Electric control of Dirac quasiparticles by spin-orbit torque in an antiferromagnet

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(Dated: October 27, 2016)

Spin-orbitronics and Dirac quasiparticles are two fields of condensed matter physics initiated independently about a decade ago. Here we predict that Dirac quasiparticles can be controlled by the spin-orbit torque reorientation of the Néel vector in an antiferromagnet. Using CuMnAs as an example, we formulate symmetry criteria allowing for the co-existence of Dirac quasiparticles and Néel spin-orbit torques. We identify the non-symmorphic crystal symmetry protection of Dirac band crossings whose on and off switching is mediated by the Néel vector reorientation. We predict that this concept, verified by minimal model and density functional calculations in the CuMnAs semimetal antiferromagnet, can lead to a topological metal-insulator transition driven by the Néel vector and to the corresponding topological anisotropic magnetoresistance.

2004 was the year when the spin Hall effect was observed in GaAs [1,3] and one-atom-thick flakes of graphene were isolated [4,5]. The former discovery marked the dawn of the field of spin-orbitronics, in which the relativistic conversion between linear momentum and spin angular momentum of conducting electrons has provided new physical concepts for spintronics devices. These include the spin-orbit torque (SOT), which has opened the path to reliable and fast information writing in a ferromagnetic random access memory [6,7], and also to efficient means of the electrical switching of an antiferromagnet (AF) by the Néel SOT [8,9]. Independently, the discovery of graphene initiated intense research of Dirac fermion quasiparticles in condensed matter systems. The field includes topological insulators, semimetals, or superconductors, which host a family of quasiparticles mimicking different flavors of fermions from relativistic particle physics [10–12]. More recently, novel phenomena have been discovered at the intersection of these two fields, such as the quantum spin Hall effect and the quantum anomalous Hall effect in non-magnetic and magnetic topological insulators [13–18]. Dirac quasiparticles, exhibiting a strong spin-momentum locking, are also considered for enhancing the efficiency of the SOT control of magnetic moments in ferromagnetic topological insulator hetero-structures [19].

In this Letter we close the loop of synergies between the fields of spin-orbitronics and Dirac quasiparticles by proposing a scheme for the electric control of Dirac band crossings via the Néel SOT in AFs. Our work addresses the outstanding problem of finding efficient means for controlling Dirac quasiparticles by external fields which may provide the desired tools for the experimental research and future practical applications in microelectronics [20]. On a specific example of the semimetal CuMnAs AF [9,21,22] we demonstrate that the Néel vector orientation is a suitable degree of freedom that can mediate on and off switching of the symmetry protection of Dirac band crossings. Based on this we also predict the topological metal-insulator transition (MIT) and the corresponding topological anisotropic magnetoresistance (AMR) in Dirac semimetal AFs.

Dirac quasiparticles and the Néel SOT can co-exist because of the serendipitous overlap of the key symmetry requirements. We illustrate this on examples shown in Figs. 1(a),(b) of the graphene lattice, representing the Dirac systems [23], and the tetragonal CuMnAs crystal where the Néel SOT has been experimentally verified [9]: (i) The two-Mn-site primitive cell of CuMnAs favors band crossings in analogy with the two-C-site graphene lattice. (ii) In the paramagnetic phase, CuMnAs has time reversal (T) and space inversion (P) symmetries. It guarantees that each band is double-degenerate forming a Kramer’s pair, in analogy to graphene. In the AF phase, this degeneracy is not lifted because the combined PT symmetry is preserved, although the T symmetry and the P symmetry are each broken [22,24,25]. This highlights antiferromagnetism as the favorable type of magnetic order for controlling Dirac quasiparticles. (iii) Finally, the combined PT symmetry also allows for the efficient SOT reorientation of the Néel vector [8,27]. Because the A and B Mn-sites in the CuMnAs primitive cell are non-centrosymmetric inversion partners, a non-equilibrium spin-polarization δSA,B with opposite sign on the two sites is generated by an electrical current J (see Fig. 1(b)) [8]. This applies to both the paramagnetic and the AF phase above and below the Néel temperature of CuMnAs. Moreover, in the AF phase, the inversion partner A and B sites are occupied by oppositely oriented Mn magnetic moments (hence the combined PT...
ties are connected by the PT symmetry extracted from CuMnAs. The two magnetic sublattices are non-centrosymmetric. This allows for the nonzero staggered non-equilibrium spin-polarizations \( \delta s \), which facilitates the manipulation of the Néel vector. (c) Top view of our quasi-2D-AFM model highlighting the non-symmorphic glide mirror plane \( G_x \) (see text). (d) 2D BZ projection with the DPs positions - for \( n \parallel [100] \) along the MX axis (blue), while for \( n \parallel [010] \) along M’Y axis (red). (e) Band dispersion of our minimal AFM model illustrating the control of the DPs and topological indexes of the DP \( D_1 \) in the inset (for the sake of clarity the degenerate bands are slightly shifted). (f) 3D model BZ with the Dirac nodal lines (colors of the planes protected for a given Néel vector orientation correspond to (d,e)).

