Spontaneous persistent currents in a quantum spin Hall insulator

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We present a mechanism for persistent charge current. Quantum spin Hall insulators hold dissipationless spin currents in their edges so that, for a given spin orientation, a net charge current flows which is exactly compensated by the counterflow of the opposite spin. Here we show that ferromagnetic order in the edge upgrades the spin currents into persistent charge currents without applied fields. For that matter, we study the Hubbard model including Haldane-Kane-Mele spin-orbit coupling in a zigzag ribbon and consider the case of graphene. We find three electronic phases with magnetic edges that carry currents reaching 0.4 nA, comparable to persistent currents in metallic rings, for the small spin-orbit coupling in graphene. One of the phases is a valley half metal.

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Ordered electronic phases can emerge in condensed matter with properties fundamentally different from those of the constituent atoms. Two main different scenarios are known that result in the emergence of nontrivial electronic order. On one side, spontaneous symmetry breaking driven by many-body interactions which accounts for the existence of the crystalline order in solids and the variety of ordered electronic phases they can present, such as superconductivity and ferromagnetism.¹ On the other side, topological order, which accounts for the robust quantized properties of the electron gas in the quantum Hall regimes, and, more recently, on the properties of the so-called topological insulators.^{2–5} Whereas integer quantum Hall state is driven by an external magnetic field, topological insulators are driven by spin-orbit (SO) interaction. They are different from conventional insulators because of their conducting surface (or edge) spin states which can be either chiral or spin filtered and are robust with respect to time-reversal symmetric perturbations.^{2–6}

The experimental finding of topological insulators^{7,8} motivates the general questions of whether and how electronic interactions could produce electronic phase transitions in their surface (or edge) states and what would be the consequences of such symmetry breaking. Here we address these questions by including the effect of the interactions into the Haldane-Kane-Mele model for quantum spin Hall insulators^{3,4,9} defined in a honeycomb lattice stripe. Some approximate physical realizations of this model are cold fermionic atoms trapped in suitably engineered optical lattices,¹⁰ a modulated two-dimensional electron gas,¹¹ the transition-metal oxide Na₂IrO₃,¹² and the most studied so far, graphene. The enormous interest in graphene ribbon with zigzag edges^{3,4,13–24} arises in the context of in the context of spintronics,^{3,4} magnetoelectronics,^{14,16,19,20,22,24} and valleytronics.¹⁸ When described with a one-orbital tight-binding model, graphene zigzag ribbons are conducting because of two degenerate almost flat bands associated to states localized at the edges.¹³ Importantly, the zigzag states preserve the valley character^{15,18} of two-dimensional graphene. When considered separately, the effect of electronic repulsion and spin-orbit interactions over the system is dramatic and has been widely studied. On one side, it was soon recognized that electron Coulomb repulsion, in the Hubbard

model, results in ferromagnetic order at the edges of the ribbon.¹⁴ In the ground state the edges are counterpolarized and according to both density-functional calculations¹⁶ and to mean-field Hubbard model,²² a gap opens so that the ribbon is insulating.

When Coulomb repulsion is neglected, SO interaction opens a gap in the spectrum of bulk graphene^{25,26} which is accompanied by the emergence of spin-filtered edge states at the Fermi energy.^{3,4} These two features, a spin-orbit driven gap and the emergence of topologically robust edge states, are the hallmark of the quantum spin Hall insulator phase.^{2–4} Thus, the Coulomb driven and the SO driven phase have very different magnetic and conducting properties. Here we address the electronic properties of the ribbon when both Coulomb repulsion and spin-orbit coupling are considered within a mean-field Hubbard model^{14,19,22} with Kane-Mele spin-orbit coupling.^{3,4,9} We report two main findings. First, in the presence of SO coupling the states with counterpolarized ferromagnetic edges break valley symmetry and, above a critical SO strength, the gap closes in one valley only, resulting in a valley half metal (HM). Second, in the presence of SO coupling ferromagnetic edges give rise to charge currents in the edges without an applied magnetic field. We consider the one-orbital Hubbard model in a honeycomb zigzag ribbon, at half filling, with the addition of the Kane-Mele SO coupling,³

$$\mathcal{H} = \sum_{i,j,\sigma} t_{ij}(\sigma) c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (1)$$

