Universal Linear Scaling of Topological Phase Transition in Band Theory

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(Dated: April 15, 2019)

Abstract

We develop a unified view of topological phase transitions (TPTs) in solids by revising the classical band theory with the inclusion of topology. Taking the TPT between normal insulators (NIs) and quantum spin Hall (QSH) insulators as an example, we demonstrate that the critical transition point is underlined by a universal linear scaling between the characteristic bond strength and average bond length. The validity of this scaling relation is verified in various two-dimensional (2D) systems including crystalline, quasicrystalline and amorphous lattices based on a generic tight-binding model. Furthermore, this universal linear scaling is shown to set an upper bound for the degree of structural disorder to destroy the topological order in a crystalline solid, as exemplified by formation of vacancies and thermal disorder. Our work formulates a simple framework for understanding the physical nature of 2D TPTs with significant implications in practical applications of topological materials.
Introduction. The study of TPT dates back to 1970s when phenomena in quantum states of matter, such as the quantum Hall effect and superfluid phase transitions in 2D, were explained using the mathematical concepts of topology. These pioneering works have since paved the way for the introduction of many new topological states such as quantum anomalous/spin Hall effects, 3D topological insulators (TIs) and topological superconductors, and revolutionized electron band theory. Generally, topological states are insensitive to a smooth change of material parameters unless the system passes through a TPT. The TPT is characterized by a sudden jump of topological invariant without symmetry breaking, which cannot be described by the Landau-Lifshitz theory of conventional phase transitions.

As a fascinating topic, the TPTs between NIs and QSH states have been studied in various theoretical models and real materials in recent years. The QSH state is manifested by an insulating bulk and topologically protected metallic edges with quantized conductance that are immune to non-magnetic “edge” impurities or defects. It is mathematically characterized by a non-zero integer $Z_2$ invariant. In general, the TPT from a NI to a QSH state requires a band inversion between conduction and valence bands. During the TPT, the bulk energy gap closes and reopens accompanied with a change of the $Z_2$ invariant. So far, various QSH systems with different band inversion mechanisms have been theoretically proposed and/or experimentally verified, either periodic or aperiodic. The critical condition of TPTs are determined on a case-by-case basis; there is no universal view on the TPT, such as its criticality, among different systems.

In this Letter, we devise a general topological band theory that underlines a universal linear scaling of TPTs in crystalline, quasicrystalline and amorphous lattices. Based on a generic tight-binding (TB) model, we demonstrate that the critical transition point for the TPT is determined by a universal linear scaling relation between the characteristic bond strength and average bond length, regardless of lattice symmetry and disorder. We validate this universal linear scaling by calculating TPTs in various 2D crystalline lattices (oblique, trigonal, square, rectangle, hexagonal, rhombic, etc.) as well as quasicrystal lattices. Furthermore, we demonstrate this universal linear scaling sets an upper bound for the degree of disorder to destroy the topological order in a crystal by the case studies of vacancy formation and thermal disorder.
Model. Our TB model consists of three orbitals \((s, p_x, p_y)\) per site \cite{29, 30},

\[
H = \sum_{i\alpha} \epsilon_\alpha c_{i\alpha}^\dagger c_{i\alpha} + \sum_{\langle i\alpha, j\beta \rangle} t_{i\alpha,j\beta} c_{i\alpha}^\dagger c_{j\beta} + i\lambda \sum_i (c_{ip_y}^\dagger \sigma_z c_{ip_x} - c_{ip_x}^\dagger \sigma_z c_{ip_y}),
\]

where \(c_{i\alpha}^\dagger = (c_{i\alpha\uparrow}^\dagger, c_{i\alpha\downarrow}^\dagger)\) are electron creation operators on the \(\alpha(= s, p_x, p_y)\) orbital at the \(i\)-th site and \(\epsilon_\alpha\) is the on-site energy of the \(\alpha\) orbital. \(t_{i\alpha,j\beta} = t_{\alpha\beta}(r_{ij})\) is the hopping integral. \(\lambda\) is the spin-orbit coupling (SOC) strength and \(\sigma_z\) is the Pauli matrix. All the length are measured in unit of the first nearest-neighbor (NN) distance \(r_1\). We set a cutoff distance \(r_{\text{cut}}\) beyond which the hopping vanishes. Within the cutoff, \(t_{\alpha\beta}(r_{ij}) = \text{SK}[\hat{r}_{ij}, V_{\alpha\beta\delta}(r_{ij})]\) follows the Slater-Koster scheme \cite{31}. The radial dependence of the bond strength \(V_{\alpha\beta\delta}(r_{ij})\) (with \(\delta = \sigma\) or \(\pi\)) is captured approximately by the Harrison relation \cite{32}:

