Study of stability of topological crystalline insulators against disorder

Bart de Leeuw,1,2 Carolin Kippersbusch,1,3 Vladimir Juričić,1 and Lars Fritz1

1Institute for Theoretical Physics and Center for Extreme Matter and Emergent Phenomena, Utrecht University, Leuvenlaan 4, 3584 CE Utrecht, The Netherlands
2Mathematical Institute, Utrecht University, Budapestlaan 6, 3584 CD Utrecht
3Institut für Theoretische Physik, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany

Noninteracting insulating electronic states of matter can be classified according to their symmetries in terms of topological invariants which can be related to effective surface theories. These effective surface theories are in turn topologically protected against the effects of disorder. Topological crystalline insulators are, on the other hand, trivial in the sense of the above classification but still possess surface modes. In this work we consider an extension of the Bernevig-Hughes-Zhang model that describes a topological crystalline insulator. We explicitly show that the surface properties of this state can be as robust as in topologically nontrivial insulators, but only if the $S_z$-component of the spin is conserved. However, in the presence of Rashba spin-orbit coupling this protection vanishes and the surface states localize, even if the crystalline symmetries are intact on average.

I. INTRODUCTION

Soon after the prediction3,4 and subsequent discovery5–8 of the quantum spin Hall insulator3 as a novel state of electronic matter with properties protected by topology, it became clear that this state fits into an even grander scheme.9–15 By now many more topological phases have been identified both theoretically and experimentally.16–19

The classification of noninteracting electronic insulating states with topological order was one of the milestones of theoretical condensed matter physics in the last decades.20–24 Within the so-called 'tenfold periodic table' states of matter with topological order are classified according to the presence or absence of symmetries of the underlying systems25 such as time-reversal, particle-hole, and chiral.

One of the prominent features of topological electronic systems is the existence of exotic gapless edge or surface states. In particular, these boundary modes can realize one-dimensional chiral or single two-dimensional Dirac fermions, usually ruled out by the fermion doubling theorem (at least if all the symmetries are preserved). Importantly, in the presence of disorder these states can be protected against localization which leads to unusually robust transport properties. An instructive point of view on the existence of these robust boundary states is that the tenfold periodic table does not require spatial symmetries such as translations or rotations to be present, which is particularly apparent in the classification scheme using non-linear $\sigma$ models.19 This implies that although the calculation of topological invariants can in general most easily be accomplished in clean band-insulators, in principle there is no need to have a well-defined crystal momentum for doing so. On the other hand, electronic states trivial according to the tenfold classification but still featuring edge or surface modes have been recently identified once crystalline symmetries, such as translations, rotations, reflections and inversions, were taken into account.20–24 These states are conventionally referred to as topological crystalline insulator25 (TCI).

Interestingly, these states, predicted to be realized in Sn- and Pb-based compounds25 have been reported to be observed first in Refs. 29–31. An urging question is therefore whether the boundary states in TCI can enjoy similar protection against the effects of disorder as they do in tenfold-wise topologically nontrivial insulators.

