Characterization of topological phase transitions via topological properties of transition points

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We study topological properties of phase transition points of topological quantum phase transitions by assigning a topological invariant defined on a closed circle or surface surrounding the phase transition point in the parameter space of momentum and transition driving parameter. By applying our scheme to the Su-Schrieffer-Heeger model and Haldane model, we demonstrate that the topological phase transition can be well characterized by the defined topological invariant of the transition point, which reflects the change of topological invariants of topologically different phases across the phase transition point.

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Introduction.- Conventional continuous quantum phase transitions (QPTs) are driven by pure quantum fluctuation effects due to the change of external parameters and generally described in terms of the spontaneous symmetry breaking and order parameters of the ground state [1]. On the contrary, topological QPTs involve the change of ground-state topological properties and accompany no symmetry breaking [2–4]. Different topological states are classified by topological quantum numbers, which take discrete numbers, in contrast to order parameters used in conventional QPTs to distinguish various phases, which generally take continuous values. Conventionally, continuous QPTs can be classified into different order QPTs by singularity properties of the ground-state energy at the phase transition point (or critical point for \( n \geq 2 \)), i.e., \( n \)th order QPTs are characterized by discontinuities in the \( n \)th derivative of the ground-state energy.

As the singularity of ground-state energy plays an important role in determining universal properties around the critical point of the QPT, however it can not distinguish whether the phase transition is a topological QPT or a conventional one within the Landau-Ginzburg paradigm [1]. Beyond the traditional energy criterion, a QPT can be also witnessed by qualitative changes of physical quantities related to the ground-state wavefunctions, e.g., the Berry phase [5,6], quantum fidelity and the fidelity susceptibility [7–10], and the quantum geometric tensor [11–13]. Although these approaches have shed light on our understanding of QPTs from the geometric aspect of the ground-state manifold, one can not identify a QPT to be a topological or trivial one solely from the singularity of particular physical quantities at the phase transition point unless additional quantities related to the topological invariant are calculated. An interesting question arising here is whether we can characterize a QPT is topological or conventional phase transition from the property of the phase transition point?

To answer the question, let us recall that a topological QPT distinguished from a trivial one is manifested by the change of topological invariant, instead of symmetry breaking, across the transition point. While the topological invariant, e.g., the quantized Berry phase for one-dimensional (1D) topological systems [14] or Chern number for two-dimensional (2D) quantum Hall systems [15], is well defined for a gapped phase apart from the QPT point and characterizes the global geometrical property of the Bloch band, it fails to work at the gapless critical point. To overcome the difficulty, in this work we propose an alternative definition for the topological invariant, which is not defined on the momentum space at the transition point, but via a closed detour path surrounding the critical point on the parameter space spanning by both the momentum and the transition driving parameter. By applying this idea to the 1D and 2D topological systems, e.g., the celebrated Su-Schrieffer-Heeger (SSH) model and Haldane model, we demonstrate these topological invariants taking nontrivial quantized numbers for topological QPTs, but some non-universal numbers or zero number for conventional QPTs. Our results suggest that we can judge topological or trivial QPTs from topological properties of the phase transition points.

1D topological models.- We begin our discussion with one of the simplest 1D topological systems, the SSH model [16], which can be described by the Hamiltonian:

\[
H = \sum_{i} \left[ (t + \delta) \hat{c}_{A,i}^\dagger \hat{c}_{B,i} + (t - \delta) \hat{c}_{A,i+1}^\dagger \hat{c}_{B,i} \right] + h.c.,
\]

where \( c_{A/B,i}^\dagger \) is the creation operator of fermion on nth A (or B) sublattice. This model has two sites in a unit cell, the hopping amplitude in the unit cell is \( t + \delta \) and that between two unit cells is \( t - \delta \). For convenience, \( t = 1 \) is taken as the energy unit. After the Fourier transformation \( \hat{c}_{i,s} = \frac{1}{\sqrt{2}} \sum_{k} e^{i k n} \hat{c}_{k,s} \), the Hamiltonian can be written as

\[
H = \psi_k^\dagger h(k) \psi_k,
\]

