Anderson localization and topological transition in Chern insulators

Eduardo V. Castro¹, M. Pilar López-Sancho², and María A. H. Vozmediano²

¹CeFEMA, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal and
²Instituto de Ciencia de Materiales de Madrid, CSIC, Sor Juana Inés de la Cruz 3, Cantoblanco, E-28049 Madrid, Spain
(Dated: February 18, 2015)

We analyse the topological transition and localization evolution of disordered two dimensional systems with non trivial topology based on bipartite lattices. Chern insulators with broken time reversal symmetry show non standard behavior for disorder realizations selectively distributed on only one of the sublattices. The Chern number survives to a much stronger disorder strength (one order of magnitude higher) than in the equally distributed disordered case and the final state in the strongly disordered case is metallic.

Introduction-summary. The metal insulator transition and the associated issue of the existence or not of metals in two dimensions [1] have fascinated physicists in the last century and have been the focus of intense debates and great advances in the understanding of low dimensional material physics. The interest of these materials is of special relevance today due to the unusual applications expected following the experimental capability of synthesising and manipulating layered compounds [2]. But also the fundamental physical aspects are still providing surprises mostly around the Dirac physics based materials and their related topologically non-trivial features. The issue of how electrons in a metal become localised by disorder in the presence of non–trivial topology started with the analysis of Landau levels in the integer quantum Hall effect and was rapidly adapted to other time reversal preserving topological matter [3–5]. The standard classification of disordered classes [6–8] based on the Altland-Zirnbauer sets of random matrices [9] was completed to include topological features and the “ten-fold way" was set in Refs. [10] and [11].

Two dimensional (2D) topological insulators belong to class A (unitary) with time reversal symmetry broken or AII (symplectic) time reversal invariant. Prominent examples in these classes are the Haldane [12] and the Kane-Mele model [13]. They are characterized by a quantized Chern (or spin Chern) number $C$. The localization transition in these cases is accompanied by a topological transition between a topological (band) insulator and a trivial (Anderson) insulator. The topological transition of these classes is assumed to be well understood. The standard mechanism is referred to as "levitation and annihilation" [14]. For moderate disorder, an impurity band of localized state forms inside the band and simultaneously the high energy states in the edges of the conduction and valence bands start to localize. As disorder increases, the gap is totally populated by localized states and the bulk extended states above and below the Fermi level carrying the Chern number shift toward one another and annihilate leading to the topological phase transition. The transition from a Chern to an Anderson insulator under a random potential disorder has been analyzed in Ref. [15].

model and methods. We use the Haldane model [12] as a generic example of a topologically non trivial system in symmetry class A. It was initially proposed as a tight binding model in the honeycomb lattice with complex next nearest neighbour (NNN) hoppings carefully adjusted so as to mimic a magnetic flux flowing in opposite directions through the two triangular sublattices. It was build to show the possibility to have Hall conductivity in zero external magnetic field and it is nowadays the prototype of a modern topological insulator. Interestingly, a physical realization of the model has been
the band edges and generate a mobility edge \[33\]. We see that Anderson disorder (local random potential) and vacancies show quantitative differences only. The crucial difference is found between the two disorder realizations analyzed: Selective and equally distributed in the two sublattices. We summarize our results in two blocks of figures. The evolution of the Chern number with disorder strength encodes the topological transition. The various cases are shown in Figure 1. The bulk DOS contains information on the localization behavior and is displayed in Figs. 2 and 3.

We will first discuss the situation when impurities or vacancies are equally distributed in the two sublattices. The upper side of Figure 1 shows the behaviour of the Chern number with potential disorder as a function of the linear lattice size \(d\) for increasing disorder strengths \(W\) in units of \(t\). In the left hand side the disorder is equally distributed among the two sublattices. We see that the Chern number is already well defined and stable at very small lattice sizes and it ceases to be quantized at a mild disorder strength (\(4t < W < 5t\)), a behavior already found in the literature \[23,34\]. Fig. 2 shows a comparison of the DOS of the Haldane model with Anderson disorder of the two cases: equal (blue) and selected disorder (red). The left hand side displays the DOS for weak disorder strength \(W = 2t\) well below the critical value for the topological transition of the case of equally distributed disorder. The two images are very similar. We see a well defined gap at zero energy and two peaks of similar intensity in the conduction and valence bands, a situation compatible with the standard picture of the mobility edge. The right hand side shows the DOS for a disorder strength \(W = 4t\) close to the critical value for the topological transition of the case of equally distributed disorder. There we see a clear difference between the two disorder distributions. For the selectively distributed case (red) the structure of the DOS is similar to the weak disorder case while in the equally distributed case (blue) the gap has disappeared and the DOS has flattened.

