Dirac fermions in an antiferromagnetic semimetal

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Analogues of the elementary particles have been extensively searched for in condensed-matter systems for both scientific interest and technological applications3–5. Recently, massless Dirac fermions were found to emerge as low-energy excitations in materials now known as Dirac semimetals3–5. All of the currently known Dirac semimetals are non-magnetic with both time-reversal symmetry $\mathcal{T}$ and inversion symmetry $\mathcal{P}T$. Here we show that Dirac fermions can exist in one type of antiferromagnetic system, where both $\mathcal{T}$ and $\mathcal{P}$ are broken but their combination $\mathcal{P}T$ is respected. We propose orthorhombic antiferromagnet CuMnAs as a candidate, analyse the robustness of the Dirac points under symmetry protections and demonstrate its distinctive bulk dispersions, as well as the corresponding surface states, by ab initio calculations. Our results provide a possible platform to study the interplay of Dirac fermion physics and magnetism.

The great success in the field of topological insulators1,2 since last decade inspired the study of topological features of metals. Topological metals have non-trivial surface states and their bulk Fermi surfaces can be topologically characterized3. Among them, Dirac semimetals3–5 have received special attention, because they host relativistic particles, the massless Dirac fermions, in a non-relativistic set-up. In such Dirac materials, two doubly degenerate bands contact at discrete momentum points called Dirac points, and disperse linearly along all directions around these points. The four-fold degenerate Dirac points are unstable by themselves; hence, symmetry protection is necessary7. Following this guideline, several three-dimensional Dirac semimetals have been theoretically proposed, and some of them have been experimentally verified recently8,9. All of these materials have time-reversal symmetry $\mathcal{T}$, inversion symmetry $\mathcal{P}$, and certain crystalline rotation symmetry.

If some of the symmetries are broken, massless Dirac fermions can in general be destroyed. For instance, when either $\mathcal{T}$ or $\mathcal{P}$ is broken, each doubly degenerate band is lifted, so that the Dirac cones can split into multiple Weyl cones10. This gives birth to Weyl semimetals11–17, and the chiral-anomaly-related transport phenomena can be observed as a signature18,19. However, the result of both $\mathcal{T}$ and $\mathcal{P}$ breaking remains obscure until now. It is thus natural to ask whether Dirac fermions can still exist in the absence of both $\mathcal{T}$ and $\mathcal{P}$.

In this letter, we answer the question in the affirmative, and provide a concrete example of such a Dirac semimetallic phase. We consider three-dimensional systems with the antiferromagnetic (AFM) order that breaks both $\mathcal{T}$ and $\mathcal{P}$ but respects their combination $\mathcal{P}T$. The low-energy physics can be explicitly captured by the following four-band effective model

$$H(k) = d_0(k) \mathbb{1}_{4 \times 4} + d_1(k) \tau_x + d_2(k) \tau_y + d_3(k) \tau_z \sigma_z + d_4(k) \tau_x \sigma_x + d_5(k) \tau_y \sigma_y$$  

where $d_i(k), i=0,1,\ldots,5$ are real functions of momentum $k$ and $\tau_x, \tau_y, \tau_z, \sigma_z$ are Pauli matrices for orbital (spin-related AFM) basis (see Supplementary Section 3 for details). The anti-unitary $\mathcal{P}T$ symmetry satisfying $(\mathcal{P}T)^2 = -1$ is given as $\mathcal{P}T = i\sigma_y K$, where $K$ is complex conjugation. Due to this symmetry, the last five terms in $H(k)$ anti-commute with one another; therefore, every band must be doubly degenerate (this degeneracy holds generally for all $\mathcal{P}T$ invariant systems, see Supplementary Section 1) with energy spectrum

$$\varepsilon = d_i(k) \pm \sqrt{\sum_{i=1,3} d_i^2(k)}$$  

If one has $d_i(q) = 0$ for $i=1,\ldots,5$ at a certain isolated momentum $k = q$, then the two doubly degenerate bands must cross each other there. The resulting four-fold degenerate point $k = q$ can be further made Dirac-like when additional constraints are enforced by crystalline symmetry.

To realize stable four-fold degenerate crossing points, the generic way is to let the pair of doubly degenerate bands carry different representations of certain symmetries in the system20,21. For our AFM model, however, there is a simpler starting point for investigation. Let us assume that the local magnetic moments are along the $z$ axis without loss of generality. When the spin–orbit coupling (SOC) effect is ignored, $d_1(k)$ and $d_2(k)$ vanish because they correspond to spin-flip processes. Thus, the crossing points must be present in general, because with three momentum components one can tune $d_3(k), d_4(k)$ and $d_5(k)$ to zero simultaneously. These points can be Dirac points as long as linear dispersion is required by certain crystalline symmetry. When SOC is included, the presence of the crossing points can still be guaranteed due to the protection of the crystalline symmetry.

