Robustness of the Spin-Chern number: An analytic proof

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Ever since introduced, the topological properties of the Spin-Chern (C_s) have been discussed and re-discussed in a fairly large number of works. On one hand the original paper by Sheng and collaborators revealed robust properties of C_s against disorder and certain deformations of the model and, on the other hand, other people pointed out that C_s can change sign under special deformations that keep the insulating gap open. This makes one wonder how far does the robustness observed in the original paper extend? In this paper we give an analytic result that allows us to state in extremely simple terms the origin of the robustness against disorder and continuous local deformations of the models. It also allows us to give several generalizations of the topological invariant.

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Quantum Spin-Hall insulators represent a new state of matter. They were predicted theoretically in Ref. [1] and soon after that they were found experimentally [2, 3]. Samples made of such materials display dissipationless spin currents at the edges, that are robust against continuous deformations and disorder [4].

The presence of the edge channels is due to the non-trivial topology of the bulk energy bands and two non-trivial topological invariants were proposed, virtually in the same time: the $Z2$ invariant proposed by Kane and Mele [5] and the Spin-Chern number proposed by Sheng and collaborators [6] (first mentioned in Ref. [4]). In this paper we focus on the later invariant, which came under sustained scrutiny because it promised a finer classification of the Spin-Hall insulators. This was later argued [7, 8] not to be the case.

The Spin-Chern number is obtained by integrating the Berry curvature of a fiber bundle obtained by imposing twisted boundary conditions on a finite sample [6]. In general, such procedure does not necessarily lead to smooth fiber bundles. However, the numerical evidence given in Ref. [6] implied that, for their case, the structure is a smooth fiber bundle and that C_s is a robust topological invariant. It was later observed, however, that one can continuously deform the model using spin rotations that keep the insulating gap unchanged but switch the sign of the Spin-Chern number [7, 8]. This argument shows that sometime the structure proposed in Ref. [6] fails to be a smooth fiber bundle and that C_s may not be well defined over the entire Spin-Hall zone of the phase diagram. The current understanding is that, whenever one crosses certain zones of the parameter space, C_s jumps, but these jumps are always by an even number. Therefore, one can still use C_s to formulate a Z2 classification of the Spin-Hall insulators and to efficiently compute the Z2 invariant. For this reason, the interest in the Spin-Chern number continues to be strong. An efficient algorithm for numerical evaluations of C_s was proposed by Fukui and Hatsugai [9]. Later, the algorithm was used to map C_s for aperiodic systems [10].

In this paper we give an analytic result that tells when C_s can be defined and how to define C_s in a manner that allows extensions to the disordered case. Once we complete this step, we show that the topological invariance of C_s can be established using the non-commutative theory of the Chern number [11]. Let us start our discussion from the concrete model of electrons in graphene [1]:

$$\begin{aligned} H_0 = &-t \sum_{\langle \mathbf{ij}\rangle,\sigma} |\mathbf{i},\sigma\rangle\langle \mathbf{j},\sigma| \\ &+i\lambda_{SO} \sum_{\langle\langle \mathbf{ij}\rangle\rangle,\sigma\sigma'} [\mathbf{s}\cdot(\mathbf{d_{kj}}\times\mathbf{d_{ik}})]_{\sigma,\sigma'} |\mathbf{i},\sigma\rangle\langle \mathbf{j},\sigma'| \\ &+i\lambda_{R} \sum_{\langle \mathbf{ij}\rangle,\sigma\sigma'} [\hat{\mathbf{z}}\cdot(\mathbf{s}\times\mathbf{d_{ij}})]_{\sigma,\sigma'} |\mathbf{i},\sigma\rangle\langle \mathbf{j},\sigma'|. \end{aligned} \quad (1)$$

Here, $\mathbf{i}$ and $\mathbf{j}$ denote the sites of the honeycomb lattice and σ and σ' the electron spin degrees of freedom, taking the values ± 1. The Hamiltonian acts on the Hilbert space $\mathcal{H}$ spanned by the orthonormal basis $|\mathbf{i},\sigma\rangle$. The simple kets denote the nearest neighbors and double kets denote the second nearest neighbours. The electrons are considered non-interacting. The three terms in Eq. 1 are the usual nearest neighbor hopping term, the intrinsic spin-orbit coupling preserving the lattice symmetries and the Rashba potential induced by the substrate supporting the graphene sheet. We assume that the parameters in the Hamiltonian are chosen so that we are in the Spin-Hall zone of the phase diagram [5].