The behaviour of vacancy disorder equally distributed among the two sublattices is similar to that of the Anderson disorder. The evolution of the Chern number as a function of linear lattice size for various densities of vacancies is shown in Fig. 1 (lower left panel). Notice the units in the vertical axis. The quantization disappears for a critical density of around 4-10 percent compatible with the standard mechanism of "levitation and pair annihilation" of the extended states carrying the Chern number \[14\]. A similar behavior has been reported in Ref. \[35\] for the case of vacancies. This mechanism is also supported by the analysis of the density of states depicted in Figure 3. The left hand side shows the DOS of the Haldane model for various density of vacancies \(nv\) randomly but equally distributed in the two sublattices. It is apparent that vacancies induce a finite spectral weight inside the gap. As the disorder density increases the impurity band widens and the center of the conduction and valence band

implemented in \[22\]. The Haldane model tight binding Hamiltonian can be written as

\[
H = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j + -t_2 \sum_{\langle\langle i,j \rangle\rangle} e^{-i\phi_{ij}} c_i^\dagger c_j + M \sum_i \eta_i c_i^\dagger c_i + \text{H.c.,}
\]

where \(c_i = A, B\) are defined in the two triangular sublattices that form the honeycomb lattice. The first term \(t\) represent a standard real nearest neighbor hopping that links the two triangular sublattices. The next term represents a complex next nearest neighbor hopping \(t_2 e^{-i\phi_{ij}}\) acting within each triangular sublattice with a phase \(\phi_{ij}\) that has opposite signs \(\phi_{ij} = \pm \phi\). This term breaks time–reversal symmetry and opens a non–trivial topological gap at the Dirac points. We have done our calculations for the simplest case \(\phi = \pi/2\). The last term represents a staggered potential \((\eta_i = \pm 1)\). It breaks inversion symmetry and opens a trivial gap at the Dirac points.

We will discuss two types of disorder: Anderson and vacancy disorder equally or selectively distributed among the two sublattices. Potential (Anderson) disorder is implemented by adding to the Hamiltonian the term \(\sum_{i \in A,B} \epsilon_i c_i^\dagger c_i\), with a uniform distribution of random local energies, \(\epsilon_i \in [-W/2,W/2]\). For selected disorder the sum runs only over one sublattice. The same is done for vacancies which are introduced by removing a given lattice site and the hopping to its neighbors.

The Haldane model belongs to symmetry class \(A\) \[10\] where the different topological phases can be characterized by a \(Z\)-topological number, the Chern number \(C\). In the clean system it can be computed from the single particle Bloch states \(u_n(k)\) as:

\[
C_n = \frac{1}{2\pi} \int_S \Omega^n_z(k) dS, \tag{2}
\]

where the integral is over the unit cell and \(\Omega^n_z(k)\) is the \(z\) component of the Berry curvature: \(\Omega^n_z(k) = \nabla_k \wedge A_n(k)\) defined from the Berry connection: \(A_n(k) = \langle u_n(k) | -i \nabla_k | u_n(k) \rangle\). When translational invariance is broken by disorder or any other perturbation, the Chern number has to be computed numerically in real space. The problem has been addressed in the literature and a number very efficient numerical techniques based on the use of twisted boundary conditions are now available \[13,23,24\]. We have calculated the Chern number for the bulk bands using the method in Ref. \[24\].

The bulk density of states (DOS) have been computed using the recursive Green’s function method as used for example in Refs. \[25\] and \[26\].

