1D SPT phases must fuse into a trivial state. One way to see this is that, after gauging the Z_2 symmetry, the vison (π flux introduced by the Z_2 gauge symmetry) preserves the symmetry G as long as G commutes with Z_2, and the vison is the boundary of the 1D decorated SPT state [26]. Since two visons fuse into a local excitation, the 1D SPT state must have a Z_2 classification. But, at a Z_2^T (time-reversal) domain wall one can decorate a lower-dimensional SPT phase with (for example) Z classification because the antidomain wall of Z_2^T is the time-reversal conjugate of a Z_2^T domain wall, which is automatically decorated with the "inverse" state of the SPT state decorated at the Z_2^T domain wall.[1] This observation is consistent with many known facts about SPT phases. For instance, in three-dimensional space, there is a Z_2^T SPT which can be viewed as Z_2^T domain walls decorated with the E_8 invertible topological order [10], but there is no such decorated domain-wall construction for 3D SPT phases with a Z_2 symmetry.

B. Spin chain with reduced symmetry

Now, one can exploit the connection between 1D spin chains and the boundary of 2D SPT states even further, and consider a spin chain with a reduced spin symmetry. For example, we can start with a spin-$\frac{1}{2}$ chain, and break the SO(3) spin symmetry down to its subgroup $G \rtimes Z_2$, where Z_2 is the spin π rotation $S^z \to -S^z$, $S^y \to -S^y$, and G is a subgroup of the in-plane U(1) spin symmetry. Whether the spin chain can be featureless or not is equivalent to the problem of whether the corresponding bulk state with $(G \rtimes Z_2) \times Z_2$ symmetry is a nontrivial SPT state or not; based on the "decorated domain-wall" picture mentioned above, this again is equivalent to the problem of whether the 1D Z_2 domain wall is a nontrivial 1D SPT state with $G \rtimes Z_2$ symmetry or not, and if it is indeed a nontrivial SPT, whether it has a Z_2 classification.

Now, we can look up the classification in Refs. [8,9]. For example, when $G = Z_{2n+1}$ with integer n, since there is no nontrivial 1D SPT state with $Z_{2n+1} \rtimes Z_2$ symmetry, the bulk SO(3)$\times Z_2$ SPT state discussed previously must be trivialized by reducing the SO(3) spin symmetry down to $Z_{2n+1} \rtimes Z_2$, thus, its boundary can in principle be gapped and nondegenerate. This observation already gives us a meaningful conclusion:

A spin chain with translation and $(Z_{2n+1} \rtimes Z_2)$ spin symmetry can have a featureless ground state.

By contrast, for $G = $ U(1) or Z_{2n}, a nontrivial 1D SPT state with $G \rtimes Z_2$ does exist, and it does have a Z_2 classification. Hence, the Haldane phase with SO(3) spin symmetry remains a nontrivial SPT state under the symmetry reduction to $G \rtimes Z_2$. Thus, the 2D bulk SPT state with $(G \rtimes Z_2) \times Z_2$ remains nontrivial, and hence the 1D boundary cannot be trivially gapped. This observation leads to the following conclusion:

A 1D spin-$\frac{1}{2}$ chain (likely) cannot have a featureless ground state, even if we break the SU(2) spin symmetry down to $(Z_{2n} \rtimes Z_2)$ symmetry.

[1]The authors thank D.-H. Lee for clarifying this important point for us.

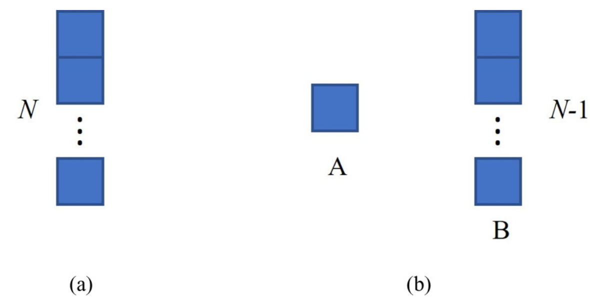

FIG. 2. (a) The self-conjugate SU($2N$) spin representation on each site considered in Sec. II C. (b) For the square, honeycomb, and cubic lattices, we consider a SU(N) spin system with a fundamental representation (FR) on sublattice A and an antifundamental representation (AFR) on sublattice B.

C. SU($2N$) spin chain

Now, let us consider spin chains with higher spin symmetries. A natural generalization of the spin-$\frac{1}{2}$ chain with translation symmetry is a SU($2N$) spin chain with self-conjugate representation on each site [Young tableau with N boxes in one column, Fig. 2(a)]. The analog of the "Néel" order parameter of this SU($2N$) spin chain is a $2N \times 2N$ Hermitian matrix order parameter $\mathcal{P}$, and it can be represented in the form

$$\mathcal{P} = V\Omega V^\dagger, \quad \Omega \equiv \begin{pmatrix} \mathbf{1}_{N\times N} & \mathbf{0}_{N\times N} \\ \mathbf{0}_{N\times N} & -\mathbf{1}_{N\times N} \end{pmatrix}, \tag{2}$$

where V is a SU($2N$) matrix. All the configurations of $\mathcal{P}$ belong to the Grassmanian manifold $\mathcal{M} = \mathrm{U}(2N)/[\mathrm{U}(N) \times \mathrm{U}(N)]$ [27,28]. To see that $\mathcal{P}$ is a natural generalization of the ordinary SU(2) Néel order parameter, we can take $N = 1$, then this Grassmanian is precisely S^2, which is the manifold of the ordinary SU(2) Néel order parameter. We can also define matrix order parameter $\mathcal{P} = \vec{n} \cdot \vec{\sigma}$ for the SU(2) spin chain, where $\vec{n}$ is the SU(2) Néel order parameter.

The effective field theory for the SU($2N$) spin chain described above can be written as [27]

$$\mathcal{S} = \int dx\, d\tau\, \frac{1}{g}\mathrm{tr}[\partial_\mu \mathcal{P} \partial_\mu \mathcal{P}] + \frac{\Theta}{16\pi}\epsilon_{\mu\nu}\mathrm{tr}[\mathcal{P}\partial_\mu \mathcal{P} \partial_\nu \mathcal{P}]. \tag{3}$$

This is the analog of the nonlinear sigma model for the SU(2) spin chain [29,30], with a Θ term which comes from the fact that for all N, the Grassmanian $\mathcal{M}$ satisfies $\pi_2[\mathcal{M}] = Z$. Under translation by one lattice constant, $\mathcal{P}$ transforms as $T_x : \mathcal{P} \to -\mathcal{P}$ ($\mathcal{P}$ and $-\mathcal{P}$ both belong to the same Grassmanian target manifold), and the coefficient Θ transforms as $T_x : \Theta \to -\Theta$, which guarantees that Θ is quantized to be multiple of π. The same field theory as Eq. (3) with a topological Θ term has been used to describe the phase diagram of the integer quantum Hall systems [31–33], while there the theory is written in the 2D real space instead of space-time. A proposed renormalization group flow for Eq. (3) is that $\Theta = 2\pi k$ are stable fixed points, while $\Theta = \pi(2k+1)$ are instable fixed points which correspond to transitions between stable fixed points $\Theta = 2k\pi$ [27].

