Inverse participation ratio and localization in topological insulator phase transitions

M Calixto\textsuperscript{1} and E Romera\textsuperscript{2}

\textsuperscript{1} Departamento de Matemática Aplicada and Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada, Fuentenueva s/n, 18071 Granada, Spain

\textsuperscript{2} Departamento de Física Atómica, Molecular y Nuclear and Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada, Fuentenueva s/n, 18071 Granada, Spain

E-mail: calixto@ugr.es and eromera@ugr.es

Received 30 April 2015
Accepted for publication 31 May 2015
Published 23 June 2015

Abstract. Fluctuations of Hamiltonian eigenfunctions, measured by the inverse participation ratio (IPR), turn out to characterize topological-band insulator transitions occurring in 2D Dirac materials like silicene, which is isostructural with graphene but with a strong spin–orbit interaction. Using monotonic properties of the IPR, as a function of a perpendicular electric field (which provides a tunable band gap), we define topological-like quantum numbers that take different values in the topological-insulator and band-insulator phases.

Keywords: quantum phase transitions (theory), electrical and magnetic phenomena (theory), fluctuations (theory), graphene (theory)
1. Introduction

In recent years, the concepts of insulator and metal have been revised and a new category called ‘topological insulators’ has emerged. In these materials, the energy gap $\Delta$ between the occupied and empty states is inverted or ‘twisted’ for surface or edge states basically due to a strong spin–orbit interaction $\Delta_{so}$ (namely, $\Delta_{so} = 4.2$ meV for silicene). Although ordinary band insulators can also support conducting metallic states on the surface, topological surface states have special features due to symmetry protection, which make them immune to scattering from ordinary defects and can carry electrical currents even in the presence of large energy barriers.

The low energy electronic properties of a large family of topological insulators and superconductors are well described by the Dirac equation \[1\]; in particular, some 2D gapped Dirac materials isostructural with graphene such as: silicene, germanene, stannene, etc. Compared to graphene, these materials display a large spin–orbit coupling and show quantum spin Hall effects \[2,3\]. Applying a perpendicular electric field $E_z = \Delta_z/l$ ($l$ is the inter-lattice distance of the buckled honeycomb structure, namely $l = 0.22$ Å for silicene) to the material sheet generates a tunable band gap (Dirac mass) $\Delta_z^\xi = (\Delta_z - s\xi\Delta_{so})/2$ ($s = \pm 1$ and $\xi = \pm 1$ denote spin and valley, respectively). There is a topological phase transition \[4\] from a topological insulator (TI, $|\Delta_z| < \Delta_{so}$) to a band insulator (BI, $|\Delta_z| > \Delta_{so}$), at a charge neutrality point (CNP) $\Delta_z^{(0)} = s\xi\Delta_{so}$, where there is a gap cancellation between the perpendicular electric field and the spin–orbit coupling, thus exhibiting the aforementioned semi-metal behavior. In general, a TI-BI transition is characterized by a band inversion with a level crossing at some critical value of a control parameter (electric field, quantum well thickness \[3\], etc).

Topological phases are characterized by topological charges like Chern numbers. For an insulating state $|\psi(k)\rangle$, a ‘gauge potential’ $a_j(k) = -i\langle\psi(k)|\partial_j\psi(k)\rangle$ can be defined in momentum space $(k_x, k_y)$, so that the Chern number $C$ is the integral $C = \int d^2k f(k)/2\pi$ of the Berry curvature $f = \partial_{k_x}a_y - \partial_{k_y}a_x$ over the first Brillouin zone. When the Hamiltonian
is given by (1), the Chern number is obtained as \( C_\xi = -\xi \text{sgn}(\Delta_\xi)/2 \), so that a topological insulator phase transition (TIPT) occurs when the sign of the Dirac mass \( \Delta_\xi \) changes [5].