To answer this question at least for one concrete example, we investigate the transport properties of an extension of the well-known Bernevig-Hughes-Zhang (BHZ) model that was recently introduced21. There, it was identified that a rotational symmetry leads to the existence of a state characterized by a trivial topological invariant, but possesses two pairs of helical edge modes. Within this note we make a comparison of this TCI with a quantum spin Hall insulator (QSHI), for which the BHZ model was originally formulated.3 For the QSHI we find, as expected and well known, very robust transport properties with a quantized lead-to-lead conductance, both in presence and absence of disorder (as long as the disorder strength is smaller than the bulk-gap scale). Importantly, this property is also robust against breaking of the spin-rotational symmetry, introduced for instance by Rashba spin-orbit coupling, and is a direct consequence of time-reversal symmetry. For the TCI, on the other hand, we find that the conductance is only quantized and robust against disorder if the $S_z$-component of the spin is conserved. However, in the presence of Rashba spin-orbit coupling disorder localizes, in the Anderson sense, the boundary modes leading to a vanishing conductance. We argue that this can be traced back to the fact that in the absence of Rashba spin-orbit coupling, the model constitutes an example of two time-reversed copies of Chern insulators with Chern numbers $C_\uparrow = -C_\downarrow = -2$ stacked on top of each other. When Rashba spin-orbit coupling is present, it mixes the $S_z$ sectors and the orthogonality of all the left-moving states with respect to the right-moving states (expect for the time reversed partners at the time-reversal-invariant momenta) at the edges is lost.
We show explicitly that this leads to a localization of the modes and agrees with the specific TCI state being trivial in the sense of the periodic table. We note here that our results concerning the stability of the edge modes in a TCI without Rashba spin-orbit coupling are in agreement with the findings recently reported in Refs. 32 and 33.

The paper is organized as follows. In Sec. II, we introduce the model and its phase diagram, and in Sec. III, we present the results concerning the transport properties in both QSHI and TCI phases. Our conclusions are drawn in Sec. IV.

II. MODEL AND PHASE DIAGRAM

The model we study was recently introduced in Ref. 21 and represents an extension of the BHZ Hamiltonian that includes next-nearest neighbor hoppings. Its Bloch Hamiltonian has the generic form

$$H = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger \left( \begin{array}{cc} H_{\mathbf{k}} & H_{SO}(\mathbf{k}) \\ H_{SO}(\mathbf{k})^* & H^*(-\mathbf{k}) \end{array} \right) \Psi_{\mathbf{k}}^\dagger,$$

where

$$H_{SO} = R_0 \left( \begin{array}{cccc} -i \sin k_x - \sin k_y & 0 \\ 0 & 0 \end{array} \right).$$

The Hamiltonian (1) obeys time reversal symmetry, which is implemented via $T = i\tau_0 \otimes \sigma_y K$, where $\sigma_y$ acts in spin space and $K$ denotes complex conjugation ($\tau_0$ is the identity in orbital space). This symmetry will be intact hereafter. Additionally, the clean system has the discrete rotational $C_4$ symmetry about the axis orthogonal to the crystal plane, represented by $R = 1/2 (\tau_0 (1 + i) + \tau_z (1 - i))$. However, this symmetry will be broken by disorder and the finite size sample.

The phase diagram for Eq. (1) is shown for $\tilde{B}/B = 1$ as a function of $M/B$ and $R_0/B$ in Fig. 1. The phase diagram for $R_0 = 0$ but all values of $\tilde{B}/B$ was introduced recently. If $R_0 = 0$, the Hamiltonian explicitly conserves the $S_z$-component of the spin and we can deduce a phase diagram by calculating the Chern numbers in the respective $S_z$ spin sectors. As a function of $M/B$ this leads to three phases. For values of $M/B < 8$ there is the $\Gamma$-phase which is the standard QSHI from the AII symmetry class with a $Z_2$ topological index $\nu$. For finite $R_0$ the spin Chern number is not well defined any more, but we instead use adiabatic continuity and the finite size spectrum to obtain the $Z_2$ topological index.

Figure 1: Phase diagram of the clean system. The phase diagram without Rashba spin-orbit coupling is obtained from the calculation of the Chern numbers of the spin subsystems, $C_\uparrow$ and $C_\downarrow$, and the corresponding $Z_2$ index $\nu$. For finite $R_0$ the spin Chern number is not well defined any more, but we instead use adiabatic continuity and the finite size spectrum to obtain the $Z_2$ topological index.
III. TRANSPORT PROPERTIES

One of the most striking properties of topological insulator states is not only the existence of boundary modes but also their stability with respect to disorder. The most prominent example is the quantum Hall state which has quantized Hall conductivity \( \sigma_H = e^2/n \), with \( n \) as an integer. The integer \( n \) can be viewed in two equivalent ways: (i) it is the cumulative Chern number of the bands below the chemical potential or (ii) the number of chiral boundary modes. The conductance then accounts for the number of channels at the boundary. Naively, one would expect disorder to localize these modes, but their chiral nature provides an escape route: disorder cannot localize them since there is no way of converting a left-mover into a right-mover and vice versa by virtue of them being unidirectional.