\[
V_{\alpha\beta\delta}(r_{ij}) = \eta_{\alpha\beta\delta} \frac{\hbar^2}{m} \left(\frac{\gamma}{r_{ij}}\right)^n,
\]

where \(\hbar\) is reduced Planck constant and \(m\) is electron mass. \(\eta_{\alpha\beta\delta}\) is a constant \cite{33, 34, 35} and \(\gamma\) represents the characteristic bond strength \cite{36, 37}. Here we chose the typical value \(n = 2\) \cite{32, 38}, however, it may take other values for different materials \cite{39}. Since only the band inversion between \(s\) and \(p\) states of different parities is important for TPT, we focus on the \(2/3\) filling of electronic states hereafter.

We define the average bond length \(L\) for a system with \(N\) atomic sites as,

\[
\frac{1}{L^n} = \frac{1}{N} \sum_{i<j} \frac{1}{r_{ij}^n},
\]

where the summation runs over all the bonds within the cutoff (i.e., \(r_{ij} < r_{\text{cut}}\)). It is worth noting that this expression is applicable to both crystal and noncrystal lattices, as discussed later.

Universal linear scaling of TPT. It is well known that isolated atomic levels will spread to form energy bands when atoms are brought together to form a solid \cite{32, 40, 41}, which provides a general band evolution process to understand metal, semiconductor and insulator states. However, an intermediate topological phase may appear during the band evolution process when the SOC effect is included. Here we consider the band inversion process induced by increasing the bond strength for a fixed SOC and atomic levels. As shown in Fig. 1 starting from the atomic limit, \(s\) and \(p\) levels are initially separated by a trivial charge gap \(\Delta_{sp}\). We illustrate the case for \(s\) level above \(p\) level with \(\Delta_{sp} \gg \lambda\), and the cases with
FIG. 1. Schematic illustration of TPT. By increasing bond strength $\gamma$, the bandwidth increases gradually and a TPT occurs at $\gamma_c$, which exhibits a linear scaling with $L$.

the reversed order and with $\Delta_{sp} \ll \lambda$ are shown in Fig. S1-S3 in Supplemental Materials [42]. $p$ levels split due to SOC effect. By increasing the bond strength $\gamma$, the orbital levels spread to form individual bands with a finite band width $W$. Consequently, the charge gap reduces and closes eventually to realize a band inversion. Then the SOC effect reopens an energy gap with nontrivial topology. Further increasing the bond strength to overcome the SOC gap will drive the system into a gapless phase before reaching a semiconducting phase with strong $s$-$p$ hybridization. Therefore, the TPT occurs when the band width $W$ is enlarged sufficiently to close the charge gap. Accordingly, the critical transition point is roughly determined by a critical band width $W_c = \frac{1}{2}(W_s + W_p - 2\lambda) = \Delta_{sp} - \lambda$, which depends only on the given atomic levels and SOC strength, independent of lattice periodicity and symmetry.

Within the TB approximation, the band width $W$ of different lattices is approximatively proportional to the summation of NN hopping integrals [43, 44], which can be tuned by the bond strength $\gamma$ in Eq. (1). Then, the critical transition point $\gamma_c$ of TPT is simply
FIG. 2. TPT in a trigonal lattice. The parameters used here are $\epsilon_s = 0.18, \epsilon_p = -0.65, \lambda = 0.08, V_{ss\sigma} = -0.04, V_{sp\sigma} = 0.09, V_{pp\sigma} = 0.18$ and $V_{pp\pi} = 0.005$ eV. The color of dots represents the relative weight of $s$ and $p$ orbitals. (a) Energy gap $E_g$ and $Z_2$ index versus bond strength $\gamma$. A TPT between a NI and a QSH insulator is clearly visible. (b) Band structure of the trigonal lattice at the QSH phase.