The model is time reversal invariant and it displays two upper and two lower bands separated by an insulating gap. The total Chern number of the lower (and for that matter also of the upper) bands is zero, as it will generically be for any time reversal invariant band model. When λ_R=0, s_z, defined by $s_z|\mathbf{i},\sigma\rangle = \frac{1}{2}\sigma|\mathbf{i},\sigma\rangle$, commutes with the Hamiltonian and the model Eq. 1 reduces to a spin up and a spin down decoupled Haldane models [12]. Thus, we can define two Chern numbers, for the spin up and for the spin down electrons, which are non-trivial in the Spin-Hall part of the phase diagram. We choose λ_{SO} so that $C_\uparrow$=1 and $C_\downarrow$=-1. The sign of these numbers will change if λ_{SO} changes sign, due to the closing of the

insulating gap at $\lambda_{SO} = 0$. When the Rashba term is turned on, s_z is no longer conserved. The question is, without such conserved quantity, how can one smoothly split the fiber bundle of the occupied states into two fiber bundles with non-trivial Chern numbers? Also, how can one tackle the disorder case, when the Brillouin torus is no longer there?

The splitting in up/down spin sectors is, of course, given by the spectral decomposition of s_z. When s_z is no longer conserved, we should look for another operator that does the same job. Let us start with the strictly periodic Hamiltonian Eq 1. We also defer certain abstractions and generalizations till later in the paper and we start with a concrete choice for this operator, which is Ps_zP, P being the projector onto the occupied states. Ps_zP changes sign after the conjugation with the time reversal operation θ:

$$\theta P s_z P \theta = -P s_z P. \tag{2}$$

For $\lambda_R = 0$, s_z commutes with the projector P, thus the spectrum of Ps_zP consists of just two points: $\pm\frac{1}{2}$. Of course, Ps_zP is zero on the un-occupied states, but here we restrict the discussion to the space $\mathcal{K} = P\mathcal{H}$ of occupied states only. When λ_R is turned on, the spectrum of Ps_zP spreads but is still contained between $-\frac{1}{2}$ and $+\frac{1}{2}$ (see Fig. 1). Moreover, for small λ_R, we can be sure that the spectrum does not cross the origin [see the technical discussion near the end of the paper]. Due to property 2, we can also be sure that the spectrum of Ps_zP is symmetric relative to the origin. If we denote by $\mathcal{K}_\pm$ and by $P_\pm$ the invariant spectral spaces and the spectral projectors corresponding to the positive/negative spectrum of Ps_zP, then:

$$\mathcal{K} = \mathcal{K}_- \oplus \mathcal{K}_+, P = P_- \oplus P_+, \quad \theta\mathcal{K}_\pm = \mathcal{K}_\mp. \tag{3}$$

In other words, the spectral spaces of Ps_zP can provide a splitting of $P\mathcal{H}$. To have a valid splitting, however, *we need to demonstrate that the kernels $\langle \mathbf{i},\sigma|P_\pm|\mathbf{j},\sigma'\rangle$ decay exponentially fast with the separation $|\mathbf{i}-\mathbf{j}|$*. The proof that this is indeed the case is at the core of our paper, but for the sake of exposition we defer the proof till the end of the paper.

