Instanton effects in lattice models of bosonic symmetry-protected topological states

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Bosonic symmetry-protected topological (SPT) states are gapped disordered phases of matter possessing symmetry-preserving boundary excitations. It has been proposed that, at long wavelengths, the universal properties of an SPT system are captured by an effective nonlinear sigma model field theory in the presence of a quantized topological θ term. By studying lattice models of bosonic SPT states, we are able to identify, in their Euclidean path integral formulation, (discrete) Berry phases that hold relevant physical information on the nature of the SPT ground states. These discrete Berry phases are given intuitive physical interpretation in terms of instanton effects that capture the presence of a θ term on the microscopic scale.

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I. INTRODUCTION

Since the prediction and discovery of topological band insulators [1–3], the relation between topology and symmetries in the realization of new phases of matter has been the focus of intense scrutiny in recent years. While the classification of noninteracting symmetry-protected topological (SPT) fermionic phases of matter appears to have been completely formulated [4–7], the quest for *interacting* SPT phases is actively being theoretically studied [8–27]. Moreover, it has been recently proposed that bosonic SPT states could be realized in periodically driven interacting systems [28], as well as in other cold-atom platforms [29,30], thus opening the interesting possibility to probe and manipulate SPT systems.

The simplest example of a bosonic SPT state is provided by the $S = 1$ antiferromagnetic Heisenberg chain, whose ground state is gapped, symmetry unbroken, and possesses twofold degenerate edge states that behave as $S = 1/2$ low energy excitations. Haldane has shown that the Euclidean path integral of the $S = 1$ antiferromagnetic chain is described by an Euclidean action that contains, in addition to a standard nonlinear sigma model term, a topological θ-term action S_θ with the coefficient θ quantized in multiples of 2π [31,32]

$$S_{D=1} = S_{\mathrm{NLSM}} + \mathrm{i} S_\theta = \int dx\, d\tau \left[\frac{1}{g}(\partial_\mu \hat{n})^2 + \mathrm{i}\,\frac{\theta}{8\pi}\epsilon_{abc}\epsilon_{\mu\nu}\hat{n}^a\partial_\mu\hat{n}^b\partial_\nu\hat{n}^c\right]. \tag{1.1}$$

($\hat{n}$ is a three-component unit vector.) Whereas the presence of the topological action does not change the partition function when periodic boundary conditions are imposed on the system [due to the fact that $\exp(\mathrm{i}\, S_\theta) = \exp(\mathrm{i}\, 2\pi \times \text{integer}) = 1$], S_θ is nevertheless directly responsible for the $S = 1/2$ excitation in the presence of edges [33–38].

Recently, Bi *et al.* [24] proposed a classification of bosonic SPT states in D-dimensional space via an extension of Eq. (1.1), whereby the gapped symmetric state is assumed to be described by an $\mathrm{O}(D+2)$ nonlinear sigma model augmented with a quantized θ-term action,

$$S_D = S_{\mathrm{NLSM}} + \mathrm{i} S_\theta = \int d^D x\, d\tau \left[\frac{1}{g}(\partial_\mu \hat{n})^2 + \mathrm{i}\,\frac{2\pi}{\Omega_{D+1}}\epsilon_{a_1\cdots a_{D+2}}\hat{n}^{a_1}\,\partial_{x_1}\hat{n}^{a_2}\,\cdots\,\partial_{x_D}\hat{n}^{a_{D+1}}\,\partial_\tau\hat{n}^{a_{D+2}}\right], \tag{1.2}$$

where Ω_{D+1} is the area of the $(D+1)$-dimensional sphere of unit radius. In the strong coupling limit $g \to \infty$, the wave function acquires the form [16]

$$|\Psi\rangle \sim \int D\hat{n}(x)\, e^{\mathrm{i}\frac{2\pi}{\Omega_{D+1}}\int d^D x \int_0^1 du\, \mathcal{W}[\hat{n}]}\,|\hat{n}(x)\rangle$$
$$\mathcal{W}[\hat{n}] = \epsilon_{a_1\cdots a_{D+2}}\hat{n}^{a_1}\,\partial_{x_1}\hat{n}^{a_2}\cdots\partial_{x_D}\hat{n}^{a_{D+1}}\,\partial_u\hat{n}^{a_{D+2}}, \tag{1.3}$$

where $\hat{n}(\boldsymbol{x},u)$ is an extension that satisfies $\hat{n}(\boldsymbol{x},0) = (0,0,\ldots,0,1)$ and $\hat{n}(\boldsymbol{x},1) = \hat{n}(\boldsymbol{x})$. The θ-term action then endows the wave function with an amplitude given by a Wess-Zumino-Witten term at level-1 [39,40]. Although the field theory approach adopted in Ref. [24] gives a useful platform for discriminating various classes of bosonic SPT states, there remains the question of how the properties encoded by the long wavelength description Eq. (1.2) are manifested at the microscopic scale.

In this paper we investigate the effects of the θ term at the microscopic level by studying the Euclidean partition function of microscopic Hamiltonians of bosonic SPT states. According to the work of Chen *et al.* [11], SPT phases can be characterized by their "short-range entanglement," in that an SPT ground state can be connected to a trivial state by the action of a unitary transformation that preserves the relevant global symmetry. Recently, one of us [26], using ideas of entanglement spectrum, has constructed explicit unitary transformations that give rise to one-dimensional SPT chains with time-reversal and $\mathbb{Z}_n\times\mathbb{Z}_n$ symmetries, as well as two-dimensional SPT paramagnets with $\mathbb{Z}_2\times\mathbb{Z}_2$ symmetry, which are a generalization of the $\mathbb{Z}_2$ paramagnet introduced by Levin and Gu in Ref. [13]. In this paper, we shall then use the unitary mappings studied in Ref. [26] to find an explicit form of the Euclidean partition function for those classes of SPT states.

