Z_N Berry Phases in Symmetry Protected Topological Phases

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We show that the Z_N Berry phase (Berry phase quantized into $2\pi/N$) provides a useful tool to characterize symmetry protected topological phases with correlation that can be directly computed through numerics of a relatively small system size. The Z_N Berry phase is defined in a $N-1$-dimensional parameter space of local gauge twists, which we call the "synthetic Brillouin zone," and an appropriate choice of an integration path consistent with the symmetry of the system ensures exact quantization of the Berry phase. We demonstrate the usefulness of the Z_N Berry phase by studying two 1D models of bosons, SU(3) and SU(4) Affleck-Kennedy-Lieb-Tasaki models, where topological phase transitions are captured by Z_3 and Z_4 Berry phases, respectively. We find that the exact quantization of the Z_N Berry phase at the topological transitions arises from a gapless band structure (e.g., Dirac cones or nodal lines) in the synthetic Brillouin zone.

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In the past decades, topology has come to the fore of the condensed matter research and it has been serving as a guiding principle to explore novel phases of matter without relying on the symmetry breaking [1]. Meanwhile, symmetry still plays an important role in an interplay with topology. For example, topological phases of noninteracting fermions have been classified according to the generic internal symmetries, i.e., time-reversal, particle-hole, and chiral symmetries [1–5], and recently, the classification has been further extended by incorporating crystal symmetries [4,6–11]. On the other hand, characterization of topological phases becomes a more difficult problem for systems of strongly interacting particles [12]. There have been active studies on classification and characterization of symmetry protected topological (SPT) phases that are supported with strong correlation effects [1,13–21]. However, the characterization of SPT phases for a given Hamiltonian remains a highly nontrivial problem. In particular, a concise way to characterize them through fairly cheap numerics has been desired.

In characterizing SPT phases, the notion of adiabatic continuation plays an essential role [13–15,22]. By adiabatically continuing a given system into a simple reference system, the topological character in the original system is easily diagnosed by studying the simple reference system. For example, a system that can be adiabatically decomposed into a set of the elementary units in the system (an atomic insulator in the case of free fermions) is identified as a trivial phase. In contrast, the requirement for keeping a finite gap and the symmetry of the system sometimes excludes the possibility of "atomic insulators" and leaves a set of finite size *entangled* clusters [13,16,23], which indicates that the state is in a SPT phase. A representative example is the Haldane phase in a spin-1 Heisenberg chain [14,17,24–26], where the entangled clusters are intersite singlets of emergent spin-1/2 degrees of freedom.

In the search of adiabatic continuation into the embedded entangled clusters, it is useful to study the Berry phase defined through the local gauge twist [as schematically illustrated in Fig. 1(a)] [13,15,22,27,28]. Since the Berry phase can be quantized by symmetry in some cases, it

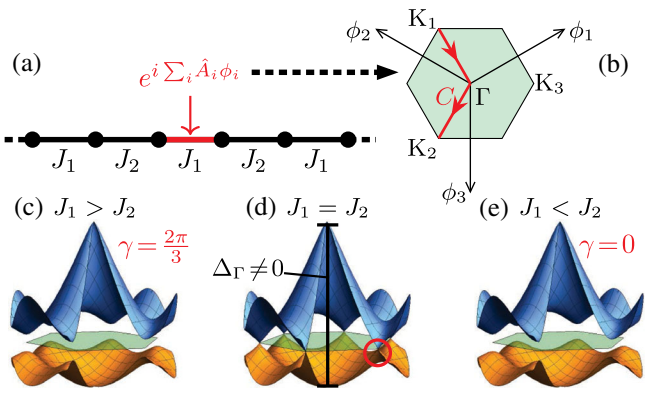

FIG. 1. (a) Schematic picture of the biquadratic model and the local gauge twist. The bonds J_i represent the biquadratic interactions. (b) Synthetic Brillouin zone and the integration path C leading to the Berry phase quantization. (c)–(e) The energy spectra for the ground state and the first excited state on the Brillouin zone. The gap at Γ point is always nonzero due to the finite size effect. At the phase transition, the gap closes at K and K' points forming Dirac cones.