A few clarifications are in place. The above splitting is not associated with slashing the Brillouin torus in half. The two spaces $\mathcal{K}_\pm$ remain fibrations over the whole Brillouin torus. Their Whitney sum gives the original fiber bundle of the occupied states. The fact that the projectors $P_\pm$ are exponentially localized assures that the splitting $P(\mathbf{k}) = P_-(\mathbf{k}) \oplus P_+(\mathbf{k})$ can be done smoothly over the entire Brillouin torus. Of course, at this point one can go ahead and compute the Chern numbers for each sectors, by integrating the corresponding Berry curvature over the Brillouin torus:

$$C\pm = \int_{\mathcal{T}} \frac{d^2\mathbf{k}}{2\pi i}\ \mathrm{Tr}\{P_\pm(\mathbf{k})[\partial_{k_1}P_\pm(\mathbf{k}), \partial_{k_2}P_\pm(\mathbf{k})]\}. \tag{4}$$

This, however, is not satisfactory because the computation will depend on the existence of the Brillouin torus, which is lost when disorder is added.

A key observation is that our construction does not involve the Bloch fibration and for that reason it can be extended to the disordered system. To be specific, let us consider the addition of a random potential

$$V_\omega = \sum_{\mathbf{i},\sigma} \lambda_{\mathbf{i}}(\omega)|\mathbf{i},\sigma\rangle\langle\mathbf{i},\sigma|, \tag{5}$$

where $\lambda_{\mathbf{i}}(\omega)$ is a random variable with $\omega \in \Omega$. We assume the existence of a probability measure $d\mu(\omega)$ on Ω and of an ergodic flow $t_{\mathbf{n}} : \Omega \to \Omega$, $t_{\mathbf{n}}t_{\mathbf{n}'} = t_{\mathbf{n}+\mathbf{n}'}$, such that $u_{\mathbf{n}}V_\omega u_{\mathbf{n}}^{-1} = V_{t_{\mathbf{n}}\omega}$, where $u_{\mathbf{n}}$ refers to the lattice translation by a vector $\mathbf{n}$ of the Bravais lattice. The probability measure is assumed invariant to this flow. At all times, we assume that the insulating gap of $H_\omega{=}H_0 + V_\omega$ remains open and consider the Fermi level inside this gap. We denote by P_ω the projector onto the occupied states. As we shall see, at least for small λ_R, $P_\omega s_z P_\omega$ continues to display a spectral gap around the origin, in which case the splitting $P_\omega = P_-(\omega) \oplus P_+(\omega)$ is still possible.

The idea is then to apply the non-commutative theory of the Chern number [11] to the projectors $P_\pm$, individually. Of course, this theory cannot be applied to any projectors. It works for the present case because $P_\pm$ are exponentially localized and because they have the covariance property: $u_{\mathbf{n}}P_\pm(\omega)u_{\mathbf{n}}^{-1} = P_\pm(t_{\mathbf{n}}\omega)$. The non-commutative version of the Chern numbers is

$$C_\pm(\omega) = 2\pi i \mathrm{tr}\{P_\pm(\omega)[[n_1, P_\pm(\omega)], [n_2, P_\pm(\omega)]]\}, \tag{6}$$

where tr is the trace over the states in the first unit cell and $\mathbf{n}$ denotes the position operator of the unit cells in the Bravais lattice. For the periodic case, this expression is equivalent to Eq. 4. The main result is

$$\int d\mu(\omega)\ C_\pm(\omega) = \pm 1, \tag{7}$$

which follows from the equality:

$$\begin{aligned} 2\pi i \textstyle\int d\mu(\omega)\ \mathrm{tr}\{P_\pm(\omega)[[n_1, P_\pm(\omega)][n_2, P_\pm(\omega)]]\} \\ = \mathrm{Index}\{P_\pm(\omega)UP_\pm(\omega)\} \end{aligned} \tag{8}$$

with U being the unitary transformation given by multiplication with $(n_1 + in_2)/\sqrt{n_1^2 + n_2^2}$. The index is well defined if $P_\pm$ are exponentially localized. If this is the case, the index is an integer by definition and is independent of ω. The index cannot change under various deformations of the Hamiltonian, as long as $P_\pm(\omega)$ remain exponentially localized. The proof of Eq. 8 can be achieved by following step by step the analysis given in Ref. 11 for the full Chern number.

