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First-order quantum phase transition in three-dimensional topological band insulators

Vladimir Juričić,¹ D. S. L. Abergel,¹ and A. V. Balatsky^{1,2,3}

¹*Nordita, KTH Royal Institute of Technology and Stockholm University, Roslagstullsbacken 23, 10691 Stockholm, Sweden*

²*Institute for Materials Science, Los Alamos National Laboratory, Los Alamos, NM 87545, USA*

³*ETH Institute for Theoretical Studies, ETH Zürich, 8092 Zürich, Switzerland.*

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Topological states of matter are characterized by global topological invariants which change their value across a topological quantum phase transition. It is commonly assumed that the transition between topologically distinct noninteracting gapped phases of fermions is necessarily accompanied by the closing of the band gap as long as the symmetries of the system are maintained. We show that such a quantum phase transition is possible without closing the gap in the case of a three-dimensional topological band insulator. We demonstrate this by calculating the free energy of the minimal model for a topological insulator, the Bernevig-Hughes-Zhang model, and show that as the band curvature continuously varies, a jump between the band gap minima corresponding to the topologically trivial and nontrivial insulators occurs. Therefore, this first order phase transition is a generic feature of three-dimensional topological band insulators. For a certain parameter range we predict a re-entrant topological phase transition. We discuss our findings in connection with the recent experimental observation of a discontinuous topological phase transition in a family of topological crystalline insulators.

Introduction. The study of topological states of matter has emerged as one of the most active topics in condensed matter physics since the theoretical prediction^{1–5} and the experimental discovery of two- and three-dimensional topological band insulators (TBIs)^{6–9}. Topological states of matter are characterized by a global order parameter that represents the topological invariant of the underlying noninteracting Hamiltonian, which distinguishes these states from the ordinary Landau-like states characterized by a local order parameter^{10,11}. In particular, topological insulators in both two and three dimensions (3D) are characterized by a $\mathbb{Z}_2$ topological invariant^{1,5}. From the point of view of the bulk band structure, this topological invariant counts the parity of the number of the band inversions occurring at the high symmetry points in the Brillouin zone. Upon the transition from a topological to a topologically trivial phase these topological invariants change.

Until recently, the topological phase transition (TPT) between trivial and nontrivial insulators was believed to be continuous (*i.e.* of second order) and accompanied by a closing of the band gap which occurs at the quantum-critical point separating the two phases. The argument for this is based on the underlying assumption that the band structure parameters continuously evolve with the external parameters, such as doping and pressure. Hence, band inversions could only occur if the band gap continuously closes and reopens across a TPT. Analysis of the thermodynamics appears to reveal universal behavior, depending on the dimensionality of the model¹². However, recent experiments¹³ on topological crystalline insulators^{14–16} appear to show a discontinuous (*i.e.* first order) TPT in Sn-doped PbSe. If these experiments are accurate, then a fundamental change in our theoretical understanding of TPTs will be required in order to explain them. Theoretical work has recently predicted a discontinuous topological quantum phase transi-

tions driven by electron–electron interactions in topological insulators^{17–20}, but in this Rapid Communication we address the much more fundamental question of whether first order TPTs can be explained within a noninteracting theory.

Using thermodynamic considerations, we establish that a first order TPT driven by a band structure parameter (such as the band curvature) or by changes in temperature, can occur even in *noninteracting* topological insulators. We compute the free energy of the Bernevig-Hughes-Zhang (BHZ) model³, which provides a minimal low energy description of a topological insulator in 3D²¹. We find that as the band curvature continuously evolves, a jump between the minima in the free energy corresponding to a topological and a trivial insulator occurs at a critical value of the band curvature. The magnitude of the band gap is comparable but not equal on the two sides of the transition. On the other hand, we find that the analogous transition in two dimensions is always second order. Our result therefore shows that the first order topological quantum phase transitions are a generic feature of 3D topological insulators. At finite temperature the TPT remains discontinuous. In a certain regime of parameters, we find a re-entrant TPT as a function of temperature. Our results qualitatively agree with the existing experiments.