Expanding on the framework formulated by Chen and coworkers [11], here we will investigate the structure of the cocycles of 1D and 2D spin SPT phases using a path-integral approach based on the standard mapping between quantum and classical spin systems using transfer matrices [41,42]. A recent treatment of 3D SPT phases has used a similarly inspired approach [27]. Instead of a triangulation of the Euclidean space-time, as used in Ref. [11], we will work with simple stacked lattices in the Euclidean direction and show how the resulting effective discrete Euclidean action embodies the Berry phases of these SPT states. Thus, on our route to computing the partition function for the microscopic SPT models considered here, we will be able to identify discrete Berry phases that originate from quantum fluctuations of the degrees of freedom, upon the evolution of the SPT system in imaginary time. (For other studies on the role of Berry phase in SPT systems, see Refs. [43–45].) To these discrete Berry phases, which can be viewed as instanton effects, we will attach a simple physical interpretation that will make the physics of the long wavelength θ-term topological action manifest at the microscopic scale in connection with the entanglement properties of the SPT ground state [11,26]. More specifically, after introducing our general approach in Sec. II, we derive explicit forms in Sec. III for the 1D time-reversal invariant and $\mathbb{Z}_n \times \mathbb{Z}_n$ invariant SPTs and for the 2D Levin-Gu model with $\mathbb{Z}_2$ symmetry and present the resulting Berry phases for each one of these cases.

II. GENERAL APPROACH

We are interested in evaluating the partition function

$$Z_{\rm SPT} = {\rm Tr}\,(e^{-\beta H_{\rm SPT}}), \tag{2.1}$$

where the spin Hamiltonian $H_{\rm SPT}$ describes a bosonic SPT phase in D-dimensional space. The partition function Eq. (2.1) encodes $(D+1)$-dimensional space-time quantum fluctuations of the many-body system, with an Euclidean time direction of length $\beta = 1/T$ (inverse temperature) satisfying periodic boundary conditions.

Our goal is to express the partition function Eq. (2.1) in a local basis, in the process of which we will be able to identify nontrivial discrete Berry phases originating from quantum fluctuations of the local spins. These Berry phases will establish a simple and intuitive picture of the SPT state from the point of view of the space-time quantum fluctuations of its microscopic degrees of freedom.

Important to our discussion is the fact that, if the D-dimensional spatial manifold on which the SPT system lives has no boundaries, the SPT Hamiltonian $H_{\rm SPT}$ can be generated from a trivial gapped paramagnetic Hamiltonian H_0 via a unitary, symmetry-preserving transformation $\mathbb{W}$ [11,26]:

$$H_{\rm SPT} = \mathbb{W}\, H_0\, \mathbb{W}^{-1}, \tag{2.2}$$

where H_0 describes a trivial paramagnet, i.e., a paramagnet whose edge states can be gapped without symmetry violation. In order to facilitate our obtaining of an explicit representation of the partition function Eq. (2.1), we choose to work with microscopic models in their zero correlation length limit [this choice will not affect the Berry phases, which are the subject of our attention in Eq. (2.1)]:

$$H_0 = -h \sum_{i=1}^{N} X_i, \quad [X_i, X_j] = 0, \quad \forall (i,j). \tag{2.3}$$

N is the number of lattice sites and h is a positive energy scale. X_i is a Hermitian operator defined solely on site i. (In its simplest form, $X_i = \sigma_i^x$ is a Pauli matrix.) Due to the zero correlation form assumed for H_0, the Hamiltonian Eq. (2.2) is a sum of mutually commuting operators,

$$H_{\rm SPT} = -h \sum_{i=1}^{N} \mathcal{O}_i = -h \sum_{i=1}^{N} \mathbb{W} X_i\, \mathbb{W}^{-1}. \tag{2.4}$$

In order for the ground state of $H_{\rm SPT}$ to possess nontrivial entanglement, the transformation $\mathbb{W}$ cannot be reduced to a product of on-site terms. As a consequence, the operator $\mathcal{O}_i$ acts on site i and the neighborhood thereof.

Despite the distinct entanglement patterns encoded by the ground states of H_0 and $H_{\rm SPT}$, when expressed in the same local basis, the unitary transformation Eq. (2.2) implies that in a closed spatial manifold, both Hamiltonians have the same spectra and, hence, the same partition function. Nevertheless, the fundamental physics of the SPT system can be unveiled by studying the quantum fluctuations of spins between intermediate Euclidean "time slices" of Eq. (2.1). These instanton events, as we will see by explicit computation, give rise to nontrivial phase factors in Eq. (2.1), whereby spin fluctuations in imaginary time are coupled to domain-wall-like configurations in a way that is consistent with the underlying global symmetry of the SPT state. We shall determine the phase factors associated to these instanton events for some cases of interest.