What did we learn? The robustness of the Spin-Chern number $C_s{=}\frac{1}{2}(C_+ - C_-)$ against deformations of the Hamiltonian and disorder *is due to the existence of two*

spectral gaps: the insulating gap of the Hamiltonian and the spectral gap of the operator Ps_zP. Is s_z special? No. In fact, C_s is invariant to deformations of H *and* s_z, as long as the spectral gaps of the two operators remain open. Closing any of the two gaps can result in jumps for the the Spin-Chern number. The jumps are always by an even number.

How does our analysis complete the previous discussions? The argument in Refs. [7, 8] was that, using rotations in the spin sector, one can connect the Hamiltonians with $+\lambda_{SO}$ and with $-\lambda_{SO}$ without changing the insulating gap. But at the end of such rotation, C_s changes sign. The change of sign was attributed to the closing of the gap of the Hamiltonian with the twisted boundary conditions. Various physical interpretations have been given to this finding, the most prevalent one being that Spin-Chern number describes the edge where the twisted boundary conditions were imposed rather than the bulk.

We now can give an alternative explanation: during the rotation in the spin sector, the gap of Ps_zP closes and then opens again. Can this problem be fixed? Yes. The solution is to deform not only the Hamiltonian but also the operator Ps_zP. For the case of spin rotations, this can be easily accomplished by applying the spin rotations to s_z inside Ps_zP. If there is such easy fix, then the old question resurfaces: does the Spin-Chern number contain more information than the Z2 invariant? The answer is no. After the continuous rotation, $Ps_zP \to -Ps_zP$ and $\mathcal{K}_\pm \to \mathcal{K}_\mp$. Thus, there is no canonical way to chose the spaces $\mathcal{K}_\pm$ and, since this choice determines the sign of C_s, the sign contains no additional information.

Can the construction be generalized? Yes. For other models, we can find operators PAP that have n islands of isolated spectrum with exponentially localized projectors. If A commutes with the translations of the unit cell, we can define a Chern number for each spectral island of PAP. A simple example is the model of Eq. 1 with spin $\frac{3}{2}$ particles. For $\lambda_0 = 0$, s_z commutes with the Hamiltonian and $P\mathcal{H}$ splits into four sectors, corresponding to $s_z = -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}$ and $\frac{3}{2}$. For each sector we can define a Cern number, which take the values: $C_{-\frac{3}{2}} = C_{-\frac{1}{2}} = -1$ and $C_{\frac{1}{2}} = C_{\frac{3}{2}} = 1$. When the Rashba interaction and disorder are turned on, the spectrum of Ps_zP spreads, but is still contained into four isolated spectral islands. Thus, we can still split $P\mathcal{H}$ into four sectors and our analysis shows that the Chern numbers for each sectors will be conserved as long as the the insulating gap remains open and the spectral islands of Ps_zP remain isolated. The spin-Chern number can be defined in various ways, depending how we group the sectors. If we repeat the construction for spin $\frac{1}{2}$ and put the negative s_z sectors into $\mathcal{K}_-$ and the positive s_z sectors into $\mathcal{K}_+$, C_s becomes 2. Other possible groupings gives $C_s = 0$ and $C_s = -2$.

It is interesting to remark that time-reversal invariance did not play a crucial role in our construction. If we consider more complex insulators, that is insulators with many atoms in the unit cell, it is very probable that one can build non-trivial operators A by combining spin and/or point group symmetry operators. Using such operators one might discover nontrivial topological structures in seemingly trivial insulators. For example, it was recently pointed out [13] that certain surface states in ordinary semiconductors can have topological origins. This is a remarkable observation since the presence of surface or interface states is paramount for the functioning of photovoltaic devices. Thus, in principle we can use topology to design better photovoltaic devices. In fact this drives our interest for this problem.