In this article we propose the use of the inverse participation ratio (IPR) of Hamiltonian eigenvectors as a characterization of the topological phases TI and BI. The IPR measures the spread of a state \( |\psi\rangle \) over a basis \( \{|i\rangle\}_{i=1}^N \). More precisely, if \( p_i \) is the probability of finding the (normalized) state \( |\psi\rangle \) in \( |i\rangle \), then the IPR is defined as \( I_\psi = \sum_i p_i^2 \). If \( |\psi\rangle \) only ‘participates’ of a single state \( |i_0\rangle \), then \( p_{i_0} = 1 \) and \( I_\psi = 1 \) (large IPR), whereas if \( |\psi\rangle \) equally participates on all of them (equally distributed), \( p_i = 1/N, \forall i \), then \( I_\psi = 1/N \) (small IPR). Therefore, the IPR is a measure of the localization of \( |\psi\rangle \) in the corresponding basis. Equivalently, the (Rényi) entropy \( S_\psi = -\ln I_\psi \) is a measure of the delocalization of \( |\psi\rangle \). We shall see that electron and hole IPR curves cross at the CNP, as a function of the electric field \( \Delta_z \), and the crossing IPR value turns out to be a universal quantity, independent of Hamiltonian parameters. Moreover, the different monotonic character (slopes’ sign) of combined (electron plus holes) IPRs in the TI and BI regions turn out to characterize both phases.

These and related information theoretic and statistical measures have proved to be useful in the description and characterization of quantum phase transitions (QPTs) of several paradigmatic models such as: the Dicke model of atom-field interactions [6–10], the vibron model of molecules [11–13] and the ubiquitous Lipkin–Meshkov–Glick model [14,15]. An important difference between QPT and TIPT is that the first case entails an abrupt symmetry change and the second one does not (necessarily). However, the use of information theoretic measures, such as Wehrl entropy [16] and uncertainty relations [17], has also proved to be useful to characterize TIPTs. Moreover, we must also say that strong fluctuations of eigenfunctions (characterized by a set IPRs) also represent one of the hallmarks of the traditional Anderson metal-insulator transition [18–22]. In fact, the phenomenon of localization of the electronic wave function can be regarded as the key manifestation of quantum coherence at a macroscopic scale in a condensed matter system.

The paper is organized as follows. Firstly, in section 2, we will introduce the low energy Hamiltonian describing the electronic properties of some 2D Dirac materials like silicene, germanene, stantene, etc, in the presence of perpendicular electric and magnetic fields. Then, in section 3, we will compute the IPR of Hamiltonian eigenvectors and discuss the (different) structure of IPR curves as a function of the electric field across TI and BI regions. Section 4 is devoted to the final comments and conclusions.

2. Low energy Hamiltonian

The low energy dynamics of a large family of topological insulators (namely, honeycomb structures) is described by the Dirac Hamiltonian in the vicinity of the Dirac points \( \xi = \pm 1 \) [23]

\[
H_\xi^Z = v(\xi \sigma_x p_x + \sigma_y p_y) - \frac{1}{2} \xi s \Delta_{so} \sigma_z + \frac{1}{2} \Delta_z \sigma_z,
\]

where \( \sigma_j \) are the usual Pauli matrices, \( v \) is the Fermi velocity of the corresponding material (namely, \( v = 4.2 \times 10^5 \text{ m s}^{-1} \) for silicene) and \( \Delta_{so} \) and \( \Delta_z \) are the spin–orbit and electric field couplings. The application of a perpendicular magnetic field \( B \) is implemented
Inverse participation ratio and localization in topological insulator phase transitions

through the minimal coupling $\vec{p} \rightarrow \vec{p} + e\vec{A}$ for the momentum, where $\vec{A} = (-By, 0)$ is the vector potential in the Landau gauge. The Hamiltonian eigenvalues and eigenvectors at the $\xi$ points are given by [23]

$$E_n^{\xi} = \begin{cases} 
\text{sgn}(n) \sqrt{|n|\hbar^2 \omega^2 + (\Delta_\xi)^2}, & n \neq 0, \\
-\xi\Delta_\xi, & n = 0, 
\end{cases}$$

and

$$|n\rangle^{\xi} = \begin{cases} 
-iA_n^{\xi}|n - \xi_+\rangle \\
B_n^{\xi}|n - \xi_-\rangle 
\end{cases},$$