The hopping matrix $t_{ij}(\sigma)$ in the first term accounts both for the standard first-neighbor spin-independent hopping (t) and the Kane-Mele-Haldane second-neighbor spin-orbit coupling.^{3,4,9} The amplitude of the latter is given by the expression $it_{KM}\sigma_z \cdot (\vec{d}_1 \times \vec{d}_2)$, where $\vec{d}_{1,2}$ are unit vectors along the direction of the bond that connect sites i and j with their common first neighbor [see Fig. 1(a)], $\hat{z}$ is the unit vector normal to the ribbon plane, and $\sigma = \pm 1$ indexes the spin projection along $\hat{z}$. For a flat ribbon, the SO term commutes with σ_z . The second term in Eq. (1) describes Coulomb repulsion between electrons in the Hubbard approximation. We

FIG. 1. (Color online) (Color online) (a) Honeycomb zigzag ribbon with $N_y=6$. The second-neighbor hopping vectors $\vec{d}_i$ are shown. (b) Low-energy bands for the spin Hall phase in $N_y=12$ ribbon ($U=0$, $t_{KM}=0.01$ eV). (c) Low-energy bands for the same ribbon with counterpolarized ferromagnetic edges ($U=3$ eV and $t_{KM}=0$). (d) Contour map of the valence-band wave function $|\Psi_{k\sigma\nu}(y)|^2$ for spin up (left panel) and spin down (right panel). (e) Same as (d) for the magnetic ribbon.

treat it in a mean-field approximation so that we end up with an effective single-particle Hamiltonian where the electrons interact with a spin-dependent potential that is calculated self-consistently, $U\sum_i(n_{i,\uparrow}\langle n_{i,\downarrow} \rangle + n_{i,\downarrow}\langle n_{i,\uparrow} \rangle)$, so that σ_z is a good quantum number. Zigzag ribbons are defined by N_y , the number of zigzag chains which yield a total of $2N_y$ atoms per unit cell in a one-dimensional crystal [Fig. 1(a)]. Importantly, the top and bottom edges belong to the two different triangular sublattices that define the honeycomb lattice. For a given wave number k and spin σ the mean-field Hamiltonian has $2N_y$ states $\Psi_{k\sigma\nu}(y)$ with energy $\epsilon_{\sigma\nu}(k)$.

We consider first the model in the two limit cases, $U=0$, $t_{KM}>0$ and $t_{KM}=0$, $U>0$ for a ribbon with $N_y=12$. The highest occupied and lowest empty energy bands of the $U=0$, $t_{KM}>0$ case are shown in Fig. 1(b). The special spin-filtered edge states are the linear bands crossing the Fermi energy (E_F). The wave function squared, $|\Psi_{k,\sigma,\nu}(y)|^2$, of the valence-band states are represented in Fig. 1(d) for $\sigma=\uparrow$ and $\sigma=\downarrow$, respectively. It is apparent that $\sigma=\uparrow$ ($\sigma=\downarrow$) electrons can only be in the top (bottom) edge for positive (negative)

FIG. 2. (Color online) Valence and conduction band of a $N_y=12$ ribbon with $U=t=3$ eV for two cases: (a) AF insulator with $t_{KM}=0.01t$, (b) AF valley half metal $t_{KM}=0.03t$. Insets: calculated magnetic density along the ribbon cell. (c) Evolution of the gaps $\Delta_0(K)$ and $\Delta_0(K')$ as a function of the SO coupling. (d) Depletion of the edge magnetic moment as the SO coupling t_{KM} is increased for two different values of U/t .

velocity states. Spin $\uparrow$ and $\downarrow$ electrons can also be in the bottom edge but with velocity opposite to that of the top edge. Thus, the ribbon is conducting, the edges are not spin-polarized but the states at the Fermi energy carry a net spin current. The electronic structure of the same ribbon, but now taking $t_{KM}=0$, $U>0$, is radically different. Instead of the linear spin-filtered bands there is a gap, Δ_0 so that the system is insulating. The wave functions of the valence band are shown in Fig. 1(e). They do not show correlation between spin and velocity but they are edge-sensitive: top (bottom) edge is ferromagnetic with spin-up (down) majority. The solution with reversed spins is equally valid.