In the case of a QSHI we do not have chiral channels but instead helical modes. This implies that there are right- and left-movers on either side of the sample which potentially allows for elastic backscattering due to scalar disorder. However, the helical modes are Kramers’ pairs related by time-reversal symmetry, which implies that scalar disorder cannot convert left-movers into right-movers and vice versa due to the orthogonality of Kramers’ pairs. The situation is schematically depicted in Fig. 3(b). Consequently, edge transport is also ballistic resulting in a quantized conductance. This has also been observed in transport experiments on \( \text{HgTe/CdTe} \) quantum wells.

In the case of the TCI we find there are two pairs of boundary modes at each sample edge, see right-hand-side of Fig. 2(b), but usually two pairs of modes are unstable since any right-mover in general is not mutually orthogonal to both left-movers and they can thus scatter into each other under generic circumstances. So the question we address here is in which sense and under which conditions the \( X-Y \) valley phase, topologically trivial according to the periodic table, has stable transport properties once disorder is added.

The setup that we probe is shown in Fig. 3(a) where we connect a central sample region to left and right leads and measure the response coefficient for transport from the left lead to the right lead in the linear response regime (we assume \( \mu_L = \mu_R + \delta V, \delta V \) being small).

In order to study the stability of the edge states with respect to disorder we resort to the well established non-equilibrium Green-function method, which we implement numerically in the linear response regime.

In the clean system we can count the boundary modes assuming ballistic transport based on the finite size spectrum (see Fig. 2) and find

\[
G = \frac{e^2}{\hbar} \times \begin{cases} 
2 & \text{in } \Gamma \text{-phase} \\
4 & \text{in } X-Y \text{ valley phase} 
\end{cases}
\]  \( (4) \)

We have modelled disorder by scalar disorder, i.e., through local variations in the chemical potential. We have chosen disorder of the box type with a strength
Counterpropagating modes at the boundary of a QSHI. Left- and right-movers are Kramers’ partners and are protected against backscattering both for $R_0 = 0$ and $R_0 \neq 0$. $V_{kk'} = V_0$ denotes a featureless elastic scatterer which mixes all momenta. The zero overlap between the counterpropagating modes stems from additional quantum numbers of the band structure. (c) Two sets of counterpropagating modes at the boundary of a TCI. While the modes crossing at the time-reversal invariant momenta cannot scatter into each other due to time-reversal symmetry for both $R_0 = 0$ and $R_0 \neq 0$, modes from different time-reversal invariant momenta can scatter if $R_0 \neq 0$.

In order to make better comparisons between the QSHI and TCI, we have chosen parameters such that bulk gaps are approximately the same in both systems. We found that a convenient parameter set is given by $B = B$, $M/B = 7$ (QSHI) or $M/B = 10$ (TCI) without Rashba coupling, while with Rashba coupling $R_0/B = 1$ we choose $M/B = 9$ for the TCI (to have comparable gaps).

In the absence of Rashba spin orbit coupling ($R_0 = 0$) with conserved spin, we find that both $\Gamma$ and the X-Y valley phase are equally stable against disorder. This is not very surprising since both in the $\Gamma$-phase as well as in the X-Y valley phase we can think of the system as two time-reversed Chern insulators with Chern numbers $C_{\uparrow, \downarrow} = \mp 1$ for the QSHI and $C_{\uparrow, \downarrow} = \mp 2$ for the TCI and the left- and right-moving channels do not mix, see Fig. 3 (b) and (c). In Fig. 4 we display a plot of the conductance of a sample of size $80 \times 80$ with the chemical potential in the bulk gap as a function of disorder strength. Our results show that both the QSHI and the TCI phases are stable against disorder, since the conductance is quantized. In Fig. 5 we plot conductance at fixed disorder strength as a function of the system size (we always study systems of transverse size 80 sites), and find again that both QSHI and TCI are stable.