determined by

$$W_c \propto \sum_{i,j} t_{\alpha\beta}(r_{ij}) = \sum_{i,j} SK[\hat{r}_{ij}, \eta_{\alpha\beta}\gamma_c r_{ij}] \left(\frac{\gamma_c}{r_{ij}}\right)^2$$

$$\propto \gamma_c^2 \sum_{i,j} \frac{1}{r_{ij}^2} = \left(\frac{\gamma_c}{L}\right)^2 = \text{const.} \quad (3)$$

Here we ignore the directional dependance of the interatomic bonding because it depends much more strongly on bond length than bond angle \cite{45}. In a sense, the critical behavior of TPTs is mainly determined by the neighboring environment due to the “nearsightedness” of quantum-mechanical interactions \cite{46–51}.

**TPTs in crystal and quasicrystal lattices.** To validate the above hypothesis, we first systemically calculated TPTs in various 2D periodic lattices. For a trigonal lattice, it was found previously to host QSH state, such as in Au/GaAs(111) and Bi/Si(111) systems \cite{52,53}. By tuning the bond strength $\gamma$, the trigonal lattice undergoes a TPT between a NI and a QSH state accompanied by an energy gap closing and reopening. Figure 2(a) shows the critical values of the TPT is $\gamma_c = 0.971$ for the trigonal lattice. In Fig. 2(b), the orbital-resolved band structure indicates a nontrivial electronic topology beyond the TPT.
It exhibits a band inversion around the Γ point between the \( s \)-orbital-derived conduction band and the \( p \)-orbital-derived valence band. The calculated \( Z_2 = 1 \), which is obtained by directly tracing the evolution of 1D hybrid Wannier charge center \( \overline{54} \), confirming the QSH state in this region. Furthermore, similar TPTs have been found in all 2D Bravais lattices including oblique (monoclinic), rectangular (orthorhombic), rhombic or centered rectangular (orthorhombic), honeycomb (hexagonal) and square (tetragonal) lattices (see Supplemental Materials \([42]\)). For each lattice, we calculated the phase diagram with the increasing \( \gamma \) and determined \( \gamma_c \).

Remarkably, we found that for more than 60 different lattices, \( \gamma_c \) exhibits a universal linear scaling with the average bond length \( L \), as shown in Fig. \([3]\). Numerical fitting gives a slope of \( k = 1.69 \) and a nearly zero intercept, which implies that the ratio \( \gamma_c/L = k \), approximates to a constant independent of specific lattices. We note that the slope \( k \) is material dependent. For example, if we use a different hopping with \( n = 3 \) in Eq. \([1]\), then \( k = 1.41 \) (see Fig. S17 and related discussion in Supplemental Materials \([42]\)). We emphasize that the calculations cover almost all kinds of 2D crystalline lattices with different symmetries. More interestingly, the universal linear scaling is also applicable to quasicrystal lattices, as demonstrated by examples of Penrose-type pentagonal \([29, 30]\) and Ammann-Beenker-type octagonal \([42]\) quasicrystal lattices (see Fig. \([3]\)). This points to a universal linear scaling of TPT in all the 2D systems, regardless of lattice symmetry and periodicity.

**TPTs in crystals with disorder.** As the definition of \( \gamma \) and \( L \) is the same for both crystal and noncrystal systems, one expects the universal linear scaling to be also applicable to define TPT in crystals with disorder. It is well known that the conducting edge state of a QSH insulator is distinguished from a normal metallic state by topological protection, so that the former is robust against non-magnetic “edge” disorder (defects or impurities). It is rooted in the bulk-boundary correspondence of a TI phase, as edge disorder cannot destroy bulk band topology. However, if bulk disorders occurred in a TI, bulk band topology and hence topological edge state could be destroyed. Thus, an intriguing and important question is how robust a TI can be against bulk disorder? Below we will answer this question by applying the universal linear scaling of TPT to 2D crystals with two kinds of possible bulk disorder, formation of vacancies and thermal displacements.