How about the edge currents? The existence of the nontrivial Chern numbers for different sectors does not automatically imply the existence of chiral edge modes. Generically, only the insulators with odd C_s display such edge modes [7].

The discussion given here hardly touches the problem of classification and of the edge modes. For this two problems one has to explore how the occupied states relate to the un-occupied states. This has to be done on solvable models. It is at this point where our analysis becomes relevant because now we have a guiding principle which tells when the realistic models, which should include disorder and will generally not be solvable, can be deformed into smooth solvable models without changing the topological invariants.

The robustness of the edge modes was also recently investigated in Ref. [14], which introduced a quantized edge index. Although this edge index was also constructed via a splitting, the connection between the edge index and C_s is not clear to us at this moment. We want to make a final remark about the edge modes. The existence of nontrivial topological sectors can indicate reach edge and surface physics. For example, for the model of spin $\frac{3}{2}$ particles, when cutting an edge we can be sure that four [which become 2] edge bands shoot out of the bulk spectrum. The bands hybridize and return back into the same part of the bulk spectrum were they originated. Nevertheless, these bands lead to edge states which can still be useful for practical applications. In the presence of disorder, these edge bands will localize, but if the localization length is large, these edge states, for example, can efficiently trap light and thus be useful in photovoltaic devices.

We now start the proof of the exponential localization of the projectors $P_\pm(\omega)$. To ease the notation we drop ω. First, let us show that the gap of the operator Ps_zP, viewed as an operator on $\mathcal{K}$, remains open and clean when the Rashba term is turned on, as opposed to immediately closing or filling with additional spectrum due to some instability. For this, we notice that the projector in the occupied space is analytic in λ_R. This property is protected by the insulating gap of the Hamiltonian H_ω. We will show that, at least for small λ_R, $Ps_zP - \zeta I_{\mathcal{K}}$ is invertible for ζ in the vicinity of 0. One could try to work

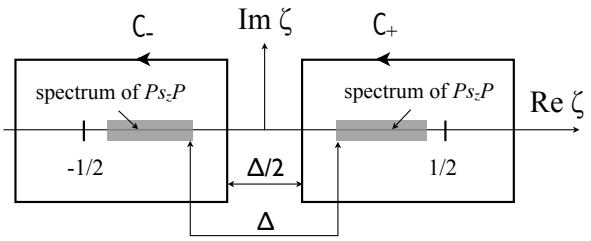

FIG. 1: The figure illustrates the spectrum of $P\sigma_3 P$ for small Rashba coupling and the contours of integrations used in the main text.

with the expression

$$(Ps_zP - \zeta I_{\mathcal{K}})^{-}1 = P(Ps_zP - \zeta I)^{-1} \tag{9}$$

and use the continuity of P, but this expression has a problem when $z = 0$, since even if $Ps_zP - \zeta I_{\mathcal{K}}$ is invertible at $z = 0$, $(Ps_zP - \zeta I)^{-1}$ diverges because we include the un-occupied states where Ps_zP is zero.

Here is an alternative approach inspired from Ref. [15]. Let $R(\zeta) = P(s_z - \zeta)^{-1}P$, with ζ in a neighborhood of zero. We have successively:

$$\begin{aligned} &R(\zeta)(Ps_zP - \zeta I_{\mathcal{K}}) = \\ &P(s_z - \zeta)^{-1}\{(s_z - \zeta)P + [P, s_z]\}P \\ &= P + P(s_z - \zeta)^{-1}[P, s_z]P \equiv I_{\mathcal{K}} + Q. \end{aligned} \tag{10}$$