When $\Theta = \pi$, Eq. (3) describes the SU($2N$) spin chain with self-conjugate representation on each site; when $\Theta = 2\pi$, Eq. (3) describes the Haldane phase of a SU($2N$) spin chain or, more precisely, it is the Haldane phase of a PSU($2N$) spin chain, as $\mathcal{P}$ is invariant under the center of SU($2N$). The

PSU($2N$) Haldane phase should have Z_{2N} classification [34], as its boundary could be $2N$ different projective representation of PSU($2N$), which is also the $2N$ different representation of the Z_{2N} center of SU($2N$). But, the particular state described by Eqs. (2) and (3) is the "Nth" PSU($2N$) Haldane phase, whose 0D boundary is a self-conjugate projective representation of PSU($2N$). This state has a Z_2 nature, namely, two copies of this state will be a trivial state, i.e., its boundary is no longer a projective representation of PSU($2N$). This 1D PSU($2N$) Haldane phase has been discussed in lattice models previously [35–37].

As we discussed before, the spin-$\frac{1}{2}$ SU(2) chain can also be described by Eq. (1), where a VBS order parameter is introduced. For the SU($2N$) spin chain with self-conjugate representation, the analog of Eq. (1) is

$$\mathcal{S} = \int dx\, d\tau\, \frac{1}{g}\mathrm{tr}[\partial_\mu U^\dagger \partial_\mu U] + \int_0^1 du\, \frac{i2\pi}{24\pi^2}\mathrm{tr}[U^\dagger dU]^3, \quad (4)$$

where $U = I_{2N\times 2N}\cos(\theta) + i\sin(\theta)\mathcal{P}$ is a SU($2N$) unitary matrix. Once again, when $N = 1$, U is a SU(2) matrix, whose manifold is S^3, the same as the target manifold of Eq. (1). For arbitrary N, under translation, $T_x : \theta \to \pi - \theta$, $T_x : U \to -U$. Thus, $\cos(\theta) \sim \phi$ is the VBS order parameter.

The same field theory Eq. (4) describes the boundary of a 2D SPT state with PSU($2N$) $\times Z_2$ symmetry, where Z_2 plays the role of T_x. And the physical picture of this 2D SPT is that we decorate every Z_2 domain wall with a Haldane phase with PSU($2N$) symmetry. Thus, as one would naively expect, the SU($2N$) spin chain with self-conjugate representation likely cannot have a featureless ground state because it can be mapped to the boundary of a nontrivial 2D SPT state.

D. SO(N) spin chain

A SO(N) spin chain with a translation symmetry may still obey a generalization of the LSM theorem. But, first let us review the current understanding of the Haldane phase of 1D SO(N) spin chain. When N is an odd integer, the double covering group of SO(N), i.e., spin(N), has a representation which is a spinor of SO(N). Thus, when N is odd, there is a Haldane phase with SO(N) symmetry with a Z_2 classification, as two spinors of SO(N) will merge into a linear representation of SO(N) [38]. Thus, in 2D space, there is a SPT state with SO(N) $\times Z_2$ symmetry, which is constructed by decorating the 1D SO(N) Haldane phase in each Z_2 domain wall. Then, the 1D boundary of this 2D SPT state with SO(N) $\times Z_2$ symmetry, has the feature that, at every Z_2 domain wall there must be a SO(N) spinor, and this 1D boundary cannot be trivially gapped without breaking the Z_2 symmetry.

Now, let us consider a spin(N) spin chain with a spinor on every site. Two spin(N) spinors with odd N can always form a singlet, thus, this spin chain naturally hosts twofold-degenerate VBS states, which transform into each other through translation by one lattice constant. The domain wall of these two VBS states is a spin(N) spinor, which is equivalently to the domain wall of the Z_2 order parameter at the 1D boundary of the 2D SO(N) $\times Z_2$ SPT state mentioned above. Based on these observations, we can conclude that *with odd N, a 1D spin(N) spin chain with spinor representation on every site likely does not permit a featureless gapped state*.

For even N, let us take $N = 2n$, then the Haldane phase has a richer structure. SO($2n$) has a Z_2 center which commutes with all the other elements, thus we can actually consider the Haldane phase with symmetry PSO($2n$) = SO($2n$)/Z_2. Then, according to Ref. [34], the center of spin($2n$) can be either Z_4 or $Z_2 \times Z_2$, for odd and even integer n, respectively. But, in either case, a Haldane phase with PSO($2n$) symmetry could have either spinor or vector representation at the boundary, both cases are nontrivial Haldane phase. And, we can construct a 2D SPT with PSO($2n$) $\times Z_2$ symmetry, by decorating the Z_2 domain wall with a PSO($2n$) Haldane phase. But, this PSO($2n$) Haldane phase must have a Z_2 nature, in the sense that two copies of the Haldane phase must be a trivial state because two Z_2 domain walls will fuse into a trivial defect. Thus, for both odd and even n, we can always decorate the Z_2 domain wall with the PSO($2n$) Haldane phase with a SO($2n$) vector at the boundary, which leads to the following conclusion:

A 1D SO($2n$) *spin chain with vector representation on every site likely does not permit a featureless gapped state.*

This conclusion is consistent with the result of Ref. [39].

III. SPIN SYSTEMS ON THE SQUARE LATTICE

A. SU(2) spin systems

The generalized LSM theorem in higher dimensions does apply to the 2D spin-$\frac{1}{2}$ system on the square lattice [2,3], i.e., there cannot be a featureless spin state on the square lattice for a spin-$\frac{1}{2}$ system with SU(2) spin symmetry. This conclusion is consistent with many observations, including a generalization of Eq. (1) to (2 + 1)D [40]:

$$\mathcal{S} = \int d^2x\, d\tau\, \frac{1}{g}(\partial_\mu \vec{n})^2 + \frac{2\pi i}{\Omega_4}\int_0^1 du\, \epsilon_{abcde} n^a \partial_\tau n^b \partial_x n^c \partial_y n^d \partial_u n^e, \quad (5)$$

where $\vec{n}$ is a five-component unit vector, which forms the target manifold S^4 with volume Ω_4. (n_1,n_2,n_3) is still the three-component Néel order parameter on the square lattice, while n_4 and n_5 are the columnar VBS states along the x and y directions, respectively. The site-centered 90° rotation of the square lattice acts on (n_4,n_5) as a Z_4 rotation, and close to the deconfined quantum critical point [41,42], one can usually embed the Z_4 into an enlarged U(1) group.

The physical meaning of the WZW term in Eq. (5) is that the vortex of (n_4,n_5) carries a spin-$\frac{1}{2}$ excitation [43], and the skyrmion of (n_1,n_2,n_3) carries lattice momentum. If we view $b \sim n_4 + in_5$ as a boson annihilation operator, then the skyrmion of (n_1,n_2,n_3) would carry nonzero boson number of b. Thus, if we destroy the ordinary Néel order by condensing the skyrmions of the Néel order parameter, the system automatically develops a columnar VBS order; and if we destroy the VBS order by condensing the (Z_4) vortex of the columnar VBS order parameter, the system automatically breaks the spin symmetry and develops the Néel order.

Equation (5) can be derived explicitly by starting with the π-flux spin-liquid state on the square lattice [44], and it was proposed as an effective field theory [40] that describes the deconfined quantum critical point between Néel and VBS order on the square lattice [41,42], and this is the critical point whose vicinity we will study and map to the boundary of a 3D system, as we discussed in the Introduction. The key physics of the intertwinement between the Néel and VBS order parameters is encoded in the WZW term. Equation (5) is capable of encapsulating a large $\mathrm{SO}(5)\times Z_2^T$ symmetry, and it also describes the boundary state of a 3D bosonic SPT state whose symmetry can be as large as $\mathrm{SO}(5)\times Z_2^T$. Equation (5) can also describe the boundary of 3D SPT states with a symmetry that is a subgroup of $\mathrm{SO}(5)\times Z_2^T$ [10,11]. According to the definition of SPT states, if the 3D bulk is a nontrivial SPT state, then the boundary cannot be a featureless state; while if the 3D bulk is a trivial direct product state after breaking the $\mathrm{SO}(5)\times Z_2^T$ to its subgroup, then the boundary in principle can be trivially gapped without degeneracy.

