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Rényi entropies and topological quantum numbers in 2D gapped Dirac materials

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ABSTRACT

New topological quantum numbers are introduced by analyzing complexity measures and relative Rényi entropies in silicene in the presence of perpendicular electric and magnetic fields. These topological quantum numbers characterize the topological insulator and band insulator phases in silicene. In addition, we have found that, these information measures reach extremum values at the charge neutrality points. These results are valid for other 2D gapped Dirac materials analogous to silicene with a buckled honeycomb structure and a significant spin-orbit coupling.

1. Introduction

Silicene is a 2D honeycomb-like lattice of silicon analogous to graphene that has attracted increasing attention during last years. It has a low buckled structure (the two sublattices in silicene are somewhat shifted in the direction perpendicular to the silicene sheet) and a significant spin-orbit coupling (due to heavier atoms and the above buckled structure). Silicene has several advantages in comparison with graphene: besides the stronger intrinsic spin-orbit coupling (useful for a better realization of quantum spin Hall effect in some cases), it has a better tunability of the band gap (useful for effective field transistors working at room temperature) and an easier valley polarization (for applications in valleytronic) [1]. There are theoretical and experimental progress in the study of silicene (see, for example, the reviews [1,2]). Theoretically, it has been verified that silicene has a stable 2D honeycomb buckled structure [3–5] with an estimated Fermi velocity $v_F = 10^6$ ms^{-1} and with a buckled height of $l = 0.44$ Å which allows to control the band structure by applying a perpendicular electric field to the silicene layer. In fact the gap decreases and increases linearly, reaching the zero value for a critical value of the electric field (for this critical value spins are perfectly polarized up or down at the two inequivalent corners of the Brillouin zone, K and K', respectively [6]). There are a lot of works to explore possible applications of silicene, among other quantum anomalous Hall effect, valleytronics, spintronics, superconductivity, band engineering field effect transistors or gas sensor [1]. Experimentally, we can stress that it has been obtained epitaxially growing silicene on metallic substrates and it has been observed a silicene field-effect transistors operating at room temperature [2,7]. Many efforts have been devoted to exploring silicene based 2D nanoelectronic (let us take into account the natural compatibility with mature silicon-based semiconductor technology [1]).

The low-energy electrons in silicene behave like massless Dirac fermions and are described by a 2D Dirac Hamiltonian. In this material there is a topological phase transition from a topological insulator (TI) phase to a trivial band insulator (BI) phase at a charge neutrality point (CNP) [8]. 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, etc). Here we would like to stress that Kane and Melle predicted theoretically the existence of 2D topological insulators [9] using a model with a 2D material isoestructural with graphene and with a stronger spin-orbit interaction. Topological insulators were firstly observed experimentally in mercury telluride quantum wells [10] and then in other materials (see [11] and references therein). A topological insulator has an energy gap but with gapless edge or surface states that are topologically protected and immune to disorders and defects, in fact it is considered a singular matter state [12–14]. There are other gapped Dirac materials with exceptional properties as germanene (Ge), tinene (Sn) or Indiene (In) [15] having a structure analogous to that of silicene and described by a 2D Dirac Hamiltonian.

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Table 1
Parameters Δ_{so} (spin-orbit coupling), l [15] and v_F (Fermi velocity) [30,31] for monolayer Si (silicene), Ge (germanene) and Sn (tinene).

	Δ_{so} (meV)	l (Å)	v_F (10^5 m/s)
Si	4.2	0.44	4.2
Ge	11.8	0.68	8.8
Sn	36.0	0.84	9.7

The band topology of an insulator is mainly characterized by the Z_2 topological invariant ($Z_2 = 0$ for a band insulator and 1 for a topological insulator, see [16–18]), by the Chern number (defined in terms of the Berry curvature), the spin-Chern number and, in honeycomb-like materials, by the valley-Chern number [19–22]. Other way to quantify these properties is by analyzing the edge energy spectrum (see [1] and references therein). Recently theoretic information measures and some properties of the time evolution of electron wave packets have been used to characterize topological phase transitions in 2D gapped Dirac materials [23–27]. In particular, it has been shown that the inverse participation ratio (IPR) is an alternative (Chern-like) measure of a topological insulator phase transition [24]. The IPR measures the delocalization of a state $|\psi\rangle$ over a basis $\{|i\rangle\}$ in terms of the probability p_i of finding the state $|\psi\rangle$ over the element $|i\rangle$ as $I = \sum p_i^2$. In this paper we propose the relative Rényi entropy and the relative complexity measure to define topological quantum numbers and characterize the topological phases TI and BI in silicene (and other 2D analogous gapped Dirac Materials) in external magnetic and electric fields. The paper is organized as follows. In the next section we have introduced the model for the description of silicene, in section 3 we introduce the new topological quantum numbers doing a numerical analysis in the silicene model. Finally, our conclusions are presented in the final section.

