Interaction driven surface Chern insulator in nodal line semimetals

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Nodal line semimetals are characterized by nontrivial bulk-band crossings, giving rise to almost flat drumhead-like surface states (DSS), which provide an attractive playground where interaction can induce symmetry-broken states and potential emergent phases. Here, we show that electronic interaction causes Stoner ferromagnetic instability in the DSS while the bulk remains non-magnetic, which together with spin-orbit coupling drive the surface states into a 2D Chern insulator. We show that each DSS carries a half-monopole charge, which for systems containing two pieces of DSS yield a net Chern number $C = -1$. We show that this phenomenology is robust against chiral-symmetry breaking, that gives a finite dispersion to the DSS. Our work shows that nodal line semimetals are a promising platform to implement surface Chern insulators and dissipation-less electron transport by exploiting enhanced interaction effects of the DSS.

Topological electronic states have motivated large research efforts due to their gapped bulk coexisting with protected gapless surface modes. Specific examples of those states are the helical edge modes in quantum spin hall insulators \cite{PhysRevLett.95.126802,PhysRevLett.96.106802}, recently also proposed as hinge states in higher-order topological insulators \cite{PhysRevX.6.021006,PhysRevX.5.041015}. In particular, chiral edge states are especially attractive as they would yield unidirectional channels lacking electric loss, representing a cornerstone in low consumption electronics. Natural compounds for Chern insulator have been proved to be rather elusive, which has motivated several proposals for its realization \cite{PhysRevX.7.041056,PhysRevLett.120.036804}, yet the most successful implementation requires a building block that is also very rare in nature: magnetically doped topological insulators \cite{PhysRevLett.115.136802,PhysRevLett.117.116804,PhysRevLett.118.236802}. Thus, a key question is whether if Chern insulators can be engineered by means of a family of materials more common in nature, which would open new possibilities in condensed matter research, apart from applications in low consumption electronics.

During the last years, the classification of topological insulators has been extended to so-called topological semimetals \cite{PhysRevX.7.031013,PhysRevLett.121.146802}, i.e., systems that are gapless in the bulk and simultaneously host topologically protected surface states. The topological band crossing may occur at discrete points or along closed loops in reciprocal space. The former case corresponds to Weyl/Dirac semimetals \cite{PhysRevLett.118.116802,PhysRevX.5.041015}, whereas the latter is referred as nodal line semimetals (NLSMs) \cite{PhysRevLett.117.186805,PhysRevX.7.011027}. The nodal line carries a $\pi$ Berry flux \cite{PhysRevLett.117.186805,PhysRevX.7.011027}, resulting in drumhead-like surface states (DSS) \cite{PhysRevLett.117.186805}. In the presence of chiral symmetry, such DSS are perfectly flat, yielding a regime where any residual electronic interaction would overcome the surface kinetic energy, which provides a perfect platform to realize strongly correlated and symmetry-broken surface states \cite{PhysRevLett.117.186805,PhysRevX.5.041015,PhysRevLett.120.036804,PhysRevLett.121.146802}.

In this Letter, we show that a surface 2D Chern insulator can emerge from electronic interaction in a NLSM. For the sake of concreteness, we focus on the NLSM containing two disconnected pieces of DSS with spin degeneracy, see Fig. 1(a). Electronic interaction results in Stoner instability in the DSS and induces a surface ferromagnetic order. The emergent exchange field together with the spin-orbit coupling (SOC) on an open surface, yield a half-monopole charge for each DSS, driving the surface band into a Chern insulator, see Figs. 1(b,c). Such spontaneously emergent 2D Chern insulator on the