provides a conserved quantity in the process of the adiabatic continuation that encodes the topological nature of the system. The Berry phase for the entangled cluster is easily obtained in the simple reference system and gives a characterization for the original system, which helps to have intuitive understanding of SPT phases. Also, the quantized nature is suitable for numerical analysis since it eliminates system size dependence. This is especially helpful in characterizing correlated SPT phases in numerical analysis. However, Berry phase analysis of correlated SPT phases have been so far mostly limited to the Haldane phase with Berry phase π [13].

In this Letter, we generalize the characterization of SPT phases with a correlation based on the Berry phase by using fractionally quantized Berry phase $2\pi/N$ (Z_N Berry phase) and propose that such Z_N Berry phase provides a useful tool to diagnose general topological phases of interacting particles [23]. We demonstrate that the Z_N Berry phase is useful in characterizing one-dimensional SPT phases classified by general Z_N topological number. Specifically, we extend the Berry phase analysis so that it can detect entangled clusters other than the conventional spin-1/2 singlets. We demonstrate that spin-1 singlets can be detected with the appropriate redefinition of the Berry phase. This can be applied to a bond-alternating spin-1 chain with biquadratic interaction (hereafter, called the biquadratic model), which supports a Z_3 SPT phase. In this case, the phase transition is captured by the Z_3 Berry phase (0 or $2\pi/3$), instead of the conventional one $\pi(=2\pi/2)$. We also show that a SU(4) symmetric spin chain supports a topological phase with a SU(4) fully antisymmetrized state being the entangled cluster, which can be diagnosed by the Z_4 Berry phase. These generalizations of the Berry phase into fractional ones involve the synthetic Brillouin zone (BZ) [see Fig. 1(b)] that parametrizes local gauge twists for a particular bond. When there exist N kinds of local gauge twists [$N=3$ for the SU(3) chain and $N=4$ for the SU(4) chain], such synthetic BZ is given by a $N-1$-dimensional space. (Note that the system itself is one dimensional.) We find that the phase transition is governed by a gapless structure that appears in the effective band structure in the synthetic Brillouin zone, such as the Dirac cones shown in Fig. 1(d). Thus, the Z_N Berry phase analysis allows us to understand the topological phase transition in the many-body system by using an analogy to that in the free-fermion system.

Let us begin with the formulation of the Berry phase. For simplicity, we focus on a one-dimensional periodic system with Hamiltonian $H=\sum_{ij}H_{ij}$. For finite size systems (either open or periodic) that are studied by numerical calculations in practice, the Berry phase is defined in the following way. First, we pick up a term on a certain bond, H_{nm}, out of the terms in the Hamiltonian. Then, it is replaced by $H_{nm}(\phi)=U_m(\phi)H_{nm}U_m^\dagger(\phi)$, where $U_m(\phi)=e^{i\hat{A}\phi}$ (the local gauge twist) acts on the mth site. While it looks like a unitary transformation, it actually is not, since the operation is selectively acting on the chosen bond. Therefore, the eigenvalues and eigenvectors change as $|G_0\rangle\to|G_\phi\rangle$. Using the set of these wave functions, the Berry phase γ is defined as

$$i\gamma=\int_0^{2\pi}d\phi\langle G_\phi|\partial_\phi G_\phi\rangle. \tag{1}$$

The choice of the gauge twist $\hat{A}$ is essential: it should make $U_m(\phi)$ periodic in ϕ and should properly capture the underlying entangled cluster [29].

