Title: Weyl Semimetal Phase in Noncentrosymmetric Transition-Metal Monophosphides

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Abstract: Based on first-principle calculations, we show that a family of nonmagnetic materials including TaAs, TaP, NbAs, and NbP are Weyl semimetals (WSM) without inversion centers. We find twelve pairs of Weyl points in the whole Brillouin zone (BZ) for each of them. In the absence of spin-orbit coupling (SOC), band inversions in mirror-invariant planes lead to gapless nodal rings in the energy-momentum dispersion. The strong SOC in these materials then opens full gaps in the mirror planes, generating nonzero mirror Chern numbers and Weyl points off the mirror planes. The transport properties obtained by the Boltzmann equation combined with the semiclassical treatments of the unique electronic structure in these materials will also be discussed in comparison with the most recent experimental data.
The Weyl semi-metal: a new topological state in condensed matter

HongMing Weng, Zhong Fang and Xi Dai
Institute of Physics, CAS

Chen Fang and Andrei Bernevig
Princeton University

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Definition of Topological Semi-Metal (TSM)

- Topological Semi-metal: metal with vanishing FS, insulator with vanishing energy gap, band crossings at Fermi level
- Semi-metals defined above can all described by Topological invariance: Weyl, Dirac, Nodal lines
- TSM has very unique and fruitful transport properties (mostly under magnetic field)
Weyl Fermion in solid

- Fermions described by massless Weyl equation with fixed chirality, half of the Dirac equation

\[ H = \bar{v}_x \cdot \bar{\sigma} k_x + \bar{v}_y \cdot \bar{\sigma} k_y + \bar{v}_z \cdot \bar{\sigma} k_z \]

Chirality = \( \text{sgn}[(\bar{v}_x \times \bar{v}_y) \cdot \bar{v}_z] \)

Principle axes:

\[ H = \sum_{\alpha \beta = x, y, z} v_{\alpha \beta} \sigma_{\alpha} k_{\beta} = \sum_{i} \lambda_{i} \tilde{k}_{i} \tilde{\sigma}_{i} \]

\[ \tilde{v} = L \lambda \tilde{R} \]

\[ \tilde{\sigma}_{i} = \sum_{\alpha} \tilde{\sigma}_{\alpha} L_{\alpha i} \]

\[ \tilde{k}_{i} = \sum_{\beta} R_{\beta i} k_{\beta} \]

\[ \chi = \text{sgn}[\text{det}(R) \cdot \text{det}(L)] \]

\[ \epsilon = \sqrt{\lambda_{1}^{2} k_{1}^{2} + \lambda_{2}^{2} k_{2}^{2} + \lambda_{3}^{2} k_{3}^{2}} \]
Weyl points and singularity of Berry's Curvature

- Weyl points are always come in pairs with opposite chirality for any lattice model.
- Weyl points are the singular point of the Berry's Curvature

\[ \vec{A}(\vec{k}) = \sum_{n} <n\vec{k}|\vec{\nabla}_{\vec{k}}|n\vec{k}> \quad \vec{B}(\vec{k}) = \vec{\nabla}_{\vec{k}} \times \vec{A}(\vec{k}) \]

\[ \vec{\nabla}_{\vec{k}} \cdot \vec{B}(\vec{k}) = \pm \delta(\vec{k} - \vec{k}_0) \]

- integral of Berry curvature over a 2D closed manifold gives Chern number:
  - Chern number for a 2D BZ: quantum Hall effect
  - Chern number for a FS in 3D: Chiral anomaly
Why Weyl points must appear in pairs?
Why Weyl points must appear in pairs?
Properties of WSM:
Fermi arcs on the surface, what protects it?

fully gapped between nth and (n+1)th bands!
Weyl points are located between nth and (n+1)th bands!

Wan et al, Phys. Rev. B 83, 205101
Properties of WSM:
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- fully gapped between n-th and (n+1)-th bands!
- Weyl points are located between n-th and (n+1)-th bands!

Wan et al., Phys. Rev. B 83, 205101
Where to find WSM?

- Remove the spin degeneracy of the band
- Spin-orbital coupling is essential
- SOC+Either breaking of time reversal or spacial inversion symmetries
- First proposed real material by X. Wan, S. Savrasov et al: Y2Ir2O7 with all in all out spin structure  *Phys. Rev. B* 83, 205101
- Ferromagnetic metal proposed by us: HgCr2Se4  *PRL* 107, 186806
- Tellurium and Selenium under pressure by S. Murakami, and T. Miyake’s groups: cond-mat:1409.7517
- critical point between normal and topological insulators by Vanderbilt’s group: PRB 90, 155316
Crystal structure of TaAs family

Symmetrical operations (in MCT conventional unit cell)

<table>
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<th>1. Mx</th>
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<td>0 0 0 0000</td>
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<td>5.</td>
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</tbody>
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There is no spatial inversion symmetry.
How to confirm if there are Weyl points or not?