\begin{figure}[h]
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\caption{(a) Nodal lines around $\bm{K}$, $\bm{K}'$ points and corresponding DSS enclosed by their projection onto the surface Brillouin zone. (b) Spin-orbit coupling (SOC) introduces opposite mass terms to the DSS around $\bm{K}$, $\bm{K}'$. Electronic interaction (e-e) inverts one of the bands. (c) Two pieces of DSS each carries a half-monopole charge, resulting in a Chern number $C = -1$ of the whole surface band. (d) Spin polarized surface states and chiral hinge current. Inset: diamond lattice with an open surface.}
\end{figure}
The Hamiltonian characterized by $H = H_0 + H_{SOC} + H_U$ (1) where $H_0$ captures the NLSM, $H_{SOC}$ is the intrinsic SOC and $H_U$ is the local Coulomb interaction term, that we will discuss in detail below. The Bloch Hamiltonian for the NLSM is $H_0 = d_x(k)\sigma_x + d_y(k)\sigma_y$ with $d_x(k) = t + t'\cos(k_xa_x) + t'\sum_{l=1}^2\cos(k_la_x)$ and $d_y(k) = t'\sin(k_xa_x) + t'\sum_{l=1}\sin(k_la_x)$, where Pauli matrices act on the AB sublattice space [inset in Fig. 1(d)], $t, t'$ are the nearest-neighbor hopping, and $t'$ denotes the hopping along the $(1, 1, 1)$ orientation, which has been set to the $z$-axes for simplicity. The corresponding lattice vectors are $a_1 = a(1 - \frac{\sqrt{3}}{2}, 0)$, $a_2 = a(-\frac{1}{2\sqrt{3}}, \frac{\sqrt{3}}{2}, 0)$, $a_3 = a(0, \frac{\sqrt{3}}{2}, \frac{\sqrt{3}}{2})$, with $a$ being the lattice constant. When $t'/t < 1$, the system is a NLSM, carrying two spiral nodal lines centered at $K = (\frac{4\pi}{3a}, 0, 0)$ and $K' = -K$ in the $k_x-k_y$ plane [49, 49], see Fig. 1(a). This can be seen in the limiting case $t' \to 0$ by expanding $H_0$ around $\pm K$ points as $h^s = d^s_x\sigma_x + d^s_y\sigma_y$, with $d^s_x = \mp vq_x + t'\cos(k_la_x/\sqrt{3})$ and $d^s_y = -qv_y + t'\sin(k_la_x/\sqrt{3})$, where the velocity is defined as $v = \sqrt{3}ta/(2\sqrt{2})$, the small wave vector $q = (q_x, q_y)$ is measured from $\pm K$. By putting $d^s_{x,x'} = 0$, we obtain the parametric equations of the spiral nodal lines around $\pm K$ as $q_x = \pm \frac{\sqrt{3}}{2}\cos(\frac{\sqrt{3}}{2}q_y), q_y = \frac{\sqrt{3}}{2}\sin(\frac{\sqrt{3}}{2}q_y)$, which have opposite chirality [Fig. 1(a)].

The nontrivial band topology of the NLSM is characterized by $\pi$ Berry phase carried by each nodal line. The Hamiltonian $H_0$ possesses time reversal ($T$) symmetry, $H_0(k) = TH_0(-k)T^{-1} = H_0(-k)$, and inversion ($P$) symmetry, $H_0(k) = PH_0(k)P^{-1} = \sigma_xH_0(-k)\sigma_x$, so that the Berry curvature vanishes everywhere away from the nodal lines [40]. Then one can choose an arbitrary integral path to calculate the Berry phase. Here we choose the integral path to be a straight line along the $z$-direction, then the Zak phase calculated inside/outside the projection of the nodal line equals $\pi/0$. This configuration of path integral is convenient to show the bulk-boundary correspondence of the NLSM, that is, DSS appear inside the projection of the nodal lines onto the surface Brillouin zone [Fig. 1(a)]. For a semi-infinite ($z < 0$) sample with an open surface lying at $z = 0$ [Fig. 1(d)], by substituting $k_z \to -id_z$ in $h^s(q)$, the zero-energy DSS around $K, K'$ can be obtained as $\psi_{\pm} \propto (0, 1)^T e^{\pm z}$, where $\lambda = \pm \frac{\sqrt{3}}{a}(\ln t' + i\theta_\pm)$, with $\theta_\pm = \tan^{-1}(a/q), \theta_\pm = \pi - \theta_\pm$. As long as $v|q| < t'$, i.e., the states lie inside the projection of the nodal loops, the wave functions $\psi_{\pm}$ decays to zero as $z \to -\infty$, indicating the existence of sublattice polarized DSS [cf. 1(a)]; Otherwise, there are no surface states. The above results hold generally in the NLSM regime $t'/t < 1$. This can be checked by numerically computing the band structure in a slab of NLSM with the Hamiltonian $H_0$, infinite in the $x-y$ plane and whose $z$-axis lies along the $(1, 1, 1)$ direction of the parent diamond lattice [inset of Fig. 1(d)]. We take a slab thick enough so that the two surfaces are decoupled, and we project the final result onto the upper half of the system to retain only the DSS on the upper surface. We show in Fig. 2(a) the band structure of the NLSM described above, where two pieces of zero-energy DSS exist. Without dispersion, the surface density of states (DOS) diverges at zero energy, see Fig. 2(b), whereas the bulk DOS vanishes.