In accordance with our analysis, we discover that the AFM semimetals orthorhombic CuMnAs and CuMnP22,23 can host the Dirac fermions around the Fermi level. Their crystal structure has the non-symmorphic space group $D_{2h}$ (Pnma) with four formula units in the primitive unit cell (see Fig. 1a,b for the structure and the first Brillouin zone). The space group consists of eight symmetry operations that can be generated by three of them: the inversion $\mathcal{P}$, the gliding mirror reflection of the $y$ plane $R_y = \{m_y\|(0,1/2,0)\}$, and the two-fold screw rotation along the $z$ axis $S_{2z} = \{C_{2z}\|(1/2,0,1/2)\}$, where the two non-symmorphic symmetries $R_y$ and $S_{2z}$ are important in our symmetry analysis (see Supplementary Section 2 for details).

CuMnAs and CuMnP have been experimentally identified as room-temperature antiferromagnets previously20,24, where non-zero magnetic moments on Mn atoms with $3d$ electrons order antiferromagnetically (see Supplementary Section 4). The magnetic configuration breaks some symmetries from the original space group. For the most energy-favoured AFM configuration in the

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orthorhombic phase (see Fig. 1a), the magnetic moments on the inversion-related Mn atoms are aligned along opposite directions; therefore, both $T$ and $P$ are broken whereas $PT$ still holds. If SOC is absent, spin internal space is decoupled from real space, so the spatial symmetries $R_i$ and $S_{2z}$ are kept. When SOC is included, however, residual symmetries depend on the orientation of magnetic moments, for example, only $S_{2y}$ will survive if magnetic moments are along the $z$ axis.

With the crystal structure and symmetry operations in mind, we begin to present our results of band structure calculations as well as effective model analysis (see Supplementary Section 9 for details of parameter choices). Figure 1d shows the electronic structures from first-principles calculations for a case where SOC is turned off in the AFM system without SOC (see Supplementary Section 3). As we mentioned above, our AFM system without SOC is described by the effective model (see Supplementary Section 2). By checking the orbital composition of the bands, we finally confirmed that the existence of such a DNL in the absence of SOC is associated with the behaviours of the underlying atomic orbitals under $R_i$ (see Supplementary Section 7).

Corresponding to the DNL in the bulk, a non-trivial surface state appears inside the projection of the DNL on the (010) surface (see Fig. 2f–h). This dispersive drumhead-like surface state can be measured as a clear signature of the DNL semimetallic.

When we still exclude SOC but break $R_z$ (see Supplementary Section 9), a bandgap opens along the entire DNL except at four discrete points. One pair of the four-fold degenerate points is located on the high-symmetry line X–U, and the other pair is in the interior of the Brillouin zone. We verified the first pair as Dirac points with linear dispersions shown in Fig. 2b. The Dirac points are guaranteed by the screw rotation symmetry $S_{2z}$. Unlike $R_z$, $S_{2z}$ anti-commutes with $PT$ along the X–U line, so the doubly degenerate states at each $k$ point on this line have the same $S_{2z}$ eigenvalues. As a result, the crossing of one pair of the doubly degenerate bands must be stable, as long as they carry different $S_{2z}$ eigenvalues. On the basis of $ab initio$ results, we calculated $S_{2z}$ eigenvalues of the bands near the Fermi level, and the results match the symmetry argument exactly (see Supplementary Sections 2 and 6).

To check the nature of the Dirac points, we derive the low-energy effective model (see Supplementary Section 3). As we mentioned above, our AFM system without SOC is described by (we ignore the overall shift $\mathbb{1}_{4\times4}$ term in the following)

$$H(k) = d_3(k) \tau_3 + d_1(k) \tau_1 + d_1(k) \sigma_3$$  \hspace{1cm} (3)

On the high-symmetry line X–U, the screw rotation symmetry $S_{2z}$ is represented by $S_{2z} = i e^{-ik_z/2} \tau_z$. Expanding the Hamiltonian around one Dirac point and enforcing the symmetry constraints, we can obtain the exact Dirac-type Hamiltonian

$$H_{\text{Dirac}} = (v_{11} k_x + v_{12} k_y) \tau_3 + v_{13} k_z \tau_5 + (v_{31} k_y + v_{32} k_z) \tau_3 \sigma_5$$  \hspace{1cm} (4)
Figure 2 | Electronic structures of CuMnAs without SOC. a, The electronic structure of orthorhombic CuMnAs around the Fermi level when $R_y$ is present. The black line gives the Dirac nodal line. b, The electronic structure of orthorhombic CuMnAs when $R_y$ is broken by shear strain. The red stars stand for the Dirac points (DPs) around the Fermi level. c–d, Schematics of the projected anisotropic Dirac cone into the $(k_x, k_z)$ space reconstructed from the fitting parameters. e, Schematics of the degenerate Weyl points (WPs) with different pseudo-spin $\sigma_z = \pm 1$. The green arrows show the orbital texture. f–h, The Fermi surface contour on the (010) surface when $R_y$ is present (f), and the corresponding electronic spectra along $k_z = \pi/a$ and $k_z = 0$ when $R_y$ is present (g,h). SS, surface state. i, The Fermi surface contours on the (010) surface for spin-up states along $k_z(2\pi/c)$ and -down (j) states when $R_y$ is broken. The red and white stars stand for the Weyl points with different topological charges. k, The corresponding electronic spectrum for spin-up states along $k_z = \pi/5c$. The Fermi level is set to zero. Colour scale bars in f–k relate to the local density of states, with warmer colours representing a higher density.