Q is small, at least for small λ_R, since

$$Q = P(s_z - \zeta)^{-1}[P - P_0, s_z]P, \tag{11}$$

where P_0 is the projector onto the occupied states for $\lambda_R = 0$. The small factor comes from $P - P_0$, which is proportional to λ_R. Above, we used the fact that s_z commutes with P_0, even in the presence of disorder. In this case, the operator $I_{\mathcal{K}} + Q$ is invertible and we find:

$$(I_{\mathcal{K}} + Q)^{-1}R(\zeta)(Ps_zP - \zeta I_{\mathcal{K}}) = I_{\mathcal{K}}, \text{ or} \tag{12}$$

$$(Ps_zP - \zeta I_{\mathcal{K}})^{-1} = (I_{\mathcal{K}} + Q)^{-1}P(s_z - \zeta)^{-1}P. \tag{13}$$

We now show that, as long as the gap Δ of Ps_zP (or any deformation of it) remains opened, the spectral projectors $P_\pm$ are exponentially localized. By exponential localization of an operator T we mean the existence of a strictly positive α such that

$$|\langle \mathbf{i}, \sigma | T | \mathbf{j}, \sigma' \rangle| \leq \text{ct. } e^{-\alpha|\mathbf{i}-\mathbf{j}|}. \tag{14}$$

We will use the following simple observation [16]. If $U_{\mathbf{q}}$ denotes the non-unitary transformation $U_{\mathbf{q}}|\mathbf{i}, \sigma\rangle = e^{\mathbf{q}\cdot\mathbf{i}}|\mathbf{i}, \sigma\rangle$, then: if T is exponentially localized, then $T_{\mathbf{q}} \equiv U_{\mathbf{q}} T U_{-\mathbf{q}}$ is a bounded operator for all orientations of $\mathbf{q}$, provided $|\mathbf{q}|$ is smaller than α, and conversely: if $T_{\mathbf{q}}$ is bounded for any orientation of $\mathbf{q}$ and $|\mathbf{q}| < \alpha$, then T is exponentially localized with a localization exponent equal or larger than α. Also, it is a fact that if T is exponentially localized, then [$\|\ \|$ denotes the operator norm]

$$\|T - T_{\mathbf{q}}\| \to 0 \text{ as } q \to 0, \tag{15}$$

i.e. the difference between T and $T_{\mathbf{q}}$ is small for q small. Since

$$P_\pm = \frac{i}{2\pi}\int_{\mathcal{C}_\pm} P(Ps_zP - \zeta I)^{-1} d\zeta, \tag{16}$$

it is enough to show the exponential localization of $P(Ps_zP - \zeta I)^{-1}$. The contours $\mathcal{C}_\pm$ are shown in Fig. 1. The projector P itself is exponentially localized. For a general proof see Ref. [17]. We have:

$$U_{\mathbf{q}} P(Ps_zP - \zeta I)^{-1} U_{\mathbf{q}} = P_{\mathbf{q}}(P_{\mathbf{q}} s_z P_{\mathbf{q}} - \zeta I)^{-1}, \tag{17}$$

and

$$P_{\mathbf{q}} s_z P_{\mathbf{q}} - \zeta I = Ps_zP - \zeta I + P_{\mathbf{q}} s_z P_{\mathbf{q}} - Ps_zP \tag{18}$$

thus

$$\|P_{\mathbf{q}} s_z P_{\mathbf{q}} - \zeta I\| \geq \frac{\Delta}{2} - \|P_{\mathbf{q}} s_z P_{\mathbf{q}} - Ps_zP\| \tag{19}$$

which is strictly positive for small q due to Eq. 15. In other words, $P_{\mathbf{q}} s_z P_{\mathbf{q}} - \zeta I$ is invertible, at least for small q, which shows that all operators appearing in the right hand side of Eq. 17 are bounded. Consequently, $P_\pm(\omega)$ are exponentially localized.

In conclusion, for the graphene model we have shown that the space of the occupied states can be robustly split into two sectors by using the spectral properties of Ps_zP. We also found that the well established non-commutative theory of the Chern number can be applied to define invariants for the two sectors and to demonstrate their robustness against deformations and disorder. We showed that the construction can be generalized in several ways, some with potential for practical applications.

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