In the presence of Rashba spin-orbit coupling ($R_0 \neq 0$), we find that the features of the QSHI phase are unchanged, as expected. However, the protection of the conductance is lost in the case of the TCI. This can explicitly seen in Fig. 4 where the conductance as a function of disorder strength at fixed sample size decreases, as soon as Rashba spin orbit coupling is switched on. Furthermore, in Fig. 5 we observe that the conductance as a function of the system size decreases and eventually would vanish if we made the sample long enough. This signals the localization of the modes in agreement with the absence of topological protection. As discussed before, this can be traced back to the loss of orthogonality of left- and right-movers at the sample edges. We have explicitly checked the loss of orthogonality under scattering from a structureless impurity ($V_{kk'} = V_0$) of the left- and right-movers in the finite size spectrum (as also discussed in Fig. 3 (c)). We can therefore conclude that the absence of protection against backscattering leads to the localization of the boundary modes.

IV. CONCLUSIONS

In this paper we have studied the stability of the edge states of a topological system outside the tenfold classification of the topological insulator states with respect to disorder. We considered a special instance of a TCI where discrete rotational $C_4$ symmetry guarantees the existence
disorder for increasing system sizes. For $R_0 = 0$ we find that both QSHI as well as TCI are equally stable, while for finite $R_0$ the conductance of the TCI decreases as a function of the system size.

of edge states in a clean system. If the $S_z$-component of the spin is a conserved quantity in this system we find that the boundary modes are protected against localization due to disorder. This protection against disorder is lost if Rashba spin-orbit coupling is present. Consequently, the system indeed behaves like a trivial insulator in the sense of the topological classification of electronic states. For the future it is an interesting prospect to study the localization properties of other systems with boundary modes which are outside the tenfold classification of topological states, such as the recently observed three-dimensional TCI phase featuring band-inversions at symmetry-related $L$-points in the Brillouin zone.

V. ACKNOWLEDGEMENT

We thank Michael Wimmer and Jason Frank for helpful discussions. We acknowledge funding from the DFG FR 2627/3-1 (C.K. and L.F.). This work is part of the D-ITP consortium, a program of the Netherlands Organisation for Scientific Research (NWO) that is funded by the Dutch Ministry of Education, Culture and Science (OCW). V. J. acknowledges financial support from NWO.