In the light of Fig. 1, the question of how these competing electronic phases merge when both the Coulomb repulsion and the SO coupling are present calls for an answer. In Fig. 2 we show the energy bands for two cases, both with $N_y=12$, $U=t=3$ eV, suitable for graphene (see supplementary material²⁷) and counterpolarized ferromagnetic edges. In Fig. 2(a) or Fig. 2(b) we take $t_{KM}=0.01t$ ($t_{KM}=0.03t$). As shown in the inset, the magnetic moments are localized in the edges. In the small t_{KM} case, the system is an insulator, but the interedge gaps Δ_0 are now valley dependent. In the large t_{KM} case, the gap in one of the valleys closes completely, yet the edges are magnetic. This phase is radically different from the SO free case: a valley half metal with magnetic edges anti-ferromagnetically (AF) oriented.

The evolution of the valley symmetry breaking, reflected by the different size of $\Delta_0(K)$ and $\Delta_0(K')$, is shown in Fig. 2(c). The valley symmetry breaking can be understood using perturbative arguments. Close to the Dirac point the Kane-Mele-Hamiltonian can be approximated³ by $V_{KM} = 3\sqrt{3}t_{KM}\sigma_z\tau_z\lambda_z$, where σ_z , τ_z , and λ_z are the spin, valley, and sublattice index, respectively. Let us consider first the ($t_{KM}=0$, $U>0$) antiferromagnetic phase [Figs. 1(c) and 1(e)] as starting point. The valence band is made of states with $\sigma_z = \uparrow$ and sublattice $\lambda_z = +$ (bottom edge) and states with $\sigma_z = \downarrow$ and sublattice $\lambda_z = -$ (top edge).

FIG. 3. (Color online) Phase diagrams for the AF insulating, AF valley HM, and nonmagnetic (NM) phases for the ribbon with $N_y=12$ (left) and $N_y=24$ (right).

$=\downarrow$ and sublattice $\lambda_z=-$ (upper edge) so that in both cases the product $\sigma_z\lambda_z$ has the same sign. Now it is apparent that the expectation value of $\sigma_z\tau_z\lambda_z$ has opposite signs in opposite valleys so that in one case the gap opens and in the other closes, as shown in Fig. 2(a).

In Fig. 2(d) we show how the magnetic moment in the edge atoms, $m = \frac{\langle n_\uparrow \rangle - \langle n_\downarrow \rangle}{2}$ is depleted as the strength of the spin-orbit coupling is increased, reflecting the competition between the two terms in the Hamiltonian. Above a certain value of t_{KM} , the magnetic moment vanishes altogether and a spin Hall insulator phase with conducting edge states identical to that with $U=0$ is obtained. The calculated phase diagram in the (t_{KM}, U) plane showing the three different phases with zero total spin is shown in Fig. 3(a) or Fig. 3(b), for the case of $N_y=12$ ($N_y=24$). The phase diagram does not depend dramatically on the ribbon width. For freestanding intrinsic graphene $t_{KM} < 10^{-4}t$ so that the ribbon would be in the insulating phase with magnetic edges.

In the noninteracting Kane-Mele model a nonequilibrium current I induces spin accumulation m in the edges.³ This can be quantified as follows. We assume that a population of nonequilibrium extra electrons occupies the positive velocity states so that the Fermi energy is increased by $\delta E_F = eV$. Using Landauer formula we have $I = 2\frac{e}{h}\delta E_F$, half of which goes on the top edge. From the noninteracting conduction-band dispersion $\epsilon_k = \hbar v_F k$, we obtain δk_F and the corresponding change in density due to δE_F , $\delta n = \frac{\delta q}{a} = \frac{1}{\pi}\delta k_F$. Since δE_F is small, this extra density goes as spin $\uparrow$ to one edge and spin $\downarrow$ to the other. Thus, half of the extra charge goes to each edge fully spin polarized so that the edge magnetic moment reads $\delta m = \frac{1}{4}\delta q = \frac{1}{4\pi}\delta k_F a$. We can write the current in a given edge as

$$I_{edge} = 4\pi \frac{ev_F}{a} m. \quad (2)$$

We now show that this picture survives in the interacting case in equilibrium. We find that in the ground state of the magnetically ordered topological insulator phases shown in Fig. 2, charge currents flow on the edges, the total current across a unit cell being null, in agreement with general theorems.²⁸ The current operator is given by the sum of link currents associated with all the sites b connected to a by single-particle hopping,