Next, we include the SOC effect by second-neighbor hopping [51] as $H_{SOC} = i\lambda \sum_{(i,j)} \sum_{\alpha\beta} s_i \cdot (d_{ik} \times d_{jk}) c_j$ where $c_i = (c_{i\uparrow}, c_{i\downarrow})$ is the Fermi operator for both spins on site $i$, $\lambda$ is the SOC strength, $s$ is the spin vector, and $d_{ik}$ is the vector connecting sites $i$ and $k$. The SOC term opens a gap in the band structure, both in the bulk and in the surface modes, lifting the spin degeneracy of the DSS [Fig. 2(c)] and introducing nontrivial spin textures to the DSS [Fig. 2(d)]. Its effect on the surface modes can be described by the following massive Dirac Hamiltonian $H_{SOC}^\pm = \alpha(s_xq_x - s_yq_y) \pm \beta s_z$, which is sufficient to characterize the surface band topology. Here, $H_{SOC}^\pm$ is induced by the bulk SOC on an open surface, so that two coefficients $\alpha, \beta > 0$ are determined by $\lambda$. Interestingly, the bulk SOC, that does not break bulk inversion symmetry, takes the form of a Rashba-type SOC on the surface. The parameter $\beta$ introduces opposite mass terms to the DSS around $K, K'$ points, see Fig. 1(b). Without SOC, the Hamiltonian for the DSS vanishes, so that $H_{SOC}^\pm$ can serve as the effective Hamiltonian of the DSS. The monopole charge carried by each DSS is calculated through $Q_\pm = \frac{1}{4\pi} \int d\varphi d\varphi d\varphi q_x(\varphi_x b^\pm \times \varphi_q q_x b^\pm \cdot b^\pm /|b^\pm|^3$, with $b^\pm = (aq_x - sq_x, \pm \beta)$, yielding $Q_\pm = \pm \frac{1}{2}$. Each DSS carries a half-monopole charge, but with an opposite sign, due to the opposite mass term. Two half-monopole charges cancel out and result in zero Chern number as imposed by time reversal symmetry. In this scenario, it is suggestive to think that, if one of the half-monopoles would be inverted, the system would show a net Chern number.

In order to have nonzero Chern number, time reversal symmetry must be broken. In the following, we will show that electronic interaction can spontaneously break time reversal symmetry on the surface, inverting one of the half-monopoles and turning the DSS into a Chern insulator. For that goal, it is convenient to first consider the case without SOC, where the system shows gapless flat
Zeeman term to the Hamiltonian for the DSS. In particular, at the \(K, K'\) points, the new term takes the form \(H_Z = -m_Z s_z\), where its strength can be evaluated as 
\[
m_Z = \frac{\hbar}{2} \int_{-\infty}^{\infty} m^2(z)|\psi_\pm(\vec{q} = 0, z)|^2 dz.
\]

Finally, we consider the simultaneous action of both electronic interaction and SOC. By numerically solving the full self-consistent model with SOC, we observe that the surface magnetization survives even in the presence of SOC, see Fig. 2(f). In this situation, the effective Hamiltonian for the DSS takes the form \(H = H_{ZSOC}^\beta + H_Z\). Now the Chern number for the whole surface bands can be defined by the mass terms at the \(K, K'\) points as
\[
C = \frac{1}{2} \left[ \text{sgn}(\beta - m_Z) + \text{sgn}(-\beta - m_Z) \right].
\]

As \(m_Z > \beta\), the surface Zeeman splitting reverses the sign of the mass term around \(K\) [compare Figs. 2(c), 2(f)], and drive the system to a Chern insulator [cf. Fig. 1(b)]. Such kind of topological phase transition resembles the scenario of the Haldane model on the graphene lattice [52], yet here the sign change of the mass around one valley is dynamically generated by electronic interaction.

Since we are solving a self-consistent problem that does not have a smooth behavior, a gap closing and reopening cannot generically be observed. Nevertheless, since the mean-field term of the original Hamiltonian effectively reduces to a site-dependent exchange field that decays as one enters the bulk [Fig. 3(a)], we may try to artificially switch on its contribution, in order to adiabatically trace the topological phase transition. This can be made concrete by taking a final self-consistent Hamiltonian realizing the Chern insulating state \(H = H_0 + H_{MF}\), and defining an adiabatic Hamiltonian of the form \(\tilde{H}(\alpha) = H_0 + \alpha H_{MF}\), where \(\alpha = 0\) corresponds to the non-interacting Hamiltonian with \(C = 0\), whereas \(\alpha = 1\) corresponds to the physical self-consistent solution with \(C = -1\). By tuning \(\alpha\) from 0 to 1, the topological phase transition can be observed [Fig. 3(b)] as a gap closing and reopening in the energy spectra, concomitant with a change of Chern number from 0 to -1.

