ゼロギャップ半導体におけるスピン物性とワイル半金属相







野村健太郎 (東北大学金属材料研究所)

outline

- 1. What is Weyl semimetal
- 2. How can it be realized
- 3. Charge transport
- 4. Novel phenomena

ゼロギャップ半導体におけるスピン物性とワイル半金属相







紅林大地(M1)



関根聡彦(D2)



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outline

What is Weyl semimetal
 How can it be realized
 Charge transport
 Novel phenomena

Insulator and Metal



small g

Insulator and Metal



Insulator and Metal



Relativistic quantum mechanics

Dirac Fermions

$$H_{Dirac} = p_x \alpha_1 + p_y \alpha_2 + p_z \alpha_3 + m \alpha_4$$



 α_i : 4x4 Dirac matrix

 $\{\alpha_i, \alpha_j\} = 2\delta_{ij}$



Relativistic quantum mechanics

Dirac Fermions

$$H_{Dirac} = p_x \alpha_1 + p_y \alpha_2 + p_z \alpha_3 + m \alpha_4$$

 α_i : 4x4 Dirac matrix

$$\{\alpha_i, \alpha_j\} = 2\delta_{ij}$$

Weyl Fermions

$$H_{Weyl} = p_x \sigma_1 + p_y \sigma_2 + p_z \sigma_3$$

 σ_i : 2x2 Pauli matrix

-Massless fermions -Parity broken





Relativistic quantum mechanics

Dirac Fermions

$$H_{Dirac} = p_x \alpha_1 + p_y \alpha_2 + p_z \alpha_3 + m \alpha_4$$

Weyl Fermions

$$\alpha_{::} 4x4 \text{ Dirac matrix}$$

$$H_{Weyl} = \begin{pmatrix} p_z & p_x - ip_y \\ p_x + ip_y & -p_z \end{pmatrix}$$

$$H_{Weyl} = p_x \sigma_1 + p_y \sigma_2 + p_z \sigma_3$$

 σ_i : 2x2 Pauli matrix

Massless fermionsParity broken





Condensed matter systems

Dirac semimetals

degenerate



Weyl semimetals

non-degenerate





Condensed matter systems

Dirac semimetals

degenerate



Condensed matter systems

Dirac semimetals

2D (graphene) Wallace (1947), ...
3D (accidental) Herring (1937), ... (symmetry protected) Wang et al., Young et al.(2012),...

Weyl semimetals

3D (I-broken) Murakami (2007)
3D (T-broken) Wan et al. (2011) Burkov&Balents (2012) degenerate







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Dirac semimetals

PHYSICAL REVIEW B 85, 195320 (2012)

Dirac semimetal and topological phase transitions in $A_3Bi(A = Na, K, Rb)$

Zhijun Wang,¹ Yan Sun,² Xing-Qiu Chen,² Cesare Franchini,² Gang Xu,¹ Hongming Weng,^{1,*} Xi Dai,¹ and Zhong Fang^{1,†} ¹Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China ²Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China (Received 6 March 2012; revised manuscript received 7 May 2012; published 22 May 2012)

Discovery of a Three-Dimensional Topological Dirac Semimetal, Na₃Bi

Z. K. Liu, ¹* B. Zhou, ^{2,3}* Y. Zhang, ³ Z. J. Wang, ⁴ H. M. Weng, ^{4,5} D. Prabhakaran, ² S.-K. Mo, ³ Z. X. Shen, ¹ Z. Fang, ^{4,5} X. Dai, ^{4,5} Z. Hussain, ³ Y. L. Chen^{2,6}†

Science 343, 864 (2014)



Dirac semimetals

Unexpected mass acquisition of Dirac fermions at the quantum phase transition of a topological insulator

T. Sato¹*, Kouji Segawa², K. Kosaka¹, S. Souma³, K. Nakayama¹, K. Eto², T. Minami², Yoichi Ando²* and T. Takahashi^{1,3}

Nat. Phys. 7, 840 (2011)