It is clear that if the symmetry $\mathrm{SO}(5)\times Z_2^T$ is reduced to $\mathrm{SO}(3)\times\mathrm{U}(1)$, where (n_1,n_2,n_3) rotates as a vector of SO(3) and singlet under U(1), while (n_4,n_5) transforms as a vector of U(1) and singlet of SO(3), the bulk is still a nontrivial SPT state. And, this state can be understood as the "decorated vortex line" construction introduced in Ref. [10]: one first breaks the U(1) symmetry by condensing the two-component vector (n_4,n_5), and decorate a Haldane phase with the SO(3) spin symmetry on each vortex loop of (n_4,n_5) with odd vorticity, then proliferate the vortex loops to restore the U(1) symmetry. The SPT state so constructed has a Z_2 classification, which is consistent with the Z_2 classification of the Haldane phase decorated in each vortex loop, and also consistent with the Z_2 nature of the fourth Steifel-Whitney class of the SO(5) gauge bundle [44]. This implies that two copies of the 3D SPT states with $\mathrm{SO}(3)\times\mathrm{U}(1)$ symmetry weakly coupled together will become a trivial 3D bulk state.

The site-centered rotation symmetry of the square lattice acts on (n_4,n_5) as the Z_4 subgroup of U(1). The 3D nontrivial SPT state with $\mathrm{SO}(3)\times\mathrm{U}(1)$ symmetry survives under the further symmetry breaking of U(1) to Z_4, as a Z_4 vortex loop is still a well-defined object in the bulk and can be decorated with a 1D Haldane phase. The same conclusion still holds if we consider a spin-$\frac{1}{2}$ system on the rectangular lattice (or a more general distorted square lattice with translation symmetry and one site per unit cell). Now, this system corresponds to the boundary of a 3D bulk SPT with $\mathrm{SO}(3)\times Z_2^x\times Z_2^y$. n_4, n_5 each changes its sign under one of these two Z_2's, while (n_1,n_2,n_3) is odd under both Z_2's. The two Z_2's correspond to translation along x and y directions, respectively. The 3D bulk SPT state can be viewed as decorating the Z_2^x domain wall with the 2D SPT with $\mathrm{SO}(3)\times Z_2^y$ symmetry or equivalently decorating the Z_2^y domain wall with the 2D $\mathrm{SO}(3)\times Z_2^x$ SPT state. This observation is consistent with the generalized LSM theorem which states that a spin-$\frac{1}{2}$ system on the rectangular lattice cannot have a featureless state.

Just like the previous section, if we break the spin symmetry down to $G\rtimes Z_2$, when $G=Z_{2n+1}$ the spin system on the square lattice allows a featureless state because the Haldane phase that we decorated in the vortex loop becomes a trivial state with only $Z_{2n+1}\rtimes Z_2$ spin symmetry.

Now, suppose we consider a spin-1 system on the square lattice, then a similar deconfined quantum critical point corresponds to Eq. (5) with a level-2 WZW term: the coefficient of the WZW term doubles. This equation with a level-2 WZW term can be derived using the π-flux spin-liquid state of a spin-1 system on the square lattice: there are twice as many Dirac fermions in the Brillouin zone compared with the case derived in Ref. [44], thus, the level of the WZW term also doubles [the difference from the spin-$\frac{1}{2}$ π-flux state is that the spin-1 π-flux state has a Sp(4) gauge fluctuation [45], while the spin-$\frac{1}{2}$ π-flux state has a SU(2) gauge fluctuation]. The physical meaning of this term is that the vortex of (n_4,n_5) now carries a spin-1 instead of spin-$\frac{1}{2}$, which is equivalent to the physics of the boundary of two weakly coupled 3D SPT states with $\mathrm{SO}(3)\times\mathrm{U}(1)$ symmetry, and as we discussed above, this state is generically a trivial state in the bulk. Thus, its boundary could be a featureless gapped state. This observation implies that *a spin-1 system on the square lattice permits a featureless state, which is consistent with the conclusion of Ref. [6]*.

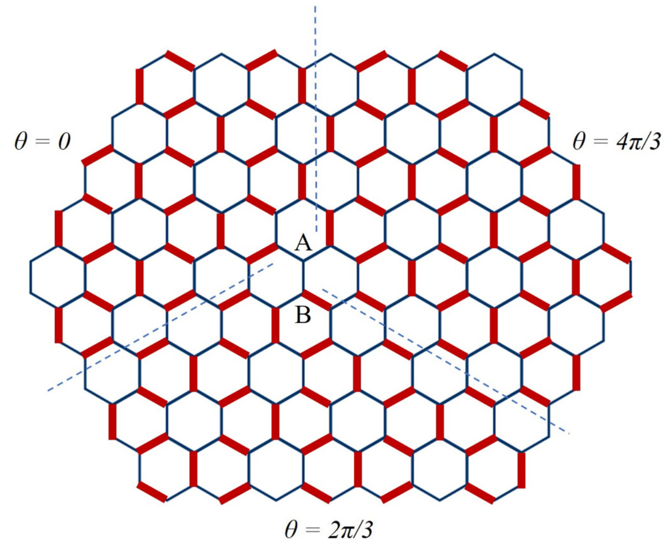

FIG. 3. A Z_3 vortex of the VBS order parameter on the honeycomb lattice has a vacant site on the sublattice A, and hence carries a fundamental representation of the SU(N) spin.

B. SU(N) and SO(N) spin systems

Now, let us consider a SU(N) spin system on the square lattice, with fundamental representation (FR) on sublattice A and antifundamental representation (AFR) on sublattice B. Since the spins on two nearest-neighbor sites can still form a SU(N) spin singlet, the columnar VBS order parameter and its Z_4 structure still naturally hold: the site-centered lattice rotation acts as a Z_4 rotation of the columnar VBS order parameter in this system. The Z_4 vortex (antivortex) of the VBS order parameter always has a vacant sublattice A (B) in the core, hence, it always carries SU(N) FR (AFR). This is consistent with the fact that a vortex-antivortex pair can always annihilate, hence, the quantum spin they carry must together form a spin singlet. An analogous effect on the honeycomb lattice is depicted in Figs. 3 and 4.

With large enough N, a Heisenberg model with the representation described above should have the fourfold-degenerate VBS state [46,47]. Now, we ask whether a featureless ground state of this spin system is in principle allowed or not. Once again, we first view the Z_4 lattice rotation as an onsite internal symmetry, and enlarge it to U(1). Then, the 2D spin system on

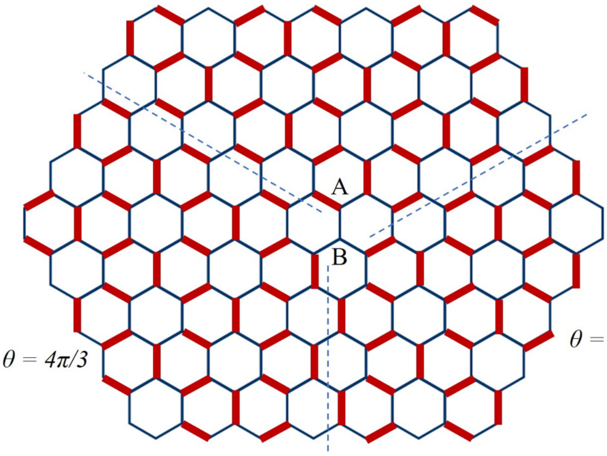

FIG. 4. An antivortex of the VBS order parameter on the honeycomb lattice has a vacant site on the sublattice B, and hence carries an antifundamental representation of the SU(N) spin.

the square lattice can be *potentially* viewed as the boundary of a 3D bosonic SPT state with PSU(N) $\times$ $U(1)$ symmetry.