Since SOC opens up a gap in the single particle spectra, it is expected that at large values of \(\lambda\) the magnetic order will be quenched and the system will remain a trivial semiconductor. This competition between SOC and electronic interaction is shown in the phase diagram in terms of interaction strength \(U\) and SOC strength \(\lambda\) in Figs. 3(c,d). Different from the band closing and reopening by continuously tuning the order parameter in Fig. 3(b), the surface magnetization [Fig. 3(c)] and the energy gap [Fig. 3(d)] change abruptly with varying interaction \(U\), indicating a phase transition with spontaneous symmetry breaking. Remarkably, such a conventional phase transition further induces and coincides with a topological phase transition on the surface. The topologically nontrivial phase with \(C = -1\) holds in a wide parametric region. For a larger SOC strength, the parametric re-
FIG. 3. (a) Real space distribution of the magnetization, where $z = 0$ corresponds to the surface. (b) Energy gap as a function of the mean-field order parameter. Phase diagram associated with (c) surface magnetization and (d) energy gap in terms of SOC strength $\lambda$ and interaction $U$. (e) Band structure including the second-neighbor hopping $t_2 = 0.03t$, in the absence of $U$ and $\lambda$. (f) Phase diagram containing chiral-symmetry breaking. We took $t' = 0.8t$, $\lambda = 0.01t$ and $U = 2t$ for (a,b), 200 layers for (a,b,c,d,f) and 600 layers for (e).

region of $U$ for a Chern insulator becomes narrower, while the energy gap increases. When the interaction becomes extremely large, the whole system becomes a trivial antiferromagnetic insulator, opening a large bulk magnetic gap.

In real materials, chiral symmetry is usually broken, and the DSS have finite dispersion. We investigate this situation by introducing a second-neighbor hopping $t_2 = 0.03t$, in the absence of $U$ and $\lambda$. (f) Phase diagram containing chiral-symmetry breaking. We took $t' = 0.8t$, $\lambda = 0.01t$ and $U = 2t$ for (a,b), 200 layers for (a,b,c,d,f) and 600 layers for (e).

A direct result of a 2D Chern insulator is the existence of chiral edge states. Here, the Chern insulator emerges on the surface of a 3D sample, resulting in chiral hinge states [Fig. 1(d)] [3–7, 53, 54]. The chiral edge states can also be achieved in a magnetic domain wall between two oppositely ordered ferromagnetic regions on the surface. The two regions are related by time reversal symmetry, so that they carry opposite Chern numbers, yielding a pair of chiral modes inside the domain wall, see Fig. 3(a). This image can be made concrete by computing the spectral function of the magnetic domain wall by means of the Dyson equation $G_D(\omega, k_\parallel) = \left[ \omega - H_D(k_\parallel) - \Sigma_L(\omega, k_\parallel) - \Sigma_R(\omega, k_\parallel) \right]^{-1}$, where $k_\parallel$ is the Bloch momentum along the direction defined by the domain wall, $\Sigma_{L,R}(\omega, k_\parallel)$ are the self-energies induced by the semi-infinite magnetic regions (taken from the self-consistent solution of the infinite problem), and $H_D(k_\parallel)$ is the local Hamiltonian of the domain wall. With the previous Green’s function, we compute the DOS at the surface as $\frac{1}{\pi} \text{Im} \text{Tr}_U [G_D(\omega)]$, where $\text{Tr}_U$ traces over the degrees of freedom of the upper surface. The interfacial spectral function is shown in Fig. 3(b), where it is seen that two gapless modes appear at the magnetic domain wall. Therefore, controlling such magnetic domain walls [55, 56] would allow to imprint chiral states on the surface of NLSMs.

To conclude, we have demonstrated that correlation effect can induce surface symmetry breaking in NLSM, which together with spin-orbit coupling further drive the surface states into a Chern insulator. Spin-degenerate NLSMs with two pieces of DSS in the surface Brillouin zone are potential candidates to achieve such interaction-driven surface Chern insulators. Interestingly, the NLSMs which are fragile to SOC and usually considered to be trivial, can serve as a promising platform to engineer surface Chern insulators, opening a venue to implement dissipation-less electronics in NLSMs.

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