Model. The continuum Hamiltonian of the BHZ model in three spatial dimensions with two orbitals and two spins can be written in momentum space as $H = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \Psi^\dagger(\mathbf{k}) H(\mathbf{k}) \Psi(\mathbf{k})$ where^{3,21}

$$H(\mathbf{k}) = v\mathbf{\Gamma} \cdot \mathbf{k} + (M - Bk^2)\Gamma_0, \quad (1)$$

and spinor $\Psi_{\mathbf{k}}^\dagger = [u_{\mathbf{k},\uparrow}^\dagger, v_{\mathbf{k},\uparrow}^\dagger, u_{\mathbf{k},\downarrow}^\dagger, v_{\mathbf{k},\downarrow}^\dagger]$, with u, v denoting annihilation operators of the low-energy valence and conduction electron bands with spin projections $\sigma = \uparrow, \downarrow$ and momentum $\mathbf{k}$; a momentum cutoff Λ is assumed and

we use natural units $\hbar = k_B = e = 1$. The Γ matrices form a set of mutually anticommuting Hermitian matrices, $\{\Gamma_\mu, \Gamma_\nu\} = 2\delta_{\mu\nu}$, $\mu, \nu = 0, 1, 2, 3$. The parameter v is the Fermi velocity, which is irrelevant for the topological considerations, and we thus set it to unity. The parameters M and B are the band gap and the band curvature, respectively, and determine the $\mathbb{Z}_2$ topological index ν of a phase as $(-1)^\nu = -\text{sign}[BM(B)]$, where $M(B)$ depends on the band curvature and is determined self-consistently by minimization of the free energy, as we describe below. If M and B have the same sign, this corresponds to the topological phase, while otherwise a phase is trivial. Notice that the band curvature term proportional to the square of the momentum, has to be included in the effective Hamiltonian for the topological invariant to be defined. This Hamiltonian describes a time-reversal symmetric insulator close to the TPT between a trivial and a topological phase. It can be thought of as a minimal continuum Hamiltonian that accounts for the $\mathbb{Z}_2$ topological invariant, and can be obtained from the lattice tight binding models after expanding the Hamiltonian about the band gap minimum. It was originally introduced to describe two-dimensional quantum spin Hall insulator state realized in HgTe/CdTe quantum wells³, and its 3D version provides an effective description of Bi-based TBIs²¹. We here use the simplest version of the BHZ Hamiltonian where full 3D rotational symmetry is present^{22,23}. This Hamiltonian is in general anisotropic, but the anisotropies are irrelevant for the topological purposes and we thus do not include them.

Discontinuous topological quantum phase transition. To study the TPT between a topological and a trivial phase, we compute the free energy density of the BHZ model at temperature $T = 0$

$$F_0 = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \varepsilon(\mathbf{k}), \quad (2)$$

with

$$\varepsilon(\mathbf{k}) = \sqrt{M^2 + (1 - 2MB)k^2 + B^2k^4}, \quad (3)$$

as the dispersion corresponding to the Hamiltonian (1). We consider the thermodynamic limit and so neglect the contribution from the surface states since it is proportional to the surface to bulk volume ratio which tends to zero in this limit. Using the rotational symmetry and introducing the substitution $x = k^2$, we obtain

$$F_0(M, B) = \frac{1}{2\pi^2} \int_0^{\Lambda^2} dx \sqrt{x[M^2 + (1 - 2MB)x + B^2x^2]}. \quad (4)$$

This integral cannot be calculated in the closed form so we expand the integrand to arbitrary order in the parameter B , and then compute it. Finally, we extract the cutoff-independent part of the integral, which therefore only depends on the parameters M and B . The result to the n^{th} order in B is

$$F_0^{(n)}(M, B) = \frac{M^4}{D_n} [A_n(MB) + C_n(MB) \log M^2], \quad (5)$$

FIG. 1. (Color online) Zero temperature free energy as a function of the band gap for different values of the band curvature. The green and red curves represent the free energy right before and after the transition from the topological to the trivial phase at the critical $B_c(T=0) \simeq 0.23$. Notice that the band gaps corresponding to the global minima in the topological and the trivial phase across the transition are similar in size, but not precisely equal. Global band gap minima are marked by a dot for each curve.

with $A_n(x) = \sum_{k=0}^n a_k x^k$ and $C_n(x) = \sum_{k=0}^n c_k x^k$, where a_k and c_k are real coefficients, and D_n is also real; for details, see the Supplemental Material²⁴. Notice that the free energy satisfies $F_0(M, B) = F_0(-M, -B)$. The term containing the logarithm of the band gap arises from the fact that Dirac fermions live in three dimensions where hyperscaling is violated²⁵, and together with odd powers of the parameters M and B in the free energy (5), is responsible for the discontinuous character of the TPT, which we discuss next. On the other hand, repeating this calculation in two spatial dimensions shows that the free energy does not contain the logarithm and the topological transition is continuous and accompanied by a closing of the band gap.

We now study the above zero temperature free energy of the BHZ model as function of the band curvature. In Fig. 1 we plot the free energy to the eighth order in B for different positive values of this parameter. The free energy has two local minima at values of the gap parameter asymmetrically located with respect to $M = 0$ with the global minimum at $M_{\text{min}} > 0$ ($M_{\text{min}} < 0$) corresponding to the topological (trivial) phase. Most importantly, as the band curvature increases, the global minimum in the free energy *discontinuously* changes from a positive value to a negative one at the critical value $B_c(T=0) \simeq 0.23$, as shown in Figs. 1 and 2. The green and red curves in Fig. 1 correspond to the free energy right before and after the transition. Notice that the absolute values of the band gap minima on the two sides of the transition are comparable in size.