The bosonic SPT states with PSU(N) $\times$ U(1) symmetry do exist in 3D, and they can be interpreted as the decorated vortex loop construction, i.e., we decorate every U(1) unit vortex loop with a 1D PSU(N) Haldane phase, whose boundary is a projective representation of the PSU(N), or a faithful representation of SU(N). As we have discussed, 1D PSU(N) Haldane phase has a Z_N classification, which corresponds to N different projective representations of the PSU(N) group, or N different representations of the Z_N center of SU(N).

In general, the $N-1$ different nontrivial Haldane phases of PSU(N) can be described by Eq. (3) with $\Theta = 2\pi$, and $\mathcal{P}$ replaced by [27]

$$\mathcal{P} = V\Omega V^\dagger, \quad \Omega \equiv \begin{pmatrix} \mathbf{1}_{m\times m} & \mathbf{0}_{m\times N-m} \\ \mathbf{0}_{N-m\times m} & -\mathbf{1}_{N-m\times N-m} \end{pmatrix} \tag{6}$$

with $m = 1, \ldots N-1$, and V is a SU(N) matrix. All the configurations of $\mathcal{P}$ belong to the Grassmanian manifold U(N)/[U(m) $\times$ U($N-m$)]. In our case, when the vortex line terminates at the boundary, the vortex at the boundary will carry a FR of SU(N), hence, for our case we need to choose $m = 1$, and $\mathcal{P}$ becomes the CP^{N-1} manifold.

However, let us not forget that eventually we need to break the U(1) symmetry down to Z_4. Then, for the 3D SPT state to survive under this symmetry breaking, the Z_N classification of the PSU(N) Haldane phase must be compatible with the Z_4 vortex. If N and 4 are coprime, then this bulk state definitely becomes trivial after breaking the U(1) to Z_4. For example, when $N = 3$, there is no consistent way we can decorate the Z_4 vortex with a PSU(3) Haldane phase. Because four Z_4 vortex loops merge together will no longer be a well-defined defect, while four PSU(3) Haldane phases merge together is still a nontrivial Haldane phase. Thus, for odd integer N, the 3D SPT phase with PSU(N) $\times$ U(1) symmetry becomes a trivial phase once U(1) is broken down to Z_4.

To further demonstrate that for odd integer N, the 3D SPT phase with PSU(N)$\times$ U(1) symmetry is trivialized with U(1) broken down to Z_4, we need to show that its 2D boundary can be trivially gapped out when U(1) is broken down to Z_4. One of the 2D boundary states of the 3D PSU(N) $\times$ U(1) SPT phase is a Z_N topological order, which can be constructed by starting with a superfluid order with spontaneous U(1) symmetry breaking at the 2D boundary, and then condense the N-fold vortex (a vortex with $2\pi N$ vorticity) of the superfluid order. The single vortex of the superfuid phase carries a FR of SU(N), hence, an N-fold vortex can carry a SU(N) singlet, and its condensate is a Z_N topological order which preserves all the symmetries. A 2D Z_N topological order has bosonic e and m excitations, while e and m have mutual statistics with statistical angle $\theta_{e,m} = 2\pi/N$. In our construction, the e excitation carries $1/N$ charge of the U(1) symmetry, and the m excitation carries a FR of SU(N).

Once U(1) is broken down to Z_4, in order to gap out the Z_N topological order, we can condense the bound state of a e particle and $3N$ Z_4 charges. This bound state carries $\frac{3N^2+1}{N}$ Z_4 charges. Under the Z_4 transformation, it acquires a phase $\exp\left(\frac{2\pi(3N^2+1)}{4N}i\right)$, which can always be canceled/compensated by a gauge transformation with odd integer N (the numerator of the phase angle is always a multiple of 8π with odd integer N). Thus, the condensate of this bound state will drive the Z_N topological order into a completely featureless gapped state without any anyons, and all the global symmetries are preserved. This is only possible when N is odd.

As a contrast, for even integer N, we can always construct a nontrivial 3D SPT by decorating the Z_4 vortex loop with the 1D SPT state with SU(N)/Z_2 symmetry, which has a Z_2 classification.

Now, we can make the following conclusion:

A SU(N) *spin system on the square lattice with fundamental and antifundamental representation on the two sublattices permits a featureless gapped ground state for odd integer N.*

We can also consider SO(N) spin systems on the square lattice. The analysis is very similar to the previous case. We can make the following conclusion:

A SO($2n$) *spin system with vector representation on every site likely does not permit a featureless gapped state on the square lattice.*

A SO($2n+1$) *spin system with spinor representation on every site likely does not permit a featureless gapped state on the square lattice.*

On the other hand, a SO($2n+1$) spin system with vector representation on every site does permit a featureless gapped state.

IV. SPIN SYSTEMS ON THE HONEYCOMB LATTICE

A. SU(2) spin systems

A spin-$\frac{1}{2}$ system on the honeycomb lattice, when tuned close to certain point, can also be described by Eq. (5). Equation (5) can be derived with the SU(2) spin liquid on the honeycomb lattice, like the one discussed in Ref. [48]. Now, the lattice symmetry, both the translation T_x and a site-centered 120° rotation, acts as a Z_3 subgroup of the U(1) transformation on (n_4,n_5).

Once again, the question of whether a featureless spin-$\frac{1}{2}$ state exists on the honeycomb lattice is equivalent to whether the 3D SPT state with SO(3)×U(1) symmetry is stable against breaking the U(1) down to Z_3. It turns out that this time the 3D bulk becomes a trivial state. The vortex loop decoration picture fails with a Z_3 symmetry. Suppose we decorate a Haldane phase on each Z_3 vortex loop, then three of the Z_3 vortex loops would be decorated with three Haldane phases, and due to the Z_2 classification of the 1D Haldane phase, three Haldane phases are still a nontrivial 1D SPT state. However, a threefold Z_3 vortex loop is no longer a well-defined defect any more. Thus, the decorated vortex loop picture is incompatible with the Z_3 symmetry. Thus, the bulk becomes a trivial state once we break the U(1) down to Z_3. This implies that the 2D boundary, which corresponds to the spin-$\frac{1}{2}$ system on the honeycomb lattice, permits a featureless spin state. This is consistent with the previous result on the honeycomb lattice [6,7].

We can also add other symmetries of the honeycomb lattice, such as reflection $P_x : y \to -y$. Under this reflection, $P_x : (n_1,n_2,n_3) \to -(n_1,n_2,n_3)$, while (n_4,n_5) is unchanged. In the Euclidean space-time, a reflection symmetry can be treated equivalently as the time-reversal symmetry. Thus, with both translation T_x and reflection P_x, we need to study whether the 3D SPT state with SO(3)×Z_2^T × U(1) symmetry is stable against symmetry breaking down to SO(3)×Z_2^T × Z_3. The analysis is the same as before: the 3D SPT state with SO(3)×Z_2^T × U(1) symmetry is constructed with proliferated vortex loops decorated with a 1D Haldane phase with SO(3)×Z_2^T symmetry. However, this construction is still incompatible with the Z_3 vortex loops because the classification of the Haldane phase with SO(3)×Z_2^T symmetry is $Z_2 \times Z_2$.