We illustrate the concept first on a minimal model of the tetragonal CuMnAs AF, considering only the Mn atoms (with one orbital per atom) that form a stack of the crinkled quasi-2D square lattices shown in Figs. 1(b),(c). We first neglect the coupling between these quasi-2D planes; their distance is larger than first and second nearest neighbor distances within the quasi-2D plane. The corresponding model Hamiltonian in the crystal momentum space,

\[
H_k = -2t \tau_x \cos \frac{k_x}{2} \cos \frac{k_y}{2} - t' \cos k_x \cos k_y + \lambda \tau_z (\sigma_y \sin k_z - \sigma_x \sin k_y) + \tau_z J_n \sigma \cdot n, \tag{1}
\]

consists of the first nearest neighbor hopping \( t \) (inter-sublattice \( A - B \) hopping), the second nearest neighbor hopping \( t' \) (intra-sublattice \( A - A \) hopping), the second-neighbor SOC of strength \( \lambda \), and the AF exchange coupling of strength \( J_n \). The wavevector \( k_{x(y)} \) is in units of the inverse lattice constant, \( n \) is the Néel vector, and \( \tau \) and \( \sigma \) are Pauli matrices describing the crystal sublattice \( A, B \) and spin degrees of freedom, respectively. We diagonalize \( H \) analytically,

\[
E_{k \pm} = -t' \cos k_x \cos k_y \pm \left| 4t'^2 \cos^2 \frac{k_x}{2} \cos^2 \frac{k_y}{2} + (J_n n_x - \lambda \sin k_y)^2 + (J_n n_y + \lambda \sin k_x)^2 + J_n^2 n_x^2 \right|^{1/2}, \tag{2}
\]

and plot in Fig. 1(e) the resulting bands measured from the Fermi level for \( \lambda = 0.8t, J_n = 0.6t, \) and \( t' = 0.08t \). For the Néel vector \( n \parallel [100] \) we found two Dirac points (DPs) \( D_1 \), and \( D_2 \) in the first Brillouin zone (BZ) along the MX axis at wave-vectors \( D_1 = (\pi, \arcsin \frac{J}{2}) \) and \( D_2 = (\pi, \pi - \arcsin \frac{J}{2}) \), as shown in Figs. 1(d-f).

For the minimal quasi-2D model of the CuMnAs AF we can now show explicitly that the DPs are protected by a non-symmorphic, glide mirror plane symmetry \( G_x \). \( G_x = \{ M_x \parallel [100] \} \). It combines the mirror symmetry \( M_x \) along the (100) plane with the half-primitive cell translation along the [100] axis (see Fig. 1(c)) and has eigenvalues \( g_{\pm} = \pm i \). The four-fold degenerate OP originates from a crossing of two Kramer’s pairs where the two bands in each pair are degenerate due to the \( \mathcal{PT} \) symmetry. Hybridization between the pairs is prohibited, i.e. the crossing is protected by \( G_x \), when the following conditions are met: (i) The crossing occurs at the BZ sub-manifold invariant under \( G_x \). This is fulfilled in \( k_x = 0, \pm \pi \) planes. (ii) The two bands forming a given Kramer’s pair, with the corresponding wavefunctions \( \psi_k \) and \( \mathcal{PT} \psi_k \), can be assigned the same eigenvalue of \( G_x \). From the commutation relation of \( G_x \) and \( \mathcal{PT} \) we obtain that this condition is fulfilled only at the BZ sub-manifold \( k_x = \pm \pi \) (cf. Figs. 1(d),(e)). (iii) One Kramer’s pair corresponds to one eigenvalue and the other Kramer’s pair to the opposite eigenvalue of \( G_x \). This can be verified by employing the \( k \cdot p \) perturbation theory. Around, e.g., the \( D_1 \) point in the \( k_x = \pi \) plane

