Zero-field and time-reserval-symmetry-broken topological phase transitions in graphene

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We propose a quantum electronic device based on strained graphene nanoribbon. Mechanical strain, internal exchange field and spin-orbit couplings (SOCs) have been exploited as principle parameters to tune physical properties of the device. We predict a remarkable zero-field topological quantum phase transition between the time-reversal-symmetry broken quantum spin hall (QSH) and quantum anomalous hall (QAH) states, which was previously thought to take place only in the presence of finite magnetic field. We illustrate as intrinsic SOC is tuned, how two different helicity edge states located in the opposite edges of the nanoribbon exchange their locations. Our results indicates that pseudomagnetic field induced by the strain could be coupled to the spin degrees of freedom through the SOC responsible for the stability of QSH state. The controllability of this zero-field phase transition with strength and direction of the strain is also demonstrated. Our prediction offers a tempting prospect of strain, electric and magnetic manipulation of the QSH effect.

Graphene has been widely studied since its realization in 2004 [1]. New classes of matters, such as quantum spin Hall (QSH) and quantum anomalous Hall (QAH) states have been theoretically predicted. Both the QSH and QAH states possess topologically protected edge states at the boundary, where the electron backscattering is forbidden, offering a potential application to electronic devices to transport current without dissipation. However, the QSH and QAH states are essentially two very different states of matter. The QSH is characterized by a full insulating gap in the bulk and helical gapless edge states where opposite spin counter-propagate at each boundary of the graphene ribbon, protected by time-reversal symmetry (TRS) [2]. Whereas in the case of QAH, the helical gapless edge states are replaced by chiral gapless edge states where one of the spin channels is suppressed, because of broken TRS [3]. Usually, an external magnetic field is needed to realize a quantum phase transition between these two exotic states of matter [4]. Here we propose a remarkable way in which spin-orbit coupling (SOC) strength, uniaxial mechanical strain and an internal exchange field (EX), instead of external magnetic field, are utilized to realize this quantum phase transition [5].

In order to reveal the underlying physics of a controllable QSH to QAH phase transition, we study graphene nanoribbons with intrinsic- and Rashba- SOCs, exchange field and subjected to an uniaxial strain. The system is schematically illustrated in the Fig. 1 and well described by the following tight-binding Hamiltonian,

\[ H = - \sum_{(i,j),\sigma\sigma'} t_{i,j} c_{i\sigma}^\dagger c_{j\sigma'} + i\lambda_R \sum_{(i,j),\sigma\sigma'} c_{i\sigma}^\dagger (\vec{\gamma}_{\sigma\sigma'} \times \vec{d}_{ij}) c_{j\sigma'} + \frac{2i}{\sqrt{3}} \lambda_{so} \sum_{\langle(i,j)\rangle,\sigma\sigma'} c_{i\sigma}^\dagger (\vec{d}_{kj} \times \vec{d}_{ik}) c_{j\sigma'} + M \sum_{(i,j)} c_{i\sigma}^\dagger \eta_{\sigma\sigma'} c_{i\sigma'}, \]

where \( t = 2.7 \text{ eV} \) is the unstrained hopping parameter, \( c_{i\sigma}^\dagger \) (\( c_{i\sigma} \)) is the creation (annihilation) operator, \( \sigma \) is a spin index and \( \vec{\gamma} \) is a vector whose components are the Pauli matrices. The first term is the nearest neighbor hopping term on the honeycomb lattice, the second one is the Rashba SOC with strength \( \lambda_R \), the third, the intrinsic
SOC with coupling $\lambda_{so}$, and the last term is the exchange field with parameter $M$.

The uniaxial strain may be induced either by an external stress applied to the nanoribbon in a particular direction or by a substrate due to deposition of graphene on top of other materials. We define the direction as $\theta = 0$ when it is parallel to the zigzag chain and $\theta = \pi/2$, when it is in the armchair direction, as shown in Fig. 1. The strain modified distances between carbon atoms, is described by $d'_l = (I + \epsilon)d_l$, with $(d_1, d_2, d_3)$ the unstrained vectors for nearest-neighbors, $I$ is the identity matrix and $\epsilon$ is the strain tensor [6], with strain modulus $\epsilon$. In this model, the hopping term is affected by the strain through $t'_l = te^{-3.37(d_l/a-1)}$.