In order to carry out this program, we evaluate the trace in Eq. (2.1) using the complete set of orthonormal many-body basis states $|\sigma\rangle = |\sigma_1,\sigma_2,\ldots,\sigma_N\rangle$, whereby the trivial, unique ground state of H_0 is represented as

$$|\Psi_0\rangle = \frac{1}{\mathcal{D}^{1/2}} \sum_{\sigma} |\sigma\rangle. \tag{2.5}$$

$\mathcal{D}$ denotes the dimension of the Hilbert space and $|\Psi_0\rangle$ is a product state expressed in the "ordered" basis $|\sigma\rangle$ satisfying $X_j\,|\Psi_0\rangle = |\Psi_0\rangle$, for every j. In the ordered basis, all the diagonal matrix elements of X_j vanish: $\langle\sigma|X_j|\sigma\rangle = 0$.

The advantage of working with the representation Eq. (2.5) for the trivial ground state is that $\mathbb{W}$ is diagonal in the $|\sigma\rangle$ basis: $\mathbb{W}|\sigma\rangle = e^{{\rm i}\,W(\sigma)}\,|\sigma\rangle$. (See examples in Sec. III.) Hence, the SPT ground state in the zero correlation limit reads

$$|\Psi_{\rm SPT}\rangle = \frac{1}{\mathcal{D}^{1/2}} \sum_{\sigma} e^{{\rm i}\,W(\sigma)}\,|\sigma\rangle. \tag{2.6}$$

Normalization factors aside, $e^{{\rm i}\,W(\sigma)}$ is the SPT ground state wave function in the $|\sigma\rangle$ basis. Hence the phase factor $e^{{\rm i}W(\sigma)}$ in Eq. (2.6) plays the role of the WZW term in Eq. (1.3).

In order to explicitly capture the nontrivial quantum fluctuations associated with the SPT Hamiltonian, we conventionally represent the trace in Eq. (2.1) as:

$$Z_{\rm SPT} = \sum_{\sigma(\tau_1)} \cdots \sum_{\sigma(\tau_M)} \prod_{k=1}^{M} Z_{\rm SPT}[\sigma(\tau_k),\sigma(\tau_{k+1})], \tag{2.7a}$$

$$Z_{\rm SPT}[\sigma(\tau_k),\sigma(\tau_{k+1})] = \langle\sigma(\tau_k)|\, e^{-\tau H_{\rm SPT}}\,|\sigma(\tau_{k+1})\rangle = e^{{\rm i}\,[W(\sigma(\tau_k)) - W(\sigma(\tau_{k+1}))]}\, Z_0[\sigma(\tau_k),\sigma(\tau_{k+1})] \equiv e^{{\rm i}\,\Delta W_{k,k+1}}\, Z_0[\sigma(\tau_k),\sigma(\tau_{k+1})], \tag{2.7b}$$

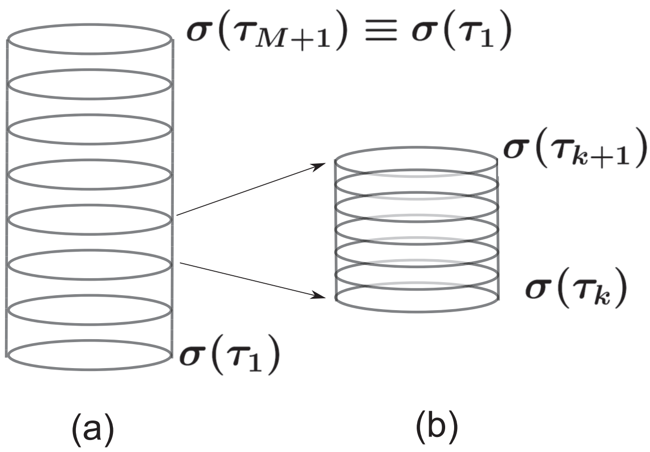

FIG. 1. Figure 1(a) depicts the slicing of the partition function into M intervals, as described by Eq. (2.7a). At each time slice, we have an instantaneous representation of the D-dimensional SPT system, which, without boundaries, is generically represented by a circle. Figure 1(b) depicts the slicing of $Z_{\text{SPT}}[\sigma(\tau_k),\sigma(\tau_{k+1})]$ into N subintervals, as described by Eq. (2.10).

where, in Eq. (2.7a), we have introduced M time intervals of length $\tau_{k+1} - \tau_k = \tau = \beta/M$ with the periodic boundary condition in imaginary time $\sigma(\tau_{M+1}) \equiv \sigma(\tau_1)$ implied. [See Fig. 1(a).] Also, in Eq. (2.7b) we have used the unitary transformation given in Eq. (2.2) to relate the imaginary time evolution of the SPT Hamiltonian at each time slice with $Z_0[\sigma(\tau_k),\sigma(\tau_{k+1})] \equiv \langle\sigma(\tau_k)|\, e^{-\tau H_0}\, |\sigma(\tau_{k+1})\rangle$.

Since $Z_0[\sigma(\tau_k),\sigma(\tau_{k+1})] > 0$, all the nontrivial Berry phases associated with quantum fluctuations of the SPT system are given by the phase factor on the second line of Eq. (2.7b). Moreover, this phase factor has the interpretation of a surface term since it only depends on the configurations at the time slices τ_k and τ_{k+1}.