In the previous studies of spin systems, $\hat{A}=S-\hat{S}_z$ has been the standard choice [13,15,27], which is suitable for detecting a spin-1/2 singlet. In this case, some symmetries constrain the Berry phase γ to quantize into 0 or π, where $\gamma=\pi$ signals the existence of a spin-1/2 singlet at the chosen bond. This is indeed the case for the Haldane phase in the spin-1 Heisenberg chain, which is a representative SPT phase, and its topological nature is captured by the valence bond solid picture, with pairs of spin-1/2 obtained from fractionalization of the original spin-1 forming *intersite* spin-1/2 singlets [30]. Then, $\gamma=\pi$ characterizes the Haldane phase, while $\gamma=0$ characterizes the topologically trivial large-D phase where fractional spin-1/2s form *intrasite* spin-1/2 singlets. Such quantization of the Berry phase (into 0 or π) allows us to observe the sharp transition between the Haldane and the large-D phases even for a chain of a relatively small number of sites. This observation can be generalized to the case of the Z_N Berry phase. Namely, the quantization of the general Z_N Berry phase indicates a sharp phase transition even for a small size system (without extrapolation to the thermodynamic limit) that can be studied in practical numerical calculations.

Next, we study a case where the entangled cluster is not a conventional spin-1/2 singlet. To this end, we consider a spin-1 chain with bond-alternating biquadratic interaction [31], which is described by the Hamiltonian

$$\hat{H}=-J_1\sum_i(\hat{\boldsymbol{S}}_{2i}\cdot\hat{\boldsymbol{S}}_{2i+1})^2-J_2\sum_i(\hat{\boldsymbol{S}}_{2i+1}\cdot\hat{\boldsymbol{S}}_{2i+2})^2. \tag{2}$$

It is known that this model supports the SU(3) Affleck-Kennedy-Lieb-Tasaki (AKLT) state [32]. In the language of the SU(3) AKLT state, the elementary object is a quark (and antiquark) and the entangled cluster characterizing the SPT phase is a meson (specifically, η meson). In the language of the spin-1 biquadratic model, the entangled cluster is mapped to a spin-1 "singlet" (two-spin state with zero total angular momentum). By writing $J_{1,2}$ as $J_1=J+\Delta$ and $J_2=J-\Delta$, the parameter Δ controls how the entangled clusters are formed. Therefore, once we fix the position of the gauge-twisted bond, the transition has to be observed by changing Δ. However, the standard choice of $\hat{A}=S-\hat{S}_z$ is inadequate for detecting the spin-1 singlet.

Instead, we use the twist operator $\hat{A} = \hat{A}_3 \equiv 1 - \hat{S}_z^2$. Since $\hat{S}_z$ ($\hat{S}_z^2$) is part of the dipole (quadrupole) moment, we call $e^{i(S-\hat{S}_z)\phi}$ ($e^{i\hat{A}_3\phi}$) dipolar (quadrupolar) twist. For our model, the twist is reflected in $H_{n,n+1}(\phi)$, and if there is a symmetry $H_{n,n+1}(\phi) = H_{n+1,n}(-\phi)$, the Berry phase should quantize into 0 or π [13]. The dipolar twist obeys this symmetry, while the quadrupolar twist does not. As a result, the latter does not lead to Z_2 quantization, but may quantize into other fractions of 2π [29].

The numerically obtained Berry phase as a function of Δ is summarized in Fig. 2. We identify two phases, which are characterized by $\gamma = 0$ for $\Delta > 0$ and $\gamma = 2\pi/3$ for $\Delta < 0$. The embedded spin-1 singlet exists on the twisted bond if $\gamma = 2\pi/3$, since an isolated singlet with a $\hat{A}_3$ twist is described by the wave function, $|\psi_\phi\rangle = (|+1,-1\rangle - e^{i\phi}|0,0\rangle + |-1,+1\rangle)/\sqrt{3}$ (by using a representation for the state of two spins, $|s_1^z, s_2^z\rangle = |s_1^z\rangle \otimes |s_2^z\rangle$ with $\hat{S}_{zi}|s_i^z\rangle = s_i^z|s_i^z\rangle$), and the second term $e^{i\phi}|0,0\rangle$ contributes to the Berry phase by $2\pi/3$. Note that, with the dipolar twist, the Berry phase is zero regardless of the sign of Δ, which means that the phase transition in Fig. 2 is captured only with our new method. The system size dependence in Fig. 2(a) suggests that the transition gets sharper as we approach the thermodynamic limit. However, the imperfect quantization degrades the advantage of the Berry phase.

