日本物理学会2010年秋季大会、大阪府立大学中百舌鳥キャンパス、2010.9.23-26

多バンド系でのディラック電子：有機導体および鉄系超伝導体

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共同研究者

兼下英司、遠山貴巳

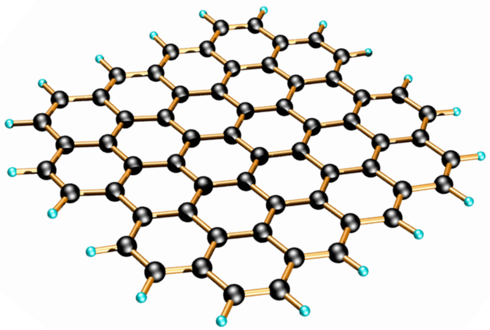
京都大学基礎物理学研究所

事の発端

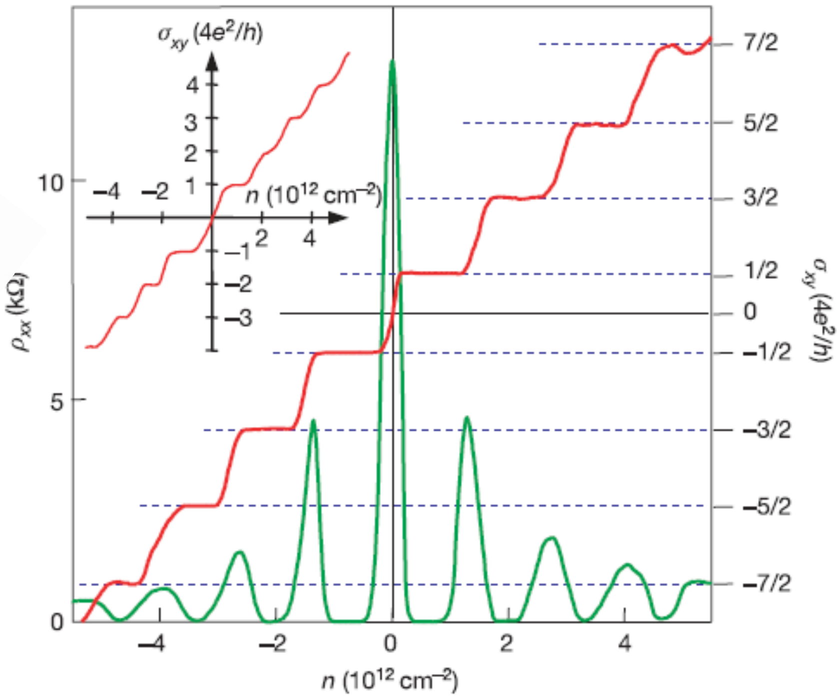
Grapheneでの
Half-Integer Quantum Hall 効果の観測

K. S. Novoselov et al., Nature **438**, 197 (2005).

Y. Zhang et al., Nature **438**, 201 (2005).



graphene



$$\sigma_{xy} = 4\left(n + \frac{1}{2}\right)\frac{e^2}{h}$$

固体中のDirac電子？

- どんなときに出てくるか？
- 普通の電子と何が違うか？
- 何が面白いか？

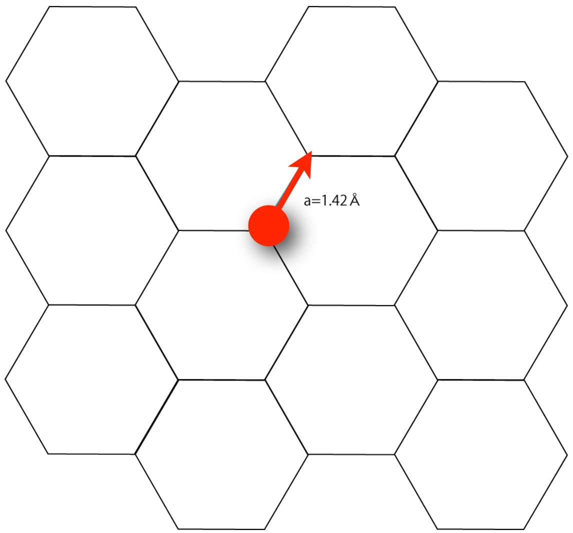
Outline

1. Dirac fermion in graphene
2. Dirac fermion in α-(BEDT-TTF)$_2$I$_3$
3. Dirac fermion in iron-based superconductors

1. Dirac fermions in graphene

出自のはっきりしたDirac電子

蜂の巣格子上の電子

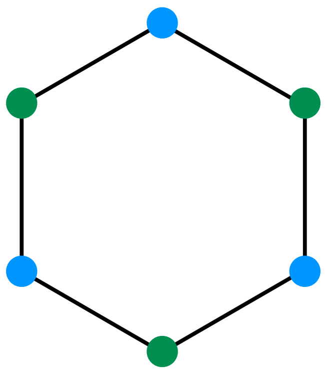


$$H = -t\sum_{j\in A}\sum_{\delta=\mathbf{a}_1,\mathbf{a}_2,\mathbf{a}_3}\left(c^\dagger_{Aj}c_{B,j+\delta} + h.c\right)$$

$$= \sum_k\left(\kappa_k c^\dagger_{Ak}c_{Bk} + h.c\right)$$

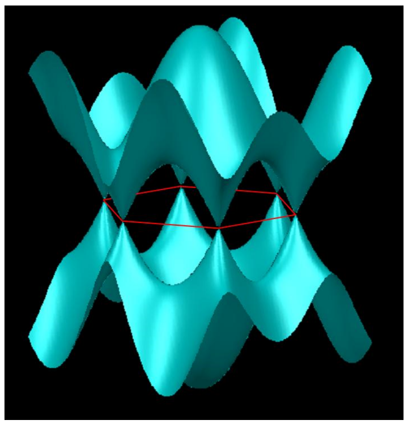
$$\kappa_k = -t\left[e^{ik_x a} + e^{i\left(-\frac{1}{2}k_x a+\frac{\sqrt{3}}{2}k_y a\right)} + e^{-i\left(\frac{1}{2}k_x a+\frac{\sqrt{3}}{2}k_y a\right)}\right]$$

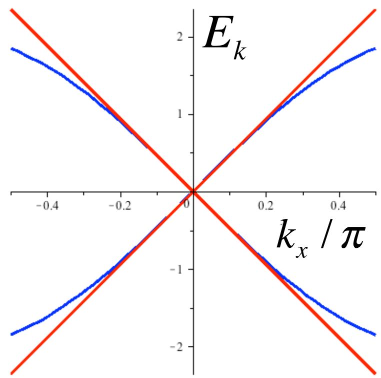
$$t = 2.8\mathrm{eV}$$



$$K = \frac{2\pi}{3a}\left(1,\frac{1}{\sqrt{3}}\right)$$

$$K' = \frac{2\pi}{3a}\left(1,-\frac{1}{\sqrt{3}}\right)$$





Dirac電子のHamiltonian

$$H = \sum_k c_k^\dagger H_k c_k$$

$$H_{K+k} = \hbar v_F \begin{pmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{pmatrix} \qquad H_{K'+k} = \hbar v_F \begin{pmatrix} 0 & k_x + ik_y \\ k_x - ik_y & 0 \end{pmatrix}$$

通常の電子

$$H_k = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2\right)$$

- 2x2行列：擬スピン空間(A,B副格子)
- 本家Dirac電子との違い？

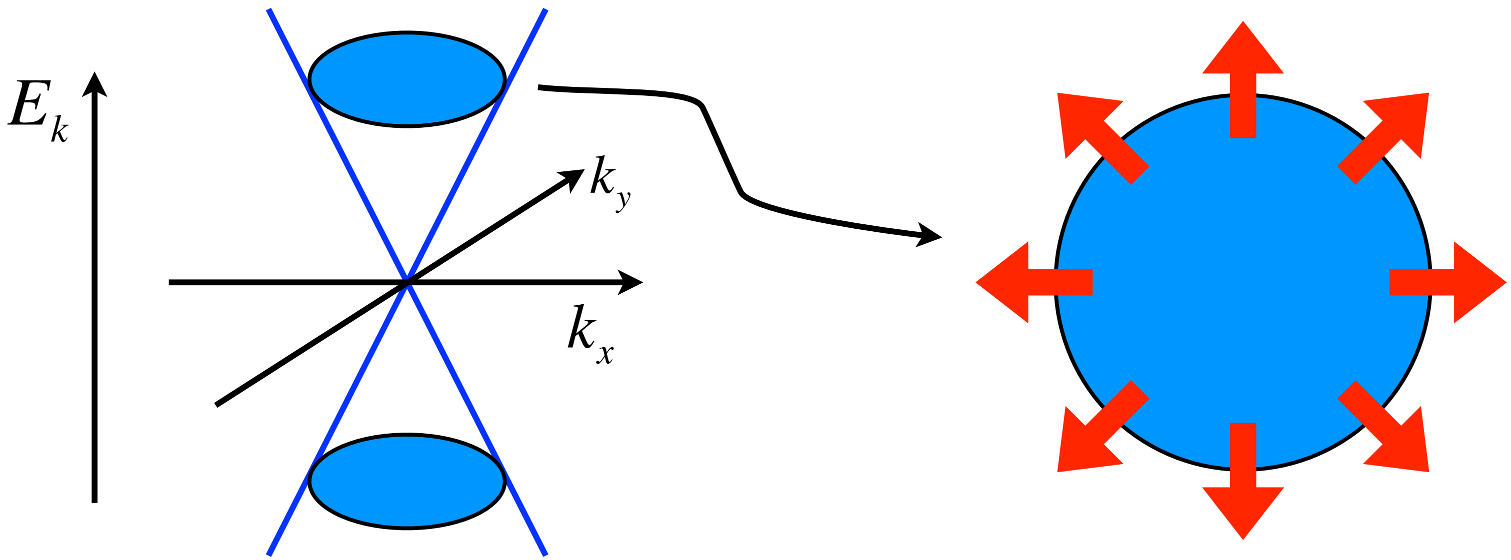
$$c \rightarrow v_F \simeq c / 300$$

普通の電子と何が違うか？

Chirality

$$H = \hbar v_F \begin{pmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{pmatrix} = \hbar v_F \mathbf{k} \cdot \boldsymbol{\sigma}$$