While the phases appearing in Eq. (2.7b) account for the space-time quantum fluctuation of the whole system [recall that $\sigma(\tau)$ refers to the many-body configuration at time τ], we can gain further information about the nature of the SPT system by studying Berry phases picked up by *local* spin fluctuations. In order to do this, we divide each time interval (τ_k,τ_{k+1}) into N subintervals $(\tau_k,\tau_k+\epsilon,\ldots,\tau_k+j\epsilon,\ldots,\tau_k+(N-1)\epsilon,\tau_{k+1}) \equiv (\tau_{k,0},\tau_{k,1},\ldots,\tau_{k,j},\ldots,\tau_{k,N-1},\tau_{k,N})$ of length $\epsilon = \tau/N = \beta/(MN)$ [see Fig. 1(b)] and rewrite Eq. (2.7b) as

$$Z_{\text{SPT}}[\sigma(\tau_k),\sigma(\tau_{k+1})] = \sum_{\sigma(\tau_{k,1})}\sum_{\sigma(\tau_{k,2})}\cdots\sum_{\sigma(\tau_{k,N-1})} \times \prod_{j=1}^{N} \langle\sigma(\tau_{k,j-1})|e^{h\epsilon\mathcal{O}_j}|\sigma(\tau_{k,j})\rangle. \tag{2.8}$$

In going from Eqs. (2.7b) to (2.8) we have used the fact that the local operators $\mathcal{O}_j$ in Eq. (2.4) commute among themselves and we have introduced the identity operator $(N-1)$ times in the form of a complete summation over intermediate many-body configurations $\sigma(\tau_{k,1}),\ldots,\sigma(\tau_{k,N-1})$.

We are now faced with the evaluation of the transfer matrices between many-body configurations of *local* operators $e^{h\epsilon\mathcal{O}_j}$, which, straightforwardly, yields

$$\langle\sigma(\tau_{k,j-1})|e^{h\epsilon\mathcal{O}_j}|\sigma(\tau_{k,j})\rangle = e^{\mathrm{i}\,\mathcal{S}_j(\tau_{k,j-1},\tau_{k,j})}\,\langle\sigma_j(\tau_{k,j-1})|e^{h\epsilon X_j}|\sigma_j(\tau_{k,j})\rangle, \tag{2.9a}$$

$$e^{\mathrm{i}\,\mathcal{S}_j(\tau_{k,j-1},\tau_{k,j})} = e^{\mathrm{i}[W(\sigma(\tau_{k,j-1}))-W(\sigma(\tau_{k,j}))]}\,\Delta_j(\tau_{k,j-1},\tau_{k,j}), \tag{2.9b}$$

where $\Delta_j(\tau_{k,j-1},\tau_{k,j}) \equiv \prod_i^{i\neq j}\,\delta_{\sigma_i(\tau_{k,j-1}),\sigma_i(\tau_{k,j})}$ enforces that all spins at time slices $\tau_{k,j-1}$ and $\tau_{k,j}$ be the same, except at site j. Thus the phase $e^{\mathrm{i}\,\mathcal{S}_j(\tau_{k,j-1},\tau_{k,j})}$ in Eq. (2.9b) accounts for the Berry phase contribution due to the quantum fluctuations of a single spin at site j in the presence of an instantaneous configuration of adjacent spins. Therefore, the contribution of the partition function between time slices τ_k and τ_{k+1}, which takes into account the Berry phases picked up by local spin fluctuations, can be cast in the form

$$Z_{\text{SPT}}[\sigma(\tau_k),\sigma(\tau_{k+1})] = \sum_{\sigma(\tau_{k,1})}\sum_{\sigma(\tau_{k,2})}\cdots\sum_{\sigma(\tau_{k,N-1})}\prod_{j=1}^{N} e^{\mathrm{i}\,\mathcal{S}_j(\tau_{k,j-1},\tau_{k,j})} \times\langle\sigma_j(\tau_{k,j-1})|e^{h\epsilon X_j}|\sigma_j(\tau_{k,j})\rangle. \tag{2.10}$$

It is worthwhile to remind the reader that, even though, by construction, the right hand sides of Eqs. (2.7b) and (2.10) are identical, the latter equation makes evident the Berry phases due to local instanton effects while the former equation captures the quantum fluctuations of the entire D-dimensional system as it propagates in imaginary time.

III. EXAMPLES

A. $D = 1$, time-reversal symmetric SPT state

A one-dimensional periodic SPT chain, invariant under time-reversal $\mathbb{Z}_2^T$ operation,

$$\Theta = \left(\prod_{j=1}^{N}\sigma_j^x\right)K, \tag{3.1}$$

(K denotes complex conjugation) can be constructed using the unitary transformation [26]

$$\mathbb{W}_{\text{TRS}} = \prod_{j=1}^{N} e^{\mathrm{i}\,\theta_{i,i+1}\,(\frac{1-\sigma_i^z\sigma_{i+1}^z}{2})}, \quad \theta_{i,i+1} = \frac{\pi}{2}, \tag{3.2}$$

where at every site of the chain there is a spin-1/2 degree of freedom represented by a Pauli operator σ_i^a with $a = 1,2,3 = x,y,z$. The unitary operator Eq. (3.2) endows a many-body basis state $|\sigma\rangle = |\sigma_1,\sigma_2,\ldots,\sigma_N\rangle$ with a phase factor $\exp\{\mathrm{i}(\pi/2)N_{\text{d}}(\sigma)\} = \pm 1$, where $N_{\text{d}}(\sigma)$ denotes the (even) number of domain walls in the state $|\sigma\rangle$. Moreover, this transformation commutes with the time-reversal operator Eq. (3.1) and each local unitary piece creates a maximally entangled state between nearest neighbor spins [26].