Weyl semimetals

Selected for a Viewpoint in Physics

PHYSICAL REVIEW B 83, 205101 (2011)

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Topological semimetal and Fermi-arc surface states in the electronic structure of pyrochlore iridates

Xiangang Wan,¹ Ari M. Turner,² Ashvin Vishwanath,^{2,3} and Sergey Y. Savrasov^{1,4}



Weyl semimetals

PRL 107, 127205 (2011)

PHYSICAL REVIEW LETTERS

week ending 16 SEPTEMBER 2011

Weyl Semimetal in a Topological Insulator Multilayer

A. A. Burkov^{1,2} and Leon Balents²

¹Department of Physics and Astronomy, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada ²Kavli Institute for Theoretical Physics, University of California, Santa Barbara, California 93106, USA (Received 27 May 2011; published 16 September 2011)

$$\mathcal{H}(\mathbf{k}) = v_F \tau^z (\hat{z} \times \boldsymbol{\sigma}) \cdot \mathbf{k} + m\sigma^z + \hat{\Delta}(k_z),$$
$$\hat{\Delta} = \Delta_S \tau^x + \frac{1}{2} (\Delta_D \tau^+ e^{ik_z d} + \text{H.c.}).$$



From Dirac to Weyl

Dirac hamiltonian

$$H = \sum_{i=1}^{3} p_i \alpha_i + m_0 \alpha_4$$





$$\alpha_{i} = \begin{bmatrix} 0 & \sigma_{i} \\ \sigma_{i} & 0 \end{bmatrix}, \qquad \alpha_{4} = \begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix}$$

From Dirac to Weyl

Dirac hamiltonian

$$H = \sum_{i=1}^{3} p_i \alpha_i + m_0 \alpha_4 + b \Sigma_z$$





$$\alpha_{i} = \begin{bmatrix} 0 & \sigma_{i} \\ \sigma_{i} & 0 \end{bmatrix}, \qquad \alpha_{4} = \begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix}$$
$$\Sigma_{i} = \begin{bmatrix} \sigma_{i} & 0 \\ 0 & \sigma_{i} \end{bmatrix} \longleftarrow \text{ spin of electron}$$





From Dirac to Weyl

Dirac hamiltonian $H_J = J \sum_{I} S(r_I) \cdot c_I^{\dagger} \Sigma c_I$ $H = \sum_{i=1}^{3} p_i \alpha_i + m_0 \alpha_4 + JM\Sigma_z$







Magnetic order?



$$1 - J^2 \chi_L \chi_e < 0 \quad \Longrightarrow \quad M \neq 0$$

 $\chi_L \simeq 1/T$

at low temperature

Magnetic order?



Experiments of magnetic TIs

Science 329, 659 (2010)

Massive Dirac Fermion on the Surface of a Magnetically Doped Topological Insulator

Y. L. Chen,^{1,2,3} J.-H. Chu,^{1,2} J. G. Analytis,^{1,2} Z. K. Liu,^{1,2} K. Igarashi,⁴ H.-H. Kuo,^{1,2} X. L. Qi,^{1,2} S. K. Mo,³ R. G. Moore,¹ D. H. Lu,¹ M. Hashimoto,^{2,3} T. Sasagawa,⁴ S. C. Zhang,^{1,2} I. R. Fisher,^{1,2} Z. Hussain,³ Z. X. Shen^{1,2}*



sive; indeed, we find that the Dirac gap can be observed in magnetically doped samples with or without bulk ferromagnetism (19). Furthermore, if $E_{\rm F}$ can be tuned into this surface-state gap, an insulating massive Dirac fermion state is formed;

Experiments of magnetic TIs

Science 339, 1582 (2013)