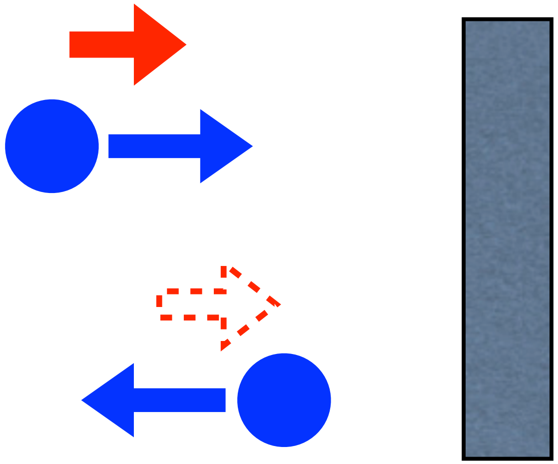
k方向の"磁場"



Chiralityの効果

後方散乱の消失

T. Ando, T. Nakanishi, and R. Saito,
J. Phys. Soc. Jpn. 67, 2857 (1998).

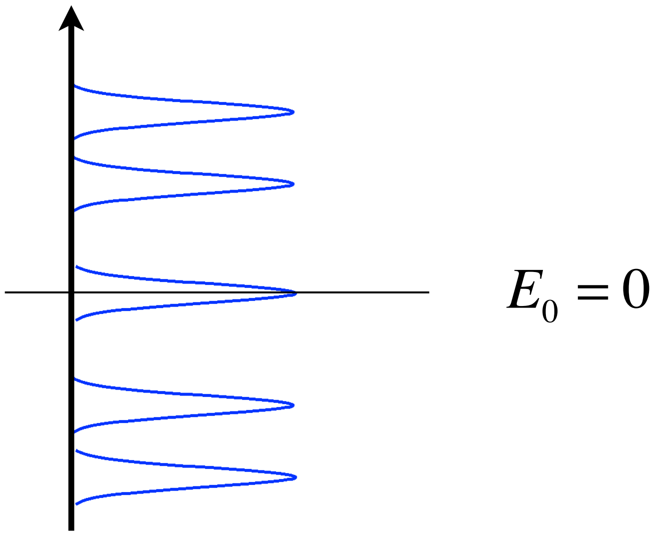


Berry 位相

$$\left|\mathbf{k},s\right\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{i\theta_{\mathbf{k}}/2} & 0 \\ 0 & e^{-i\theta_{\mathbf{k}}/2} \end{pmatrix}\begin{pmatrix} 1 \\ s \end{pmatrix} \longrightarrow \pi$$

Landau準位

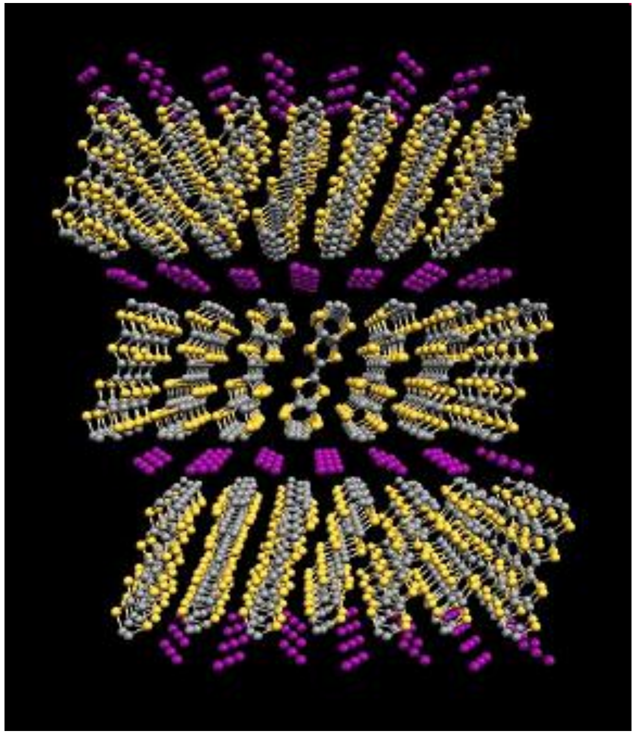
$$E_n = \mathrm{sgn}(n)\sqrt{2e\hbar v_F^2 |n| B}$$



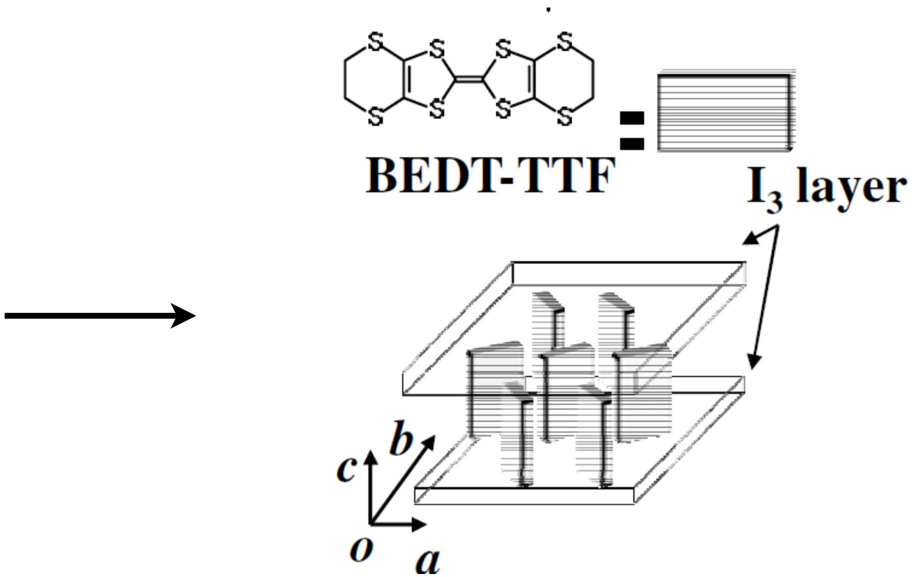
2. Dirac fermion in α-(BEDT-TTF)$_2$I$_3$

bulkのDirac電子

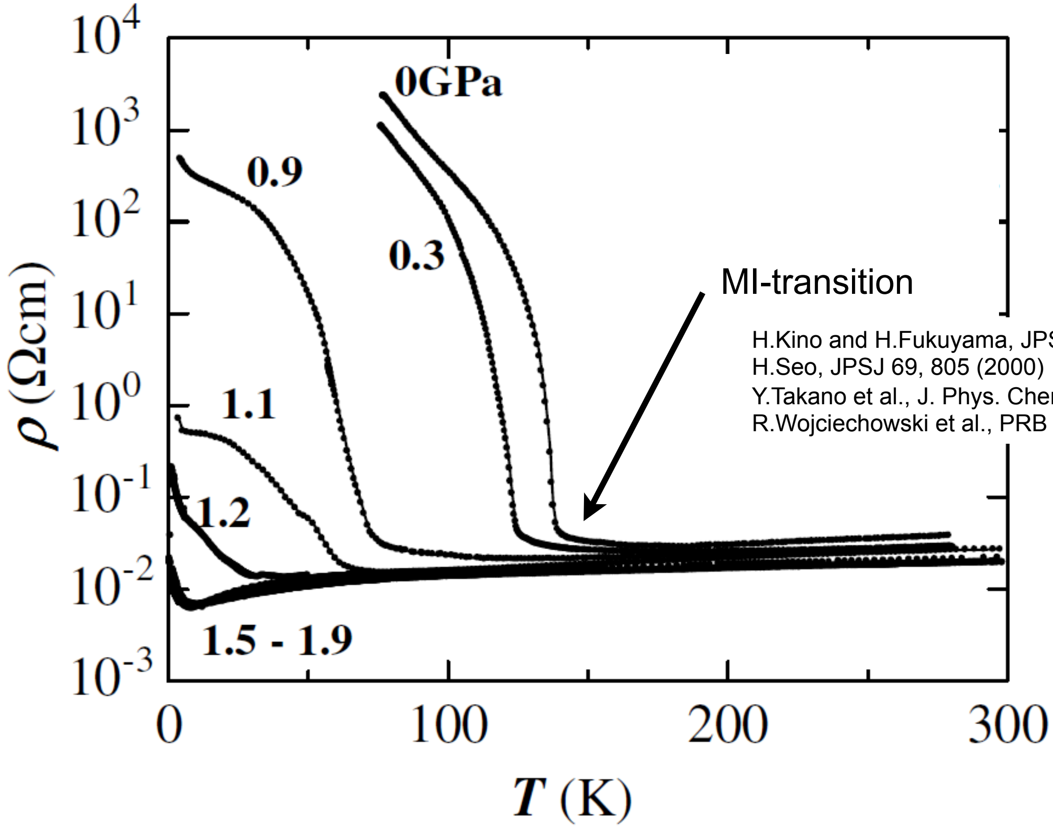
有機導体α-(BEDT-TTF)$_2$I$_3$の構造



Courtesy of N. Tajima (RIKEN)



