Band inversion at critical magnetic fields in a silicene quantum dot

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Abstract – We have found out that the band inversion in a silicene quantum dot (QD), in perpendicular magnetic $B$ and electric $\Delta_z$ fields, drastically depends on the strength of the magnetic field. We study the energy spectrum of the silicene QD where the electric field provides a tunable band gap $\Delta$. Boundary conditions introduce chirality, so that negative and positive angular-momentum $m$ zero Landau level (ZLL) edge states show a quite different behavior regarding the band-inversion mechanism underlying the topological insulator transition. We show that, whereas some ZLLs suffer band inversion at $\Delta = 0$ for any $B > 0$, other ZLLs only suffer band inversion above critical values of the magnetic field at nonzero values of the gap.

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Introduction. – It is believed that silicene opens new opportunities for electrically tunable nanoelectronic devices $^{[1,2]}$. The quantum spin Hall effect $^{[3]}$, chiral superconductivity $^{[4]}$, giant magnetoresistance $^{[5]}$ and other exotic electronic properties have been predicted in silicene. Silicene takes part in an emerging category of materials called “topological insulators”. 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, $\Delta_{so} = 4.2 \text{meV}$ for silicene).

The low-energy electronic properties of a large family of topological insulators and superconductors are well described by the Dirac equation $^{[6]}$, in particular, some 2D gapped Dirac materials isostructural with graphene like silicene, germanene, stannene, etc. Compared to graphene, these materials display a large spin-orbit coupling and show quantum spin Hall effects $^{[7,8]}$. Applying a perpendicular electric field $E_z$ to the material sheet, generates a tunable band gap (Dirac mass) $\Delta = (\Delta_z - s\xi\Delta_{so})/2$, with $s = \pm 1$ the spin, $\xi = \pm 1$ the valley and $\Delta_z = 2\ell E_z$ the electric potential (see fig. 1). There is a topological phase transition $^{[9]}$ 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, $\Delta = 0$, between the perpendicular electric field and the spin-orbit coupling, thus exhibiting a semimetal 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 $^{[8]}$, etc.). In silicene, in the absence of boundary conditions, the zero Landau level (ZLL) energy is given by $E_0 = -\xi\Delta$ and the band inversion at the CNP ($\Delta_z^{(0)} = s\xi\Delta_{so} \Rightarrow \Delta = 0$) entails a topological phase transition. Actually, the transition in silicene is associated with a nonanalytic contribution to the conductivity from the zero Landau level (ZLL) topological edge or surface states, as a result of a band inversion. Indeed, in ref. $^{[9]}$ it has been shown that the Hall conductivity jumps from 0 to $e^2/h$ at the CNP, by tuning the electric field, thus reflecting the transition from a trivial insulator to a Hall insulator at the CNP. We address the reader to ref. $^{[9]}$ for further details on the relation between the topological phase transition in silicene and the change in the character of the ZLL at the CNP.

Finite-size and boundary conditions on the effective field theory describing these materials bring some extra features $^{[10]}$. In this letter we study Berry-Mondragon $^{[11]}$
boundary conditions for a circular silicene QD of radius $R$, which introduces some novelties with regard to the previous discussion and leads to additional interesting physical phenomena. In ref. [12] the authors studied the energy spectrum of a circular graphene QD with radius $R$ subjected to a perpendicular magnetic field $B$. Here we consider a circular silicene QD subjected to perpendicular magnetic and electric fields, the last one providing a tunable band gap and introducing new interesting physics with potential applications in nanotechnology.