Topology-Driven Magnetic Quantum Phase Transition in Topological Insulators

Jinsong Zhang,¹* Cui-Zu Chang,^{1,2}* Peizhe Tang,¹* Zuocheng Zhang,¹ Xiao Feng,² Kang Li,² Li-li Wang,² Xi Chen,¹ Chaoxing Liu,³ Wenhui Duan,¹ Ke He,²† Qi-Kun Xue,^{1,2} Xucun Ma,² Yayu Wang¹†

 $Bi_{2-y}Cr_{y}(Se_{x}Te_{1-x})_{3}$







$$H_{total} = H_e^{MF} + H_L^{MF} - N_i JMm$$

D. Kurebayashi 27pBF-3

Electron

$$\boldsymbol{H}_{e}^{MF} = \sum_{\boldsymbol{k}} \boldsymbol{c}_{\boldsymbol{k}}^{+} \left[\boldsymbol{H}_{0}(\boldsymbol{k}) + \boldsymbol{X} \boldsymbol{J} \boldsymbol{M} \boldsymbol{\Sigma}_{z} \right] \boldsymbol{c}_{\boldsymbol{k}}$$

 Σ_{z} : spin matrix

$$H_0(\mathbf{k}) = \sum_{i=1}^3 R_i(\mathbf{k})\alpha_i + m_0(\mathbf{k})\alpha_4 + \varepsilon(\mathbf{k})I$$

Bi₂Se₃ family Hexagonal lattice model

$$R_{1}(\mathbf{k}) = \frac{2}{\sqrt{3}}A_{1}\sin\left(\frac{\sqrt{3}}{2}k_{x}\right)\cos\left(\frac{1}{2}k_{y}\right)$$

$$R_{2}(\mathbf{k}) = \frac{2}{3}A_{1}\left[\cos\left(\frac{\sqrt{3}}{2}k_{x}\right)\sin\left(\frac{1}{2}k_{y}\right) + \sin\left(k_{y}\right)\right]$$

$$R_{3}(\mathbf{k}) = A_{2}\sin(k_{z})$$

$$m(\mathbf{k}) = m_{0} - B_{2}\left[2 - 2\cos(k_{z})\right]$$

$$-\frac{4}{3}B_{1}\left[3 - 2\cos\left(\frac{\sqrt{3}}{2}k_{x}\right)\cos\left(\frac{1}{2}k_{y}\right) - \cos(ky)\right]$$

$$\varepsilon(\mathbf{k}) = -\epsilon_{F} + D_{2}\left[2 - 2\cos(k_{z})\right]$$

$$+\frac{4}{3}D_{1}\left[3 - 2\cos\left(\frac{\sqrt{3}}{2}k_{x}\right)\cos\left(\frac{1}{2}k_{y}\right) - \cos(ky)\right]$$

$$H_{total} = H_e^{MF} + H_L^{MF} - N_i JMm$$

D. Kurebayashi 27pBF-3

<u>Electron</u>

Local spin

$$H_{e}^{MF} = \sum_{k} C_{k}^{+} \left[H_{0}(k) + XJM\Sigma_{z} \right] C_{k}$$

$$H_L^{MF} = Jm \sum_{l=1}^{N_{imp}} S_z(r_l)$$





Virtual crystal approximation

D. Kurebayashi

27pBF-3





Phase diagram

D. Kurebayashi 27pBF-3



Dirac semimetals

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outline

What is Weyl semimetal
 How can it be realized
 Charge transport
 Novel phenomena

Charge transport of Weyl fermions

From 2d to 3d

topics

- Impurity scattering
- Quantum effect (localization)
- Anomalous Hall effect

Charge transport of Weyl fermions

From 2d to 3d

topics

- Impurity scattering
- Quantum effect (localization)
- Anomalous Hall effect

$$\hbar / \tau = 2\pi \sum_{\boldsymbol{k}} \left| \left\langle \boldsymbol{k} \mid \boldsymbol{V} \mid \boldsymbol{k}' \right\rangle \right|^2 (1 - \hat{\boldsymbol{k}} \cdot \hat{\boldsymbol{k}}') \delta(\boldsymbol{E}_F - \boldsymbol{v}_F \mid \boldsymbol{k} \mid)$$