電気抵抗の圧力依存性

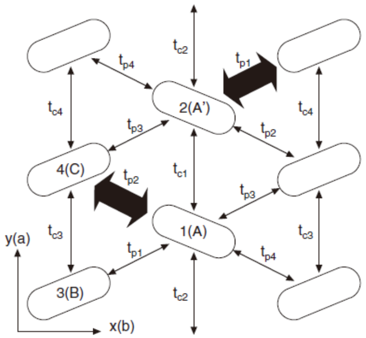


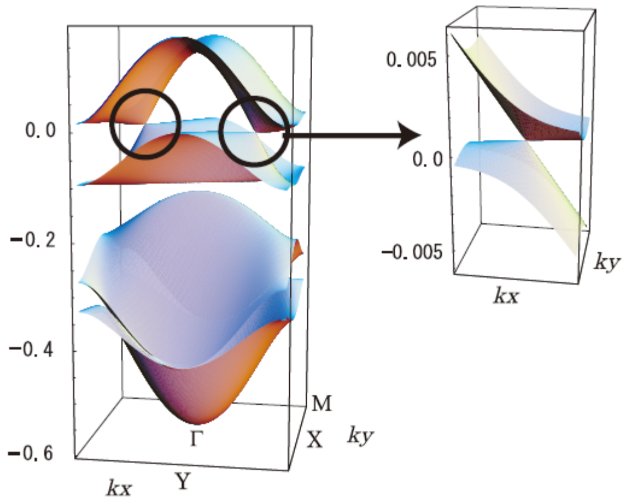
H.Kino and H.Fukuyama, JPSJ 64, 1877 (1995)
H.Seo, JPSJ 69, 805 (2000)
Y.Takano et al., J. Phys. Chem. Solid 62, 393 (2001)
R.Wojciechowski et al., PRB 67, 224105 (2003)

N. Tajima *et al*., Europhys. Lett. **80**, 47002 (2007)

圧力下の理論計算

Tight-binding model





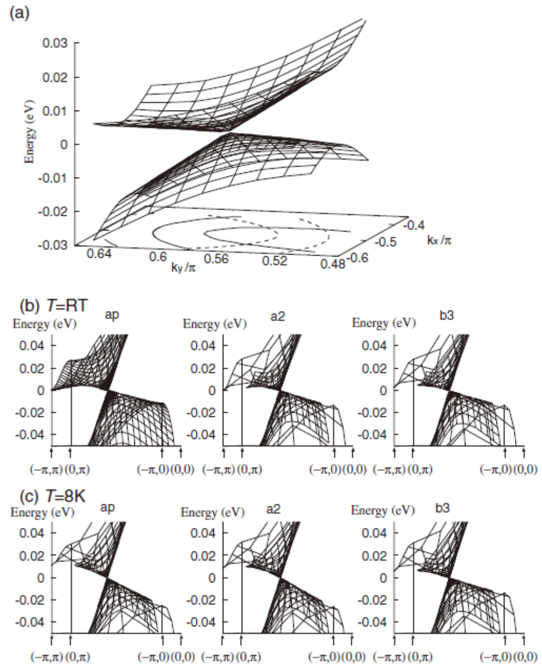
A. Kobayashi et al., JPSJ **73**, 3135 (2004)

S. Katayama, A. Kobayashi, and Y. Suzumura,
JPSJ **75**, 054705 (2006)

hoppingの圧力依存性

R. Kondo, S. Kagoshima, and J. Harada,
Rev. Sci. Instrum. 76, 093902 (2005).

第一原理計算

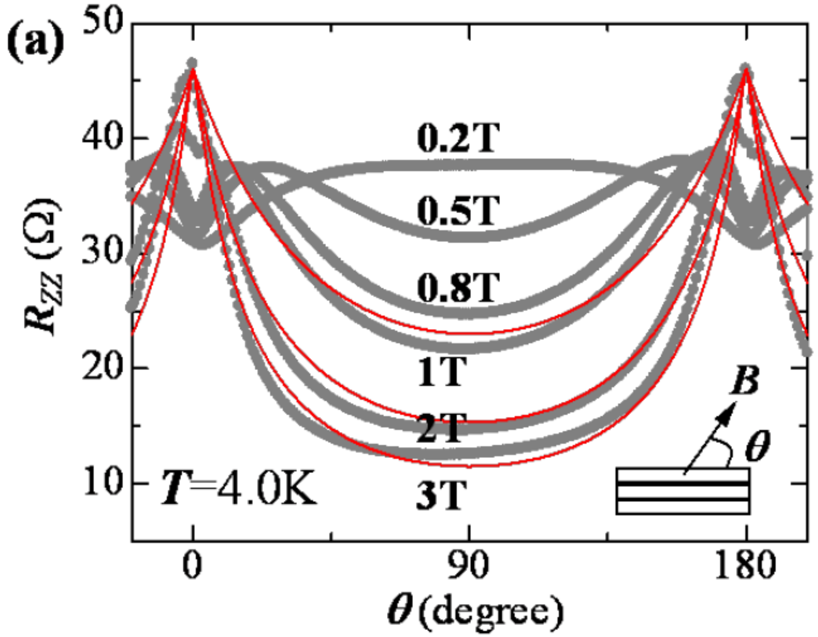


H. Kino and T. Miyazaki, J. Phys. Soc. Jpn. **75**, 034704 (2006)

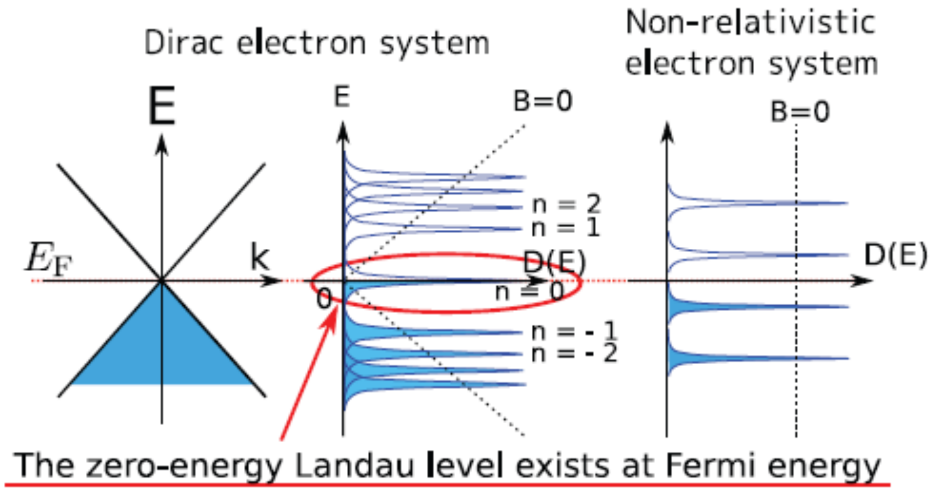
S. Ishibashi *et al*, J. Phys. Soc. Jpn. **75** ,015005 (2006)

実験？

面間磁気抵抗



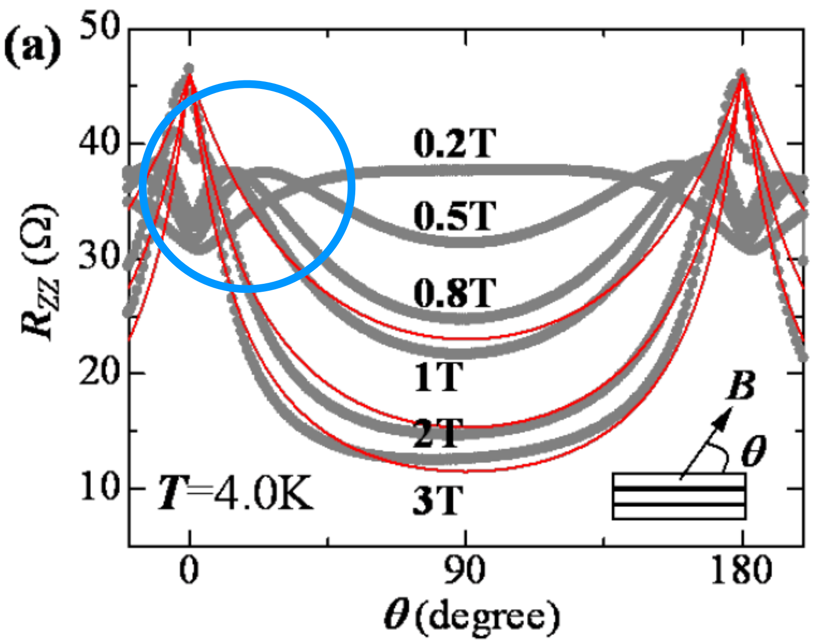
N. Tajima *et al*., PRL **102**, 176403 (2009).