symmetry). The current-induced non-equilibrium spin-polarization and the equilibrium AF moments are therefore both staggered and commensurate. In combination with the exchange interaction that couples them, the resulting current-induced Néel SOT can efficiently orient the Néel vector [8,9].

An additional crystal symmetry is now needed to mediate the dependence of Dirac quasiparticles on the Néel vector orientation. In graphene there is no symmetry that protects the four-fold degeneracy of Dirac crossings of two Kramer’s pair bands in the presence of spin-orbit coupling (SOC) [13]. Inspired by recent predictions of the symmetry protection of band-crossings in Dirac semimetals [28,30], we identify non-symmorphic symmetries that can be turned on and off by reorienting the Néel vector in CuMnAs and by this can close and open a gap at the Dirac crossing. Recall that non-symmorphic space groups contain point group operations coupled with non-primitive lattice translations.
we obtain, \( E_{\mathbf{D}_1 + k_y \pm} = \pm \hbar v_F \sqrt{x^2 + y^2} \) with the two Kramer’s pairs fulfilling, \( G_x \psi_{k_x \pm} = G_x \mathcal{P} T \psi_{k_x \pm} = \mp i \psi_{k_x \pm} \). This is highlighted in the inset of Fig. 1(e).

Because of the combined \( \mathcal{P} T \) symmetry we can define the topological index of our DPs analogously to the paramagnetic Dirac semimetals [31]. The topological index \( N(k_y) \) at the crystal momentum \( k_y \), invariant under \( G_x \), is given by: \( N(k_y) = [N^\text{c}(k_y) - N_y^\text{v}(k_y)] - [N^\text{c}(k_y) - N_y^\text{v}(k_y)] \). Here \( N^\text{c,v}(k_y) \) is the number of conduction (valence) bands at \( k_y \) with the eigenvalue \( g_\pm = \pm i \). An integer value and a discontinuity of the topological index when crossing the DP in our model is highlighted in the inset of Fig. 1(e). The corresponding topological charge at e.g. the DP \( D_1 \), obtained by approaching \( D_1 \) from left and right [31], is \( Q = [N(D_1 + \delta) - N(D_1 - \delta)] / 8 = -1 \).

Following the symmetry analysis of Néel SOTs in Refs. [8, 27], we obtain for our CuMnAs model that the lowest-order (\( n \)-independent) component of \( \delta \psi_{A,B} \) is staggered, i.e., can generate an efficient field-like SOT. The field allows for the rotation of \( n \) in the (001)-plane in the direction perpendicular to the applied in-plane current. In Figs. 1(d),(e) we show that for \( n \parallel [010] \) the DPs move to the \( M'Y \) axis. They are now protected by the \( \mathcal{G}_y = \{ M_y | 0 \} \) symmetry, as expected for the square quasi-2D lattice.

At intermediate in-plane angles, no DP protecting symmetry remains and the entire spectrum is gapped (see the \( n \parallel [110] \) bands in Fig. 1(e)). As highlighted on the full spectra of the minimal quasi-2D model in Fig. 2(a),(b), this leads to the topological MIT driven by the Néel vector reorientation. The band-gap at the DP is a continuous function of the in-plane Néel vector angle, \( \Delta(D_1) \sim J_n \sqrt{1 - \cos^2(\phi)} \), where \( \phi \) is measured from the [100] axis. The transport counterpart of the MIT is the topological AMR which we define as, \( \text{AMR} \equiv \frac{\sigma(\phi) - \sigma_{\text{min}}}{\sigma_{\text{max}}} \). Here \( \sigma(\phi) \) is the \( \phi \)-dependent conductivity with current along the [100] axis and \( \sigma_{\text{min}}(\text{max}) \) referring to the conductivity minimum (maximum). The topological AMR in our Dirac semimetal AF is schematically illustrated in Fig. 2(c). High AMR values correspond to \( \phi = 0, \pi / 2 \) with the closed gap of the DPs at \( \mathbf{M}' \). For comparison, we illustrate in Fig. 2(c) a characteristic harmonic angular dependence of the conventional AMR in a normal magnetic metal [32].