where we denote by $\xi_\pm = (1 \pm \xi)/2$, the Landau level index $n = 0, \pm 1, \pm 2, \ldots$, the cyclotron frequency $\omega = v\sqrt{2eB/\hbar}$, the lowest band gap $\Delta_\xi \equiv (\Delta_z - s\xi\Delta_{so})/2$ and the coefficients $A_n^{\xi}$ and $B_n^{\xi}$ are given by [23]

$$A_n^{\xi} = \begin{cases} 
\text{sgn}(n) \sqrt{\frac{|E_n^{\xi}| + \text{sgn}(n)\Delta_\xi}{2|E_n^{\xi}|}}, & n \neq 0, \\
\xi_-, & n = 0, 
\end{cases}$$

$$B_n^{\xi} = \begin{cases} 
\sqrt{\frac{|E_n^{\xi}| - \text{sgn}(n)\Delta_\xi}{2|E_n^{\xi}|}}, & n \neq 0, \\
\xi_+, & n = 0, 
\end{cases}$$

The vector $|n\rangle$ denotes an orthonormal Fock state of the harmonic oscillator. We are discarding a trivial plane-wave dependence $e^{ikx}$ in the $x$ direction that does not affect our IPR calculations, which only depend on the $y$ direction in this gauge.

As already stated, there is a prediction (see e.g. [24–27]) that when the gap $|\Delta_\xi|$ vanishes at the CNP $|\Delta_z| = \Delta_{so}$, silicene undergoes a phase transition from a topological insulator (TI, $|\Delta_z| < \Delta_{so}$) to a band insulator (BI, $|\Delta_z| > \Delta_{so}$). This topological phase transition entails an energy band inversion. Indeed, in figure 1 we show the low energy spectra (2) as a function of the external electric potential $\Delta_z$ for $B = 0.01$ T. One can see that there is a band inversion for the $n = 0$ Landau level (either for spin up and down) at both valleys. The energies $E_{1,0}^{1,\xi}$ and $E_{0,1}^{-1,\xi}$ have the same sign in the BI phase and a different sign in the TI phase, thus distinguishing both regimes. We will provide an alternative description of this phenomenon in terms of IPR relations for the Hamiltonian eigenstates (3), thus providing a quantum-information characterization of TIPT.

3. IPR and topological insulator phase transition

The IPR of a given state $I_\psi$ is related to a certain basis. In this article we will choose the position representation to write the Hamiltonian eigenstates (3). We know that Fock (number) states $|n\rangle$ can be written in position representation as

$$\langle y|n\rangle = \frac{\omega^{1/4}}{\sqrt{2^n n!\sqrt{\pi}}} e^{-y^2/2} H_n(\sqrt{\omega}y)$$

where $H_n$ are the Hermite polynomials of degree $n$. The number-state density in position space is $\rho_n(y) = |\langle y|n\rangle|^2$, which is normalized according to $\int \rho_n(y)dy = 1$. Now, taking

doi:10.1088/1742-5468/2015/06/P06029
Inverse participation ratio and localization in topological insulator phase transitions

Figure 1. Low energy spectra of silicene as a function of the external electric potential $\Delta_z$ for $B = 0.01$ T. Landau levels $n = \pm 1, \pm 2$ and $\pm 3$, at valley $\xi = 1$, are represented by dashed (electrons) and solid (holes) thin lines, black for $s = -1$ and red for $s = 1$ (for the other valley we simply have $E^s_{n,-\xi} = E^{-s,\xi}$). The lowest Landau level $n = 0$ is represented by thick lines at both valleys: solid at $\xi = 1$ and dashed at $\xi = -1$. The vertical blue dotted grid lines indicate the CNPs separating BI ($|\Delta_z| > \Delta_{so}$) from TI ($|\Delta_z| < \Delta_{so}$) phases.

into account equation (3), the density for the Hamiltonian eigenvectors (3) in position representation is given by

$$\rho_n^\xi(y) = (A_n^\xi)^2|\langle y|n| - \xi_+\rangle_\xi|^2 + (B_n^\xi)^2|\langle y|n| - \xi_-\rangle_\xi|^2.$$  