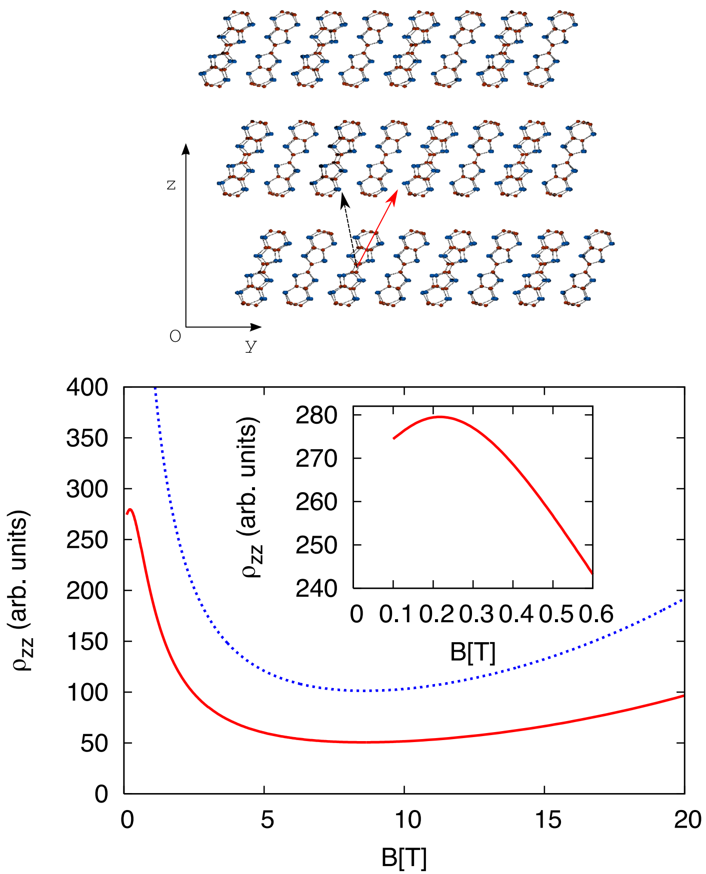
ゼロエネルギーLandau準位！

T. Osada, JPSJ **77**, 084711 (2008).

正の磁気抵抗領域？



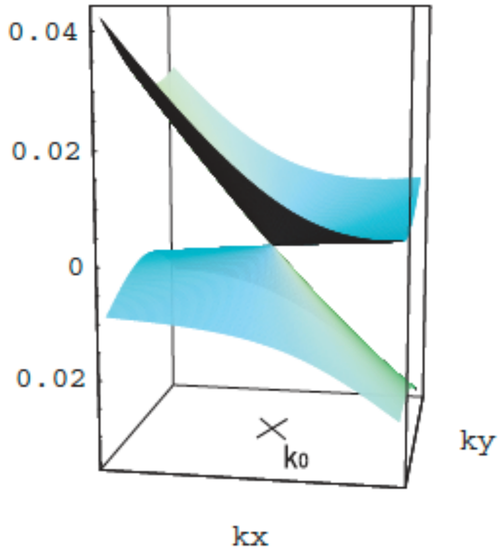
N. Tajima *et al.*, PRL **102**, 176403 (2009).

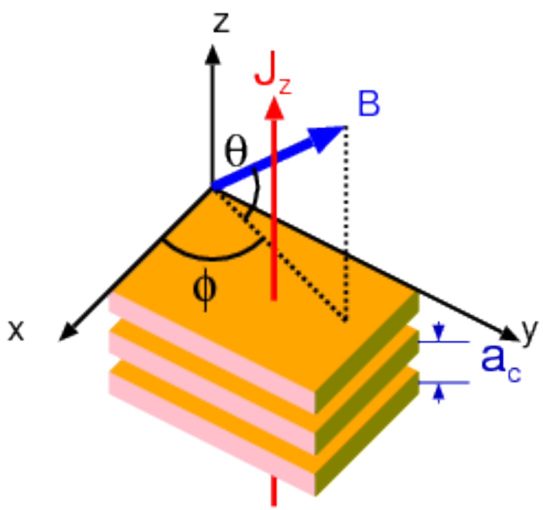


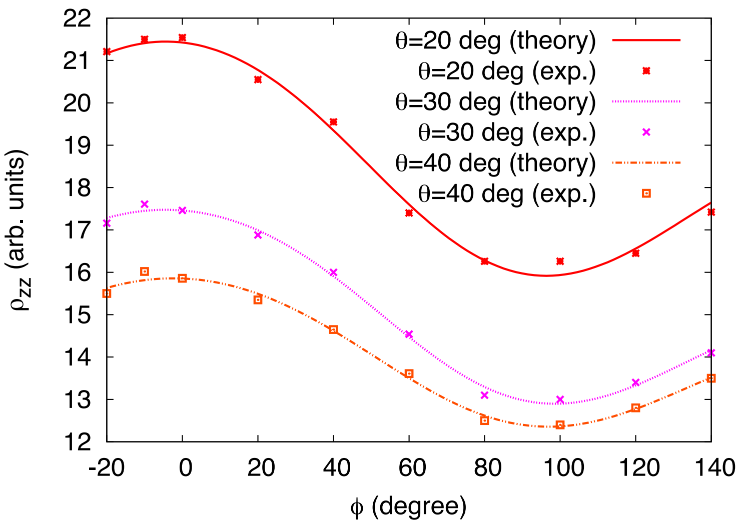
TM and T. Tohyama, J. Phys. Soc. Jpn. 79, 044708 (2010)

Landau準位間遷移

Dirac coneの傾き？

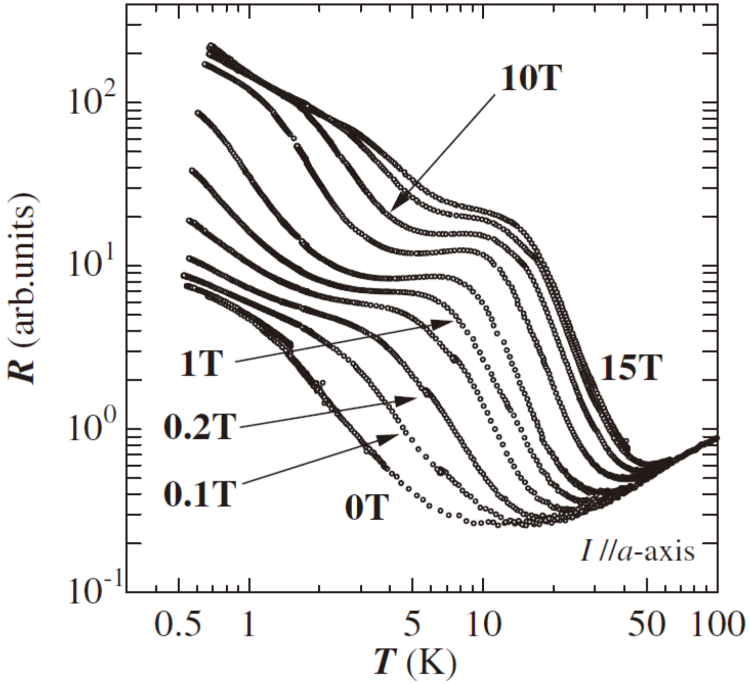




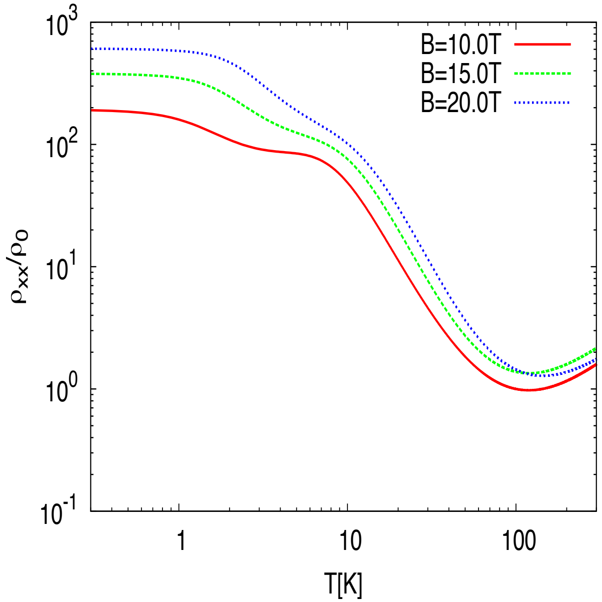


TM, T.Himura, and T. Tohyama,
J. Phys. Soc. Jpn. 78, 023704 (2009)