We again considered a trigonal lattice with random vacancies in a wide range of concentration \( n \) [see Fig. \([4]\)(a) for example], and studied the TPT induced by increasing \( \gamma \).
FIG. 3. The linear scaling relation between critical bond strength $\gamma_c$ and the average bond length $L$ for TPT in all the studied 2D periodic lattices [oblique (monoclinic), rectangular (orthorhombic), rhombic or centered rectangular (orthorhombic), honeycomb (hexagonal), square(tetragonal)], quasicrystal lattices [Penrose-type and Ammann-Beenker-type (AB)] and disordered lattices (random-vacancy and thermal-disorder). The calculation parameters are the same as those in Fig. 2. The superscript “∗” represents lattices with a larger $r_{cut}$.

As shown in Fig. 4(b), TPTs between NI and QSH states may occur for different vacancy concentration $n_v$ and the critical point $\gamma_c$ increases with increasing $n_v$. Correspondingly, the region of the QSH phase becomes smaller with increasing $n_v$ and eventually disappears beyond a critically large $n_v$. Figure 4(d) shows the phase diagram in the $\gamma$-$n_v$ parameter space. Apparently, the NI and QSH phases are divided by a curve of zero energy gap. In order to confirm the TPT, we calculated the spin Bott index, a topological invariant we developed recently for QSH systems with disorder [29, 30]. It is found that there is a concomitant
FIG. 4. (a) Atomic configuration of a trigonal lattice with random vacancies at $n = 0.15$. (b) Energy gap $E_g$ versus bond strength $\gamma$ for samples with difference $n$. (c) Average bond length $\bar{L}$ as a function of $n$, the red dashed line represents the fitted line $\bar{L} = 1/\sqrt{a(1-n)}$. The inset shows the average coordination number $\bar{z}$ versus $n$. (d) Phase diagram of trigonal lattices with random vacancies in the parameter space of $n$ and $\gamma$. The color represents the size of energy gap. The white dashed curve represents the trend $\gamma = k\bar{L} = k/\sqrt{a(1-n)}$ derived from the universal linear scaling.

sharp jump in the spin Bott index $B_s$ across the phase boundary, confirming a TPT. With the increasing $n$ (i.e., decreasing of atomic density $\rho = 1 - n$), the average coordination number decreases linearly $\bar{z} = a(1-n)$. Thus, the average bond length required for TPT increases $\bar{L} = 1/\sqrt{a(1-n)}$, as shown in Fig. 4(c). Then, the critical value $\gamma_c$ should follow the trend $k/\sqrt{a(1-n)}$, according to the universal linear scaling. As shown in Fig. 4(d),
the trend (white dashed curve) indeed agrees with the phase boundary very well. Thus, the universal linear scaling is also valid in lattices with random vacancies.

In addition, there is a large region of parameters in $n$ and $\gamma$ where the system is gapless [55], as shown in Fig. 4(d). An important point is that there is a critical vacancy concentration $n_c$ below which a QSH phase can exist. The QSH region shrinks and disappears at $n_c \approx 0.22$, which defines a upper bound for TPT in a 2D trigonal lattice with vacancies. This is expected to be a general phenomenon although the precise value of $n_c$ depends on specific model parameters. For $n < n_c$, the system is driven from a NI into a gapless phase through the intermediate QSH region with the increasing $\gamma$; while for $n > n_c$, there is no QSH region no matter how large $\gamma$ is. We also investigated the samples with different sizes and found similar phase transitions [42]. This confirms the applicability of the universal linear scaling of TPT in the thermodynamic limit of infinite lattice size.

We next investigate the effect of thermal disorder in destroying the topological phase in a 2D crystal. Due to thermal fluctuation, the neighboring bond distance $r_i$ varies locally, which broadens the discrete peaks of the radial distribution function $g(r)$ [56–58]. It is noted that the melting transition from perfect crystalline to paracrystalline [59–61] and amorphous lattices [62, 63] with increasing thermal fluctuation can be complicated. As an illustrative example, we adopted the quasi-lattice model [64–67] which assumes that the atomic displacements ($u$) away from their equilibrium positions follow a Gaussian distribution:

$$p(u) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{u^2}{2\sigma^2}\right).$$ (4)

