Zₙ Berry Phases in Symmetry Protected Topological Phases

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We show that the Zₙ Berry phase (Berry phase quantized into 2π/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 Zₙ Berry phase is defined in a N − 1 dimensional parameter space of local gauge twists, which we call “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 Zₙ Berry phase by studying two 1D models of bosons, SU(3) and SU(4) AKLT models, where topological phase transitions are captured by Z₃ and Z₄ Berry phases, respectively. We find that the exact quantization of the Zₙ Berry phase at the topological transitions arises from a gapless band structure (e.g., Dirac cones or nodal lines) in the synthetic Brillouin zone.

In the past decades, topology has come to the fore of the condensed matter research and it has been realized that it serves 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]. The topological classification of noninteracting fermions 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 concave 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 possibility of “atomic insulators”, and leaves a set of finite-size entangled clusters [13, 16, 23], which indicates that the state is in an SPT phase. A representative example is 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 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 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. For instance, the spin-1/2 singlet in Haldane phase in spin chain is characterized by Berry phase π [13]. While the analysis based on Berry phase is useful in characterizing SPT phases, studies of correlated systems so far have mainly focused on those phases characterized by Berry phase π.

In this paper, we generalize the characterization of SPT phases with correlation based on Berry phase by using fractionally quantized Berry phase 2π/N (Zₙ Berry phase), and propose that such Zₙ Berry phase provides a useful tool to diagnose general topological phases of interacting particles [23]. We demonstrate that the Zₙ Berry phase is useful in characterizing one-dimensional SPT phases classified by general Zₙ 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 Z₃ SPT phase. In this case, the phase transition is captured by the Z₃ Berry phase (0 or 2π/3), instead of the conventional one π (= 2π/2). We also show that an SU(4) symmetric spin chain supports a topological phase with an SU(4) fully antisymmetrized state being the en-
tangled cluster, which can be diagnosed by $Z_4$ Berry phase. These generalizations of the Berry phase into fractional ones involve “synthetic” Brillouin zone (BZ) [see Fig. 1(b)] that parameterizes 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 appears in the effective band structure in the synthetic Brillouin zone such as 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 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 $U_m(\phi) H_{nm} U^\dagger_m(\phi)$, where $U_m(\phi) = e^{iA\phi}$ (the local gauge twist) acts on the $m$th 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 $|G_0\rangle \rightarrow |G_\phi\rangle$. Using the set of these wave functions, the Berry phase $\gamma$ is defined as

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

The choice of the gauge twist $\hat{A}$ is the most important part of this scheme. It should make $U_m(\phi)$ periodic in $\phi$, and should properly capture the underlying entangled cluster.

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 $\gamma$ to quantize into 0 or $\pi$, 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. The topological nature of the Haldane phase is captured by the valence bond solid picture, where pairs of spin-1/2 obtained from fractionalization of the original spin-1 form intersite spin-1/2 singlets [29]. The Berry phase quantizes into $\gamma = \pi$ in the Haldane phase, while it quantized into $\gamma = 0$ in the topologically trivial large-D phase where fractional spin-1/2’s form intrasite spin-1/2 singlets. Such quantization of the Berry phase (into 0 or $\pi$) 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 $Z_N$ 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 [30], which is described by the Hamiltonian,

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

It is known that this model supports the SU(3) AKLT state [31]. In the language of the SU(3) AKLT state, the elementary object is a quark (and antiquark) and the entangled cluster characterizing SPT phase is a meson (specifically, $\eta$-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 \( \Delta \) controls how the entangled cluster are formed. Therefore, once we fix the position of the gauge-twisted bond, the transition has to be observed by changing \( \Delta \). However, the standard choice of \( \Delta = S - \bar{S}_2 \) is inadequate for detecting the spin-1 singlet. Instead, we use the twist operator \( \hat{A} = \hat{A}_3 \equiv 1 - \hat{S}_2^z \). If the bond with the biquadratic interaction is twisted by \( e^{i\hat{A}_3\phi} \), each term acquires the phase as summarized in Table I. For comparison, we list the phase factors acquired in the conventional twist with \( e^{i(S - \bar{S}_2)\phi} \). Since \( \bar{S}_z \) (\( \bar{S}_2^z \)) is the part of the dipole (quadrupole) moment, we call \( e^{i(S - \bar{S}_2)\phi} \) (\( e^{i\hat{A}_3\phi} \)) dipolar (quadrupolar) twist. An important feature that we can see from the phase factors in Table I is their symmetry. If they are symmetric with respect to the combined operation of the complex conjugation and \( n \leftrightarrow m \), the Berry phase should be quantized into 0 or \( \pi \) [13]. Indeed the dipolar twist obeys this symmetry (e.g., the operation on the term 2 results in the term 3, leaving the term unchanged in total). On the other hand, the quadrupolar twist breaks this symmetry, and hence, it does not show \( Z_2 \) quantization, but may quantize into other fractions of \( 2\pi \).