(6)

The IPR of a Hamiltoninan eigenstate in position representation is then calculated as

$$I_n^\xi \equiv \int_{-\infty}^{\infty} (\rho_n^\xi(y))^2 dy.$$  

(7)

As a previous step, we need the following integrals of Hermite density products:

$$M_{n,m} \equiv \int_{-\infty}^{\infty} \rho_n(y) \rho_m(y) dy = \sqrt{\frac{2\pi}{\omega}} \left( \begin{array}{c} 1 & 1 & 3 & 8 & 16 & \cdots \\ 1 & 3 & 7 & 16 & 32 & \cdots \\ 3 & 7 & 41 & 64 & 128 & \cdots \\ 1 & 4 & 11 & 51 & 147 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{array} \right),$$  

(8)

for $n, m = 0, 1, 2, 3 \ldots$ we will also restrict ourselves to the valley $\xi = 1$, omitting this index from (3) and (4). All the results for the valley $\xi = 1$ are straightforwardly translated to the valley $\xi = -1$ by swapping electrons for holes (i.e. $n \leftrightarrow -n$) and spin up for down (i.e. $s \leftrightarrow -s$). Taking into account all these considerations, the IPR of a Hamiltonian eigenstate is explicitly written as

$$I_n^s \equiv (A_n^s)^4 M_{|n|,-1,|n|-1} + (B_n^s)^4 M_{|n|,|n|} + 2(A_n^s B_n^s)^2 M_{|n|,|n|-1}.$$  

(9)
Figure 2. IPR $I_n^{\xi}$ in position space at valley $\xi = 1$ as a function of the electric potential $\Delta_z$ for the Landau levels: $n = \pm 1, \pm 2$ and $\pm 3$ and magnetic field $B = 0.01$ T. The electron IPR curves are dashed and the hole curves are solid, black for spin down $s = -1$ and red for spin up $s = 1$. The electron and hole IPR curves cross at the critical value of the electric potential $\Delta_z^{(0)} = s\Delta_{so}$; the vertical blue dotted grid lines indicate these CNPs and the horizontal blue dotted grid lines indicate the crossing IPR values (10).

In figure 2 we plot $I_n^{\xi}$ as a function of the external electric potential $\Delta_z$ for the Landau levels: $n = \pm 1, \pm 2$ and $\pm 3$. The electron and hole IPR curves cross at the CNPs $\Delta_z^{(0)} = s\Delta_{so}$, where they take the values:

$$I_1 = \sqrt{\frac{2\pi}{\omega} \frac{11}{16}}, \quad I_2 = \sqrt{\frac{2\pi}{\omega} \frac{145}{256}}, \quad I_3 = \sqrt{\frac{2\pi}{\omega} \frac{515}{1024}}.$$  \tag{10}

Note that, except for $\omega$, the critical crossing IPR value $I_n$ only depends on the Landau level $n$, and not on any other physical magnitude, thus providing a universal characterization of the topological insulator transition. We have checked that the smaller the magnetic field strength, the greater the slope of the electron-hole IPR curves at the CNP. The asymptotic values $I_n(\pm\infty) = \lim_{\Delta_z \to \pm\infty} I_n(\Delta_z)$ also exclusively depend on $n = 1, 2, \ldots$ and $\omega$, and are:

$$I_1(\infty) = \sqrt{\frac{2\pi}{\omega}}, \quad I_2(\infty) = \sqrt{\frac{2\pi}{\omega} \frac{3}{4}}, \quad I_3(\infty) = \sqrt{\frac{2\pi}{\omega} \frac{41}{64}}, \ldots$$  \tag{11}

fulfilling $I_{-n}(\infty) = I_n(\infty)$ and $I_{-|n|}(\infty) = I_{|n|+1}(\infty)$.