面内磁気抵抗？



N.Tajima *et al.*, JPSJ **75**, 051010 (2006)



TM and T. Tohyama, arXiv:1006.0567

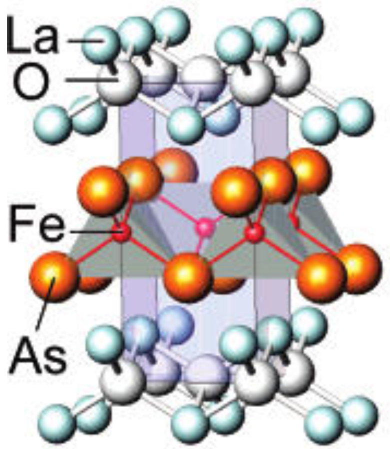
Dirac電子のLandau準位構造＋相互作用

3. Dirac fermion in iron-based superconductors

軌道に関連したDirac電子

鉄系超伝導体

$LaFeAsO_{1-x}F_x$ (1111)



Y. Kamihara, T. Watanabe, M. Hirano, and H. Hosono, J. Am. Chem. Soc. 130, 3296 (2008)

$$T_c \sim 26\mathrm{K}$$

$R\mathrm{FeAs}(\mathrm{O}_{1-x}\mathrm{F}_x)$ K.Ishida, Y.Nakai, and H.Hosono, J. Phys. Soc. Jpn. 78, 062001 (2009)

	R							
	La	Ce	Pr	Nd	Sm	Gd	Tb	Dy
T_c^{Max} (K)	28	41	52	52	55	36	46	45
x	0.11	0.16	0.11	0.11	0.1	0.17	0.1	0.1
			[3]	[2]	[1]		[4]	

[1] Z.-A.Ren et al., Chin. Phys. Lett. 25, 2215 (2008)
[2] Z.-A.Ren et al., Europhys. Lett. 82, 57002 (2008)
[3] Z.-A.Ren et al., Mater. Res. Innovations 12, 106 (2008)
[4] J.-W.G.Bos et al., Chem. Commun. 3634 (2008)
…

122 $B^+[(A_{1-x}B_x)Fe_2As_2]$ (A=Ba,Sr,Ca, B=K,Cs,Na)

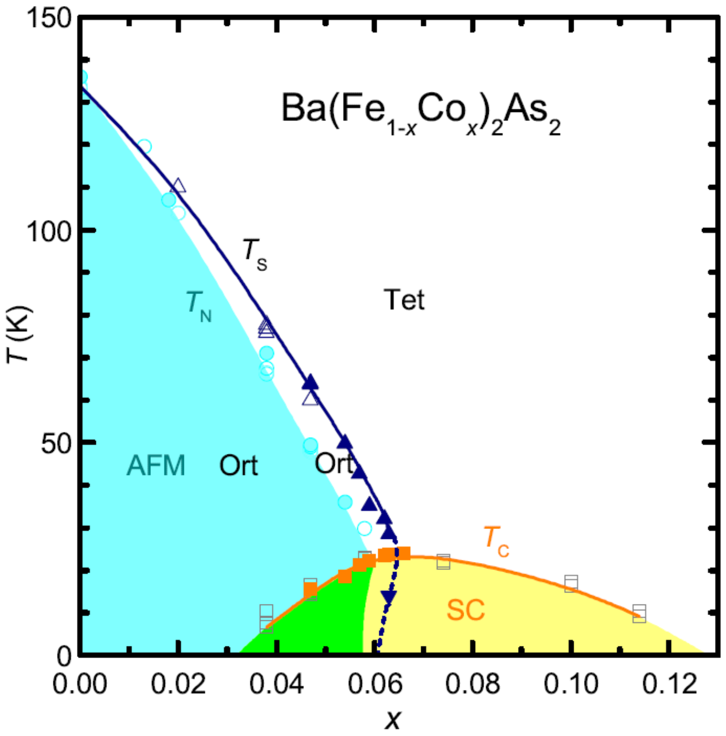
111 LiFeAs, NaFeAs

11 $FeSe_{0.5}Te_{0.5}$

相図

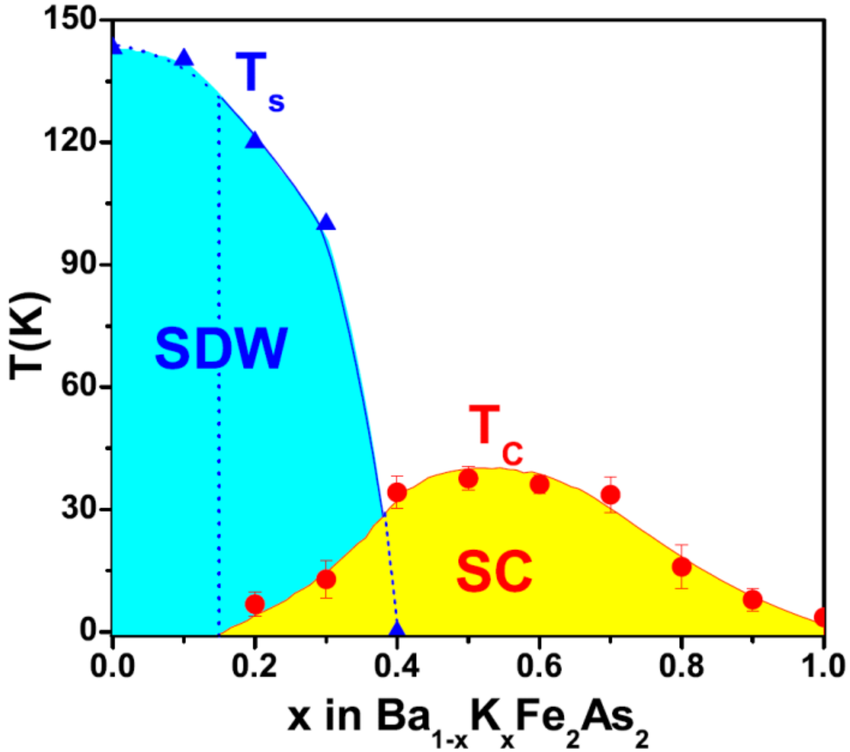
$Ba(Fe_{1-x}Co_x)_2As_2$ Electron “doping”

S. Nandi *et al.*, PRL **104**, 057006 (2010)

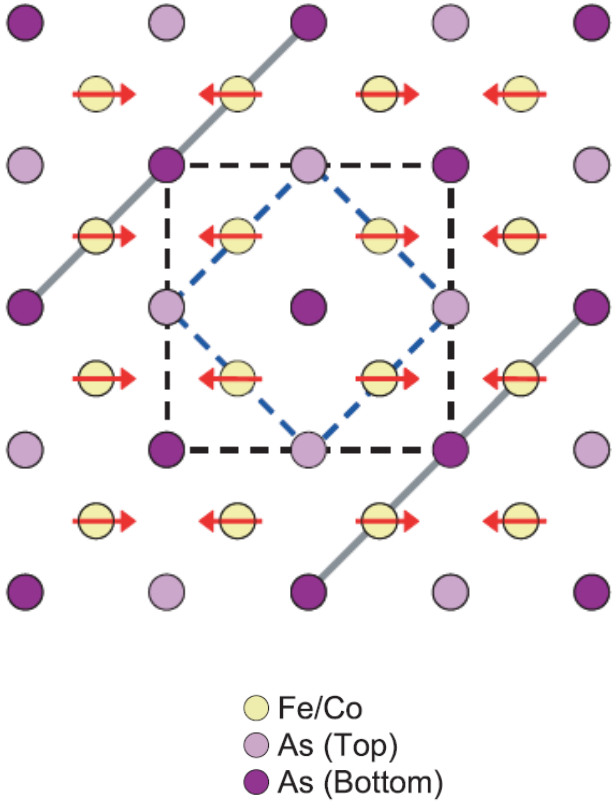


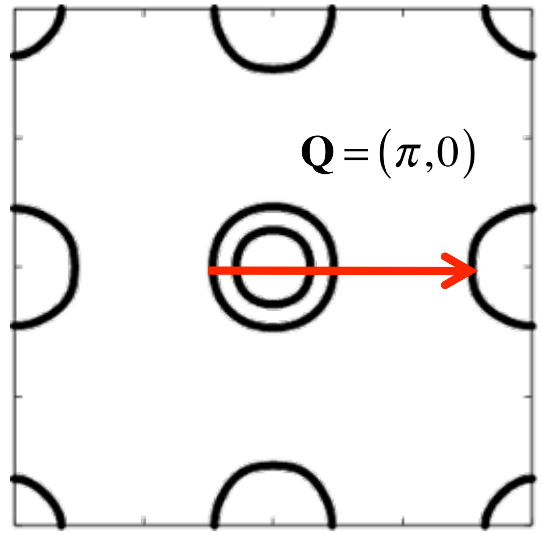
$Ba_{1-x}K_xFe_2As_2$ Hole “doping”