Results. As shown by many authors, a single vacancy induces a midgap bound state in the Haldane or Kane Mele model \[27,32\], while a density of vacancies induces an impurity band inside the gap \[32\]. Increasing the density of vacancies enhances the spectral weight inside the gap, which eventually closes for high enough vacancy density. In contrast, potential disorder localizes states near
that host the extended states carrying the Chern number (1 and -1 respectively) move closer. At a density of vacancies around $n v_c \approx 3\%$ the gap closes (inset of Figure 3 left). The Chern number remains quantized up to a density of $\approx 8\%$ where the ‘annihilation’ occurs. Similar behavior has been found in Ref. [35] although the critical density reported there is a bit different.

We will now discuss the results obtained for disorder selectively located in one of the sublattices. A comparison of the behaviour of the Chern number as a function of Anderson disorder strength for the two types of disorder: Selective and equally distributed in the sublattices is shown in the upper right hand side of Fig. 1. The transition described above in the evenly distributed case (red squares) occurs sharply around $W = 5t$. For this value, the Chern number in the selective disorder case (blue circles) is still quantized to one. The topological transition occurs for disorder strengths one order of magnitude bigger (inset of Figure) ($40t < W_c < 50t$) than in the equally distributed case.

Similarly, for the case of disorder in the form of vacancies selectively distributed (lower panel right) the Chern number is still very close to one for a density of vacancies of around 30 percent. This is to be compared with the equally distributed disorder in the two sublattices (left hand side) where the graphic departs from 1 already at a critical density around 12 percent. The density of states (right hand side of Figure 3) for selective vacancy disorder is also very different than in the previous case. Valence and conduction peaks do not move substantially as disorder increases and the behavior of the gap between the valence (conduction) and midgap bands is also different. As can be seen in the inset of Figure 3 (right) the gap decreases and reopens well before the Chern number ceases to be quantized what happens at a density of vacancies of around 30 percent ( right hand side of Figure 1). At this density there is a noticeable gap separating the midgap band from the conduction and valence bands.

The case of disorder distributed in only one sublattice requires an alternative explanation. We believe that both the topological transition and the localization mechanism are different in this case. The robustness to disorder of the extended states carrying the Chern number is related to the fact that one of the sublattices remains perfect. The component of the wave function corresponding to the “clean” sublattice stays delocalized in a way similar to the vacancy states of bilayer graphene described in reference [25]. The fact that the topological transition in the vacancies case coincides with the percolation transition of the honeycomb lattice [36] (around 30 percent)
points to the possibility that the topological transition occurs when the disordered sublattice is destroyed and the extended (Bloch) state is driven by the underlying triangular lattice that is topologically trivial.

The case of vacancies is very intuitive: In the limit when we have removed all the atoms in one of the triangular sublattices what remains is the extended wave function corresponding to the triangular sublattice. Let us emphasize that we should not confuse the triangular lattice with homogeneous complex hoppings, which break time reversal symmetry, with the familiar triangular (or hexagonal) lattice with real hoppings. A discussion of the transition between the honeycomb and two independent triangular lattices is done in the supplementary material.

**Discussion and open issues.** It is by now clear that topological features can change the localization behavior of the disordered electronic lattice systems. The topological transition (topological index going to zero or to a non-quantised value) and the localization transitions are related but do not occur, in general, at the same critical value of the disorder. In the “ten-fold” way classification of topological insulators \[10\] chiral classes (with well defined sublattice symmetry) do not support topological features in two dimensions and the issue of selective disorder (affecting only one sublattice) has only started to be explored \[21\]. The topological transition in the 2D (non chiral) classes is assumed to occur through “levitation and annihilation” \[14\] of the extended states carrying the topological index. The mechanism is less understood in the chiral (sublattice symmetry) classes \[37\]. In the one dimensional chiral case analyzed recently in Ref. \[38\], the topological index \( C \) remains quantized and non-fluctuating even when the bulk energy-spectrum is completely localized and after the insulating gap has closed. \( C \) changes abruptly to a trivial value when disorder is further increased.

We observe a similar behavior for the Chern number \( C \) for selective vacancy disorder: \( C \) remains quantized up to a large disorder strength but in our case extended states remain present possibly all the way until one of the sublattices is totally destroyed. This type of disorder realizes the transition from honeycomb lattice physics with topologically nontrivial features to the two topologically trivial uncoupled triangular lattices. Our results
for the selective disorder do not convey with the standard description of the topological transition based on “levitation and annihilation” of the extended states carrying the topological index.