We conclude the discussion of the minimal model of the CuMnAs AF by taking into account the coupling between the quasi-2D planes. The coupling leads to the following renormalization of the model Hamiltonian [1]:

\[
2t_x \rightarrow 2(t_x + t_z \cos k_x) \tau_x + t_z \sin k_x \tau_y, \quad t'(\cos k_x + \cos k_y) \rightarrow t' + (\cos k_x + \cos k_y) \quad \lambda \rightarrow \lambda - \lambda_z \cos k_x.
\]

As a result, the \( G_x (G_y) \) protected DPs in 2D transform into protected nodal lines in 3D. For example, \( D_1 \rightarrow (\pi, \arcsin \frac{\lambda_z}{\lambda - \lambda_z \cos k_x}, k_z) \) gives an open nodal line for \( \lambda_z < \lambda / 2 \), as shown in Fig. 1(f) for \( \lambda_z = 0.2t \). Note that in our Dirac AF, the nodal lines are dispersive in contrast to the paramagnetic \( J_n = 0 \) model [31].

We now verify all observations made in the minimal model by performing full-potential relativistic \textit{ab initio} calculations as implemented in FLEUR and ELK packages [33]. The exchange correlation potential is parametrized by the Perdew-Burke-Ernzerhof generalized gradient approximation (GGA) [34, 35]. The full crystal of tetragonal CuMnAs, including also the Cu and As atoms, is shown in Fig. 3(a) [36, 37]. Results without SOC are summarized in Figs. 3(b),(c). They show the semimetallic character with the dip in the density of states near the Fermi level and numerous band crossings. Note that their position is sensitive to the com-

![FIG. 2. Topological MIT in our minimal model driven by Néel vector reorientation from (a) [100] to (b) [110] by the Néel SOT. (c) Schematics of the corresponding angular dependence of the topological AMR contrasted to the normal AMR.](image-url)
model and, therefore, allows for the current-induced ro-
symmetric protection in paramagnetic ZrSiS [38].
nal CuMnAs AF distinct from the earlier identified non-tries. Note that the
in Fig. 3(e), excluding the protection by these symme-
However, the nodal lines become gapped, as illustrated
vector to
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PT
metry elements: Identity, non-symmorphic glide planes
of the tetragonal CuMnAs lattice reduces to eight sym-
mal model. Instead of assigning the
to the
conjugated symmetries. By rotating the Néel
D
1
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(see also the comparison of GGA and GGA+U calcula-
cally at these four sites we obtain that they contain
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level and we now discuss the properties of the three Fermi
level DPs seen in Fig. 4(b),(c). Without SOC they are part of an ungauged nodal line in the $k_x = 0$ plane [22].
In the presence of SOC and for $n || [001]$, the DPs along the $\Gamma X$ and $ZX$ axes become gapped. The gap opening applies to the entire nodal line, except for the DP along the $XU$ axis (and also $X'U$), as shown in Figs. 4(d),(f),(h). Using the same method as in the $ab initio$ calculations for the tetragonal CuMnAs, we identified that the $XU$ DP protection is due to the screw-axis symmetry $S_z = \{C_{2z}, [\frac{1}{2} \frac{1}{2} 0] \}$ [22]. The corresponding state at $n || [001]$ is then a topological AF Dirac semimetal with the topological charge of the $XU$ DP $Q = +1$. For $n || [101]$, all DPs (the entire nodal line) are gapped and the system becomes an AF semiconductor, as seen in Figs. 4(e)-(h). Finally, for $n || [100]$, the spin-orbit gap is nearly but not fully closed at the $\Gamma X$ DP, as shown in Fig. 4(f). This "trivial" AF Dirac semimetal phase is reminiscent of graphene. Since the DPs can appear at the Fermi level (see also the comparison of GGA and GGA+U calculations in Fig. 4(b)), orthorhombic CuMnAs represents a realistic material candidate for observing the topological MIT and AMR driven by the Néel vector reorientation.