H. Chen *et al.*, Europhys. Lett. **85**, 17006 (2009)



反強磁性相





5-band tight-binding model
[K. Kuroki *et al.*, PRL **101**, 087004 (2008)]

反強磁性相におけるDirac電子？

JPSJ Online—News and Comments [May 12, 2008]

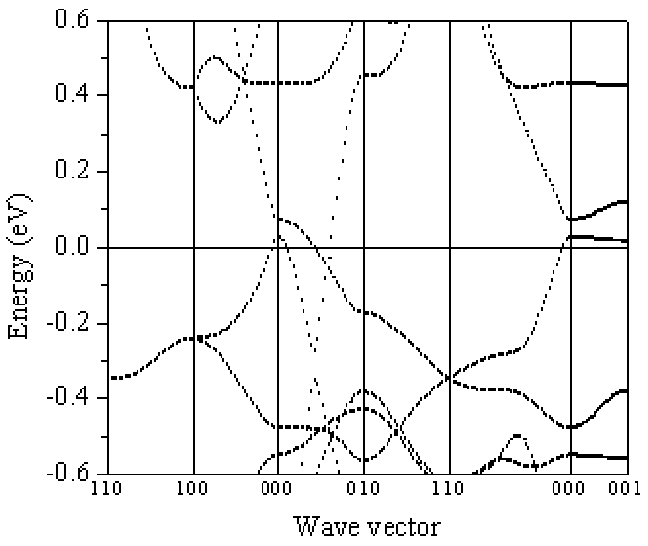
High-Temperature Superconductivity in Another Beautiful Crystal Structure

by **Hidetoshi Fukuyama** (Faculty of Science and Research Institute of Science and Technology, Tokyo University of Science)
Published May 12, 2008

…

When closely examined, the band dispersion near the Fermi energy, as observed in Fig. 2 (taken from Fig. 7 of Ishibashi *et al*. [5]), indicates the very intriguing feature that the system is semimetallic and the crossing of energy bands occurs in the energy region very close to the Fermi energy; the latter appears to be similar to that in molecular solids, αET_2I_3 [9,10], and shows strong enhancement of mobility toward low temperatures, as observed in ref. 7. The fact that the

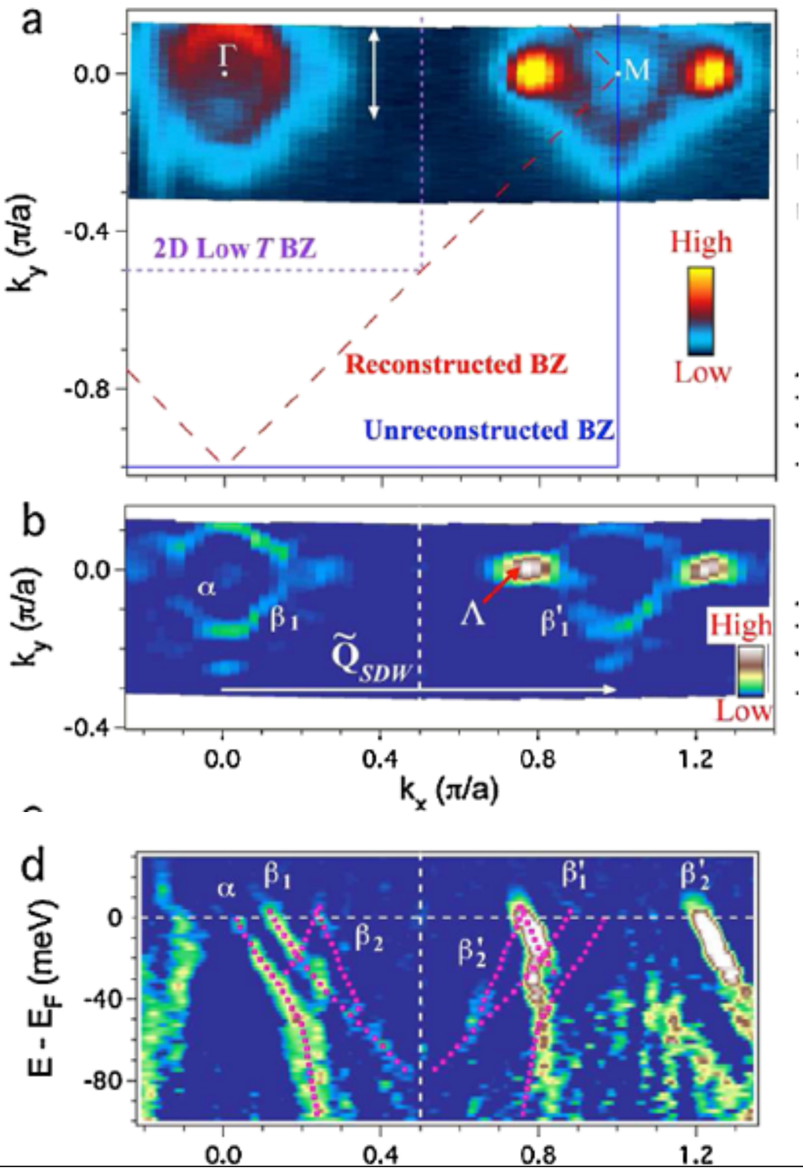
…



S. Ishibashi *et al*.: J. Phys. Soc. Jpn. **77** (2008) 053709.

反強磁性相で現れるDirac電子！

ARPES: $BaFe_2As_2$ P. Richard et al., Phys. Rev. Lett. 104, 137001 (2010).



$$\left(k_x, k_y\right)_{\exp} = (0.785, 0)$$

反強磁性相のバンド分散

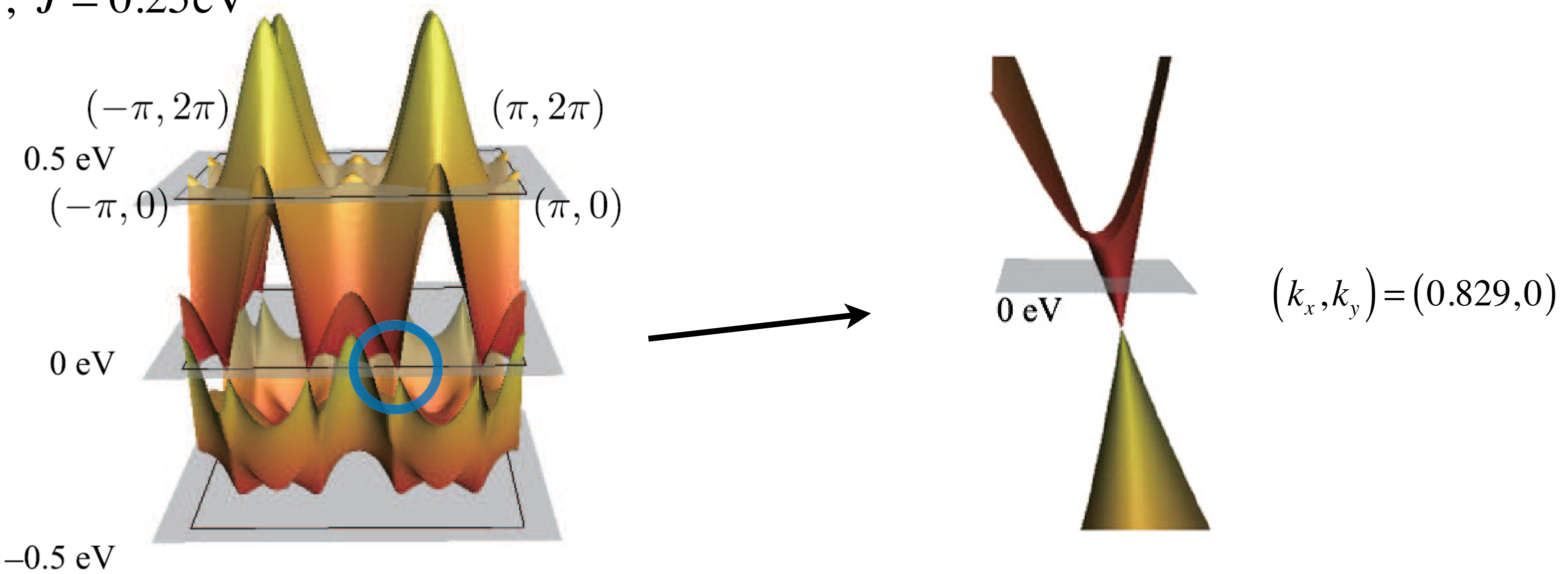
5-band model + SDW mean field theory

Y. Ran et al., PRB 79, 014505 (2009).

E. Kaneshita, TM, and T. Tohyama, PRL 103, 247202 (2009).

$$H_{\mathrm{int}} = U\sum_{j,\mu} n_{j\mu\uparrow}n_{j\mu\downarrow} + (U-2J)\sum_{j,\mu<\nu} n_{j\mu}n_{j\nu}$$
$$+J\sum_{j,\mu<\nu,\alpha,\beta=\uparrow,\downarrow} d^{\dagger}_{j\mu\alpha}d^{\dagger}_{j\nu\beta}d_{j\mu\beta}d_{j\nu\alpha} + J\sum_{j,\mu<\nu}\left(d^{\dagger}_{j\mu\uparrow}d^{\dagger}_{j\mu\downarrow}d_{j\nu\downarrow}d_{j\nu\uparrow} + h.c.\right)$$

$U = 1.2\mathrm{eV},\ J = 0.25\mathrm{eV}$



TM, E. Kaneshita, and T. Tohyama, PRL 105, 037203 (2010).