So, under Eq. (3.1), one can map the trivial time-reversal symmetric ground state

$$|\Psi_0\rangle = \left(\frac{|\uparrow\rangle + |\downarrow\rangle}{\sqrt{2}}\right)^{\otimes N} = \frac{1}{2^{N/2}} \sum_{\sigma} |\sigma\rangle \tag{3.3a}$$

of

$$H_0 = -h \sum_{j=1}^{N} \sigma_j^x \tag{3.3b}$$

into

$$|\Psi_{\mathrm{TRS}}\rangle = \mathbb{W}_{\mathrm{TRS}}\,|\Psi_0\rangle = \frac{1}{2^{N/2}} \sum_{\sigma} e^{\mathrm{i}\,\frac{\pi}{2} N_{\mathrm{d}}(\sigma)}|\sigma\rangle, \tag{3.4a}$$

which is the unique ground state of the SPT Hamiltonian

$$H_{\mathrm{SPT}} = \mathbb{W}_{\mathrm{TRS}}\, H_0\, \mathbb{W}_{\mathrm{TRS}}^{-1} = h \sum_{j=1}^{N} \sigma_{j-1}^z\, \sigma_j^x\, \sigma_{j+1}^z. \tag{3.4b}$$

It is immediate to see that the SPT Hamiltonian Eq. (3.4b), when open boundary conditions are imposed, possesses twofold degenerate states per edge.

Now, applying our discussion of Sec. II to the time-reversal symmetric SPT Hamiltonian Eq. (3.4b) yields the phase contribution Eq. (2.9b) due to a single spin fluctuation to be

$$e^{\mathrm{i}\,\mathcal{S}_j(\tau_{k,j-1},\tau_k,j)} = e^{\mathrm{i}\,\pi\left(\frac{\sigma_j(\tau_{k,j-1})-\sigma_j(\tau_{k,j})}{2}\right)\left(\frac{\sigma_{j+1}(\tau_{k,j})-\sigma_{j-1}(\tau_{k,j})}{2}\right)}, \tag{3.5}$$

[the product of delta functions $\Delta_j(\tau_{k,j-1},\tau_{k,j})$ in Eq. (2.9b) is omitted in Eq. (3.5)]. Combining the result Eq. (3.5) due to single spin processes yields, according to Eq. (2.7b), the total Berry phase as the one-dimensional SPT chain evolves in imaginary time:

$$e^{\mathrm{i}\,\Delta\, W_{k,k+1}} = e^{\mathrm{i}\,\frac{\pi}{2}[N_{\mathrm{d}}(\sigma(\tau_k))-N_{\mathrm{d}}(\sigma(\tau_{k+1}))]}. \tag{3.6}$$

Equation (3.5) implies that a single spin fluctuation at site j contributes a phase -1 to the partition function if the neighbor spins are antiparallel and $+1$ if they are parallel to each other. Summing up these individual phase contributions throughout the chain gives $e^{\mathrm{i}\,\Delta\, W_{k,k+1}} = -1$ if the change in domain wall number is $4m+2$ ($m \in \mathbb{Z}$) and $e^{\mathrm{i}\,\Delta\, W_{k,k+1}} = +1$ if the change in domain wall number is $4m$.

B. $D = 1, \mathbb{Z}_n \times \mathbb{Z}_n$ symmetric SPT state

We consider a periodic chain with an even number N of sites where, at every site j, there exists a clock operator σ_j and its conjugate operator τ_j satisfying the algebra

$$\sigma_j^n = \tau_j^n = 1, \quad \sigma_j^\dagger = \sigma_j^{n-1}, \quad \tau_j^\dagger = \tau_j^{n-1},$$
$$\tau_j^\dagger\, \sigma_j\, \tau_j = \omega\, \sigma_j, \quad \omega \equiv e^{i\,\frac{2\pi}{n}}. \tag{3.7}$$

For the $n=2$ case, Eq. (3.7) admits a Hermitian representation in terms of Pauli matrices $\sigma_j = \sigma_j^z$ and $\tau_j = \sigma_j^x$; otherwise these clock operators are not Hermitian (see Ref. [46] for a recent discussion). We shall denote by $|\sigma_i\rangle$, for $\sigma_i \in \{1,\omega,\ldots,\omega^{n-1}\}$, the eigenstates of σ_i, and by $|\sigma\rangle = |\sigma_1,\ldots,\sigma_N\rangle$ the corresponding many-body state. (The distinction between operators and their eigenvalues should be clear from the context.)

We choose to work with a representation in which the generators of the $\mathbb{Z}_n \times \mathbb{Z}_n$ symmetry implement transformations $\sigma_j \to \omega\, \sigma_j$ independently for the operators on even and odd sublattices, and hence are given by

$$\widehat{S}_{\mathbb{Z}_n}^{(1)} = \prod_{j\in\mathrm{even}} \tau_j, \quad \widehat{S}_{\mathbb{Z}_n}^{(2)} = \prod_{j\in\mathrm{odd}} \tau_j. \tag{3.8}$$