TPT at finite temperature. The free energy at finite temperature has an additional contribution coming from the entropy, $F(M, B, T) = F_0(M, B) - TS(M, B, T)$,

with

$$S(M, B, T) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \log \left(1 + e^{-\frac{\epsilon(\mathbf{k})}{T}} \right), \quad (6)$$

with the dispersion given by Eq. (3), and is also even under the combined operation $M \rightarrow -M$ and $B \rightarrow -B$. Furthermore, it has been demonstrated by recent numerical studies of topological insulator crystals^{26,27} that the band curvature parameter B may also depend on temperature. Therefore, we generalise B to the form $B(T) = B_0 - B_1T$, where B_1 is a positive parameter which describes the response of the lattice to finite temperature. The negative sign is chosen since we assume that the lattice expands with increasing temperature, *i.e.* it has a positive thermal expansion coefficient, indicating that the effective lattice constant increases, hence weakening the confining potential which generates the band curvature and so B decreases. We choose linear temperature dependence of the band curvature for simplicity to demonstrate the effect of temperature on the TPT. However, only its monotonic behavior with temperature is important in this regard. At finite temperature, the full $B(T)$ is substituted into Eqs. (2)–(6) to compute the free energy.

The finite temperature phase diagram is shown in Fig. 2. Most importantly, the discontinuous character of the TPT remains unchanged at finite temperature, so that all lines in the phase diagram correspond to first order phase transitions. A system in the trivial phase at $T = 0$ always undergoes a first order transition into the topological phase at high temperature as a result of the entropic contribution to the free energy. However, the low temperature regime is more subtle, and depends on the competition between the entropic contribution and the temperature dependence of the band curvature.

Let us first address the situation $B_0 > 0$, which corresponds to TBIs with a positive thermal expansion coefficient, shown in the right half of Fig. 2. We observe that as the value of the zero temperature band curvature (B_0) increases, the critical temperature (T_c) for the phase transition from the trivial to the topological phase increases. This occurs because as temperature increases, band curvature decreases and therefore the transition to the topological phase should occur at $B_0 > B_c(T = 0)$, *i.e.*, at a value of B_0 higher than the critical one at $T = 0$. By neglecting the entropy contribution in the free energy (6), we can estimate critical temperature T_c from the value of the critical band curvature at zero temperature, $B_c(T = 0) \approx B_0 - B_1T_c$, yielding $T_c \approx [B_0 - B_c(T = 0)]/B_1$. We see in Fig. 2 that this trend indeed holds when T_c is low enough and the effects from the band curvature dominate. At higher temperatures, thermal fluctuations take over and bend the phase boundary to favor the topological phase. As a result, there is a region in the phase diagram $0.23 \lesssim B_0 \lesssim 0.28$ where, as temperature increases from zero, the system begins in the topological phase, undergoes a first-order transition to the trivial phase and then re-enters the

FIG. 2. (Color online) Finite temperature phase diagram of the BHZ model as a function of the zero temperature band curvature B_0 . The trivial phase remains stable at finite temperature up to a critical value of the zero temperature band curvature. Notice that there is a region where a re-entrant behavior in the topological phase through the trivial phase is possible, highlighted by the vertical dashed black line. For larger absolute values of B_0 topological phase is stable at any temperature. The topological and trivial phases are separated by a first-order phase transition.

topological phase at some higher temperature, as marked by a dashed black line in Fig. 2. The size of the region where this re-entrant behavior takes place scales with the slope of the band curvature at low temperature. The case $B_0 < 0$ describes TBIs with a negative thermal expansion coefficient since $F(M, B) = F(-M, -B)$ and is shown in the left half of Fig. 2. The previous argument suggests that the T_c decreases linearly with $|B_0|$, which is seen in the low temperature regime. At higher temperature, we observe that T_c crosses over from linear to nonlinear (quadratic) dependence on $|B_0|$ as the thermal fluctuations start to become important.