1. C. L. Kane, E. J. Mele, Phys. Rev. Lett. 95, 146802 (2005).
2. C. L. Kane, E. J. Mele, Phys. Rev. Lett. 95, 226801 (2005).
3. B. A. Bernevig, T. L. Hughes, S. C. Zhang, Science 314, 1757 (2006).
4. M. König, et al., Science 318, 766 (2007).
5. J. E. Moore, L. Balents, Phys. Rev. B 75, 121306 (2007).
6. L. Fu, C. L. Kane, Phys. Rev. B 74, 195312 (2006).
7. L. Fu, C. L. Kane, Phys. Rev. Lett. 98, 106803 (2007).
8. L. Fu, C. L. Kane, Phys. Rev. B 76, 045302 (2007).
9. D. Hsieh, et al., Nature 452, 970 (2008).
10. D. Hsieh, et al., Science 323, 919 (2009).
11. Y. Xia, et al., Nature Phys. 5, 398 (2009).
12. H. Zhang, et al., Nature Phys. 5, 438 (2009).
13. Y. L. Chen, et al., Science 325, 178 (2009).
14. M. Z. Hasan, C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
15. X. L. Qi, S. C. Zhang, Rev. Mod. Phys. 83, 1057 (2011).
16. A. P. Schnyder, S. Ryu, A. Furusaki, A. W. W. Ludwig, Phys. Rev. B 78, 195125 (2008).
17. A. Kitaev, AIP Conf. Proc. 22, 1132 (2009).
18. X.-L. Qi, T. Hughes, S.-C. Zhang, Phys. Rev. B 78, 195424 (2008).
19. S. Ryu, A. P. Schnyder, A. Furusaki, A. Ludwig, New J. Phys. 12, 065010 (2010).
20. L. Fu, Phys. Rev. Lett. 106, 106802 (2011).
21. R.-J. Slager, A. Mesaros, V. Juričić, and J. Zaanen, Nature Phys. 9, 98 (2013).
22. C.-K. Chiu, H. Yao, and S. Ryu, Phys. Rev. B 88, 075142 (2013).
23. T. Morimoto and A. Furusaki, Phys. Rev. B 88, 125129 (2013).
24. K. Shiozaki and M. Sato, Phys. Rev. B 90, 165114 (2014).
25. T. H. Hsieh, H. Lin, J. Liu, W. Duan, A. Bansil, L. Fu, Nat. Comm. 3, 982 (2012).
26. Y. Tanaka, Z. Ren, T. Sato, K. Nakayama, S. Souma, T. Takahashi, K. Segawa, and Y. Ando, Nature Phys. 8, 800 (2012).
27. S.-Y. Xu, C. Liu, N. Alidoust, M. Neupane, D. Qian, I. Belopolski, J. D. Denlinger, Y. J. Wang, H. Lin, L. A. Wray, G. Landolt, B. Slomski, J. H. Dil, A. Marcinkova, E. Morosan, Q. Gibson, R. Sankar, F. C. Chou, R. J. Cava, A. Bansil, and M. Z. Hasan, Nature Commun. 3, 1192 (2012).
28. P. Dziawa, B. J. Kowalski, K. Dymbko, R. Buczko, A. Szczerbakow, M. Szot, E. Lusakowska, T. Balasubramanian, B. M. Wojek, M. H. Berntsen, O. Tjernberg, and T. Story, Nature Mater. 11, 1023 (2012).
29. Y. Tanaka, T. Sato, K. Nakayama, S. Souma, T. Takahashi, Z. Ren, M. Novak, K. Segawa, and Y. Ando, Phys. Rev. B 87, 155105 (2013).
30. Y. Okada, M. Serbyn, H. Lin, D. Walkup, W. Zhou, C. Dhitial, M. Neupane, S. Xu, Y. J. Wang, R. Sankar, F. Chou, A. Bansil, M. Z. Hasan, S. D. Wilson, L. Fu and V. Madhavan, Science 341, 6153 (2014).
31. I. Zeljkovic, Y. Okada, C. Y. Huang, R. Sankar, D. Walkup, W. Zhou, M. Serbyn, F. Chou, W. F. Tsai, H. Lin, A. Bansil, L. Fu, M. Z. Hasan, and V. Madhavan, Nature Phys. 10, 572 (2014).
32. H. Jiang, H. Liu, J. Feng, Q. Sun, and X. C. Xie, Phys. Rev. Lett. 112, 176601 (2014).
33. M. Ezawa, New J. Phys. 16, 065015 (2014).
34. D. G. Rothe, R. W. Reithaler, C.-X. Liu, L. W. Molenkamp, S.-C. Zhang, and E. M. Hankiewicz, New J. Phys. 12, 065012 (2010).
35. D. J. Thouless, M. Kohmoto, M. P. Nightingale, M. den Nijs, Phys. Rev. Lett. 49, 405 (1982).
36. F. D. M. Haldane, Phys. Rev. Lett. 61, 2015 (1988).
S. Datta, *Electronic Transport in Mesoscopic Systems*, Cambridge University Press (1997).