Fortunately, the exact quantization is restored if the symmetry of the system is fully appreciated. The key symmetry of Eq. (2) is the spin rotational symmetry, in particular, the symmetry under the interchange of x, y, and z directions in the spin space. [This corresponds to the interchange of three flavors of quarks that forms a Z_3 subgroup of the SU(3) symmetry [32].] Accordingly, our formulation of the Berry phase can be symmetrized by considering the other twist operators $\hat{A}_1 = 1 - \hat{S}_x^2$ and $\hat{A}_2 = 1 - \hat{S}_y^2$ in addition to $\hat{A}_3$, and we define the generalized local gauge twist as $\exp(i\sum_i \hat{A}_i\phi_i)$ with three parameters $\phi_{1,2,3}$. Because $\hat{A}_1 + \hat{A}_2 + \hat{A}_3 = \hat{1}$, only two of three parameters are independent, namely, a twist by $e^{i\hat{A}_3\phi}$ has the same effect as a twist by $e^{-i(\hat{A}_1+\hat{A}_2)\phi}$ since $e^{i\hat{1}\phi}$ is trivial. This means that the generalized local gauge twist is defined on the two-dimensional periodic parameter space, which we call the synthetic Brillouin zone, with the hexagonal symmetry as shown in Fig. 1(b). In terms of the synthetic BZ, we can see that the Berry phase defined for a straight line along the ϕ_3 axis in the synthetic BZ leads to deviation from the quantization [Fig. 2(a)]. Instead, we now consider the path C (K_1-Γ-K_2) in Fig. 1(b), which is more symmetric in the synthetic BZ. Figure 2(b) shows the Berry phase obtained with the path C. In this case, the Berry phase shows an exact quantization into 0 and $2\pi/3$, leading to the sharp transition. The origin of the quantization is understood by considering the Berry phases defined with three different paths, γ_1 with K_1-Γ-K_2, γ_2 with K_2-Γ-K_3, and γ_3 with K_3-Γ-K_1. By the threefold rotational symmetry in the synthetic BZ, we obtain $\gamma_1 = \gamma_2 = \gamma_3$. At the same time, if the three paths are combined, they result in a trivial path, giving us $\sum_i \gamma_i = 0 \pmod{2\pi}$. The consequence of this symmetry consideration is that the Berry phase γ_i should quantize into $2\pi/3$ [23]. This argument does not rely on full SU(3) symmetry; we have confirmed the quantization with perturbation that breaks SU(3), but preserves $Z_3 \times Z_3$ symmetry (see Supplemental Material [29]).

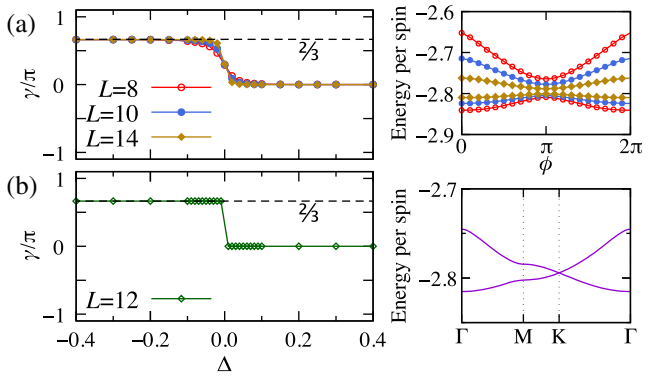

FIG. 2. (a) The Berry phase with $e^{i\hat{A}_3\phi}$ for several system sizes (L denotes the number of the spins). (Right) The energy spectra as functions of ϕ at $\Delta = 0$. (b) The Berry phase with $e^{i\sum_i \hat{A}_i\phi_i}$ using C in Fig. 1(b) as an integration path. (Right) The energy spectrum along the high symmetry lines in the synthetic Brillouin zone. L is set to 12. The energies are in the unit of J.