where \( \psi_k = (\hat{c}_{k,A}^\dagger, \hat{c}_{k,B}^\dagger) \) and \( h(k) = h_x \sigma_x + h_y \sigma_y \) with \( \sigma \) the Pauli matrix acting on the vector \( \psi_k \), \( h_x = (1 + \delta) + (1 - \delta) \cos k \), \( h_y = (1 - \delta) \sin k \). It is well known that this model has two topologically distinct phases for \( \delta > 0 \) and \( \delta < 0 \) with the phase transition point at \( \delta = 0 \), where the gap closes at \( k = \pi \). Under the open boundary condition (OBC), these two phases can be distinguished by the presence and absence of degenerate zero-mode edge states [17], as shown in Fig 1(a).
played in Fig. 1(b)-(d), the topological property of the distinct phase can be characterized by the Zak phase [18, 19], i.e., the winding of $\phi$ varies a period. The arrows in (e)-(g) show the winding of $\phi$ at $\gamma$ varies a period. The arrows in (e)-(g) show the direction of the Hamiltonian $h(k)$ and $\gamma$. 

While the spectrum under periodic boundary condition (PBC) shows a similar structure for $\delta < 0$ or $\delta > 0$, as displayed in Fig. 1(b)-(d), the topological property of the distinct phase can be characterized by the Zak phase [18, 19], i.e., the Berry phase across the the Brillouin zone, which is defined as

$$\gamma = i \int_{-\pi}^{\pi} dk (w(k) \partial_k w(k)),$$

with $w(k)$ the eigenstate of the occupied Bloch band. While the topological phase is characterized by $\gamma = \pi$ for $\delta < 0$, the trivial phase corresponds to $\gamma = 0$ for $\delta > 0$. The geometrical meaning of the Zak phase can be understood as the winding angle of $h(k)$ as $k$ varies across the Brillouin zone [20], as shown in Fig. 1(c) and (g). For the topological nontrivial case with $\delta = -0.5$, the direction of $h(k)$ winds an angle of $2\pi$, whereas for the trivial case with $\delta = 0.5$ the winding angle is zero. However, when $\delta = 0$, the two bands are degenerate at $k = \pi$ (Fig. 1(c)), and the Zak phase is ill-defined.

To describe the topological property of state at the phase transition point, here we defined the Berry phase on a circle around the gap closing point in the parameter space of $k$ and $\delta$. Introducing $\theta$ as the varying angle and $A$ as radius of the circle, we have $k = A \sin \theta + \pi$ and $\delta = A \cos \theta$, hence the Hamiltonian around the circle can be represented as $h(\theta)$, and the Berry phase is defined as

$$\gamma_d = i \int_{-\pi}^{\pi} d\theta (\dot{\varphi}(\theta) \dot{\theta}_\theta | \varphi(\theta)),$$

After some algebras, one can obtain $\gamma_d = \pi$, which corresponds to the topological phase transition at $\delta = 0$. In Fig. 1(d), we also show the winding of $h(\theta)$ as $\theta$ varies a period, giving rise to a winding angle of $2\pi$.

As a comparison, we next consider a topologically trivial two-band model with alternating on-site potentials, described by the Hamiltonian:

$$H = \sum_i [\hat{c}_i^\dagger \hat{c}_{i+1} + \hat{c}_i^\dagger \hat{c}_{i+1} + h.c.] + \mu (\hat{c}_i^\dagger \hat{c}_i - \hat{c}_i^\dagger \hat{c}_i).$$

This model has alternating chemical potential $\mu$ and $-\mu$ for site A and B, and has a similar spectrum as the SSH model with a phase transition occurring at $\mu = 0$. However, as $\mu$ breaks the inversion symmetry, the Berry phase of each band is no longer quantized and no degenerate edge states emerge under the OBC. Similarly, we can also calculate the Berry phase around the gap closing point at $\mu = 0$ and $k = \pi$. The numerical result shows that $\gamma_d$ is not a quantized invariant and is associated with the radius $A$ of the integral path. On the contrary, the $\gamma_d$ for the SSH model is always $\pi$ regardless of the value of $A$, which suggests that $\gamma_d$ is a topological invariant. This difference means that we can judge whether the QPT is a topological phase transition from values of the Berry phase $\gamma_d$ around the critical point.