The crossing of the IPR curves for the electron and holes characterizes the CNPs. However, in order to properly characterize the TI and BI phases, the combined IPR of
Inverse participation ratio and localization in topological insulator phase transitions

Figure 3. Combined IPR $I_s^{\xi} + I_{-s}^{\xi}$ of electron plus holes at valley $\xi = 1$ as a function of the electric potential $\Delta_z$ for the Landau levels: $n = \pm 1, \pm 2$ and $\pm 3$ and magnetic field $B = 0.01$ T. Black curves for $s = -1$ and red for $s = 1$. The vertical blue dotted grid lines indicate the CNPs and the horizontal blue dotted grid lines indicate the minimum combined IPR values.

the electrons plus holes, $Y_s^n = I_s^n + I_{-s}^n$, offers a better indicator of the corresponding transition (see figure 3). Indeed, on the one hand, $Y_s^n$ displays the global minima at the CNPs (highly delocalized states); on the other hand, the quantity

$$C(\Delta_z) = \text{sgn} \left( \frac{\partial Y_s}{\partial \Delta_z} \frac{\partial Y_{-s}}{\partial \Delta_z} \right),$$

plays the role of a ‘topological charge’ (like a Chern number) so that

$$C(\Delta_z) = \begin{cases} 1, & |\Delta_z| > \Delta_{so} \text{ BI}, \\ -1, & |\Delta_z| < \Delta_{so} \text{ TI}. \end{cases}$$

That is, the sign of the product of the combined IPR slopes for spin up and down clearly characterizes the two (TI and BI) phases.

The product $I_s^n \times I_{-s}^n$ of the electron times hole IPRs also exhibits a critical behavior at the CNPs and characterizes both phases. Actually, the combined entropy ($S = -\ln I$)

$$S_s^n + S_{-s}^n = -\ln(I_s^n \times I_{-s}^n),$$

is minimal at the CNPs (highly delocalized states), as can be seen in figure 4. For the quotient $Q_s^n = I_s^n/I_{-s}^n$ we have that the quantity

$$\text{sgn} \left( \frac{Q_s^n(\Delta_z) - 1}{Q_s^{-s}(\Delta_z) - 1} \right) = \begin{cases} 1, & |\Delta_z| > \Delta_{so} \text{ BI}, \\ -1, & |\Delta_z| < \Delta_{so} \text{ TI}. \end{cases}$$

also characterizes both phases, as can be clearly seen in figure 5.

doi:10.1088/1742-5468/2015/06/P06029
4. Conclusions

We have studied the localization properties of the Hamiltonian eigenvectors \(|n\rangle^\xi_s\) \((n, \xi, s\) denote: Landau level, valley and spin, respectively) for 2D Dirac materials isostructural with graphene (namely, silicene) in the presence of perpendicular magnetic \(B\) and electric \(\Delta_z\) fields. The electric field provides a tunable band gap \(\Delta^\xi_s = (\Delta_z - s\xi\Delta_{so})/2\) which is ‘twisted’ at the charge neutrality points (CNP) \(|\Delta_z| = \Delta_{so}\), for surface states, due to a strong spin–orbit interaction \(\Delta_{so}\). The topological insulator (TI) and band insulator (BI) phases are then characterized by \(|\Delta_z| < \Delta_{so}\) and \(|\Delta_z| > \Delta_{so}\), respectively, or by the sign of \(\Delta^\xi_s\) (the Chern number).

We have proposed information-theoretic measures, based on the inverse participation ratio \(I_n^\xi_s\) (IPR), as alternative signatures of a topological insulator phase transition. The IPR measures the localization of a state in the corresponding basis (position representation in our case). We have seen that IPR curves \(I_n^\xi_s(\Delta_z)\) of electrons \((n > 0)\) and holes \((n < 0)\) cross at the CNPs, the crossing value being a universal quantity basically depending on the Landau level \(n\). The combined IPR \(Y_n^\xi_s = I_n^\xi_s + I_{-n}^\xi_s\) of the electrons plus holes is minimal at the CNPs; i.e. the combined state is highly delocalized (maximum entropy) at the transition point. The different monotonic behavior of the combined \(Y_n^\xi_s\) and quotient \(Q_n^s \equiv I_n^s/I_{-n}^s\) IPR curves across the BI and TI regions provides topological (Chern-like) numbers \((12)\) and \((15)\) which characterize both phases.