The introduction of the synthetic BZ reveals another notable aspect of the transition, i.e., an emergent gapless structure in the effective band structure. Generally speaking, quantization of the Berry phase indicates a jump in the value of γ at the phase transition, and such a jump requires a singularity in the wave function that is associated with gap closing. In this case, the energy gap above the ground state should close somewhere on the integration path. Conversely, no sharp transition is expected when the gap remains finite over the entire integration path. The right panel of Fig. 2(a) plots the energy spectrum as a function of ϕ for the $e^{i\hat{A}_3\phi}$ twist at $\Delta = 0$, which shows the absence of any gap closure. This accounts for the smooth change of γ at Δ in Fig. 2(a). In contrast, we indeed have a gap closing point on the path C at $\Delta = 0$. More specifically, the gapless points are found at K and K' points in the synthetic Brillouin zone. [See Figs. 1(c)–1(e) and the right panel of Fig. 2(b).] Interestingly, the energy spectrum at $\Delta = 0$ shows Dirac cones in a similar way to the band structure of graphene. This reminds us of the fact that the topological transition in free-fermion systems is often associated with a gapless band structure, such as Dirac cones. In an analogy, the topological phase transition in our model, although it is a correlated one-dimensional model, is associated with the Dirac cones that appear in the synthetic Brillouin zone. Note that the gap at Γ point, representing the state without

any twist, is always finite, including the case with $\Delta = 0$. In passing, we note that it is known that the ground state is doubly degenerate in the thermodynamic limit for $\Delta = 0$ [31]. This means that the "band structures" in Figs. 1(c)–1(e) collapse in the infinite size limit, and the jump in γ gets sharper with $L \to \infty$ in any case. However, as we have stressed earlier, the advantage of the quantized Berry phase lies in the usefulness in the finite size calculation of a relatively small system size.

Next, we show the usefulness of the Z_N Berry phase by applying it to another example of 1D SPT phases. We consider a SU(4) symmetric Hamiltonian [33]

$$H = -\sum_i \sum_{a=1}^{15} [J_1 \Lambda_a(2i)\bar{\Lambda}_a(2i+1) + J_2 \bar{\Lambda}_a(2i+1)\Lambda_a(2i+2)]. \quad (3)$$

Here, the fundamental representations of SU(4) and its conjugate representations are assigned on the $(2i)$th sites and $(2i+1)$th sites, respectively [see Fig. 3(a)]. The explicit form of the Λ_a is found in Ref. [34]. For convenience, we parametrize $J_{1,2}$ as $J_1 = J_0 + \delta J$ and $J_2 = J_0 - \delta J$. With the appropriate parameter choice, the ground state of this Hamiltonian shares the majority of properties with the SU(4) AKLT state [32]. In this case, the entangled cluster is the completely antisymmetrized state formed by a pair of the fundamental and its conjugate representations [which is analogous to the η meson in the SU(3) case]. In a similar manner to the case of Δ for the biquadratic model, δJ controls how the entangled clusters are formed, and the phase transition takes place by changing δJ. For the detection of the pattern of entangled clusters, we adopt $U(\boldsymbol{\phi}) = \exp(i \sum_{n=1}^{4} \check{A}_n \phi_n)$ as a gauge twist, where $(\check{A}_n)_{ij} = \delta_{ij}\delta_{in}$. Independent local gauge twists are defined on the three-dimensional synthetic BZ with the symmetry of the fcc BZ.