A trivial ground state and its parent Hamiltonian, both invariant under the action of the operators in Eq. (3.8), are given by

$$|\Psi_0\rangle = \left(\frac{|1\rangle + |\omega\rangle + \cdots + |\omega^{n-1}\rangle}{\sqrt{n}}\right)^{\otimes N}$$
$$= \frac{1}{n^{N/2}} \sum_{\{\sigma\}} |\sigma\rangle, \tag{3.9a}$$

$$H_0 = -h \sum_{j=1}^{N} (\tau_j + \tau_j^\dagger). \tag{3.9b}$$

There exist $n-1$ unitary transformations $\mathbb{W}_n^{(p)}, p \in \{1,\ldots,n-1\}$ that (i) map the product state Eq. (3.9a) into a new state where every spin is maximally entangled with its nearest neighbors and (ii) commutes with the symmetries Eq. (3.8) [26]:

$$\mathbb{W}_n^{(p)} = e^{i\,\frac{2\pi p}{n}\,\sum_j \sum_{a=1}^{n-1} \frac{(\sigma_{2j}^\dagger\, \sigma_{2j+1})^a - (\sigma_{2j-1}^\dagger\, \sigma_{2j})^a}{(\omega^a-1)\,(\bar{\omega}^a-1)}}$$
$$\mathbb{W}_n^{(p)}\,|\sigma\rangle \equiv e^{\mathrm{i}\, W_n^{(p)}(\sigma)}\,|\sigma\rangle, \quad W_n^{(p)}(\sigma) \in \mathbb{R}. \tag{3.10}$$

Each of the $\mathbb{W}_n^{(p)}$ for $p \neq 0$ gives rise to an SPT ground state, and hence, there are $n-1$ SPT classes [11,24].

With the transformation Eq. (3.10), one then arrives at the SPT Hamiltonian [26]

$$H_n^{(p)} = \mathbb{W}_n^{(p)}\, H_0\, \left(\mathbb{W}_n^{(p)}\right)^{-1} = -h \sum_j \{[\tau_{2j}\, (\sigma_{2j-1}\, \sigma_{2j+1}^\dagger)^p$$
$$+ \tau_{2j+1}\, (\sigma_{2j}^\dagger\, \sigma_{2j+2})^p] + \mathrm{H.c.}\} \tag{3.11}$$

and its ground state

$$\left|\Psi_n^{(p)}\right\rangle = \mathbb{W}_n^{(p)}\,|\Psi_0\rangle = \frac{1}{n^{N/2}} \sum_{\{\sigma\}} e^{\mathrm{i}\, W_n^{(p)}(\sigma)}|\sigma\rangle. \tag{3.12}$$

The SPT Hamiltonian Eq. (3.11), when open boundary conditions are imposed, possesses n-fold degenerate states per edge.

Now, applying our discussion of Sec. II to the SPT Hamiltonian Eq. (3.11) yields the phase contribution Eq. (2.9b) due to a single spin fluctuation to be

$$e^{\mathrm{i}\,\mathcal{S}_j(\tau_{k,j-1},\tau_k,j)} = e^{\eta_j\,\mathrm{i}\,\frac{2\pi}{n}\,p\,\sum_{a=1}^{n-1}\left[\frac{\bar{\sigma}_j^a(\tau_{k,j-1})-\bar{\sigma}_j^a(\tau_{k,j})}{\bar{\omega}^a-1}\right]\left[\frac{\sigma_{j+1}^a(\tau_{k,j})-\sigma_{j-1}^a(\tau_{k,j})}{\omega^a-1}\right]}, \tag{3.13}$$

where $\eta_j = 1$ if j is even, and $\eta_j = -1$ if j is odd. [The product of delta functions $\Delta_j(\tau_{k,j-1},\tau_{k,j})$ in Eq. (2.9b) is omitted in Eq. (3.13).] According to Eq. (3.13) the Berry phases due to a single spin fluctuation in imaginary are nonzero provided the neighbor spins are not parallel to each other. Using the expression Eq. (A6) in the appendix, one can show that if the spin at site j fluctuates between values $\sigma_j(\tau_{k,j-1}) = \omega^{\ell_0+\ell}$ and $\sigma_j(\tau_{k,j}) = \omega^{\ell_0}$, for $\ell_0,\ell \in \{0,\dots,n-1\}$, then the expression Eq. (3.13) reduces to the simple form $e^{\mathrm{i}\,S_j(\tau_{k,j-1},\tau_{k,j})} = (\bar{\sigma}_{j+1}\,\sigma_{j-1})^{\eta_j\,\ell\,p}$.

Combining the result Eq. (3.13) due to single spin processes yields, according to Eq. (2.7b), the total Berry phase as the one-dimensional $\mathbb{Z}_n\times\mathbb{Z}_n$ symmetric SPT system evolves in imaginary time:

$$e^{\mathrm{i}\,\Delta\,W_{k,k+1}} = e^{\mathrm{i}\,[W_n^{(p)}(\sigma(\tau_k)) - W_n^{(p)}(\sigma(\tau_{k+1}))]}. \tag{3.14}$$

C. $D = 2, \mathbb{Z}_2$ symmetric SPT state

We now analyze the 2D $\mathbb{Z}_2$ SPT model proposed by Levin and Gu. [13] This is an exactly solvable model where spin-1/2 degrees of freedom are defined on the vertices of a triangular lattice. The Hamiltonian of the system is

$$H_{\mathbb{Z}_2} = h \sum_j \sigma_j^x\, e^{\mathrm{i}\frac{\pi}{4}\sum^{j}_{\langle\ell,\ell'\rangle}(1-\sigma^z_\ell\sigma^z_{\ell'})}, \quad h > 0, \tag{3.15}$$

where the summation $\sum^{j}_{\langle\ell,\ell'\rangle}$ extends over nearest neighbor spins around the site j. The ground state of the Levin-Gu model is

$$|\Psi_{\mathbb{Z}_2}\rangle = \frac{1}{2^{N/2}}\sum_\sigma (-1)^{L(\sigma)}|\sigma\rangle, \tag{3.16}$$

where $L(\sigma)$ counts the number of loops, defined in the dual (hexagonal) lattice, associated with domain wall configurations of the the many-body state $|\sigma\rangle$ in the σ^z basis.