Uniaxial mechanical strain does not break the sublattice symmetry, but rather causes a shift of the Dirac cones at $K$ ($K'$)-points of graphene in the opposite directions due to strain-induced, pseudomagnetic field $B_S$ [2]. Since $B_S$ has opposite signs for graphene’s two valleys $K$ and $K'$, it does not violate the TRS [7]. Very recently, new classes of materials, topological insulators (TI) [8–10] and topological crystalline insulators (TCIs) [11–17] were theoretically discovered and experimentally demonstrated. Novel exotic states of 2D TIs, such as the QSH which is characterized by a full insulating gap in the bulk and pseudo-helical gapless edges protected either by TRS [7–9] or by a symmetry of planar spin rotations [11], have been reported. The former is induced by intrinsic SOC and is protected by both inversion and TRS in graphene. By breaking these symmetries, a topological quantum phase transition takes place. For instance, staggered potential that breaks sublattice symmetry, produces a topological phase transition in graphene from a QSH state to a band insulator; subjecting graphene to a strong magnetic field which breaks TRS, replaces the helical gapless edge states with chiral gapless edge states and consequently, the QSH state vanishes, with a quantum Hall (QH) state emerging [15]. Unlike the QH state, which arises from Landau-level quantization in a strong magnetic field, the interplay of an internal EX and SOC interactions suppresses one of the spin channels in the QSH system, naturally leading to a QAH state, where the TRS is broken by the EX [18] [19]. On the other hand, the strain-induced $B_S$ leads to Landau quantization and edges states that circulate in opposite directions. Thus without breaking TRS, the strain can induce the gap in the bulk and helical gapless edges, i.e., QSH state [7–9]. Therefore, strain, exchange field and SOC can be used as versatile tools to trigger topological quantum phase transitions [19].

Intrinsic SOC respects all the symmetries of graphene. If the mirror symmetry about the graphene-plane is preserved then it is the only allowed spin dependent term in the Hamiltonian, which opens gap around Dirac points. Otherwise, if the mirror symmetry is broken (either by a perpendicular electric field or by interaction with a substrate) then a Rashba term is allowed, which mixes spin-up and spin-down states around the band crossing points. Thus the spin is no longer a good quantum number, and then the resulting angular momentum eigenstates are indexed by the spin chirality $\nu = \pm 1$ which is defined as the expectation value of $z$-component of electron spin. Besides, Rashba SOC pushes the valence band up and the conduction band down, reducing the bulk gap. Fig. 2 shows the effects of intrinsic- and Rashba- SOC terms (a), intrinsic SOC and exchange field (b), Rashba SOC and exchange field (c), and intrinsic- and Rashba- SOCs and exchange field (d). The Fermi level is assumed to be above zero, as indicated by the dashed horizontal line, and thus has four intersections with the conduction bands. This gives rise to four edge currents on the ribbon edges. The following parameters are used in the calculations: (a) $\lambda_{so} = 0.06t, \lambda_R = 0.20t$; (b) $\lambda_{so} = 0.06t, M = 0.20t$; (c) $\lambda_R = 0.20t, M = 0.20t$; (d) $\lambda_{so} = 0.06t, \lambda_R = 0.20t$ and $M = 0.20t$ for the ZGNR with width $W = 48$. The arrows represent the major components of spin.
The nanoribbon with a strong intrinsic SOC is composed of two integer quantum Hall subsystems, namely, ($\nu = +1 \oplus (\nu = -1)$), and has $\nu = (+1) + (-1) = 0$. Therefore, the nanoribbon is in the TRS broken QSH phase. In the case of weak intrinsic SOC, however, both edge states A and B, consequently $I_A$ and $I_B$, are located at the same edge, as indicated in Fig. 3(c). Since the two edge current pairs have the same chirality, the Chern number of the system with a weak intrinsic SOC is $+2$ or $-2$. Therefore, the system is equivalent to two integer quantum Hall subsystems, namely, ($\nu = +1 \oplus (\nu = +1)$, and has $\nu = (+1) + (+1) = 2$ or $(\nu = -1) \oplus (\nu = -1)$, and has $\nu = (-1) + (-1) = -2$, i.e., the system is in the QAH phase.

To profoundly understand the quantum phase transition and demonstrate intuitively how it takes place, we introduce the expectation value of position $x$ as a parameter for specifying the angular momentum of the current in the system, and define $\langle x \rangle = \sum_n x_i |\psi_n(x_i)|^2$, where $n$ represents the edge states in Fermi level and $i$ is the site index along the width of ribbon. We chose the origin of $x$-axis at the left boundary of the ribbon. Fig. 3 shows the expectation values $\langle x \rangle$ of edge states as a function of $\lambda_{so}$ in the ribbon with the width $W = 48$, $\lambda_R = 0.20t$, $M = 0.20t$, $\varepsilon = 0.10$ and $\theta = 0$. The Fermi level is at $E_F = 0.05t$. The corresponding edge state probability distributions across the width of the ribbon for the four edge states are shown in the middle panel. While the right panel illustrates schematic diagrams of charge current distributions on the edges of ZGNR.