FIG. 4. (Color online) Current and magnetization maps for the $N_y=12$ ribbon with two solutions: (a) the counterpolarized insulating and (b) the copolarized and conducting, both with $t_{KM}=0.03t$ and $U=t$. The current between two atoms $\vec{r}_a$ and $\vec{r}_b$ is plotted as a vector along the line $\vec{r}_b - \vec{r}_a$, starting in the midpoint. (c) Edge charge current, in units of $\frac{e}{h}t_{KM}$, as a function of the magnetic moment of the edge, for three values of $t_{KM}=10^{-2}$, 10^{-1} , and 1 meV, for the AF phases.

$$\hat{I}_a = \frac{ei}{\hbar} \left[\sum_{b\sigma} t_{a,b}(\sigma) c_{a,\sigma}^\dagger c_{b,\sigma} - t_{b,a}(\sigma) c_{b,\sigma}^\dagger c_{a,\sigma} \right]. \quad (3)$$

For a given eigenstate $\Psi_{k\sigma\nu}$ of the mean-field Hamiltonian the current across the link ab reads

$$I_{ab}[\Psi] = 2\frac{e}{\hbar N} \text{Im}[\Psi_{k\sigma\nu}^*(b) \Psi_{k,\sigma,\nu}(a) t_{ab}(\sigma) e^{i\phi_{ab}}], \quad (4)$$

where $\phi_{ab}=0$ for a and b in the same cell, $\phi_{ab} = \pm ka$ if a and b are in adjacent cells, and N is the number of cells in the crystal. The expectation value of this operator in the many-body ground state is obtained summing over all occupied bands: $\langle I_{ab} \rangle = \sum_{k,\nu,\sigma} f[\epsilon_{\nu\sigma}(k)] I_{ab}$. The average current is defined in the links of any pair of atoms connected by hopping in the one-body Hamiltonian. In Fig. 4 we plot the ground-state current map for the $N_y=12$ ribbon for the AF insulating phase [Fig. 2(a)] and the ferromagnetic conducting phase (supplementary material²⁷). The AF valley half metal (not shown) is very similar to the AF insulator. The two electronic phases described in Fig. 2 as well as the ferromagnetic phase, present edge current of similar magnitude. Whereas in the FM case, currents flow in opposite directions in opposite edges, in the AF phases current runs parallel at the two edges. These results can be rationalized as if the magnetization plays the role of an external magnetic field. Thus, in the ferromagnetic case current flow is the same as in a quantum Hall bar. In the antiferromagnetic phases, though, current flows parallel at the two edges, as if a magnetic field was

pointing along opposite directions at the two edges.

The magnitude of the top-edge current, normalized by $\frac{e}{h}t_{KM}$, as a function of the top-edge magnetization m collapses for several values of t_{KM} [Fig. 4(c)]. For small m the curve is linear, $I_{edge} \approx -4\frac{e}{h}t_{KM}m$, in qualitative agreement with the analytical result of Eq. (2), since $v_F = \gamma t_{KMA}/\hbar$ with $\gamma \approx 6.5$. At larger m the edge current saturates to $|I_{edge}| \approx 0.4\frac{e}{h}t_{KM}$. If we take $t_{KM} = 10 \mu\text{eV}$, close to the small values obtained by *ab initio* calculations for freestanding graphene,²⁹ we obtain an edge current of $\approx 0.4 \text{ nA}$, well within reach of state-of-the-art persistent current detection.³⁰

In conclusion, we propose a mechanism for persistent charge currents. It occurs when Coulomb interaction gives rise to magnetic order in the edge states of the quantum spin Hall insulator model proposed by Kane and Mele.^{3,4} We study this scenario in graphene zigzag ribbons but it could occur in other systems as well.^{10–12} We find three new elec-

tronic phases in that system that combine ferromagnetic order and spontaneous charge current flow, both localized in the zigzag edges. They arise from the interplay of Coulomb repulsion and spin-orbit coupling. When the ferromagnetic edges are counterpolarized, the valley symmetry is broken and, above a critical strength of the spin-orbit coupling, the system goes from an insulating to a valley-half-metal phase. In the three phases, current flows as if there was a real magnetic field perpendicular to the sample along the direction of the magnetization edge.