Dirac点まわりのHamiltonian

Contact point周りで展開　　A. Kobayashi et al., JPSJ 76, 034711 (2007).

$$H_k = H_{k_0+\delta k} = H_{k_0} + \frac{\partial H}{\partial k_x}\delta k_x + \frac{\partial H}{\partial k_y}\delta k_y$$

$$H_k = v_0 k_x + \begin{pmatrix} v_x k_x & v_y k_y \\ v_y k_y & -v_x k_x \end{pmatrix} + E_c$$

$$E_c - E_F = 20\mathrm{meV}$$

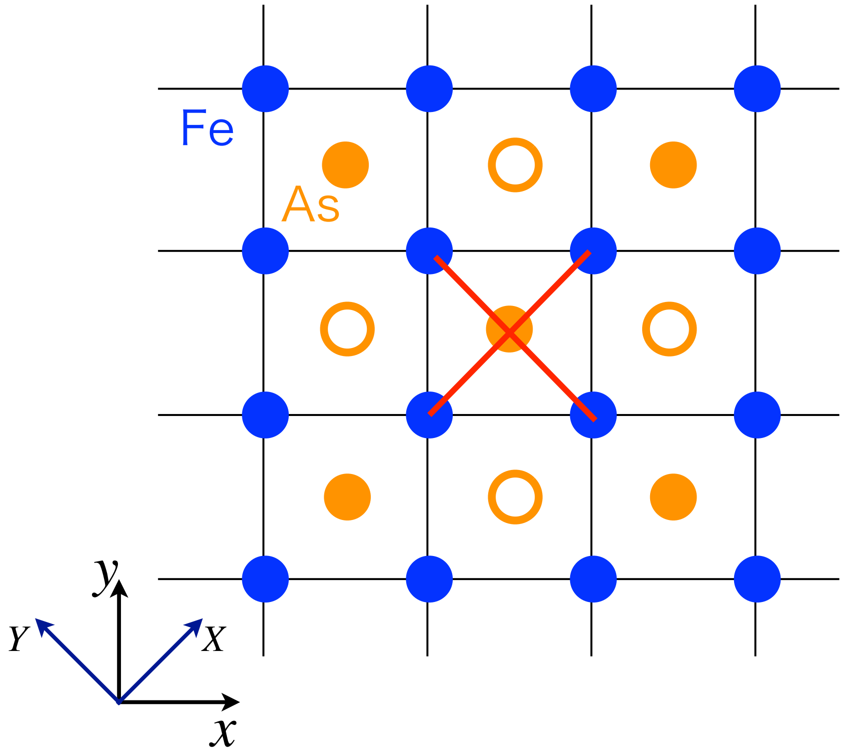
$$v_x / a = 0.672\mathrm{eV}$$

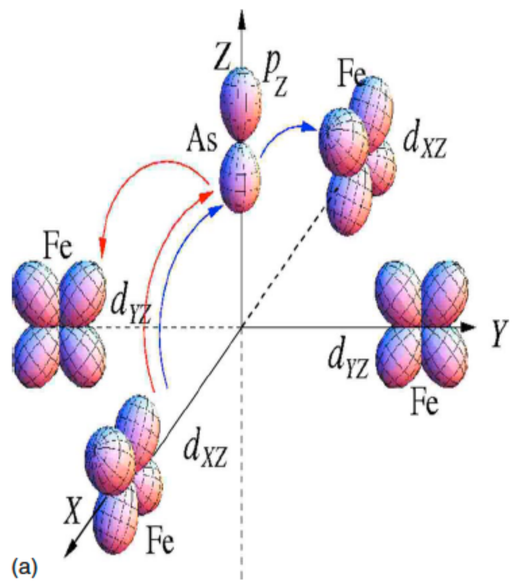
$$v_y / a = 0.229\mathrm{eV}$$

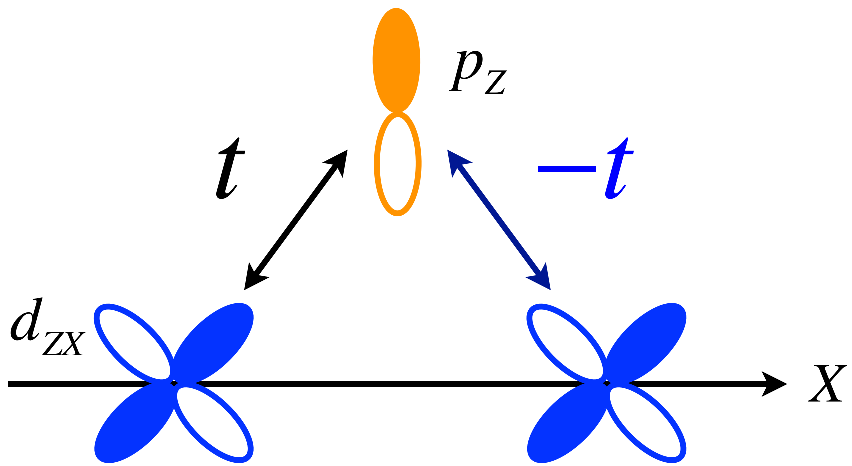
$$v_0 / a = 0.286\mathrm{eV}$$

Dirac電子があらわれるタネ

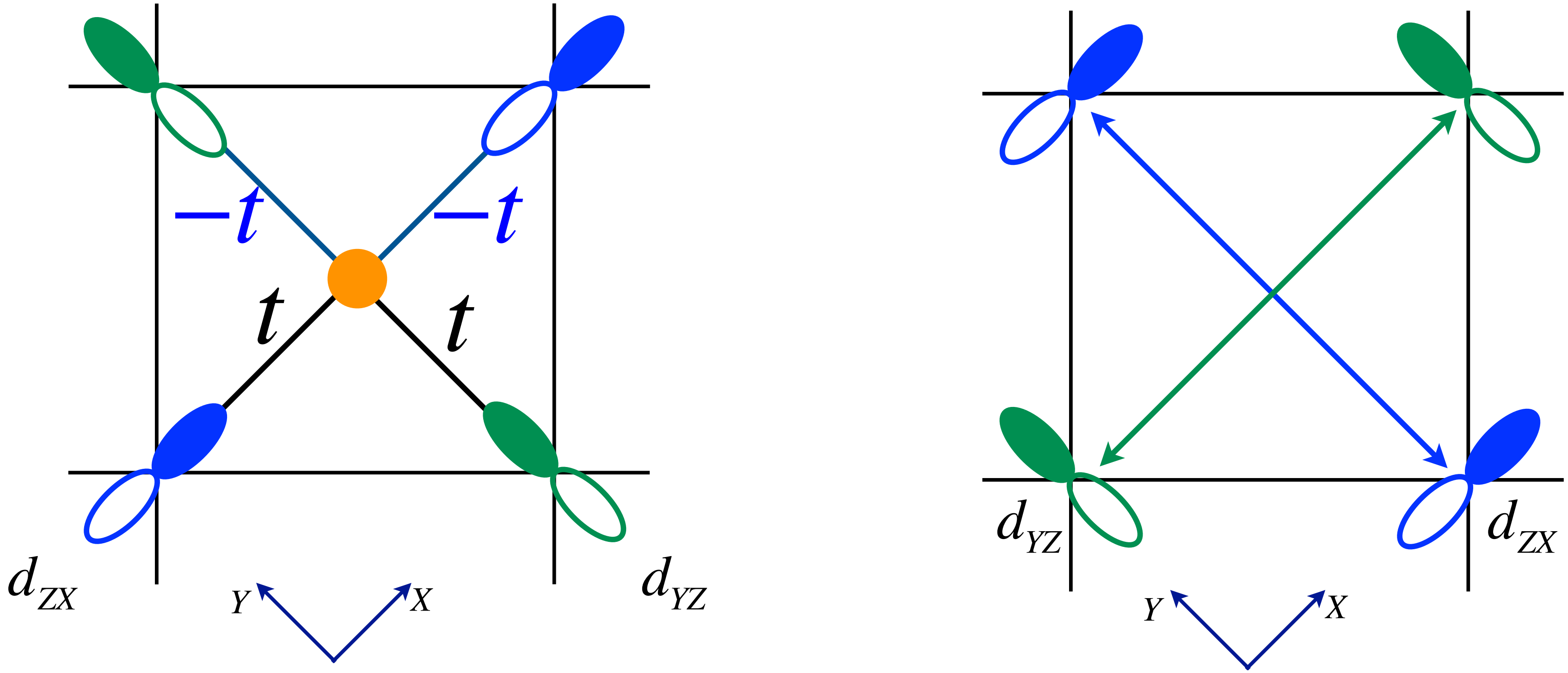
Y. Ran et al., PRB 79, 014505 (2009).