B. SU(*N*) and SO(*N*) spin systems

Now, let us consider a SU(N) spin system on the honeycomb lattice, again with FR on sublattice A and AFR on sublattice B. This system can still form the threefold-degenerate VBS states, and the vortex (antivortex) of the VBS order parameter has a vacant site in sublattice A (B), which carries a FR (AFR) of SU(N) (Figs. 3 and 4).

Now, we want to ask whether the 3D SPT state with PSU(N) × $U(1)$ symmetry is stable against breaking the U(1) down to Z_3. This depends on whether the PSU(N) SPT state decorated on the vortex line is compatible with the Z_3 nature of the vortex line, i.e., N at least cannot be coprime with 3. Thus, when N is coprime with 3, the 3D SPT state PSU(N) × $U(1)$ symmetry is trivialized by breaking U(1) down to Z_3.

Just like the case in the previous section, the boundary of a 3D SPT with PSU(N) × $U(1)$ symmetry could be a 2D Z_N topological order, whose e particle carries $1/N$ charge of U(1) and m particle carries a FR of SU(N). Once U(1) is broken down to Z_3, if N is coprime with 3, by condensing a bound state of e and certain number of Z_3 charges, this 2D boundary Z_N topological order is driven into a featureless gapped state.

We can now make the following conclusion:

SU(N) *spin systems on the honeycomb lattice with fundamental and antifundamental representation on the two sublattices permit a featureless gapped ground state when* N *is not a multiple of 3.*

Also, similar conclusions can be made for SO(N) spin systems:

A SO($2n$) *spin system with vector representation on every site permits a featureless state on the honeycomb lattice.*

A SO($2n+1$) *spin system with spinor or vector representation on every site also permits a featureless state on the honeycomb lattice.*

V. 3D SPIN SYSTEMS ON THE CUBIC LATTICE

A spin-$\frac{1}{2}$ system on the cubic lattice is subject to the generalized LSM theorem, thus, it cannot have a featureless state. Aside from the common Néel ordered state, another natural spin-$\frac{1}{2}$ state on the cubic lattice is the columnar VBS state. The "hedgehog monopole" of the VBS order parameter carries a spin-$\frac{1}{2}$, and the monopole of the Néel order parameter carries lattice momentum [49], whose condensate is precisely the VBS order. This system enjoys a nice self-duality structure. We can introduce the vector Néel order parameter $\vec{n}^e$ and vector VBS order parameter $\vec{n}^m$, as well as their CP^1 fields [49,50]:

$$\vec{n}^e \sim \tfrac{1}{2} z^{e\dagger}\vec{\sigma} z^e, \quad \vec{n}^m \sim \tfrac{1}{2} z^{m\dagger}\vec{\sigma} z^m. \tag{7}$$

When the spin system is driven into a photon phase, which is stable in (3 + 1)D, z^e and z^m are the gauge charge and the Dirac monopole of the dynamical U(1) gauge field a_μ, respectively.

The cubic lattice symmetry acts on $\vec{n}^m$ as the octahedral subgroup of SO(3),[2] and z^e, z^m carry projective representation of the SO(3) spin and (enlarged) SO(3) lattice symmetry, respectively. The intertwinement between the Néel and VBS orders is captured by a (3 + 1)D WZW term of a six-component vector which contains both $\vec{n}^e$ and $\vec{n}^m$ [51].

The same physics can be realized at the boundary of a 4D SPT state with SO(3)^e × SO(3)^m symmetry. This state can be understood as the "decorated monopole line" construction. In the 4D space, a SO(3)^e hedgehog monopole is a line defect, and we can decorate it with a 1D Haldane phase with SO(3)^m symmetry. The CP^1 field z^m can be viewed as the termination of the SO(3)^e hedgehog monopole line at the 3D boundary, which is also the boundary state of the 1D SO(3)^m Haldane phase. The self-duality of the boundary QED implies that the decoration construction is necessarily mutual, i.e.. we must simultaneously decorate the SO(3)^m hedgehog monopole with a Haldane phase with the SO(3)^e symmetry.

The "mutual decoration" construction can also be perceived as follows. In the 4D space, we can discuss the braiding process of two loops. Imagine we create two loops L^e and L^m from vacuum, and annihilate them at a later time, then the world sheets of both loops are topologically two-dimensional spheres, labeled as S_e^2 and S_m^2. If these two loops are braided, their world sheets are linked in the five-dimensional space-time. This linking can be interpreted as the intersection of S_e^2 with the interior of S_m^2 (which is a three-dimensional ball) at one point in the space time. Now suppose S_e^2 and S_m^2 are

[2]The octahedral group O does not include the spatial mirror (reflection) symmetry. The mirror symmetry is equivalent to time-reversal symmetry in the analysis of SPT states, as we explained previously. Including the mirror symmetry does not change our conclusions because the SO(3) Haldane phase with or without an extra time-reversal symmetry always has a Z_2 nature, i.e., two of these Haldane phases coupled together become a trivial state.

the world sheets of the $\mathrm{SO}(3)^e$ and $\mathrm{SO}(3)^m$ monopole lines respectively, if the $\mathrm{SO}(3)^m$ monopole line is decorated with the $\mathrm{SO}(3)^e$ Haldane phase, then this linking will accumulate phase 2π, which comes from the Θ term of the $\mathrm{SO}(3)^e$ Haldane phase.

The linking mentioned above is also symmetric under interchanging e and m, namely, it can be viewed as the intersection of S_m^2 with the interior of S_e^2 at another point in the space-time. Thus, if this linking accumulates phase 2π, then consistency demands that the $\mathrm{SO}(3)^e$ monopole line be decorated with the $\mathrm{SO}(3)^m$ Haldane phase too.

The 4D SPT state so constructed obviously has a Z_2 classification, as both the $\mathrm{SO}(3)^e$ and $\mathrm{SO}(3)^m$ SPT phases have Z_2 classification. To make an explicit connection with the $(3+1)$D QED state discussed in Ref. [49], one can first start with fractionalizing $\vec{n}^e$ in the bulk, and introduce a $(4+1)$D U(1) gauge field a_μ. The hedgehog monopole line of $\vec{n}^e$ becomes the Dirac monopole line of a_μ, which is decorated with the $\mathrm{SO}(3)^m$ Haldane phase. Now, we condense the Dirac monopole line in the bulk, but do not condense the termination of the Dirac monopole line at the 3D boundary, which becomes the Dirac monopoles (point like defects) at the 3D boundary. This will lead to a gapped 4D bulk state, while the 3D boundary is the QED state discussed in Ref. [49] with z^e and z^m being the gauge charge and Dirac monopole, respectively.

The picture above can again be generalized to the PSU(N) spin system with FR and AFR on the two sublattices. Whether this spin system permits a featureless gapped state or not is equivalent to whether the corresponding 4D bulk state is a trivial state or a SPT state. The CP^{N-1} manifold, i.e., the SU(N) generalization of the Néel order parameter, has $\pi_2[\mathrm{CP}^{N-1}] = Z$, and hence also has a "hedgehog monopole" line in the 4D space. Thus, we can again decorate the $\mathrm{SO}(3)^m$ monopole line with the PSU(N) Haldane phase, and simultaneously decorate the PSU(N) monopole line with the $\mathrm{SO}(3)^m$ Haldane phase. But, now this 4D state is *not* always a nontrivial SPT state. Because the $\mathrm{SO}(3)^m$ Haldane phase has a Z_2 classification, hence, even-number copies of the 4D state must be a trivial state, while odd-number copies of the states are equivalent to the state itself. On the other hand, the PSU(N) Haldane phase has a Z_N classification, namely, N copies of the states must be trivial. Thus, the 4D bulk state so constructed has a $Z_{(2,N)}$ classification: the "mutual monopole line decoration" gives us a nontrivial 4D SPT state only with even N.