Effective Hamiltonian and eigenfunctions. – The low-energy dynamics of silicene in the presence of a perpendicular electric field $E$, is described by the Dirac Hamiltonian in the vicinity of the Dirac points $\xi = \pm 1$

$$H^E = v(\sigma_z p_x + \xi \sigma_y p_y) - \frac{1}{2} \xi s \Delta_0 \sigma_z + \frac{1}{2} \Delta_z \sigma_z,$$

where $\sigma_j$ are the usual Pauli matrices, $s = ±1$ is the spin, $v$ is the Fermi velocity of the corresponding material (namely, $v = 4.2 \times 10^5$ m/s for silicene), $\Delta_0$ is the spin-orbit coupling and $\Delta_z$ is the electric potential. We shall combine spin-orbit coupling and electric potential into the band gap $\Delta = (\Delta_z - s \xi \Delta_0)/2$, so that the explicit dependence of $H^E$ on the spin $s$ is masked and we can simply write $H^E$. We also consider a perpendicular magnetic field $B$, which is implemented through the minimal coupling $\vec{p} \to \vec{p} + eA$ for the momentum, where $\vec{A} = B(-y,x)/2$ is the vector potential in the symmetric gauge. Since $H^E$ commutes with angular momentum, in order to solve the eigenvalue problem $H^E \Psi^E = E \Psi^E$, we choose energy eigen-spinors (we use polar coordinates $(r, \theta)$)

$$\Psi^E_m(r, \theta) = e^{i \xi m \phi} [\psi^E_m(r), e^{i \xi \theta} \chi^E_m(r)]^T,$$

$(t$ stands for transpose) which also are eigenstates of angular momentum with eigenvalue $m$ (an integer). The regular solutions at the origin are

$$\psi^E_m(r) = \frac{e^{-\frac{B r^2}{2}}}{2^{m-\frac{1}{2}} \Gamma(m+\frac{1}{2})} \left\{ \begin{array} {l} L^{m-1}_{-(m+\frac{1}{2})} \left( \frac{B r^2}{\phi} \right), \\ \xi L^{m-1}_{-(m+\frac{1}{2})} \left( \frac{B r^2}{\phi} \right), \end{array} \right. \quad (3),$$

$$\chi^E_m(r) = \frac{e^{-\frac{B r^2}{2}}}{2^{m-\frac{1}{2}} \Gamma(m+\frac{1}{2})} \left\{ \begin{array} {l} L^{m-1}_{-(m+\frac{1}{2})} \left( \frac{B r^2}{\phi} \right), \\ \xi L^{m-1}_{-(m+\frac{1}{2})} \left( \frac{B r^2}{\phi} \right), \end{array} \right. \quad (4)$$

where $\phi = 2\pi \hbar/e$ is the magnetic Dirac flux quantum, $L^m$ are the associated Laguerre polynomials and we are denoting by $a = (E^2 - \Delta^2) \phi/(B \pi^2 \hbar^2)$ and $\xi = (\xi - 1)/2$. The Berry-Mondragon [11] boundary condition $\chi^E_m(R) / \psi^E_m(R) = i \xi$ at radius $r = R$ provides the characteristic equation for the allowed energies $E$ of the QD.

Energy spectrum: analytic and numerical study. – We have numerically solved the Berry-Mondragon boundary condition

$$\beta^E_m(E, \Delta, B, R) = \chi^E_m(R) - i \xi \psi^E_m(R) = 0 \quad (5)$$

and computed the energy spectrum of a silicene QD of radius $R = 70$ nm as a function of the gap $\Delta$ for magnetic field $B = 0.1$ T (fig. 2, top panel) and $B = 0.6$ T (fig. 2, bottom panel). We have restricted ourselves to angular momentum $m = ±3, ±2, ±1, 0$ and valley $\xi = 1$. For the valley $\xi = -1$ the results are equivalent swapping $m \to -m$ and the gap $\Delta \to -\Delta$.