The direction of an edge current, denoted by an arrow, is given by $I = -|\psi_x| v_x$ where the electron group velocity $v_x$ is determined by $v_x = \partial E(k)/\partial k_x$. Notice that the A and B states have the same velocity direction, which is opposite to that of the C and D states. At ribbon boundaries, the pair A and D would form a single handed loop (the turning point is at infinity in the x-direction), meanwhile the pair B and C would constitute the other loop of the opposite handedness, as shown in the right panel of Fig. 3. For a strong intrinsic SOC, the two edge states A and C are on the same edge, and so are the B and D states, as shown in Fig. 3(f). The handedness of the current loop due to the A and D edge states would produce a Chern number of $-1$ while that of the pair B and C would give a Chern number of $+1$. Then the nanoribbon with a strong intrinsic SOC is composed of two integer quantum Hall subsystems, namely, ($\nu = +1 \oplus (\nu = -1)$, and has $\nu = (+1) + (-1) = 0$. Therefore, the nanoribbon is in the TRS broken QSH phase. In the case of weak intrinsic SOC, however, both edge states A and B, consequently $I_A$ and $I_B$, are located at the same edge, as indicated in Fig. 3(c). Since the two edge current pairs have the same chirality, the Chern number of the system with a weak intrinsic SOC is $+2$ or $-2$. Therefore, the system is equivalent to two integer quantum Hall subsystems, namely, ($\nu = +1 \oplus (\nu = +1)$, and has $\nu = (+1) + (+1) = 2$ or $(\nu = -1) \oplus (\nu = -1)$, and has $\nu = (-1) + (-1) = -2$, i.e., the system is in the QAH phase.

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![Fig. 3. (Color online) Energy spectrum of ZGNR with $W = 48$, $\lambda_R = 0.20t$, $M = 0.20t$, $\varepsilon = 0.10$ and $\theta = 0$, for (a) $\lambda_{so} = 0.035t$ and (d) $\lambda_{so} = 0.055t$, respectively. The Fermi level $E = 0.05t$ corresponds to four different edge states, as indicated by A, B, C, and D. The corresponding probability distributions $|\psi|^2$ across the width of the ribbon, and schematic diagrams of charge current distributions are shown in the middle and right panels, respectively. The direction of arrow indicates current flux.](image-url)
FIG. 4. Mean positions of edge states versus $\lambda_{so}$ in ZGNR with $W=48$, $\lambda_R = 0.20t$, $M = 0.20t$, subjected to a strain with $\varepsilon = 0.10$ and $\theta = 0$. Vertical axis is the Fermi velocity $V_F$ modulus. The arrows point in the directions of band velocities and their lengths present the magnitudes of $V_F$.

FIG. 5. Phase diagrams (strain vs intrinsic SOC) of a ribbon with $W=48$, $\lambda_R = 0.20t$, $M = 0.20t$, subjected to a strain with $\varepsilon = 0.10$ and $\theta = 0$. Vertical axis is the Fermi velocity $V_F$ modulus. The arrows point in the directions of band velocities and their lengths present the magnitudes of $V_F$.

The underlying physics of the strain tuned phase diagram is as follows. It is well established that mechanical strain does not break the sublattice symmetry, but rather deforms the Brillouin zone, such as, the Dirac cones located in graphene at points $K (K')$ being shifted in the opposite directions. This is reminiscent of the effect of pseudomagnetic field $B_S$ induced by the strain on charge carriers, i.e., accumulating charge in place where the $B_S$ is maximum. Because the $B_S$ does not break TRS, the strain will have not any direct effect on the spin degrees of freedom of the electrons, even though it couples with sublattice pseudospin. Therefore, at first glance, it seems that the strain only induces a renormalization of the energy scales. Actually, this is not true for graphenes with SOC. Since SOC couples the spin and the momentum degrees of freedom of the carriers, the $B_S$ could affect real spin of an electron through the SOC. Therefore, a strong pseudomagnetic field should lead to Landau quantization and a QSH state due to opposite signs of $B_S$ for electrons in valleys $K (K')$. In this context, the strain enhances the carrier localization and pushes the edge states much closer to the boundaries of the ribbon. Hence, the QSH state could be stabilized by the strain.

In summary, a zero-field topological phase transition between QSH and QAH states in graphene nanoribbons is reported in the presence of internal exchange field, uniaxial strain, intrinsic and Rashba SOCs. Both strength and direction of the strain can be exploited to tune the $\lambda_{so}$ at which the phase transition takes place. The pseudomagnetic field induced by the strain couples the spin degrees of freedom through SOC, enhances the carrier localization in edge states, stabilizes and even leads to formation of a QSH state. Rashba-SOC and exchange field, on the other hand, break inversion- and time-reversal-symmetry of the graphene, respectively. In the regime of small SOC and EX, they only induce an instability of the QSH state. The large Rashba-SOC SOC or EX, however, can even lead the QSH state to be destroyed, producing the QAH states. Our results offer a tempting prospect of strain, electric and magnetic manipulation of the QSH effect.

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