The natural 3D boundary state of the 4D bulk based on the "mutual" monopole line decoration construction is a U(1) photon phase whose e excitations carry SU(N) fundamental, and m carries a spin-$\frac{1}{2}$ of SO(3). When N is odd, we can drive the 3D boundary into a featureless state by condensing the dyon which is a bound state of N e particles and two m particles. We label this dyon as the $(N,2)$ dyon. This $(N,2)$ dyon is a boson, and its condensate will gap out the photons, while confining all the point particles because there is no point particle that is mutual bosonic with this dyon, except for the dyon itself. Also, the $(N,2)$ dyon could be a singlet of SU(N), and singlet of SO(3), thus its condensate does not break any global symmetry. This means that for odd integer N, the 3D boundary of the 4D bulk state can be driven into a featureless gapped state, which again demonstrates that the 4D bulk state constructed above is trivial when N is odd.

By contrast, if N is even, then the $(N/2,1)$ dyon [with nontrivial representation of SU(N) and SO(3)] is still deconfined in the condensate of $(N,2)$ dyon, and this condensate has topological order.

Now, we can conclude the following:

For odd N, the SU(N) spin system on the cubic lattice with FR and AFR spins on two sublattices permits a featureless spin state.

Here, we propose a low-energy effective field theory for the 4D SPT state that captures the "mutual decorated monopole line" construction. We first define a U($2N$) matrix field U as

$$U = \cos(\theta)\mathcal{P} \otimes I_{2\times 2} + i\sin(\theta) I_{N\times N} \otimes \vec{n}\cdot\vec{\tau}, \tag{8}$$

where $\mathcal{P}$ is the CP^{N-1} matrix field given by Eq. (6). The "mutual decoration" picture is captured by a topological term in the nonlinear sigma model of U which reads as

$$\mathcal{L}_{\mathrm{5D}}^{\mathrm{topo}} = \int d^4x\, d\tau\, \frac{2\pi}{480\pi^3}\mathrm{Tr}[(U^\dagger dU)^5]. \tag{9}$$

We will show that if we manually create a monopole line of $\vec{n}$, the topological term (9) precisely reduces to the topological term of the $(1+1)$D PSU(N) SPT. Let us parametrize the $(4+1)$D space-time by Cartesian coordinates (x,y,z,w,τ) and consider a static monopole line of $\vec{n}$ whose core line lies on the w axis. For any fixed w and τ, we will see a monopole configuration of $\vec{n}$ centered at origin in the xyz space. For a monopole configuration in the xyz space, we have

$$\begin{aligned} &\theta(r=0) = 0,\\ &\theta(r\to\infty) = \pi/2,\\ &\int_{r=r_0>0} d^2\Omega\, \frac{1}{8\pi}\epsilon_{ijk}\epsilon_{\alpha\beta} n^i\partial_\alpha n^j\partial_\beta n^k = 1, \end{aligned} \tag{10}$$

where $r = \sqrt{x^2+y^2+z^2}$. We also assume $\mathcal{P}$ is a function of w and τ. Now, we plug in this configuration of $\vec{n}$ into Eq. (9) and integrate over x, y, and z directions. This topological term reduces to the following $(1+1)$D topological term in the (w,τ) space:

$$\mathcal{L}_{\mathrm{2D}}^{\mathrm{topo}} = \int dw\, d\tau\, \frac{2\pi}{16\pi}\epsilon_{\mu\nu}\mathrm{Tr}(\mathcal{P}\partial_\mu\mathcal{P}\partial_\nu\mathcal{P}), \tag{11}$$

which is precisely the topological Θ term for the PSU(N) Haldane phase. This indicates that Eq. (9) implies there is a PSU(N) SPT decorated on the monopole line of $\vec{n}$.

If we consider a monopole line of $\mathcal{P}$ along w axis, then in the xyz directions we have

$$\begin{aligned} &\theta(r=0) = \pi/2,\\ &\theta(r\to\infty) = 0,\\ &\int_{r=r_0>0} d^2\Omega\, \frac{i}{16\pi}\epsilon_{\mu\nu}\mathrm{Tr}(\mathcal{P}\partial_\mu\mathcal{P}\partial_\nu\mathcal{P}) = 1. \end{aligned} \tag{12}$$

Now, integrating over x, y, and z directions will give us the following topological term in the $(1+1)$D space-time of the monopole line world sheet:

$$\mathcal{L}_{\mathrm{2D}}^{\mathrm{topo}} = \int dw\, d\tau\, \frac{2\pi i}{8\pi}\epsilon_{abc}\epsilon_{\mu\nu} n^a\partial_\mu n^b\partial_\nu n^c, \tag{13}$$

which exactly corresponds to the topological term of the $(1+1)$D SO(3) Haldane phase. Therefore, the topological term in

Eq. (9) captures the "mutual decoration" construction of the $(4+1)$D SPT phase with $PSU(N) \times SO(3)$ symmetry.

VI. FURTHER PROOF OF OUR CONCLUSIONS

A. Explicit construction of featureless spin states

Let us first restate our main conclusions about $SU(N)$ spin systems on the square, honeycomb, and cubic lattices:

1. A $SU(N)$ *spin system on the square lattice with fundamental (FR) and antifundamental representation (AFR) on the two different sublattices, respectively, permits a featureless gapped ground state when* N *is an odd integer.*

2. A $SU(N)$ *spin system on the honeycomb lattice with FR and AFR on two different sublattices permits a featureless gapped ground state when* N *is coprime with 3.*

3. A $SU(N)$ *spin system on the cubic lattice with FR and AFR spins on two different sublattices permits a featureless spin state when* N *is odd.*

For all the spin systems listed above, we can construct explicit featureless tensor product spin states similar to the AKLT states. All these states will be discussed in a future work [52]. Here, we discuss some of the examples of this construction.

On the honeycomb lattice, in the case of $N = 3k+1$, we introduce $3k$ auxiliary spins on each site. We also introduce a tensor on each site:

$$T^{\alpha}_{i_1 i_2 \ldots i_{3k}} = \varepsilon_{\alpha i_1 i_2 \ldots i_{3k}}, \tag{14}$$

where $\varepsilon_{\alpha i_1 i_2 \ldots i_{3k}}$ is the total antisymmetric tensor with $N = 3k+1$ indices. Here, the $i_1, i_2, \ldots i_{3k}$ labels the $3k$ auxiliary FR (or AFR) spin degrees of freedom on each site in sublattice B (or A) before the projection. Each label i_n takes value in $1,2,\ldots N$ representing the N states in each FR (or AFR). The label α, which also takes value $1,2,\ldots N$, represents the physical states in AFR (or FR) spin degrees of freedom on each site in sublattice B (or A). Physically, on each site of sublattice A, the tensor in Eq. (14) projects the $3k$ auxiliary AFR spins into a totally antisymmetric channel which, due to the nature of $SU(3k+1)$, becomes the physical FR spin. The analysis for sites in the sublattice B is similar. Now, we can use the auxiliary spins to construct a featureless gapped state on the honeycomb lattice with k $SU(N)$ singlet bonds along each link of the lattice, which is reminiscent of the AKLT state.