 $\boldsymbol{\tau}$: relaxation time





f(k) : distribution function in non-equilibrium

$$\hbar / \tau = 2\pi \sum_{\mathbf{k}} \left| \left\langle \mathbf{k} \mid \mathbf{V} \mid \mathbf{k}' \right\rangle \right|^2 (1 - \hat{\mathbf{k}} \cdot \hat{\mathbf{k}}') \delta(E_F - \mathbf{v}_F \mid \mathbf{k} \mid)$$

Short-range scatterers

2d case

$$V(\boldsymbol{r}) = \sum_{j} u_{j} \delta(\boldsymbol{r} - \boldsymbol{R}_{j})$$

 τ : relaxation time



$$\hbar / \tau = 2\pi \sum_{\boldsymbol{k}} \left| \left\langle \boldsymbol{k} \mid \boldsymbol{V} \mid \boldsymbol{k}' \right\rangle \right|^2 (1 - \hat{\boldsymbol{k}} \cdot \hat{\boldsymbol{k}}') \delta(\boldsymbol{E}_F - \boldsymbol{V}_F \mid \boldsymbol{k} \mid)$$

Short-range scatterers

2d case



 $\boldsymbol{\tau}$: relaxation time

$$1/\tau_0 \propto \rho(E_F) \propto E_F$$

$$\sigma = \frac{2e^2}{h}E_F \tau \propto \frac{E_F}{E_F}$$



Shon & Ando (1998)

$$\hbar / \tau = 2\pi \sum_{\boldsymbol{k}} \left| \left\langle \boldsymbol{k} \mid \boldsymbol{V} \mid \boldsymbol{k}' \right\rangle \right|^2 (1 - \hat{\boldsymbol{k}} \cdot \hat{\boldsymbol{k}}') \delta(\boldsymbol{E}_F - \boldsymbol{V}_F \mid \boldsymbol{k} \mid)$$

Short-range scatterers

 $V(\boldsymbol{r}) = \sum_{j} u_{j} \delta(\boldsymbol{r} - \boldsymbol{R}_{j})$

2d case

$$1/_{\tau_0} \propto \rho(E_F) \propto E_F$$

$$\sigma = \frac{2e^2}{h}E_F \tau \propto \frac{E_F}{E_F}$$

Coulomb scatterers

$$V(\boldsymbol{q}) = \sum_{j} \frac{2\pi \boldsymbol{e}^2}{\boldsymbol{q}^{d-1}} \exp(-i\boldsymbol{q}\cdot\boldsymbol{R}_j)$$

$$\frac{1}{\tau_c} \propto (1/k_F^2) \rho_F \propto \frac{1}{E_F}$$

$$\sigma = \frac{2e^2}{h} E_F \tau \propto E_F^2 \propto k_F^2 \propto n$$

KN-MacDonald (2006) Ando (2006)



$$\hbar / \tau = 2\pi \sum_{\boldsymbol{k}} \left| \left\langle \boldsymbol{k} \mid \boldsymbol{V} \mid \boldsymbol{k}' \right\rangle \right|^2 (1 - \hat{\boldsymbol{k}} \cdot \hat{\boldsymbol{k}}') \delta(\boldsymbol{E}_F - \boldsymbol{V}_F \mid \boldsymbol{k} \mid)$$