The mean-squared displacement $\sigma^2$, which represents the strength of thermal fluctuation, is approximately proportional to temperature $\sigma^2 \propto k_B T$ according to the compressibility equation [64, 67]. By increasing temperature $T$, the lattice transforms from a crystal to an amorphous gradually. We studied the TPT in trigonal lattices with thermal fluctuation-induced bond disorder [see Fig. 5(a)]. As shown in Fig 5(b), the energy gaps $E_g$ for the QSH region decrease and eventually disappear with increasing $\sigma$, indicating that the thermal disorder can actually destroy the nontrivial topology. Surprisingly, $\gamma_c$ of TPT decreases with increasing $\sigma$. Figure 4(d) shows the the phase diagram of the thermal disorder system in the $\gamma$-$\sigma$ parameter space [68]. The NI and QSH states are separated by a curve of closed energy gap. In strongly-disordered region, i.e., $\sigma > 0.16$ which represents a upper bound of thermal disorder for TPT, the intermediate QSH phase disappears and the phase transition
FIG. 5. (a) Atomic configuration of a trigonal lattice with thermal disorder at $\sigma = 0.16$. (b) Energy gap $E_g$ versus bond strength $\gamma$ for samples with different $\sigma$. (c) Average bond length $\bar{L}$ as a function of $\sigma$, the red dashed line represents the fitted line. The inset shows the first peak of the radial distribution function $g(r)$ at $\sigma = 0.1$. (d) Phase diagram of trigonal lattices with thermal disorder in the parameter space of $\sigma$ and $\gamma$. The color represents the size of energy gap. The white dashed curve represents the trend $\gamma = k\bar{L}(\sigma)$ derived from the universal linear scaling.

occurs between a NI and a gapless state directly. To check the validity of the universal linear scaling in the thermally disordered lattice, we calculated the average bond length $\bar{L}$ at different $\sigma$ and found that $\bar{L}$ decreases monotonically with $\sigma$, as displayed in Fig. 5(c), which explains why $\gamma_c$ decreases with the increasing $\sigma$. We then fitted $\bar{L}$ as a function of $\sigma$ in Fig. 5(a) and plotted $k\bar{L}(\sigma)$ in the phase diagram [white dashed curve in Fig. 5(d)], which is consistent with the phase boundary.
Finally, we presented all the critical transition points ($L$, $\gamma_c$) of both random-vacancy and thermal-disorder lattices into Fig. 3. Remarkably, they follow the same universal linear scaling relation as obtained above for various crystal and quasicrystal lattices.

Fundamentally, the universal linear scaling we discover will help us to better understand the physical nature of TPTs in terms of local atomic environment. The topological state can persist as long as on average the characteristic bond strength per bond length attains a critical value. And there exists a critical atomic density below which the average bond length is too large so that the topological state would never occur [69]. Experimentally, our finding suggests that topological states can be quite robust against a high degree of structural disorder that usually occurs during a non-equilibrium growth process. This may significantly ease the fabrication of topological materials for practical applications. Our finding provides also a useful guidance for experimental manipulation of topological materials, such as to induce topological transition in a semiconductor or insulator through strain [70, 71] and alloying [72] to tune the bond strength (length).

**Conclusion.** We have investigated the general behavior of TPTs in various 2D lattices and discovered a universal linear scaling relation between the characteristic bond strength and average bond length in governing the TPTs. The universal linear scaling is found robust regardless of the lattice periodicity, symmetry and disorder. It should be applicable to any TPT that is triggered by a band-inversion mechanism [73, 74], such as 2D/3D NI to topological (crystalline) insulator and 2D NI to Chern insulator transitions. However, it shouldn’t apply to TPTs that do not involve band inversion, such as quantum Hall effect hosted by a topological flat band [75–78] or a transition from a Dirac semimetal to TI upon opening a SOC gap like in graphene. We believe our work will stimulate future studies along these lines. Finally, our discovery may also shed lights on understanding topological effects in other fields such as topological photonics, phononics, mechanics, metamaterials, and topolectrical circuits.

This work was supported by U.S. DOE-BES (Grant No. DE-FG02-04ER46148). The calculations were done on the CHPC at the University of Utah and U.S. DOE-NERSC.

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We note that there are only NI and gapless states in the region of large $\sigma$ and small $\gamma$, which is not shown.

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