Obviously, the so-constructed tensor product state respects the translation symmetry of the lattice. Now, we analyze the compatibility between the point group C_{3v} and the site tensor in Eq. (14). Here, notice that we include not only the C_3 rotation symmetry, but also the mirror reflection symmetry of the honeycomb lattice into consideration. We notice that the point group only induces a permutation of the singlet bonds before the projection. Therefore, the action of the point group permutes the $3k$ spins on each site. Since we project the $3k$ spins into a totally antisymmetric channel using the site tensor, the point-group induced permutation keeps the site tensor invariant up to a global sign which is unimportant for the global tensor network wave function. Therefore, we can conclude that the choice of projection tensor in Eq. (14) preserves the space symmetries.

On the square lattice, in the case of $N = 4k+1$, we introduce $4k$ auxiliary spins on each site and let the auxiliary spins form a state with k $SU(N)$ singlet bonds along each link of the square lattice. We can choose the site tensors to be

$$T^{\alpha}_{i_1 i_2 \ldots i_{4k}} = \varepsilon_{\alpha i_1 i_2 \ldots i_{4k}}, \tag{15}$$

where $\varepsilon_{\alpha i_1 i_2 \ldots i_{4k}}$ is the total antisymmetric tensor with $N = 4k+1$ indices. Based on analysis completely in parallel with the honeycomb lattice, we conclude that the physical spin carries AFR (FR) under $SU(N)$ if the auxiliary spins transform as FR (AFR). Also, we can conclude that the tensors in Eq. (15) are invariant under the C_{4v} point-group action up to an unimportant sign because the actions of the C_{4v} point group on the site tensor are only permutation of the tensor indices. Now, we can use the $4k$ auxiliary spins on each site to construct a featureless spin state on the square lattice.

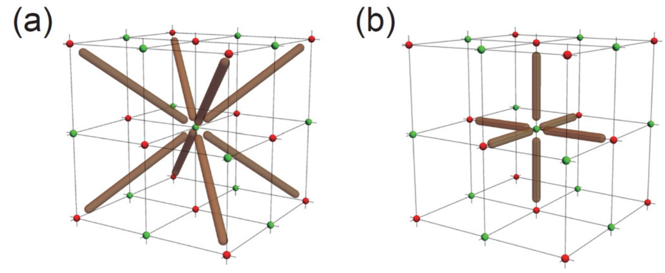

FIG. 5. (a) The schematic featureless $SU(N)$ spin state on the cubic lattice when $N = 8p+1$; (b) the schematic featureless $SU(N)$ spin state on the cubic lattice when $N = 6q+1$. More general spin systems with $N = 8p+6q+1$ have valence bonds extended along both the link and diagonal directions of the cubic lattice.

On the cubic lattice, for any odd integer N that is not 3, 5, or 11, we can write N as $N = 8p+6q+1$ with p and q non-negative integers. Again, we introduce $N-1$ auxiliary spins, and an onsite tensor $T^{\alpha}_{i_1 i_2 \ldots i_{N-1}} = \varepsilon_{\alpha i_1 i_2 \ldots i_{N-1}}$. Namely, on sublattice B, we represent the AFR with $N-1$ auxiliary FRs, and on sublattice A we represent the FR with $N-1$ AFRs. Now, these auxiliary spins can form featureless states with valence bonds extended either along the link (for $N = 6q+1$) or the diagonal directions (for $N = 8p+1$), or both directions (when p and q are both nonzero) on the cubic lattice (Fig. 5).

The point group O_h of the cubic lattice will induce a permutation among the $N-1$ auxiliary spins on each site which at most leads to an unimportant sign change of the site tensor. Therefore, this site tensor is compatible with the point-group O_h symmetry. In fact, the O_h point group is isomorphic to $S_4 \times Z_2$. The Z_2 part is the spatial inversion which takes the point (x,y,z) to $(-x,-y,-z)$. S_4 is the permutation group of four elements, which can be generated by a Z_3 cyclic permutation and a Z_4 cyclic permutation. In the language of the point group, the S_4 part is the part of O_h that preserves the spatial orientation. It can be generated by a C_3 rotation about the $(1,1,1)$ axis and a C_4 rotation about the z axis. This S_4 part alone (without the spatial inversion) is usually referred to the point group O.

The construction of these featureless tensor product wave functions does provide strong evidence to our conclusions in previous sections. Nevertheless, we need to comment that, to eventually confirm the featurelessness of these tensor product wave functions, numerical simulation of these states is demanded, in order to rule out possible spontaneous symmetry breaking, etc. For instance, it is known that the AKLT wave function on a three-dimensional lattice could have long-range spin order.

B. Connection to "lattice homotopy class"

In fact, we can also simplify all the discussions by just considering a $Z_N \times Z_N$ subgroup of PSU(N) and analyzing how the FR and AFR of SU(N) transform under this $Z_N \times Z_N$ subgroup. To specify this $Z_N \times Z_N$ subgroup, we first consider two SU(N) matrices in the FR:

$$g_1 = e^{i\pi(N-1)} \begin{pmatrix} 0 & 1 & 0 & \dots & 0 & 0 \\ 0 & 0 & 1 & \ddots & & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 1 & 0 \\ 0 & & \ddots & 0 & 0 & 1 \\ 1 & 0 & \dots & 0 & 0 & 0 \end{pmatrix},$$

$$g_2 = e^{i\pi(N-1)} \begin{pmatrix} e^{\frac{i2\pi}{N}} & & & & \\ & e^{\frac{i4\pi}{N}} & & & \\ & & \ddots & & \\ & & & e^{\frac{i2\pi(N-1)}{N}} & \\ & & & & 1 \end{pmatrix}, \quad (16)$$

where g_1 only has nonzero entries on a subdiagonal and the bottom left corner, and g_2 is a diagonal matrix. It is straightforward to check that

$$g_1^N = g_2^N = 1_{N\times N}, \quad g_1 g_2 = e^{-i2\pi/N} g_2 g_1. \quad (17)$$

We denote the elements of PSU(N) corresponding to g_1 and g_2 as $\tilde{g}_1$ and $\tilde{g}_2$. Obviously, $\tilde{g}_{1,2}$ are elements of order N. Since the phase factor $e^{-i2\pi/N}$ in the commutation relation between g_1 and g_2 is one of the center elements in SU(N), $\tilde{g}_1$ and $\tilde{g}_2$ should commute in PSU(N). Therefore, $\tilde{g}_1$ and $\tilde{g}_2$ generate a $Z_N \times Z_N$ subgroup of PSU(N). We will focus on this subgroup in the following. Notice that a physical FR spin, which transforms according to $g_{1,2}$ under this $Z_N \times Z_N$ subgroup of PSU(N), can be viewed as a projective representation of $Z_N \times Z_N$. In the classification of the projective representation $H^2(Z_N \times Z_N,\mathrm{U}(1)) = Z_N$, the FR spins actually correspond to the generating element in $H^2(Z_N \times Z_N,\mathrm{U}(1))$. The AFR spins then correspond to the conjugate of the FR spins in terms of projective representations of $Z_N \times Z_N$.