where $v_{ij}(i,j = 1,2,3)$ are velocity coefficients for different directions. These parameters are obtained from our calculations, and the resulting Dirac cones are anisotropic (see Fig. 2c,d). Splitting $H_{\text{Dirac}}$ into two blocks that correspond to $\sigma_z = \pm 1$, we can decouple each Dirac cone into two Weyl cones with opposite chiralities (see Fig. 2e)

$$H_{\text{Weyl}}^+ = (v_{11}k_x + v_{12}k_y)\tau_x + v_{13}k_z\tau_z + (v_{23}k_x + v_{24}k_y)\tau_y$$

$$H_{\text{Weyl}}^- = (v_{11}k_x + v_{12}k_y)\tau_x + v_{13}k_z\tau_z - (v_{23}k_x + v_{24}k_y)\tau_y$$

Since SOC is absent, the AFM basis $\sigma_z = \pm 1$ is almost equivalent to the physical spin basis (see Supplementary Section 1). We thus calculated the surface states on the (010) surface for each spin component, as shown in Fig. 2i–k. It is clear that Fermi arcs emerge on the surface, and they connect pairs of Weyl points with opposite chiralities. For either spin component, the chiralities of the Weyl points on the X–U line are found to be the same; therefore, it is reasonable that the other two Weyl points that carry opposite chiralities exist in the Brillouin zone such that the total chirality vanishes.

When SOC is turned on, the presence of the crossing points sensitively depends on the orientation of the local magnetic moments on Mn atoms, as crystalline symmetries can be broken by the magnetism. If the magnetic moments are aligned along the z axis, only $S_{2z}$ symmetry from the space group survives. In this case, the symmetry argument for the robust crossing points along the X–U line still holds, so the four-fold degenerate points on this line are intact under the protection of $S_{2z}$, while the other pair of crossing...
the Dirac fermions in AFM systems. Similar to normal Dirac and relativistic particles, Weyl fermions, and these relativistic particles might contribute to electric control of local magnetization in $PT$ invariant antiferromagnets\(^2\). In addition, AFM fluctuations are inevitably present in CuMnAs and CuMnP, although our current treatment assumes that the magnetic configuration is frozen. If the Dirac fermions are massive, the fluctuations not only directly couple to the massless Dirac fermions, but also produce fermion masses through breaking crystalline symmetries. The exact description of interplay between Dirac fermions, the AFM fluctuations, and the symmetry breaking at the moment remains an open question.

**Methods**

Methods, including statements of data availability and any associated accession codes and references, are available in the online version of this paper.
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Author contributions

P.T., Q.Z., G.X. and S.-C.Z. conceived and designed the project. P.T. performed the first-principles calculations; Q.Z. performed theoretical analysis; P.T. and Q.Z. analysed the data and wrote the manuscript. All authors commented on the manuscript.

Additional information

Supplementary information is available in the online version of the paper. Reprints and permissions information is available online at www.nature.com/reprints. Correspondence and requests for materials should be addressed to S.-C.Z.

Competing financial interests

The authors declare no competing financial interests.
**Methods**

*Ab initio calculations.* The first-principles calculations were carried out by the density functional theory method with the projector augmented-wave method\(^{32}\), as implemented in the Vienna *ab initio* simulation package\(^{33}\). The Perdew–Burke–Ernzerhof exchange–correlation functional and the plane-wave basis with energy cutoff of 300 eV were employed. The lattice parameters (see Fig. 1a) were chosen from experimental values\(^{22}\), which are \(a = 6.577\ \text{Å}, b = 3.854\ \text{Å}\) and \(c = 7.310\ \text{Å}\) for orthorhombic CuMnAs, and \(a = 6.318\ \text{Å}, b = 3.723\ \text{Å}\) and \(c = 7.088\ \text{Å}\) for orthorhombic CuMnP respectively; and the inner atomic positions were allowed to be fully relaxed until the residual forces are less than \(1 \times 10^{-3}\ \text{eV Å}^{-1}\). The Monkhorst–Pack \(k\) points were \(9 \times 15 \times 9\), and SOC was included in self-consistent electronic structure calculations. The maximally localized Wannier functions\(^{34}\) were constructed to obtain the tight-binding Hamiltonian, which is used to calculate the bulk Fermi surface, surface electronic spectrum and surface states.

**Data availability.** The data that support the plots within this paper and other findings of this study are available from the corresponding author on request.

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