We acknowledge support from the Grant Agency of the Charles University no. 280815 and of the Czech Republic no. 14-37-427, Humbold foundation, EU ERC Synergy Grant No. 610115, and the Transregional Collaborative Research Center (SFB/TRR) 173 SPIN+X. Access to computing and storage facilities owned by parties and projects contributing to the National Grid Infrastructure MetaCentrum provided under the programme "Projects

FIG. 4. (a) Crystallographic and magnetic structure of the orthorhombic CuMnAs with Néel SOT spin-polarization $\delta s$ for the current $J || [100]$. Atom-resolved (b) point-semimetal density of states, and (c) band structure without SOC within GGA. GGA+U shows DPs position shifts. (d-e) Topological MIT. Manipulation of the Dirac fermions along the (f) $TX$, (g) $XU$, and (h) $ZX$ axis (units $d = \sqrt{a^2 + c^2}$ with $a \neq c$ being the lattice constants) by the Néel SOT from GGA+SOC calculations reveals: topological ($n || [001]$), and ”trivial” Dirac semimetal ($n || [100]$), and semiconductor ($n || [101]$).

putational details; as an illustration we plot in Fig. 3(c) shifted bands obtained in the GGA+U approximation with the correlation potential $U = 3$ eV. When SOC is included in the $ab initio$ calculations and $n || [100]$, protected nodal lines are obtained in the $k_x = \pm \pi$ planes, as illustrated in Figs. 3(d). The nodal lines have the open geometry (cf. Fig. 1(f)). The protection is due to the $G_x$ symmetry, also in agreement with the minimal model. Instead of assigning the $G_x$ eigenvalues in the complex $ab initio$ band structure, we verify this by excluding all other relevant symmetries as the origin of the protection. For $n || [100]$, the space group $P4/nmm$ of the tetragonal CuMnAs lattice reduces to eight symmetry elements: Identity, non-symmorphic glide planes $G_x$, and $G_z = \{M_x, [\frac{1}{2} \frac{1}{2} 0] \}$; screw-axis $S_y = \{C_{2z}, [0 \frac{1}{2} 0] \}$, and four $PT$ conjugated symmetries. By rotating the Néel vector to $n || [110]$ and $n || [101]$, $G_x$ and $S_y$ remain symmetries of the AF crystal, respectively. In both cases, however, the nodal lines become gapped, as illustrated in Fig. 3(e), excluding the protection by these symmetries. Note that the $G_x$ protection makes our tetragonal CuMnAs AF distinct from the earlier identified non-symmorphic protection in paramagnetic ZrSiS [83].

The field-like Néel SOT in the full tetragonal crystal of CuMnAs has the same symmetry as in the minimal model and, therefore, allows for the current-induced ro-

tation of the Néel vector [9][27]. This opens the prospect of electric control of Dirac crossings in an experimentally relevant AF material. However, the tetragonal CuMnAs is not optimal for observing the corresponding topological MIT due to other non-Dirac bands present around the Fermi level (see Fig. 3(c)). These can be removed e.g. by lowering the lattice symmetry from tetragonal to orthorhombic [21][22], as we now discuss in the remaining paragraphs.

The non-symmetric $Pnma$ primitive cell of the orthorhombic CuMnAs [39] is shown in Fig. 4(a). It has four Mn sites consisting of the two inversion-partner pairs $A-B$ and $A'-B'$. From the symmetry analysis of the current-induced spin-polarizations [27] generated locally at these four sites we obtain that they contain components which are commensurate with the AF order: $A$ and $A'$ sites with one sign of the current-induced spin-polarizations belong to one AF spin-sublattice and $B$ and $B'$ sites with the opposite sign of the current-induced spin-polarizations belong to the opposite AF spin-sublattice. This makes the Néel SOT efficient for reorienting AF moments in orthorhombic CuMnAs.

GGA electronic structure calculations without SOC are shown in Fig. 4(b),(c). Consistent with earlier reports [21][22], the density of states vanishes at the Fermi level and we now discuss the properties of the three Fermi level DPs seen in Fig. 4(b),(c). Without SOC they are part of an ungauged nodal line in the $k_x = 0$ plane [22].

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of Projects of Large Research, Development, and Innovations Infrastructures” (CESNET LM2015042), is greatly appreciated.

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