2D topological models.- Next we apply a similar scheme to study the topological property of phase transition points of 2D systems. We begin our discussion with the famous Haldane model [21], which supports a rich phase diagram, exhibiting either topological or trivial phase transitions. The Haldane model is a prototype model which may realize the anomalous quantum Hall effect in a 2D honeycomb lattice without any net magnetic flux through a unit cell of the system. The Hamiltonian of the Haldane model is given by:

$$H = \sum_i t_i \hat{c}_i^\dagger \hat{c}_i + \sum_{(i,j)} t_{ij} \hat{c}_i^\dagger \hat{c}_j + \sum_{(i,j)} t_{ij} \hat{c}_i^\dagger \hat{c}_j,$$

where the summation is defined on the 2D honeycomb lattice, which is composed of two sublattices labeled by A and B, respectively. Here $t_0 = M$ for site A and $t_0 = -M$ for site B, $t_1$ denotes the nearest-neighbor hopping amplitude, and $t_2$ denotes the next-nearest-neighbor (NNN) hopping amplitude. The magnitude of the phase is set to be $|\sigma_{i, j}| = \alpha$, and the direction of the positive phase is clockwise, following Haldane’s work. This model is well known for its three topologically different phases characterized by the Chern number $C$ ($C = \pm 1$ or 0), which is defined as the integral of the Berry curvature $\mathbf{V}$ for each band in the Brillouin zone, with $\mathbf{V}$ defined as $\nabla \times \dot{i} (\varphi(k) / |\nabla \varphi(k)|)$, where $\varphi(k) = \varphi(x, k) = \varphi(x, k)$ is the eigenstate of the occupied Bloch band.

Consider the case with $|t_2/t_1| < 1/3$, for which the two bands never overlap and only touch at the Brillouin zone corner when $M = \mp 3 \sqrt{3} t_2 \sin \alpha$. Expanding the Hamiltonian in the momentum space around the Dirac point $K_x = (\pm 4 \sqrt{2} / 3 \sqrt{3})$, i.e., $k_x = \pm 4 \sqrt{2} / 3 \sqrt{3} + x$ and $k_y = y$, we get the effective Hamiltonian:

$$h(k) = \mp 3 t_1 x \sigma_x + t_1 y \sigma_y + (M \mp 3 \sqrt{3} t_2 \sin \alpha) \sigma_z.$$
The phase diagram of Haldane model is displayed in Fig.3 (a) and (b) show the phase diagram of the Haldane model with $C_d$ on the phase boundary being marked. (a) is for the case with $C_d$ defined in the space of momentum and $\alpha$; (b) is for the case with $C_d$ defined in the space of momentum and $M$. (c)-(e) show the direction of $h(k)$ near the gap closing point in (a) with different $\alpha_0$: (c) $\alpha_0 = \pi/3$, $M = 9t_2/2$, $C_d = 1$; (d) $\alpha_0 = \pi/2$, $M = 3\sqrt{3}t_2$, $C_d = 0$; (e) $\alpha_0 = 2\pi/3$, $M = 9t_2/2$, $C_d = -1$.

The gap closing points are at $x = y = 0$ and $M \pm 3\sqrt{3}t_2 \sin \alpha = 0$. While the gap closes at both of $K_a$ when $M = 0$ and $\alpha = 0$ or $\pi$, there can be no more than one gap closing point for other value of $\alpha$, i.e., the gap closes at $K_a$ when $M = 3\sqrt{3}t_2 \sin \alpha$ or at $K_b$ when $M = -3\sqrt{3}t_2 \sin \alpha$. Different situations of band touching are shown in Fig.2.

The phase diagram of Haldane model is displayed in Fig.3 (a) or (b) with different phases characterized by the Chern number $C$. At the phase boundary, the gap between the upper and lower energy bands closes, and the Chern number is ill-defined therein. Similar to the 1D case, we can define a topological invariant on a closed surface surrounding the phase transition point in the parameter space of $k$ and transition driving parameter $\delta$ to describe the topological property of the transition point. Different from the 1D case, here the topological invariant is given by

$$C_d = -\frac{1}{2\pi} \oint \oint \mathbf{V} \cdot d\mathbf{S},$$

with $\mathbf{S}$ a sphere surface around the gap closing point $(k_0^+, T_0^+, \delta_0)$. Following Berry’s work, the Berry curvature for the lower band can be expressed as:

$$\mathbf{V} = Im \left( \langle -|\nabla h(k, \delta)|+\rangle \times \langle +|\nabla h(k, \delta)|-\rangle \right) \left( E_+ - E_- \right)^2,$$

with $|+$ |$($-$$)$ the eigenstate of the upper (lower) band. With some further calculations, the Berry curvature can be written as:

$$V^x = -\frac{1}{2R^3} \left( \frac{\partial h_x}{\partial k_x} \right)^2 + \left( \frac{\partial h_x}{\partial k_y} \right)^2 + \left( \frac{\partial h_x}{\partial k_z} \right)^2,\quad V^y = -\frac{1}{2R^3} \left( \frac{\partial h_y}{\partial k_x} \right)^2 + \left( \frac{\partial h_y}{\partial k_y} \right)^2 + \left( \frac{\partial h_y}{\partial k_z} \right)^2,\quad V^z = -\frac{1}{2R^3} \left( \frac{\partial h_z}{\partial k_x} \right)^2 + \left( \frac{\partial h_z}{\partial k_y} \right)^2 + \left( \frac{\partial h_z}{\partial k_z} \right)^2.$$

Here the Hamiltonian $h(k) = h_x \sigma_x + h_y \sigma_y + h_z \sigma_z$ and $R = \sqrt{h_x^2 + h_y^2 + h_z^2}$. For convenience, we choose a spherical surface surrounding the gap closing point with a radius of $A$, i.e., $k_x = k_0^+ + x$, $k_y = k_0^+ + y$, $\delta = \delta_0 + z$ with $x = A \sin \theta \cos \phi$, $y = A \sin \theta \sin \phi$, and $z = A \cos \theta$, where $\theta$ is the polar angle and $\phi$ is the azimuthal angle of the spherical surface. The integral then becomes:

$$C_d = -\frac{1}{2\pi} \oint \oint \mathbf{V} \cdot (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) A^2 \sin \theta d\theta d\phi.$$
**K._** as an example, and the case at **K.** can be analyzed similarly. Defining \( \alpha = \alpha_0 + z \) with \( M - 3 \sqrt{3} t_2 \sin \alpha_0 = 0 \) and expanding the Hamiltonian near \( \alpha_0 \), we have
\[
h(k) = -\sqrt{3} t_1 x \sigma_x + t_1 y \sigma_y - 3 \sqrt{3} t_2 \cos \alpha_0 z \sigma_z \quad (10)
\]
when \( |M| < 3 \sqrt{3} t_2 \), and the Chern number around \( \text{K.} \) is \( C_d(\alpha) = \text{sgn}(\cos \alpha_0) \). When \( |M| = 3 \sqrt{3} t_2 \), i.e., the case with \( \alpha_0 = \pm \pi/2 \) marked by the “cross” in Fig.3(a), however, the expansion becomes
\[
h(k) = -\sqrt{3} t_1 x \sigma_x + t_1 y \sigma_y + 3 \sqrt{3} t_2 \sigma_z^2 \quad (11)
\]
and the integral results in \( C_d(\alpha) = 0 \) as the integrand is an odd function in the interval. In Fig.3(a), we show the value of \( C_d \) around the phase boundary: except \( C_d = 0 \) at the four points marked by “crosses”, it takes either 1 or -1. We can see that \( C_d(\alpha) \) shows the change of the band Chern number \( C \) across the transition point by varying \( \alpha \). For the case of \( C_d = 0 \), the change of \( C \) is zero when varying \( \alpha \), which indicates a topologically trivial phase transition. On the other hand, the case of \( C_d = \pm 1 \) corresponds to a topological phase transition from the trivial (topological) phase to topological (trivial) phase. Particularly, when \( M = 0 \) and \( \alpha = 0 \) (or \( \pi \)), there are two gap closing points in the Brillouin zone, and the change of \( C \) is \( \pm 2 \) when varying \( \alpha \), which corresponds to the summation of \( C_d \) around these two points.