Sublattice symmetry plays a very subtle role in 2D topological insulators. It is a necessary ingredient in a minimal model to support non trivial topology (a single band is necessarily trivial) but at the same time non trivial topology requires it to be broken by NNN hoppings or otherwise. Ultimately, it is this broken chiral symmetry that is responsible for the sensitivity to selective disorder.

We understand the topological transition as a transition from the honeycomb (topologically non–trivial for finite Haldane mass) to the two uncoupled triangular (trivial) sublattices within the same symmetry class. The “localization transition” is more complicated but in the limiting cases it is also between a Chern insulator (topologically non trivial) to a metal, again without changing symmetry or dimensionality. The localization transition in graphene with vacancies equally distributed among the two sublattices has been explored in some detail as a special example of chiral class [18–20] presenting some difficulties. Apart from being responsible for the topological features with emphasis on the selected dilution case. Ref. 21 analyses the localization properties of a 2D chiral systems (in particular in graphene) without topological features with emphasis on the selected dilution.

We gratefully acknowledge useful conversations with Belén Valenzuela on the transition from the honeycomb to the Hexagonal lattice. We also thank Fernando de Juan for a critical reading of the manuscript and useful suggestions. EC acknowledges the financial support of FCT-Portugal through grant no. EXPL/FIS/Flagship.00512, and by the European Union Seventh Framework Programme under grant agreement no. 604391 Graphene Flagship.

References

[1] P. W. Anderson, Phys. Rev. 109, 1492 (1958).
[2] A. K. Geim and I. V. Grigorieva, Nature 499, 419 (2013).
[3] B. A. Bernevig, T. L. Hughes, and S. Zhang, Science 314, 1757 (2006).
[4] H. Obuse, A. Furusaki, S. Ryu, and C. Mudry, Phys. Rev. B 76, 075301 (2007).
[5] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
[6] X. Qi and S. Zhang, Rev. Mod. Phys. 83, 1057 (2011).
[7] E. Abrahams, P. W. Anderson, D. C. Licciardello, and T. W. Ramakrishnan, Phys. Rev. Lett. 42, 673 (1979).
[8] P. W. Anderson, D. J. Thouless, E. Abrahams, and D. S. Fisher, Phys. Rev. B 22, 3519 (1980).
[9] A. Altland and M. R. Zirnbauer, Phys. Rev. B 55, 1142 (1997).
[10] A. P. Schnyder, S. Ryu, A. Furusaki, and A. W. W. Ludwig, Phys. Rev. B 78, 195120 (2008).
[11] F. Evers and A. D. Mirlin, Rev. Mod. Phys. 80, 1355 (2008).
[12] F. D. M. Haldane, Phys. Rev. Lett. 61, 2015 (1988).
[13] C. Kane and E. Mele, Phys. Rev. Lett. 95, 226801 (2005).
[14] M. Onoda, Y. Avishai, and N. Nagaosa, Phys. Rev. Lett. 98, 076802 (2007).
[15] E. Prodan, T. L. Hughes, and B. A. Bernevig, Phys. Rev. Lett. 105, 115501 (2010).
[16] R. Gade and F. Wegner, Nuclear Physics B 360, 213 (1991).
[17] E. J. König, P. M. Ostrovsky, I. V. Protopopov, and A. D. Mirlin, Phys. Rev. B 85, 195130 (2012).
[18] P. M. Ostrovsky, M. Titov, S. Bera, I. V. Gornyi, and A. D. Mirlin, Phys. Rev. Lett. 105, 266803 (2010).
[19] V. Häßner, J. Schindler, N. Weik, T. Mayer, S. Balakrishnan, R. Narayanam, S. Bera, and F. Evers, Phys. Rev. Lett. 113, 186802 (2014).
[20] Z. Fan, A. Uppstu, and A. Harju, Phys. Rev. B 89, 245422 (2014).
[21] P. M. Ostrovsky, I. V. Protopopov, E. J. König, I. V. Gornyi, A. D. Mirlin, and M. A. Skvortsov, Phys. Rev. Lett. 113, 186803 (2014).
[22] G. Jotzu, M. Messer, R. Desbuquois, M. Lebrat, T. Uehlinger, D. Greif, and T. Esslinger, Nature 515, 237 (2014).
[23] T. Fukui, Y. Hatsuigui, and H. Suzuki, J. Phys. Soc. Jpn. 74, 1674 (2005).
[24] Y. F. Zhang, Y. Y. Yang, Y. Ju, L. Sheng, D. N. Sheng, R. Shen, and D. Y. Xing, Chinese Phys. B 22, 117312 (2013).
[25] E. V. Castro, M. P. López-Sanchez, and M. A. H. Vozmediano, Phys. Rev. Lett. 104, 036802 (2010).
[26] E. V. Castro and J. M. B. Lopes dos Santos, J. Phys.: Condens. Matter 22, 075601 (2010).
[27] M. Inglot and V. Dugaev, J. Appl. Phys. 109, 123709 (2011).
[28] W. Shan, J. Lu, H. Lu, and S. Shen, Phys. Rev. B 84,
Supplementary material