Short-range scatterers

 $V(\boldsymbol{r}) = \sum_{j} u_{j} \delta(\boldsymbol{r} - \boldsymbol{R}_{j})$

2d case

3d Weyl SM

$$1/_{\tau_0} \propto \rho(E_F) \propto E_F$$

$$\frac{1}{\tau_0} \propto \rho(E_F) \propto E_F^2$$

$$\sigma = \frac{2e^2}{h}E_F \tau \propto \frac{E_F}{E_F}$$

 $\sigma \propto \frac{E_F^2}{E_F^2}$

Coulomb scatterers

$$V(\boldsymbol{q}) = \sum_{j} \frac{2\pi \boldsymbol{e}^2}{\boldsymbol{q}^{d-1}} \exp(-i\boldsymbol{q}\cdot\boldsymbol{R}_j)$$

$$\frac{1}{\tau_c} \propto (1/k_F^2) \rho_F \propto \frac{1}{E_F}$$

$$\sigma = \frac{2e^2}{h} E_F \tau \propto E_F^2 \propto k_F^2 \propto n$$

$$\frac{1}{\tau_c} \propto (1/k_F^4) \rho_F \propto \frac{1}{E_F^2}$$

 $\sigma \propto E_{F} \propto n^{1/3}$

Burkov-Hook-Balents (2011)

Charge transport of Weyl fermions

From 2d to 3d

topics

- Impurity scattering
- Quantum effect (localization)
- Anomalous Hall effect

Anderson localization?

$$H = -i\vec{\sigma} \cdot \vec{\nabla} + V_0(\boldsymbol{x}) + \vec{\sigma} \cdot \vec{a}(\boldsymbol{x})$$



Anderson localization?

 $H = -i\vec{\sigma}\cdot\vec{\nabla} + V_0(\mathbf{x}) + \vec{\sigma}\cdot\vec{a}(\mathbf{x})$



Anderson localization?

 $H = -i\vec{\sigma}\cdot\vec{\nabla} + V_0(\mathbf{x}) + \vec{\sigma}\cdot\vec{a}(\mathbf{x})$



 No numerical study has been done for 3d Weyl SM systems

-Effective field theory (class A)

$$S = \int d^{2}x \, \frac{g}{8} \operatorname{tr} \left[(\partial_{\mu} Q)^{2} \right] + S_{\text{Prueskin}}^{\text{topo}}$$

$$\operatorname{3d case} S = \int d^{3}x \, \frac{g}{8} \operatorname{tr} \left[(\partial_{\mu} Q)^{2} \right] + S_{WZW}^{\text{topo}}$$

Charge transport of Weyl fermions

From 2d to 3d

topics

- Impurity scattering
- Quantum effect (localization)
- Anomalous Hall effect

AHE = Hall effect without external B field



 $H_{2d}(k_x,k_y) = \vec{R}(k_x,k_y) \cdot \vec{\sigma}$

2d case

Massive Dirac -> AHE



 $H_{2d}(k_x,k_v) = \vec{R}(k_x,k_v)\cdot\vec{\sigma}$





$$H_{weyl}(k_x, k_y, k_z) = k_x \sigma_1 + k_y \sigma_2 + \Delta_m(k_z) \sigma_3$$

3d Weyl SM





$$H_{weyl}(k_{x'},k_{y'},k_{z}) = k_{x}\sigma_{1} + k_{y}\sigma_{2} + \Delta_{m}(k_{z})\sigma_{3}$$



$$H_{weyl}(k_{x'},k_{y'},k_{z}) = k_{x}\sigma_{1} + k_{y}\sigma_{2} + \Delta_{m}(k_{z})\sigma_{3}$$
$$\sigma_{xy}^{2D}(k_{z}) = \frac{e^{2}}{2h}[1 - \operatorname{sgn}(\Delta_{m}(k_{z}))]$$



$$H_{weyl}(k_x,k_y,k_z) = k_x\sigma_1 + k_y\sigma_2 + \Delta_m(k_z)\sigma_3$$

$$\sigma_{xy}^{2D}(k_z) = \frac{\mathbf{e}^2}{2h} [1 - \operatorname{sgn}(\Delta_m(k_z))]$$

Kubo formula by D. Kurebayashi



$$\sigma_{xy}^{3D} = \int \frac{dk_z}{2\pi} \sigma_{xy}^{2D}(k_z)$$
$$= \frac{e^2}{h} 2K_w$$