There exists a unitary transformation $\mathbb{W}_{\mathbb{Z}_2}$, connecting the Levin-Gu Hamiltonian to a trivial $2D$ paramagnetic Hamiltonian

$$H_0 = -h\sum_j \sigma_j^x, \tag{3.17}$$

whose ground state is a simple product state

$$|\Psi_0\rangle = \frac{1}{2^{N/2}}\sum_\sigma |\sigma\rangle. \tag{3.18}$$

Such transformation, having the property

$$\mathbb{W}_{\mathbb{Z}_2}\,|\sigma\rangle = (-1)^{L(\sigma)}\,|\sigma\rangle, \tag{3.19}$$

reads

$$\mathbb{W}_{\mathbb{Z}_2} = \prod_j e^{-\mathrm{i}\,\frac{\pi}{6}\,\sigma_j^z\,D_j(\{\sigma^z\})}, \tag{3.20}$$

where $D_j(\{\sigma^z\}) = \sum^{j}_{\langle\ell\ell'\rangle}(\frac{1-\sigma^z_\ell\sigma^z_{\ell'}}{2})$ defines the domain wall operator around the close loop formed by the six sites nearest neighbors of site j.

One verifies that

$$\begin{aligned}
\pi_j^x &\equiv \mathbb{W}_{\mathbb{Z}_2}\,\sigma_j^x\,\mathbb{W}_{\mathbb{Z}_2}^{-1} = -\sigma_j^x\,e^{\mathrm{i}\frac{\pi}{4}\sum_{(ik);j}(1-\sigma_i^z\sigma_k^z)},\\
\pi_j^y &\equiv \mathbb{W}_{\mathbb{Z}_2}\,\sigma_j^y\,\mathbb{W}_{\mathbb{Z}_2}^{-1} = -\sigma_j^y\,e^{\mathrm{i}\frac{\pi}{4}\sum_{(ik);j}(1-\sigma_i^z\sigma_k^z)},\\
\pi_j^z &\equiv \mathbb{W}_{\mathbb{Z}_2}\,\sigma_j^z\,\mathbb{W}_{\mathbb{Z}_2}^{-1} = \sigma_j^z.
\end{aligned} \tag{3.21}$$

As seen in Eq. (3.21), the unitary transformation Eq. (3.20) gives rise to a new set of Pauli operators whose phase factors depend on the domain wall operator $D_j(\{\sigma^z\})$ surrounding site j. Notice that since this domain wall operator takes even integer values, the phase factors in Eq. (3.21), and hence π_j^a, are Hermitian.

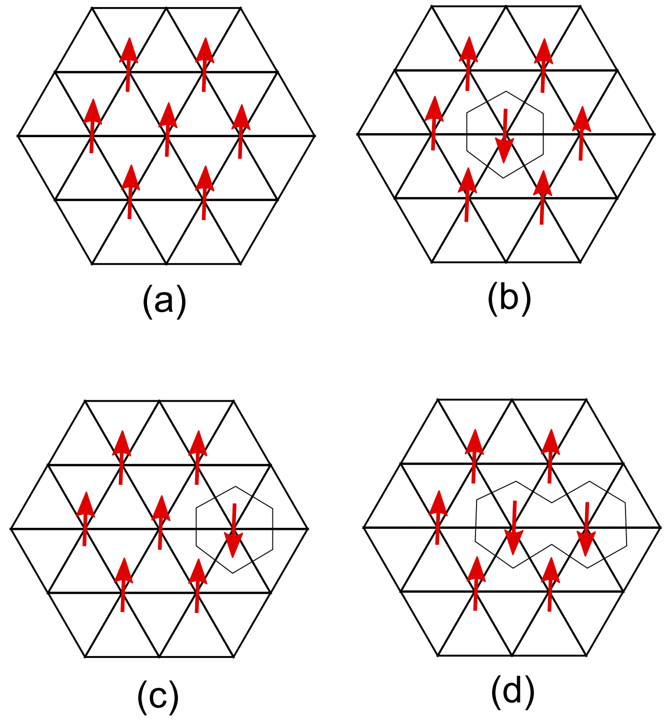

FIG. 2. Figures 2(a) and 2(b) capture the fluctuation of the middle spin giving a phase $e^{\mathrm{i}S_j} = -1$ [Eq. (3.22)], as the configuration of nearest neighbor spins has $D_j = 0$. Figures 2(c) and 2(d) capture the fluctuation of the middle spin giving a phase $e^{\mathrm{i}S_j} = +1$ [Eq. (3.22)], as the configuration of nearest neighbor spins has $D_j = 2$.