Mirror Chern Number and Z2 invariance for some special planes in momentum space
Fermi circle or arcs?

\[ \text{MCN \& } Z_2=1 \]

\[ Z_2=0 \]
Fermi circle or arcs?

M-xy  Mx  Mxy

MCN & Z2=1

Z2=0
Surface arcs obtained from tight binding calculation

(a) (001) surface

(b) (001) surface FS@0.05 eV

(c) (100) surface

(d) (100) surface FS@0.0 eV
Fermi arc pattern obtained by ab initio calculation
Chiral anomaly under U(1) gauge field: E and B
Full quantum mechanical(strong field) point of view

The Chiral density $(N_L - N_R)$ won’t be conserved under parallel magnetic and electric fields: adiabatic pumping of particles from One Weyl point to another one with opposite chirality

\[
\begin{align*}
\epsilon_n &= v_F \text{sign}(n) \sqrt{2\hbar|eB| + (\hbar k \cdot \dot{B})^2}, \ n = \pm 1, \pm 2, \ldots \\
\epsilon_0 &= -\chi \hbar v_F k \cdot \dot{B}
\end{align*}
\]

The equation of motion for the zeroth Landau level

\[
\hbar \frac{dk}{dt} = -eE
\]

Will generate negative Magneto-resistance in WSM materials
Chiral anomaly under U(1) gauge field: E and B
Full quantum mechanical(strong field) point of view

The Chiral density($N_L-N_R$) won't be conserved under parallel magnetic and electric fields:
adiabatic pumping of particles from One Weyl point to another one with opposite chirality

\[ \Psi = \frac{\text{sign}(n)\sqrt{2h\pi}\epsilon\hat{E} + (\hat{h}k - \hat{B})^2, n = \pm1, \pm2, \ldots} \]

The evolution of motion for the zeroth Landau level
\[ \hbar \frac{dk}{dt} = -eE \]
will generate negative Magneto-resistance in WSM materials
Chiral anomaly:  
Semi-classic(weak field) point of view

- Semi-classic equation of motion

\[ \begin{align*} 
\vec{k} &= qE + q\vec{\dot{r}} \times \vec{B} \\
\dot{\vec{r}} &= \frac{\partial E(\vec{k})}{\partial \vec{k}} - \vec{k} \times \Omega 
\end{align*} \]  

\[ j = \int d^4k \cdot n_{F\pi} (1 - qB \cdot \Omega) \dot{\vec{r}} = \int d^4k \cdot n_F \cdot [qE(k) - E \times \Omega - (\Omega \cdot \vec{v}(k))B] \]  

- Boltzmann equation:

\[ \begin{align*} 
[qE - (B \cdot E)\Omega] \cdot \vec{v}_k \frac{\partial f_0}{\partial \vec{v}_k} + [qE \times B] \cdot \frac{\partial f_1}{\partial \vec{k}} &= -(1 - qB \cdot \Omega) \left( \frac{f_1}{\tau_s} + \frac{f^{rs}_1}{\tau_{rs}} \right) \\
f_1 &= f^n_1 + f^{rs}_1 \\
\dot{j}_\parallel &= \sigma_0 \left( E_\parallel + \beta (B \cdot E) B \right) \\
\dot{j}_\perp &= \sigma_0 \left( \frac{E_\perp + q\alpha E \times B}{1 + (\alpha B)^2} \right) 
\end{align*} \]
Chiral anomaly:  
Semi-classic(weak field) point of view

- Semi-classic equation of motion

\[
\begin{align*}
  \mathbf{k} &= qE + q\mathbf{r} \times \mathbf{B} \\
  \mathbf{r} &= \frac{\partial \mathbf{c}(\mathbf{k})}{\partial \mathbf{k}} - \mathbf{k} \times \Omega
\end{align*}
\]

\[
j = \int d^4k \cdot n_F q (1 - qB \cdot \Omega) \mathbf{r} = \int d^4k \cdot n_F [q \mathbf{v}(k) - E \times \Omega - (\Omega \cdot \mathbf{v}(k)) \mathbf{B}]
\]

- Boltzmann equation:

\[
qE - (B \cdot E) \Omega \cdot \mathbf{v}_h \frac{\partial f_0}{\partial \mathbf{v}_h} + [q \mathbf{v}_h \times \mathbf{B}] \cdot \frac{\partial f_1}{\partial \mathbf{v}_h} = -(1 - qB \cdot \Omega) \left( \frac{f_1}{\tau_s} + \frac{f_{1s}}{\tau_{ns}} \right)
\]

\[
f_1 = f_t^s + f_t^{ns}
\]

\[
j_{\parallel} = \sigma_0 \left( E_{\parallel} + \beta (B \cdot E) B \right)
\]

\[
j_{\perp} = \sigma_0 \frac{E_{\perp} + qaE \times B}{1 + (\alpha B)^2}
\]
Negative MR in Dirac semi-metal: Na3Bi

P. Ong's group, Science 2015
Summary

- Mirror Chern number and Z2 invariance can be used to identify WSM
- TaAs family materials are WSM with broken inversion but keep TRS
- There will be more of those materials.