As we have commented, the topological phase transition in silicene is associated with a nonanalytic contribution to the conductivity from the zero Landau level (ZLL). In the absence of boundary conditions, the ZLL corresponds to the energy $E = -\xi \Delta$ [13-17], and the band inversion at zero gap $\Delta = 0$ entails a topological phase transition. The ZLL still remains in the QD (note the straight diagonal line along the second and fourth quadrants of fig. 2 for $\xi = 1$), but boundary conditions introduce chirality, which means that positive and negative angular-momentum $m$ states have a different behavior. For low magnetic fields, below a critical value $B_c = \phi/(2\pi R^2)$ (see later on eq. (6) for a semiclassical explanation), there only exists a band inversion (that is, the ordering of the conduction and valence bands is inverted by the tunable band gap which depends on the spin-orbit coupling and the electric field) for positive angular-momentum $(m \geq 0)$ ZLLs at $\Delta = 0$; all these levels are degenerate with common energy $E = -\Delta$ at valley $\xi = 1$ (see fig. 2). Actually, this can also be analytically checked by realizing that $\beta^E_m(0,0,B,R)$ vanishes only if $m \geq 0$, using properties of associated Laguerre polynomials. On the contrary, negative angular-momentum ZLLs detach more an more from the line $E = -\Delta$ as $\Delta \to -\infty$ (large negative electric field), forming an equally spaced energy band with inter-level spacing of $\epsilon = \hbar v/R$ (they correspond to the energy levels labeled by negative $m$’s in fig. 2).
Band inversion at critical magnetic fields in a silicene quantum dot

In going from $B = 0.1\, \text{T}$ (fig. 2, top panel) to $B = 0.6\, \text{T}$ (fig. 2, bottom panel) we find a band inversion of some negative angular-momentum ZLLs at certain nonzero gaps $\Delta_m$ (corresponding to given negative electric fields). For the case $R = 70\, \text{nm}$, this band inversion starts for the ZLL $m = -1$ at the particular critical magnetic field $B_c = \phi/(2\pi R^2) \approx 1.36\, \text{T}$. Summing up, for a given $R$ and for $B < B_c$, there only exists a band inversion for positive angular-momentum ZLLs at $\Delta = 0$. The situation changes for $B > B_c$, when more and more $m < 0$ ZLLs become conductive, $E_m > 0$, at a given gap $\Delta_m < 0$, for increasing values of the magnetic field. For example, as can be appreciated in fig. 2, bottom panel, for $B = 0.6 > B_c$, the ZLLs $m = -1$ and $m = -2$ have suffered a band inversion at certain values of $\Delta < 0$ (i.e., at certain values of the electric potential $\Delta_e = 2\Delta + s\xi\Delta_m$). These states must contribute to the conductivity for these critical values of the magnetic field.

Let us provide a semiclassical argument that explains the aforementioned band-inversion phenomenon for negative angular-momentum ZLLs and provides an analytical expression of the magnetic field critical values $B^m_c(R)$ at which $m < 0$ ZLLs suffer a band inversion for a given QD radius $R$. Massless Dirac electrons in silicene make a cyclotron motion with frequency $\omega = \sqrt{2}\hbar v/\ell_B$ in an external magnetic field $B$, where $\ell_B = \sqrt{\hbar/(2\pi|B|)}$ is the magnetic length (the “radius” of the cyclotron motion for the ground state). The probability of finding the electron with angular momentum $m$, at a given radius $r$ in the lowest Landau level, has a sharp peak at $r_m = \sqrt{2|m| + 1}\ell_B$. It is clear that the corresponding circular trajectory does not fit the QD when $r_m > R$ (the QD size). This threshold provides a critical magnetic field depending on $R$ and $m$ given by

$$B^m_c(R) = -\xi(2m + 1)\phi_{B}/2\pi R^2,$$

where we have also introduced the valley index $\xi = \pm 1$ for completeness. Note that, as we have mentioned before, chiral symmetry is broken, which means that, for positive magnetic fields $B > 0$, only negative (respectively, positive) angular-momentum $m < 0$ ZLLs suffer band inversion at valley $\xi = 1$ (respectively, $\xi = -1$) at certain negative (respectively, positive) values $\Delta_m$ of the gap. For negative magnetic fields we have the complementary situation, according to the general formula (6). We have numerically checked the semiclassical formula (6) for different negative angular momenta $m$ and QD radii $R$ at valley $\xi = 1$. The band inversion for $m < 0$ ZLLs occurs for $B > B^m_c(R)$ at certain negative gaps $\Delta_m(B)$ (see figs. 2 (bottom panel) and 4). At the critical point $B = B^m_c(R)$, we have that the energy $E_m$ of the $m < 0$ ZLL vanishes only for large (negative) electric fields, that is, $\Delta_m \to -\infty$. Therefore, in order to check the prediction (6), we have numerically solved the boundary condition (5) for large (negative) electric potentials and several values of $m$ and $R$. The numerical results (points) in fig. 3 confirm the semiclassical prediction (lines) in eq. (6) with high accuracy for several $m$ and $R$.