2. Low energy Hamiltonian

Let us consider the effective Hamiltonian for a monolayer silicene in the vicinity of the Dirac points in externals electric and magnetic fields, $\mathcal{E}_z$ and B which are perpendicular to the silicene sheet [28,29]:

$$H_s^{\xi} = v_F(\xi\sigma_x(p_x - eBy) - \sigma_y p_y) - \frac{1}{2}\xi s\Delta_{so}\sigma_z + \frac{1}{2}\Delta_z\sigma_z, \qquad (1)$$

where $\xi = 1$ or $\xi = -1$ corresponds to the two inequivalent points K and K', respectively, σ_j are the Pauli matrices, $s = \pm 1$ is the spin, v_F is the Fermi velocity of the Dirac fermions, Δ_{so} is the spin-orbit interaction, which provides an effective mass to the Dirac fermions, $\Delta_z = l\mathcal{E}_z$ the gap associated to the constant electric field $\mathcal{E}_z$ (the electric field provides a tunable gap that produce a potential difference between both sub-lattices) and where we have taken into account the standard minimal coupling $\vec{p} \to \vec{p} + e\vec{A}$ with the Landau gauge vector potential $\vec{A} = (-By, 0, 0)$.

This is the effective Hamiltonian for other 2D Dirac materials (for example tinene or germanene) taking into account the different values of the interlattice distance, l, the intrinsic spin-orbit coupling, and the Fermi velocity. In Table 1 are the parameters (theoretically calculated in [15,28,32,33]). We will do the study in silicene and all the results that we have obtained in this paper can be applied to the other 2D Dirac materials. These 2D Dirac materials suffer a topological phase transitions from the known as TI phase, for $|\Delta_z| < \Delta_{so}$, to the called BI phase, for $|\Delta_z| > \Delta_{so}$, when the value of the effective gap $|\Delta_{s\xi}|$ (with $\Delta_{s\xi} \equiv (\Delta_z - s\xi\Delta_{so})/2$, the lowest band gap) goes to zero at the charge neutrality points [6,28,32,33].

The solution of the eigenvalue problem for the Hamiltonian (1) can be obtained analytically by [8,23–27,29]

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

and

$$|n\rangle_{s\xi} = \begin{pmatrix} -iA_n^{s\xi}||n| - \xi_+\rangle \\ B_n^{s\xi}||n| - \xi_-\rangle \end{pmatrix}. \qquad (3)$$

Where, $\xi_\pm = (1 \pm \xi)/2$, $||n|\rangle$ are the orthonormal eigenstate of the harmonic oscillator with $n = 0, \pm 1, \pm 2, \ldots$, $\omega = v_F\sqrt{2eB/\hbar}$ is the cyclotron frequency, and the constants $A_{n,}^{s\xi}$ and $B_n^{s\xi}$ are given by [29]

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

$$B_n^{s\xi} = \begin{cases} \sqrt{\frac{|E_n^{s\xi}| - \mathrm{sgn}(n)\Delta_{s\xi}}{2|E_n^{s\xi}|}}, & n \neq 0, \\ \xi_+, & n = 0. \end{cases} \qquad (4)$$

We will used the position representation of the Fock (number) states $|n\rangle$, which is given by

$$\langle x|n\rangle = \frac{\omega^{1/4}}{\sqrt{2^n n!\sqrt{\pi}}} e^{-\omega x^2/2} H_n\left(\sqrt{\omega}x\right) \qquad (5)$$

here, $H_n(x)$ are the Hermite polynomials of degree n. Let us introduce the position density

$$\rho_n(x) = |\langle x|n\rangle|^2 \qquad (6)$$

(with $\int \rho_n(x)dx = 1$) and the position density for the eigenvectors (3)

$$\rho_n^{s\xi}(x) = (A_n^{s\xi})^2|\langle x||n| - \xi_+\rangle_{s\xi}|^2 + (B_n^{s\xi})^2|\langle x||n| - \xi_-\rangle_{s\xi}|^2. \qquad (7)$$

3. Topological quantum numbers

3.1. Relative Rényi entropy

Let us consider two nonnegative distribution functions $f(\mathbf{r})$ and $g(\mathbf{r})$ normalized to 1. We can define the relative Rényi entropy of order α as [34,35]

$$R_{f,g}^{(\alpha)} = \frac{1}{\alpha - 1}\ln\int \frac{f^\alpha(\mathbf{r})}{g^{\alpha-1}(\mathbf{r})}d\mathbf{r} \qquad (8)$$

provided that the integral exists and $\alpha > 0$. The relative Rényi entropy is an increasing function of the parameter α [36] and in the limit $\alpha = 1$ it gives us the so-called Kullback–Leibler entropy [37]. Both entropies provide a distance between the functions f and g, although they are not true metrics. In fact when $f = g$, $R_{f,g}^{(\alpha)} = 1$ and $R_{f,g}^{(\alpha)} > 1$ in any other case (the more different f and g are, the lager $R_{f,g}^{(\alpha)}$). The Relative Rényi entropy gives a local comparison of the distribution functions.

If we take the function $f = \rho_n^{s\xi}$ and $g = \rho_0^{s\xi} = \rho_0$, we can define a combined relative Rényi entropy in terms of the sum of the relative Rényi entropy for electrons and holes:

$$\hat{R}_{\rho_n^{s\xi},\rho_0}^{(\alpha)} = R_{\rho_n^{s\xi},\rho_0}^{(\alpha)} + R_{\rho_{-n}^{s\xi},\rho_0}^{(\alpha)} \qquad (9)$$

Now we plot the combined relative Rényi entropy (Eq. (9)) for silicene in terms of the external electric potential Δ_z for different values of the parameters. In Fig. 1 we have shown the results for $\alpha = 2.5$, an external perpendicular magnetic field $B = 0.01$ T, the Landau levels $n = 2, 3, 4$ and 5 and for spin up (magenta lines) and down (green lines) Dirac fermions, in the valley $\xi = 1$. The curves

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