If we choose \( M \) as the third parameter besides the momentum \( k \) by keeping \( \alpha \) fixed and define \( M \equiv M_0 + z \) with \( M_0 \equiv 3 \sqrt{3} \sin \alpha = 0 \), the expansion of the Hamiltonian becomes:
\[
h(k) = \mp \sqrt{3} t_1 x \sigma_x + t_1 y \sigma_y + z \sigma_z, \quad (12)
\]
and the Chern number around the gap closing point of \( \text{K.} \) (\( \text{K.} \)) is always \( C_d(M) = -1(1) \), as shown in Fig.3(b). The value of \( C_d(M) \) also indicates the change of \( C \) when varying \( M \). When \( M = 0 \) and \( \alpha = 0 \) and \( \pi \), the change of \( C \) is zero, which also matches the summation of \( C_d(M) \).

To visualize the Chern number \( C_d \), we show the direction of \( h(k) \) around the gap closing point with different \( \alpha_0 \) in Fig.3(c)-(e). One can see that all the arrows point to \( z = 0 \) in (c), and to the opposite direction in (e), but the \( z \)-component of \( h(k) \) in (d) is always positive. The value of \( C_d \) is associated with the direction of \( h(k) \). In Fig.3(c), the direction of \( h(k) \) is always toward \( x = z = 0 \) and away from \( y = 0 \), which corresponds \( C_d = 1 \). In Fig.3(c), the direction of \( h(k) \) is opposite to the one in Fig.3(c) only in the \( z \)-direction, corresponding to \( C_d = -1 \). However, in Fig.3(d), the \( z \)-component of \( h(k) \) follows the same direction, corresponding to \( C_d = 0 \).

Our theory can be applied to study other 2D topological systems. To give an additional example, we next investigate a lattice model on a square lattice described by the Hamiltonian

\[
H = h \cdot \sigma \quad \text{with} \quad \sigma = (\sigma_x, \sigma_y, \sigma_z, \sigma_z)
\]

the Pauli matrices and \( h = (\sin k_x, \sin k_y, \beta [\mu - \cos k_x - \cos k_y]) \), which is known as the Qi-Wu-Zhang (QWZ) model [23]. Depending on the value of \( \mu \), this model has three different topological phases characterised by the band Chern number \( C \). Setting \( \beta = 1 \), the band Chern number \( C = 0 \) when \( |\mu| > 2 \), and \( C = -\text{sgn}(\mu) \) when \( |\mu| < 2 \). There are three phase transition points for this model: \( \mu = -2 \), \( \mu = 0 \) and \( \mu = 2 \). As shown in Fig.3(a)-(c), when \( \mu = \pm 2 \), there’s only one gap closing point \((k_x = k_y = \pi) \) for \( \mu = -2 \) and \( k_x = k_y = 0 \) for \( \mu = 2 \) in the Brillouin zone, but when \( \mu = 0 \), there are two gap closing points \((k_x = \pi, k_y = 0) \) and \( (k_x = 0, k_y = \pi) \). By choosing \( \mu \) as the third parameter beside the momentum, the expansion of the Hamiltonian near the gap closing points results in

\[
h(k) = \pm x \sigma_x - y \sigma_y + z \sigma_z, \quad \mu = -2;
\]

\[
h(k) = \pm x \sigma_x + y \sigma_y + z \sigma_z, \quad \mu = 0;
\]

\[
h(k) = x \sigma_x + y \sigma_y + z \sigma_z, \quad \mu = 2.
\]

In Fig.3(d)-(f) we show the direction of \( h(k) \) in the \( x - y \) plane, as the \( z \)-component of \( h(k) \) is always away from \( z = 0 \). The result shows that \( C_d = 1 \) for \( \mu = \pm 2 \), and \( C_d = -1 \) for both gap closing points when \( \mu = 0 \), hence the summation of \( C_d \) at each phase transition point also corresponds to the change of the band Chern number \( C \).

**Summary.** In summary, we proposed a scheme to study the topological properties of phase transition point for various topological QPTs by introducing a topological invariant defined on a closed curve in the parameter space surrounding the transition point. By studying several typical topological models, we demonstrated that the topological or trivial phase transition can be distinguished by the introduced topological invariant around the transition point, which takes nontrivial quantized numbers for topological QPTs but non-universal numbers or zero number for conventional QPTs. Our theory provides a way to discriminate topological or trivial QPTs by directly studying the properties of the phase transition point.

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