When we restrict to the global internal symmetry $Z_N \times Z_N$ [which is a subgroup of PSU(N)], we can apply the lattice homotopy classification introduced in Ref. [20]. It was proven for 1D and 2D, partially proven for 3D, and conjectured for general dimensions that the generalized Lieb-Schultz-Mattis (LSM) theorems will forbid the existence of any featureless states on lattices of "nontrivial lattice homotopy class." In fact, the lattice homotopy classification proposed in Ref. [20] also covers the cases with continuous internal symmetry group. However, the proof of the relations between nontrivial lattice homotopy classes and the existence of generalized LSM theorems is less comprehensive for the most general continuous symmetry group than for the general Abelian finite group. Therefore, we will focus on the lattice homotopy classification with Abelian finite group in this section.

For a lattice with n FR spins on each site of the sublattice A and n AFR spins on each site of the sublattice B, we will refer to it as the (n,n) lattice. The fundamental-antifundamental lattices can then also be referred to as the $(1,1)$ lattice. In addition to the global internal symmetry, the lattice homotopy classification depends on the choice of space-group symmetry. Let us specify the minimal space-group symmetry for the $(1,1)$ honeycomb, $(1,1)$ square, and $(1,1)$ cubic lattices we want to consider. For the $(1,1)$ honeycomb lattice, we want to at least include the C_3 spatial rotation symmetry into consideration. Therefore, the minimal choice of space group is the wallpaper group $p3$ (No. 13). For the $(1,1)$ square lattice, we want to at least consider the C_4 spatial rotation symmetry. Therefore, the minimal choice of space group is the wallpaper group $p4$ (No. 10). For the $(1,1)$ cubic lattice, we want to at least consider the symmetry of the point group O. Therefore, the minimal choice of the 3D space group is $F432$ (No. 209). The wallpaper group and 3D space-group numbers can be found in Ref. [53].

With the global $Z_N \times Z_N$ internal symmetry and the minimal space-group symmetry given above, the $(1,1)$ honeycomb lattice belongs to a nontrivial lattice homotopy class when N is a multiple of 3. Similarly, $(1,1)$ square and $(1,1)$ cubic lattices are also nontrivial when N is even. Therefore, according to Ref. [20], there are generalized LSM theorems obstructing any featureless state compatible with the global and space-group symmetries on these lattices. Of course, when we enlarge the $Z_N \times Z_N$ symmetry back to PSU(N), such obstructions still exist.

Hence, the analysis of lattice homotopy class also indicates that *there is no featureless state with* PSU(N) *global symmetry on the* $(1,1)$ *honeycomb lattice with N being a multiple of 3, or on* $(1,1)$ *square or cubic lattices with even integer N*. These conclusions are completely consistent with those obtained from the analysis in the previous sections.

One can perform a similar lattice homotopy analysis for SO($2N$) spin systems with spins carrying the vector representation with $N \geqslant 1$. We focus on a $Z_2 \times Z_2$ subgroup of PSO($2N$). When $N = 4k$, we construct the SO($4k$) matrices

$$g_1 = i\sigma^y \otimes I_{2k\times 2k}, \quad g_2 = \sigma^z \otimes I_{2k\times 2k}, \quad (18)$$

and notice that

$$g_1^2 = -1, \quad g_2^2 = 1, \quad g_1 g_2 = -g_2 g_1. \quad (19)$$

We denote the elements of PSO($4k$) that correspond to g_1 and g_2 as $\tilde{g}_1$ and $\tilde{g}_2$. Since $-I_{4k\times 4k}$ is a nontrivial center element of $SO(4k)$, the elements $\tilde{g}_{1,2}$ generate a $Z_2 \times Z_2$ subgroup of PSO($4k$). The vector representation, which transforms according to $g_{1,2}$ under this $Z_2 \times Z_2$ subgroup, can be viewed as a nontrivial projective representation of $Z_2 \times Z_2$. If we restrict our attention to this $Z_2 \times Z_2$ subgroup of PSO($4k$), we notice that a square lattice with a SO($4k$) spin in the vector representation per site and with the space group $p4$ belongs to a nontrivial lattice homotopy class.

When $N = 4k + 2$, we construct the SO$(4k + 2)$ matrices

$$g_1 = \begin{pmatrix} \sigma^z & & & \\ & \sigma^z & & \\ & & i\sigma^y & \\ & & & i\sigma^y \otimes I_{2(k-1)\times 2(k-1)} \end{pmatrix},$$

$$g_2 = \begin{pmatrix} \sigma^x & & & \\ & i\sigma^y & & \\ & & \sigma^x & \\ & & & \sigma^z \otimes I_{2(k-1)\times 2(k-1)} \end{pmatrix} \quad (20)$$

which satisfy

$$g_1^4 = g_2^4 = 1, \quad g_1 g_2 = -g_2 g_1. \quad (21)$$

By similar reasoning in the SO$(4k)$ case, we find that the vector presentation of SO$(4k + 2)$ can be viewed as a nontrivial projective representation of a $Z_4 \times Z_4$ subgroup in PSO$(4k + 2)$. In fact, the classification of projective representation of $Z_4 \times Z_4$ is given by $H^2(Z_4 \times Z_4, U(1)) = Z_4$ in which the vector representation belongs to the "second" nontrivial class. When we consider the space group $p4$ and the $Z_4 \times Z_4$ subgroup of PSO$(4k + 2)$ given above, we notice that the square lattice with a spin in the vector representation on each site also belongs to a nontrivial lattice homotopy class, just like that case of SO$(4k)$.

Hence, we can conclude that *a* SO$(2N)$ *spin system with vector representation on every site does not permit a featureless gapped state on the square lattice.* This result completely agrees with the analysis in the previous sections.

Lastly, we consider SO$(2N + 1)$ spin systems with spinor representations. SO$(2N + 1)$ is the group of rotations in $\mathbb{R}^{2N+1}$. Let $x_{1,2,\ldots,2N+1}$ denote the $2N + 1$ axes of $\mathbb{R}^{2N+1}$. We would like to focus on a $Z_2 \times Z_2$ subgroup of SO$(2N + 1)$ generated by the π rotation in the $x_1 - x_2$ plane and the π rotation in the $x_1 - x_3$ plane. The spinor representation of SO$(2N + 1)$ can be viewed as a nontrivial projective representation of this $Z_2 \times Z_2$ subgroup. When we consider the space group $p4$ and the $Z_2 \times Z_2$ subgroup of SO$(2N + 1)$ given above, we notice that the square lattice with a spin in the spinor representation on each site belongs to a nontrivial lattice homotopy class. Therefore, *a* SO$(2N + 1)$ *spin system with spinor representation on every site does not permit a featureless gapped state on the square lattice.* Again, this statement is consistent with the analysis given in the previous sections.

VII. SUMMARY

In this work, we made connection between two seemingly different subjects: the (generalized) Lieb-Shultz-Matthis theorem for d-dimensional quantum spin systems and the boundary of $(d + 1)$-dimensional symmetry-protected topological states with onsite symmetries. This connection has led to fruitful results: we identified a series of quantum spin systems that permit a featureless spin state, as well as spin systems with a generalized LSM theorem, i.e., spin systems that likely do not permit a featureless spin state. The former cases correspond to trivial bulk states, while the latter correspond to nontrivial SPT states in one higher spatial dimension. We have also tested and verified our conclusions by other methods. For example, we explicitly constructed featureless tensor product spin states of those systems whose corresponding $(d + 1)$-dimensional bulk are trivial states (most of this construction will be presented in an upcoming paper [52]). We expect the main logic and method used in this paper can be generalized to other related problems. For example, one can study SU(N) spin systems with more general representations.

Note added. Recently, we became aware of a few upcoming independent works which may overlap with part of our results [54,55].

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