The numerically obtained Berry phase as a function of \( \Delta \) 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, \( |\psi_0\rangle = (|+1, -1\rangle - e^{i\theta}|0, 0\rangle + |-1, +1\rangle)/\sqrt{3} \) (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 \( \bar{S}_2 = |s_2^z\rangle \), and the second term \( e^{i\theta}|0, 0\rangle \) 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 \( \Delta \), 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 quantization of the Berry phase is not perfect. Thus it does not ensure the advantage of using the Berry phase, i.e., quantization even for a relatively small size system.

Fortunately, we have a remedy to this deviation from the perfect quantization. The reason why it does not show quantization is that the symmetry of the system is not 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 which forms a \( Z_3 \) subgroup of the SU(3) symmetry [31].) Accordingly, our formulation of Berry phase can be symmetrized by considering the other twist operators \( \hat{A}_1 = 1 - \hat{S}_x \) and \( \hat{A}_2 = 1 - \hat{S}_y \) in addition to \( \hat{A}_3 \), and we define the generalized local gauge twist as \( \exp[i\sum_i \phi_i] \) with three parameters \( \phi_{1,2,3} \). Because of \( \hat{A}_1 + \hat{A}_2 + \hat{A}_3 = 1 \), only two of three parameters are independent, namely, a twist by \( e^{i\theta_3} \) has the same effect as a twist by \( e^{-i\theta_1 - i\theta_2} \) since \( e^{i\Phi_3} \) is trivial. This means that the generalized local gauge twist is defined on the two-dimensional periodic parameter space, which we call “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 \( \phi_3 \) axis in the synthetic BZ leads to deviation from the quantization [Fig. 2(a)]. Instead, we now consider the path \( C \) (\( K_1 \Gamma K_2 \)) 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, \( \gamma_1 \) with \( K_1 \Gamma K_2 \), \( \gamma_2 \) with \( K_2 \Gamma K_3 \), and \( \gamma_3 \) with \( K_3 \Gamma K_1 \). By the three-fold 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 \( \sum \gamma_i = 0 \) (mod \( 2\pi \)). The consequence of this symmetry consideration is that the Berry phase \( \gamma_i \) should quantize into \( 2\pi/3 \) [23].

The introduction of the synthetic BZ reveals another notable aspect of the transition, i.e., an emergent gapless structure in the effective field structure. Generally speaking, quantization of the Berry phase indicates a jump in the value of \( \gamma \) at the phase transition, and such a jump requires a singularity in the wave function which 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 $\phi$ for the $e^{i\lambda_1\phi}$ twist at $\Delta = 0$, which shows the absence of any gap closure. This accounts for the smooth change of $\gamma$ at $\Delta$ 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-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 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 $\Gamma$ 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 $\Delta = 0$ [30]. This means that the "band structures" in Figs. 1(c-e) collapse in the infinite size limit, and the jump in $\gamma$ 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 an SU(4) symmetric Hamiltonian [32],

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

(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 $\Lambda_a$ is found in Ref. 33. For convenience, we parameterize $J_{1,2}$ 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 becomes to share the majority of properties with the SU(4) AKLT state [31]. 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 $\eta$-meson in the SU(3) case). In a similar manner to the case of $\Delta$ for the biquadratic model, $\delta J$ controls how the entangled clusters are formed, and the phase transition takes place by changing $\delta J$. For the detection of the pattern of entangled clusters, we adopt $U(\phi) = \exp[i \sum_{n=1}^{4} \Lambda_n \phi_n]$ as a gauge twist, where $(\Lambda_n)_{ij} = \delta_{ij} \delta_{in}$. By using $\sum_n \Lambda_n = 1$, we notice that a twist $e^{i\lambda_1\phi}$ is essentially equivalent to a twist $e^{-i(\Lambda_1 + \Lambda_2 + \Lambda_3)\phi}$ and consequently, the local gauge twist is defined on the three-dimensional synthetic BZ with the symmetry of the fcc BZ.

The numerically obtained Berry phase is plotted in Fig. 3. Again, the exact quantization of the Berry phase is achieved for a symmetric integration path $W_1\Gamma-W_2$ 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, 34]. Similarly to the SU(3) case, the symmetry protecting the quantization of $Z_4$ Berry phase is the invariance under the interchange of the four components of the fundamental representation of SU(4). When the straight integration path along one of the $\phi_i$ axis is used naively, the Berry phase is no longer quantized and it does not show a sharp transition at $\delta J = 0$ [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. 4]. Interestingly, the
energy spectrum resembles the band structure for the single orbital tight-binding model on the diamond lattice.

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 ingredient is a suitable choice of $\hat{A}$ for the local gauge twist, and the introduction of the synthetic Brillouin zone reflecting the symmetry of the system. The topological transitions are captured by jumps in the Berry phase, and the associated singularities (Dirac cones/nodal lines) in the synthetic Brillouin zone. It would be an interesting future problem to explore the relationship between Dirac cones/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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