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Adler-Bell-Jackiw anomaly

1D Weyl fermions

$$H_{1D} = \int dx \ \psi^{+} \left[-i(\partial_{x} + ieA_{x}) \right] \psi$$
$$\frac{dN}{dt} = \int dx \frac{-e}{2\pi} E$$



N: particle number

3D Weyl fermions

$$H_{3D} = \int d^{3}x \ \psi^{+} \Big[-i\vec{\sigma} \cdot (\vec{\nabla} + ie\vec{A}) \Big] \psi$$
$$\frac{dN}{dt} = \int d^{3}x \frac{e^{2}}{(2\pi)^{2}} \boldsymbol{E} \cdot \boldsymbol{B}$$

3D Weyl semimetals

$$H = \begin{pmatrix} \vec{\sigma} \cdot (\vec{p} + e\vec{A} + \underline{J}\vec{M}) & 0 \\ 0 & -\vec{\sigma} \cdot (\vec{p} + e\vec{A} - \underline{J}\vec{M}) \end{pmatrix}$$

"chiral vector potential"

$$\partial_{\mu} j^{\mu} = \frac{\mathbf{e}^{2}}{4\pi^{2}} \varepsilon^{\mu\nu\rho\lambda} F_{\mu\nu} \partial_{\rho} (\underline{J}\underline{M}_{\lambda})$$
$$= \partial_{\mu} \left(\frac{\mathbf{e}^{2}}{4\pi^{2}} \varepsilon^{\mu\nu\rho\lambda} JM_{\lambda} F_{\rho\nu} \right)$$

Zyusin & Burkov (2012)

3D Weyl semimetals $H = \begin{pmatrix} \vec{\sigma} \cdot (\vec{p} + e\vec{A} + J\vec{M}) & 0 \\ 0 & -\vec{\sigma} \cdot (\vec{p} + e\vec{A} - J\vec{M}) \end{pmatrix}^{E}$

"chiral vector potential"

$$\partial_{\mu} j^{\mu} = \frac{\mathbf{e}^{2}}{4\pi^{2}} \varepsilon^{\mu\nu\rho\lambda} F_{\mu\nu} \partial_{\rho} (\underline{JM}_{\lambda})$$
$$= \partial_{\mu} \left(\frac{\mathbf{e}^{2}}{4\pi^{2}} \varepsilon^{\mu\nu\rho\lambda} JM_{\lambda} F_{\rho\nu} \right)$$
$$j^{\mu}_{AHE}$$

 $\vec{j}_{AHE} = \frac{\mathbf{e}^2}{2\pi h} J \vec{M} \times \vec{E}$ $\rho_{AHE} = \frac{\mathbf{e}^2}{2\pi h} J \vec{M} \cdot \vec{B}$

k_z

Zyusin & Burkov (2012)

k_x





Liu, Ye, Qi (2013)

Interaction effects

Topological Mott insulators

Raghu et. al. (2006) Shitade et. al. (2008) Pesin&Balents (2010) Kurita, Yamaji, Imada (2011) Yoshida et al. (2013) Miyakoshi&Ohta (2013)

On-site U enhances SOC, causing a "topological Mott insulator" phase

Other ground states

Li, Wang, Qi, Zhang (2010) Ooguri&Oshikawa (2012) Sekine&KN (2014)

> Axion Magneto-electric effect, Aoki phase (QCD analogy)





Interaction effects



Summary

Weyl semimetal is a novel gapless topological state

Weyl semimetal could be realized in Bi_2Se_3 family (Cr-doped $Bi_2(Se_xTe_{1-x})_3$)

Novel quantum transport phenomena are expected

- Anderson (de)localization
- Anomalous Hall effect (chiral anomaly)

Effects of electron-electron interaction

- short range repulsion
- long range Coulomb interaction