The absence of the band gap closing is shown in Fig. 3 where we plot $M_{\min}$, the value of the band gap at the global minimum of the free energy as a function of $B_0 > 0$ and T . In panel (a) we observe that as the temperature increases for $0 < T \lesssim 0.3$, the critical value of B_0 for the transition into the topological phase, $B_{0c}(T)$, increases. This can be understood, neglecting the entropy contribution (low temperature), by noticing that the total band curvature at the transition is equal to the critical one at $T = 0$, and therefore $B_{0c}(T) = B_c(T = 0) + B_1T$. However, at higher temperature, the effects of thermal fluctuations start to be important, which leads to a stable topological phase, after a narrow region of parameters where a re-entrant behavior is possible. In Fig. 3(b), we plot the band gap as a function of temperature, from which we can infer that at values of $B_0 < B_c(T = 0)$, trivial phase is stable up to $T \sim 0.4$. When $B_0 \approx B_c(T = 0)$, we observe the re-entrant behavior described previously, where the system undergoes two discontinuous topological transitions as the temperature increases. Finally, for

even higher values of B_0 , the system is always topological, since already at $T = 0$ the system in this regime is topological and thermal fluctuations further stabilize it.

Comparison with experiments. To demonstrate the utility of this theory, we make a qualitative comparison of our findings with recent experiments in Ref. 13, where a phase transition without an associated closing of the band gap has been reported in $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$, as a function of both doping and temperature. This alloy has a face-centered cubic structure on both sides of the TPT, up to a doping level of $x \approx 0.4$ ¹⁴. We first consider the doping dependence. For doping $x \lesssim x_c = 0.17$ and at low temperature, the experiments show that this compound is topologically trivial, while for $x > x_c$ it features band inversions at four inequivalent L points in the Brillouin zone and is therefore a topological crystalline insulator^{14,28}. The Hamiltonian in Eq. (1) describes the band inversion at each of these L points. The band curvature is linked to the doping x in the $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$ materials. This is due to the Sn doping decreasing the effective lattice constant a and hence stiffening the confining potential which generates the band curvature²⁸. Therefore, $B_0 \propto x$, and our theory gives precisely the behavior observed in the experiment.

FIG. 3. (Color online) Evolution of the global band gap minimum $M_{\min}$ as a function of $B_0 > 0$ corresponding to the phase diagram in Fig. 2. $M_{\min}$ vs. B_0 at different temperatures; (b) $M_{\min}$ vs. T for different B_0 . Notice that in both panels the magnitude of the band gap is comparable across the transition. The red curve in both panels corresponds to the re-entrant TPT.

We now move on to the temperature dependence. When the material is in the topological phase at low temperature, the experiments show that raising the temperature at a fixed doping drives a first-order TPT to the trivial phase. We propose that the relevant B_0 parameter for $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$ at maximum doping is in the range $0.23 < B_0 < 0.28$, with $B_1 > 0$ so that this transition is the initial (low temperature) part of the re-entrant behavior we mark in Fig. 2 with a dashed line. Indeed, for $x > x_c$, the experimental results show that as the doping increases, the critical temperature also increases, which is in agreement with our results in Fig. 2. Moreover, as the temperature increases, the doping region with the topological phase shrinks up to a temperature above which the trivial phase is realized, also consistent with the experimental results. We suspect that the range of temperatures accessed in Ref. 13 does not go high enough to see the second part of the re-entrant behavior which manifests as a phase transition back to the topological phase. Indeed, the T_c of the first transition at $T_c \approx 250\text{K}$ is already close to the maximum temperature of $T = 300\text{K}$ reported in the experiment.

When $x < x_c$, the material is in the trivial phase at low temperature. The experiments show that it never undergoes a phase transition to the topological phase up to approximately $T = 300\text{K}$. Again, we suggest that a topological phase may reappear due to its stabilization by the entropic contribution to the free energy at higher temperatures. Finally, we point out that our calculation gives sizes of the band gaps in the trivial and the topological phases which are comparable in magnitude immediately on either side of the TPT, also consistent with the experimental findings.

Conclusions. Here we have established the first-order nature of the topological quantum phase transition in *noninteracting* 3D TBIs. We also show that at finite temperature the transition remains discontinuous. Gross features of the finite temperature phase diagram depend on the behavior of the band curvature with temperature. We find that there is a regime of parameters for which our theoretical findings qualitatively agree with experiments. However, we point out that the temperature and doping dependence of the band curvature for topological insulators will vary between different materials^{26,27}, with phonons possibly playing an important role^{29,30}. We therefore hope that our findings will motivate *ab initio* calculations to ascertain these details. We also show that it is possible to infer the temperature dependence of the band curvature from the experimental behavior of T_c as a function of B_0 near to $B_c(T=0)$, since in this regime the entropy contribution due to thermal fluctuations is expected to be subdominant. Therefore, this work motivates further experiments to probe the nature of the quantum and finite temperature TPTs in insulators, as well as in superconductors. Indeed, a first-order TPT has been also found in Sn-doped PbTe, with an even more pronounced discontinuity than in the case of PbSe³¹.

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