I. FROM HONEYCOMB TO TWO TRIANGULAR LATTICES

Dilution of a single sublattice leads, after 100% dilution, to the triangular lattice. Since the latter has a single band, the Chern number must be zero. In this section we analyze whether the transition found for the selected dilution case can be attributed to the fact that, for some critical density of vacancies, the system is already more triangular lattice like and therefore the Chern number is zero.

To address this possibility we study how the gap and Chern number evolves with the NN hopping $t$. For $t = 0$ we end up with the triangular lattice. The spectrum and the eigenvectors are obtained by the $2 \times 2$ Hamiltonian given by

$$ H_k = \begin{pmatrix} m(k) & f(k) \\ f^*(k) & -m(k) \end{pmatrix}, $$

where

$$ m(k) = -2t_2[\sin(k \cdot a_1) - \sin(k \cdot (a_1 - a_2)) - \sin(k \cdot a_2)], $$

$$ f(k) = t(1 + e^{i k \cdot a_1} + e^{i k \cdot a_2}). $$

The spectrum is easily obtained and reads

$$ E_k = \pm \sqrt{m(k)^2 + |f(k)|^2}. $$

In the limit $t/t_2 \to 0$ we get two decoupled triangular lattices with imaginary hoppings related by complex conjugation, the spectrum being $E_k = \pm m(k)$. In Fig. 4 we show the spectrum $E_k = m(k)$ for the triangular lattice with imaginary hoppings (left), the spectrum $E_k = \pm m(k)$ for two decoupled triangular lattices with imaginary hoppings (center), and the spectrum given by Eq. (3) when the system is perturbed by a finite $t$ leading to a finite gap (right).

It is apparent that any finite NN hopping parameter $t$ lifts the degeneracy that can be seen in the middle panels of Fig. [4] and opens a finite gap in the spectrum. Since we know by inspection that the gap remains open for any $t/t_2$, including $t/t_2 \gg 1$ where the system in topologically non-trivial, then we conclude that it must be non-trivial for any finite $t$. This is explicitly shown in the left panel of Fig. [4] where we represent the Chern number for the Haldane model as a function of $t/t_2$. The Chern number has been obtained using Fukui’s method [23]. So, the system is trivial only for $t = 0$, when the two triangular lattices are decoupled.

Let us emphasize that we should not confuse the triangular lattice with homogeneous complex hoppings, which breaks time reversal symmetry, with the familiar triangular (or hexagonal) lattice with real hoppings. The spectrum for the latter reads

$$ E_k = -t_2(\cos(k \cdot a_2) + \cos(k \cdot a_1) + \cos(k \cdot (a_1 - a_2))) $$

$$ = -t_2 \left( 2 \cos \left( \frac{ak_x}{2} \right) \cos \left( \frac{\sqrt{3}}{2} ak_y \right) + \cos(ak_z) \right). $$

Such energy spectrum is shown in Fig. [5] (middle and right panels).
Figure 4. Energy spectrum for the triangular lattice with imaginary hoppings (left), two decoupled triangular lattices with imaginary hoppings related by complex conjugation (center), and coupled triangular lattices as given by Eq. (3). Bottom panels are the same as top panels along a particular path in the BZ.

Figure 5. (left) Chern number for the Haldane model as a function of the parameter $t/t_2$. (middle, right) Energy spectrum for the triangular lattice with real hoppings.