From the explicit form of the unitary transformation Eq. (3.20), we find, according to Eq. (2.9b), that the Berry phase contribution due to a single spin fluctuation at site j is given by

$$\begin{aligned}
e^{\mathrm{i}\,S_j(\tau_{k,j-1},\tau_{k,j})} &= e^{-\mathrm{i}\pi(\frac{\sigma_j(\tau_{k,j-1})-\sigma_j(\tau_{k,j})}{2})[1+\frac{1}{2}\sum^{j}_{\langle\ell,\ell'\rangle}(\frac{1-\sigma_\ell(\tau_{k,j})\sigma_{\ell'}(\tau_{k,j})}{2})]}\\
&= e^{-\mathrm{i}\pi(\frac{\sigma_j(\tau_{k,j-1})-\sigma_j(\tau_{k,j})}{2})(1+\frac{1}{2}D_j(\tau_{k,j}))}.
\end{aligned} \tag{3.22}$$

Hence, the spin fluctuation at site j contributes with -1 to the partition function if the configuration of surrounding spins has $D_j = \{0,4\}$, while it contributes with $+1$ to the partition function if the configuration of surrounding spins has $D_j = \{2,6\}$ (see Fig. 2). Moreover, as the full two-dimensional system evolves in imaginary time, it picks a phase factor

$$e^{\mathrm{i}\,\Delta\,W_{k,k+1}} = e^{\mathrm{i}\,\pi\,[L(\sigma(\tau_k)) - L(\sigma(\tau_{k+1}))]}, \tag{3.23}$$

which is -1 if $\Delta\,L = 1$ (mod 2), or $+1$ if $\Delta\,L = 0$ (mod 2).

IV. SUMMARY AND DISCUSSION

We have studied the path integral of bosonic SPT systems, focusing on the manifestation of the so called topological θ terms on the lattice scale. We did so by investigating lattice models of bosonic SPT states, which allowed us to compute the Berry phase contributions appearing in the path integral due to the quantum fluctuations of local degrees of freedom.

In the examples we have considered, these nontrivial Berry phases involve the coupling of local spin fluctuations with surrounding domain wall like configurations, and thus illustrate, in a intuitive way, the connection between Berry phase effects and the nontrivial entanglement characteristic of SPT states.

Although here we have focused entirely on bosonic systems, we close by mentioning some works that address the character of Berry phases in fermionic systems. At the level of relativistic free field theories (coupled to gauge fields) this problem has been studied in the high-energy literature in the context of anomalies and obstruction to gauging certain symmetries [47–49]. It has been known from that work that there is indeed a connection between these anomalies and Berry phases. Also, a recent discussion of Berry phases in fermionic SPT systems that can be described by band theory and free fermions has been given in Ref. [50]. The bosonic cases studied here are strongly coupled and cannot be examined by the same methods as in the field-theoretic anomalies. The nature of Berry phases in strongly coupled fermionic systems is an interesting open problem.

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APPENDIX: $\mathbb{Z}_n$ OPERATORS

A possible representation for the (σ,τ) operators satisfying Eq. (3.7) is as follows

$$\sigma_j = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \omega & 0 & 0 \\ & & & \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & \omega^{n-1} \end{pmatrix}, \quad \tau_j = \begin{pmatrix} 0 & 0 & 0 & \dots & 0 & 1 \\ 1 & 0 & 0 & \dots & 0 & 0 \\ 0 & 1 & 0 & \dots & 0 & 0 \\ 0 & 0 & 1 & \dots & 0 & 0 \\ \vdots & 0 & 0 & \dots & 1 & 0 \end{pmatrix}, \tag{A1}$$

where σ is a clock variable (in the diagonal representation) and τ is a raising and lowering operator. Consider the following Hermitian operator:

$$q(\sigma) = \frac{n-1}{2} + \sum_{a=1}^{n-1} \frac{\sigma^a}{\bar{\omega}^a - 1}. \tag{A2}$$

We now prove that this operator satisfies

$$q\big(\sigma = \omega^\delta = e^{\mathrm{i}\frac{2\pi}{n}\delta}\big) = \delta, \quad \delta = 0,\dots,n-1. \tag{A3}$$

In order to prove Eq. (A3), we start by showing that $q(\omega^0) = 0$:

$$q(\omega^0) = \frac{n-1}{2} + \sum_{a=1}^{n-1} \frac{1}{\bar{\omega}^a - 1} = \frac{n-1}{2} + \mathrm{Re}\left[\sum_{a=1}^{n-1} \frac{\omega^a - 1}{|\omega^a - 1|^2}\right] = \frac{n-1}{2} + \sum_{a=1}^{n-1}\left(-\frac{1}{2}\right) = 0. \tag{A4}$$

Now it is simple to verify that the following relation holds:

$$q(\bar{\omega}\sigma) = q(\sigma) + \sum_{a=1}^{n-1} \sigma^a. \tag{A5}$$

From the fact that $\sum_{a=1}^{n-1} \sigma^a = n-1$ if $\sigma = \omega^0 = 1$ and $\sum_{a=1}^{n-1} \sigma^a = -1$ if $\sigma = \omega^\delta$, $\delta \in \{1,\dots,n-1\}$, then it is possible to use Eq. (A5) to establish Eq. (A3) by induction. Thus combining Eq. (A2) and Eq. (A3) yields

$$\exp\left\{\mathrm{i}\,\frac{2\pi p}{n}\left[\frac{n-1}{2} + \sum_{a=1}^{n-1} \frac{(\sigma_j^\dagger \sigma_{j'})^a}{\bar{\omega}^a - 1}\right]\right\} = (\sigma_j^\dagger \sigma_{j'})^p, \tag{A6a}$$

$$\exp\left\{-\mathrm{i}\,\frac{2\pi p}{n}\left[\frac{n-1}{2} + \sum_{a=1}^{n-1} \frac{(\sigma_j^\dagger \sigma_{j'})^a}{\omega^a - 1}\right]\right\} = (\sigma_j^\dagger \sigma_{j'})^p, \tag{A6b}$$

for $p \in \{0,\dots,n-1\}$ (mod n).

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