The numerically obtained Berry phase is plotted in Figs. 3(b) and 3(c). Again, the exact quantization of the Berry phase is achieved for a symmetric integration path W_1-Γ-W_2 in the synthetic BZ as shown in Figs. 3(d) and 3(e). With this setup, the phase transition is captured by a jump from $\gamma = 0$ to $\gamma = \pi/2 = (2\pi/4)$ [23,35,36]. Similar to the SU(3) case, the exact quantization is realized by integration paths that are symmetric against the interchange of $\check{A}_i$'s and forming a trivial path as a combination. On the other hand, a straight integration path and its symmetric counterparts do not form a trivial path, giving imperfect quantization [Fig. 3(c)]. The jump in the Z_4 Berry phase is again associated with the gapless point on the integration path. In this case, the gap closes on the X-W line; i.e., nodal lines appear in the three-dimensional Brillouin zone for $\delta J = 0$ [see Fig. 3(f)]. Interestingly, the energy spectrum resembles the band structure for the single orbital tight-binding model on the diamond lattice [see Fig. 3(g)].

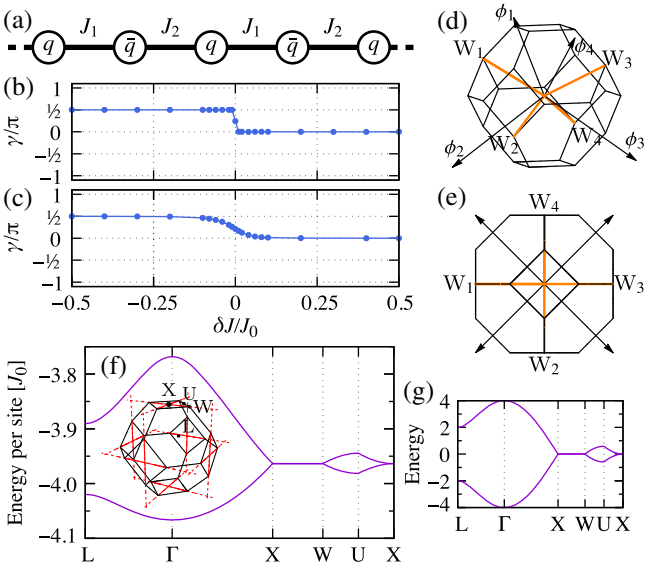

FIG. 3. (a) Schematic picture of the SU(4) model. q and $\bar{q}$ denote the fundamental representation and the conjugate representation, respectively. (b),(c) The Berry phases obtained with (b) the path W_1-Γ-W_2 and (c) the straight integration path along the ϕ_1 axis. (d),(e) The synthetic Brillouin zone and the integration path. (f) The energy spectrum on the symmetric lines in the synthetic BZ for $\delta J = 0$. (Inset) The location of the nodal lines. (g) The band structure of the single orbital tight-binding model on the diamond lattice.

Before closing, we compare the present characterization of SPT phases with the other known characterization that is based on projective representations of symmetry operation in the matrix product state representation of ground states [37]. The projective representation (and associated factor sets) extracts information of fractional excitations at the edge and is known to provide complete classification of 1D SPT phases. The Berry phase method has a similarity in that it detects entangled clusters, where the fractional excitations are interpreted as broken pieces of a cluster at the edge. Whether the Berry-phase-based theory can be as complete as the projective group method is an interesting future problem. As a first step, we give an alternative expression for the Z_3 Berry phase, which better clarifies the relation to the other theory, in the Supplemental Material [29]. This formula makes a clearer relationship between the quantized Berry phase and the general classification theory based on group cohomology [38]. Interestingly, the alternative formula uses only the wave functions at Γ and K_1 [see Fig. 1(d)], which is advantageous also in numerical evaluation.

To summarize, we have demonstrated the usefulness of the Z_N Berry phase as a topological invariant for SU(N) symmetric SPT phases. The key is the multiparameter local gauge twist, revealing that the topological transitions are associated with Dirac cones or nodal lines in the parameter space. It would be an interesting future problem to explore

the relationship between Dirac cones or nodal lines found here and those in free-fermion systems at the topological transition, for example, in terms of the criticality. Another promising direction would be an extension of the Z_N Berry phase to topological phases in higher spatial dimensions. The major task in doing so will be finding proper ways of applying the local gauge twist to ensure exact quantization. Once they are found, it will provide a tractable way to characterize general SPT phases based on the Hamiltonians explicitly.

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