\[\text{doi:10.1088/1742-5468/2015/06/P06029}\]
Figure 5. Electron-hole IPR quotients $I^\xi_n/I^\xi_{-n}$ at valley $\xi = 1$ as a function of the electric potential $\Delta_z$ for the Landau levels: $n = \pm 1, \pm 2$ and $\pm 3$ and magnetic field $B = 0.01$ T. The same color code as in figure 3. The electron-hole IPR ratios are increasing functions of $\Delta_z$.

Therefore, as already happens for the traditional Anderson metal–insulator transition, we have shown that fluctuations of Hamiltonian eigenfunctions (characterized by IPRs) also describe topological-band insulator transitions.

Acknowledgments

The work was supported by the Spanish projects: MINECO FIS2014-59386-P, CEIBIOTIC-UGR PV8 and the Junta de Andalucía projects P12-FQM.1861 and FQM-381.

References

[1] Shen S-Q 2012 Topological Insulators: Dirac Equation in Condensed Matters (Berlin: Springer)
[2] Kane C L and Mele E J 2005 Phys. Rev. Lett. 95 226801
[3] Bernevig B A, Hughes T L and Zhang S-C 2006 Science 314 1757–61
[4] Tahir M and Schwingschlägl U 2013 Sci. Rep. 3 1075
[5] Ezawa M 2015 Monolayer topological insulators: silicene, germanene and stanene J. Phys. Soc. Jap. (arXiv: 1503.08914) at press
[6] Romera E and Nagy Á 2011 Phys. Lett. 375 3066
[7] Romera E, Sen K and Nagy Á 2011 J. Stat. Mech. P09016
[8] Romera E, Calixto M and Nagy Á 2012 Europhys. Lett. 97 20011
[9] Calixto M, Nagy Á, Paradela I and Romera E 2012 Phys. Rev. 85 053813

doi:10.1088/1742-5468/2015/06/P06029
Inverse participation ratio and localization in topological insulator phase transitions

[10] Romera E, del Real R and Calixto M 2012 Phys. Rev. 85 053831
[11] Calixto M, del Real R and Romera E 2012 Phys. Rev. 86 032508
[12] Calixto M, Romera E and del Real R 2012 J. Phys. A: Math. Theor. 45 365301
[13] Calixto M and Pérez-Bernal F 2014 Phys. Rev. 89 032126
[14] Romera E, Calixto M and Castaños O 2014 Phys. Scr. 89 095103
[15] Calixto M, Castaños O and Romera E 2014 Europhys. Lett. 108 47001
[16] Calixto M and Romera E 2015 Europhys. Lett. 109 40003
[17] Romera E and Calixto M 2015 J. Phys.: Condens. Matter 27 175003
[18] Anderson P W 1958 Phys. Rev. 109 1492
[19] Wegner F 1980 Z. Phys. 36 209
[20] Brandes T and Kettemann S 2003 Anderson Localization and Its Ramifications: Disorder, Phase Coherence and Electron Correlations (Lecture Notes in Physics vol 630) (Berlin: Springer)
[21] Evers F and Mirlin A D 2008 Rev. Mod. Phys. 80 1355
[22] Aulbach C, Wobst A, Ingold G-L, Hanggi P and Varga I 2004 New J. Phys. 6 70
[23] Tabert C J and Nicol E J 2013 Phys. Rev. Lett. 110 197402
  Tabert C J and Nicol E J 2013 Phys. Rev. 88 085434
[24] Drummond N D, Zólyomi V and Fal’ko V I 2012 Phys. Rev. 85 075423
[25] Liu C C, Feng W and Yao Y 2011 Phys. Rev. Lett. 107 076802
[26] Liu C C, Jiang H and Yao Y 2011 Phys. Rev. 84 195430
[27] Ezawa M 2012 New J. Phys. 14 033003

doi:10.1088/1742-5468/2015/06/P06029