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- ¹P. W. Anderson, *Basic Notions of Condensed Matter Physics* (Benjamin/Cummings, Menlo Park, CA, 1983).
 - ²M. Hasan and C. Kane, [arXiv:1002.3895](#) (unpublished); J. E. Moore, *Nature (London)* **464**, 194 (2010).
 - ³C. L. Kane and E. J. Mele, *Phys. Rev. Lett.* **95**, 226801 (2005).
 - ⁴C. L. Kane and E. J. Mele, *Phys. Rev. Lett.* **95**, 146802 (2005).
 - ⁵B. A. Bernevig, T. L. Hughes, and S. C. Zhang, *Science* **314**, 1757 (2006); X. L. Qi, Y. S. Wu, and S. C. Zhang, *Phys. Rev. B* **74**, 085308, (2006); D. N. Sheng, Z. Y. Weng, L. Sheng, and F. D. M. Haldane, *Phys. Rev. Lett.* **97**, 036808 (2006).
 - ⁶N. A. Sinitsyn, J. E. Hill, H. Min, J. Sinova, and A. H. MacDonald, *Phys. Rev. Lett.* **97**, 106804 (2006).
 - ⁷M. König *et al.*, *Science* **318**, 766 (2007).
 - ⁸Y. L. Chen *et al.*, *Science* **325**, 178 (2009).
 - ⁹F. D. M. Haldane, *Phys. Rev. Lett.* **61**, 2015 (1988).
 - ¹⁰K. L. Lee, B. Gremaud, R. Han, B. G. Englert, and C. Miniatura, *Phys. Rev. A* **80**, 043411 (2009).
 - ¹¹M. Gibertini, A. Singha, V. Pellegrini, M. Polini, G. Vignale, A. Pinczuk, L. N. Pfeiffer, and K. W. West, *Phys. Rev. B* **79**, 241406 (2009).
 - ¹²A. Shitade, H. Katsura, J. Kuneš, X. L. Qi, S. C. Zhang, and N. Nagaosa, *Phys. Rev. Lett.* **102**, 256403 (2009).
 - ¹³K. Nakada, M. Fujita, G. Dresselhaus, and M. S. Dresselhaus, *Phys. Rev. B* **54**, 17954 (1996).
 - ¹⁴M. Fujita, K. Wakabayashi, K. Nakada, and K. Kusakabe, *J. Phys. Soc. Jpn.* **65**, 1920 (1996).
 - ¹⁵L. Brey and H. A. Fertig, *Phys. Rev. B* **73**, 235411 (2006).
 - ¹⁶Y.-W. Son, M. L. Cohen, and S. G. Louie, *Nature (London)* **444**, 347 (2006).
 - ¹⁷A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, *Rev. Mod. Phys.* **81**, 109 (2009).
 - ¹⁸A. Rycerz, J. Tworzydo, and C. W. J. Beenakker, *Nat. Phys.* **3**, 172 (2007).
 - ¹⁹D. Gunlycke *et al.*, *Nano Lett.* **7**, 3608 (2007).
 - ²⁰O. V. Yazyev and M. I. Katsnelson, *Phys. Rev. Lett.* **100**, 047209 (2008).
 - ²¹X. Li, X. Wang, L. Zhang, S. Lee, and H. Dai, *Science* **319**, 1229 (2008).
 - ²²J. Fernández-Rossier, *Phys. Rev. B* **77**, 075430 (2008).
 - ²³W. Y. Kim and K. S. Kim, *Nat. Nanotechnol.* **3**, 408 (2008).
 - ²⁴F. Muñoz-Rojas, J. Fernández-Rossier, and J. J. Palacios, *Phys. Rev. Lett.* **102**, 136810 (2009).
 - ²⁵H. Min, J. E. Hill, N. A. Sinitsyn, B. R. Sahu, L. Kleinman, and A. H. MacDonald, *Phys. Rev. B* **74**, 165310 (2006).
 - ²⁶Y. Yao, F. Ye, X. L. Qi, S. C. Zhang, Z. Fang, *Phys. Rev. B* **75**, 041401(R) (2007).
 - ²⁷See supplementary material at <http://link.aps.org/supplemental/10.1103/PhysRevB.82.161302> for a detailed comparison of the electronic structure and atomic magnetic moments obtained using the mean-field Hubbard approximation for the zigzag ribbon used throughout this report with those obtained using first principles.
 - ²⁸D. Bohm, *Phys. Rev.* **75**, 502 (1949).
 - ²⁹M. Gmitra, S. Konschuh, C. Ertler, C. Ambrosch-Draxl, and J. Fabian, *Phys. Rev. B* **80**, 235431 (2009).
 - ³⁰A. C. Bleszynski-Jayich *et al.*, *Science* **326**, 272 (2009).