For a given QD size (for example, $R = 70\, \text{nm}$) we have found out that, when the value of the magnetic field increases, there are more and more band inversions of $m < 0$ ZLLs at certain gaps $\Delta_m < 0$ (see fig. 4), corresponding to increasing values of $|m|$ with $m < 0$. Moreover, for a given

**Fig. 2:** (Colour on-line) Low-energy spectrum (for angular momenta $m = -3, \ldots, 3$ and valley $\xi = 1$) of a silicene quantum dot of radius $R = 70\, \text{nm}$ in the presence of a perpendicular magnetic field of $B = 0.1\, \text{T}$ (top panel) and $B = 0.6\, \text{T}$ (bottom panel), below and above the critical value $B_c = 0.136\, \text{T}$, respectively. Energy is given as a function of the gap $\Delta$, which is tuned by applying a perpendicular electric field. Energy and gap are measured in $\Delta_m$ units.

**Fig. 3:** (Colour on-line) Critical values of the magnetic field $B_c$ (in tesla), as a function of the silicene QD radius $R$ (in nanometers), at which angular-momenta ($m = -1, -2, -3$ and $-4$) ZLLs suffer band inversion. Points correspond to the numerical results for $R = 30, 50, 70, 90, 110$ and $130\, \text{nm}$. The lines correspond to the semiclassical prediction in eq. (6).
m < 0, $\Delta_m$ goes to zero as $B$ increases. This calculation has been done by numerically solving the boundary condition (5) for $E = 0$ and valley $\xi = 1$. We have illustrated this result in Fig. 4 for angular-momentum ZLLs $m = -1, −2, −3, −4$ and for a silicene QD of radius $R = 70\text{ nm}$.

**Conclusions.** – We have studied the energy spectrum of a silicene QD of radius $R$ in the presence of perpendicular magnetic $B$ and electric $\Delta_z$ fields, the last one providing a tunable band gap $\Delta$. We have established the existence of critical magnetic fields, given by the semiclassical formula $B^c_m(R) = −\xi(2m+1)\phi/(2\pi R^2)$, above which angular momentum $m$ ZLLs of a silicene QD of radius $R$ suffer band inversion and contribute to the conductivity. Boundary conditions introduce chirality, thus distinguishing positive and negative angular-momentum edge states. When sign$(m) = \text{sign}(\xi)$, all angular-momentum ZLLs are degenerate, with energy $E = −\xi\Delta$, and all of them suffer a band inversion at gap $\Delta = 0$ for any value of the magnetic field. When sign$(m) = −\text{sign}(\xi)$ (matching the formula for $B^c_m(R)$), the degeneracy is broken and a band inversion occurs at nonzero gap $\Delta_m(B)$ for $|B| > |B^c_m(R)|$. As $B$ increases, more and more angular-momenta $m$ ZLLs suffer band inversion at gaps $\Delta_m(B)$, which go to zero as $B$ increases.

We have performed our calculations in the continuous model, which is a long-wave approximation of the more fundamental tight-binding model. Therefore, we have disregarded the effect of lattice termination on the energy spectrum [18]. Nevertheless, we hope that the effect of the boundary irregularities on the spectrum is negligible when the radius $R$ is much larger than the lattice constant, and our results on band inversion at critical magnetic fields remain valid at least in this regime. Of course, a more detailed calculation inside the tight-binding framework with more realistic edge termination, like the one done in ref. [18] for silicene in magnetic field, is necessary to account for the robustness of the band inversion phenomenon. We think that this question deserves a separate study and will be considered elsewhere.

Anyhow, we believe that these critical phenomena in a silicene QD can lead to interesting nanotechnological applications.

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