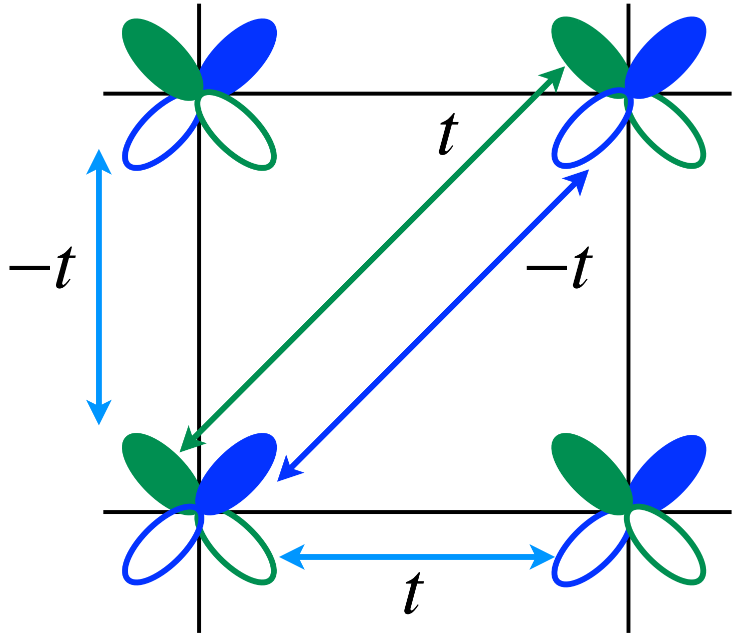
軌道間のhopping



$$\mathcal{H} = \sum_k \begin{pmatrix} d_{ZX}^\dagger(k) & d_{YZ}^\dagger(k) \end{pmatrix} K(k) \begin{pmatrix} d_{ZX}(k) \\ d_{YZ}(k) \end{pmatrix}$$

$$K(k) = \begin{pmatrix} 2t_2 \cos(k_x + k_y) + 2t_2' \cos(k_x - k_y) & 2t_1 (\cos k_x - \cos k_y) \\ 2t_1 (\cos k_x - \cos k_y) & 2t_2 \cos(k_x + k_y) + 2t_2' \cos(k_x - k_y) \end{pmatrix}$$

Chirality



$$K(k) = 4t\begin{pmatrix} \sin k_x \sin k_y & \cos k_x - \cos k_y \\ \cos k_x - \cos k_y & -\sin k_x \sin k_y \end{pmatrix}$$

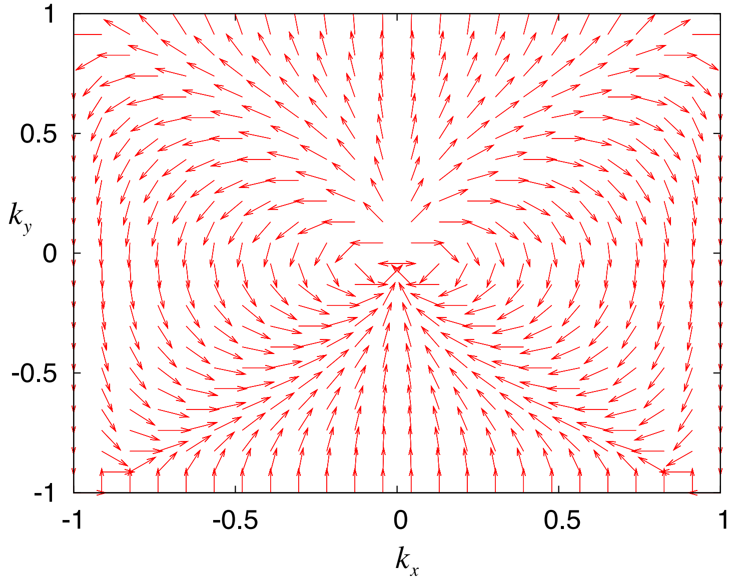
Graphene bilayer

$$|k,+\rangle = \frac{1}{\sqrt{2E_k(E_k + a_k)}}\begin{pmatrix} a_k + E_k \\ b_k \end{pmatrix}$$

$$a_k = \sin k_x \sin k_y$$
$$b_k = \cos k_x - \cos k_y$$
$$E_k = \sqrt{a_k^2 + b_k^2}$$

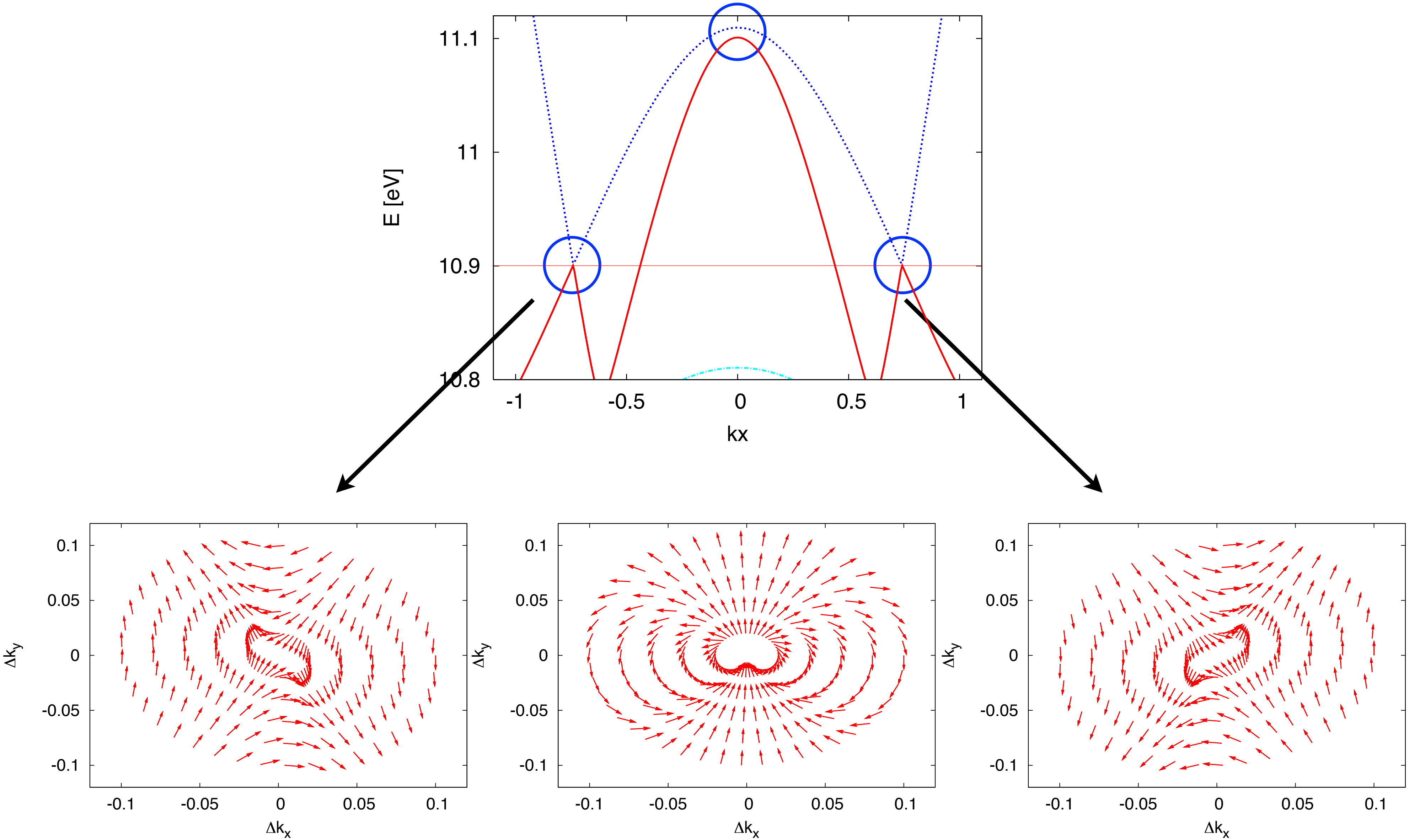
$$n_z = \langle k,+|\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}|k,+\rangle = \frac{a_k}{\sqrt{a_k^2 + b_k^2}}$$

$$n_x = \langle k,+|\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}|k,+\rangle = \frac{b_k}{\sqrt{a_k^2 + b_k^2}}$$



反強磁性状態でのchirality

5-band model + SDW mean field theory

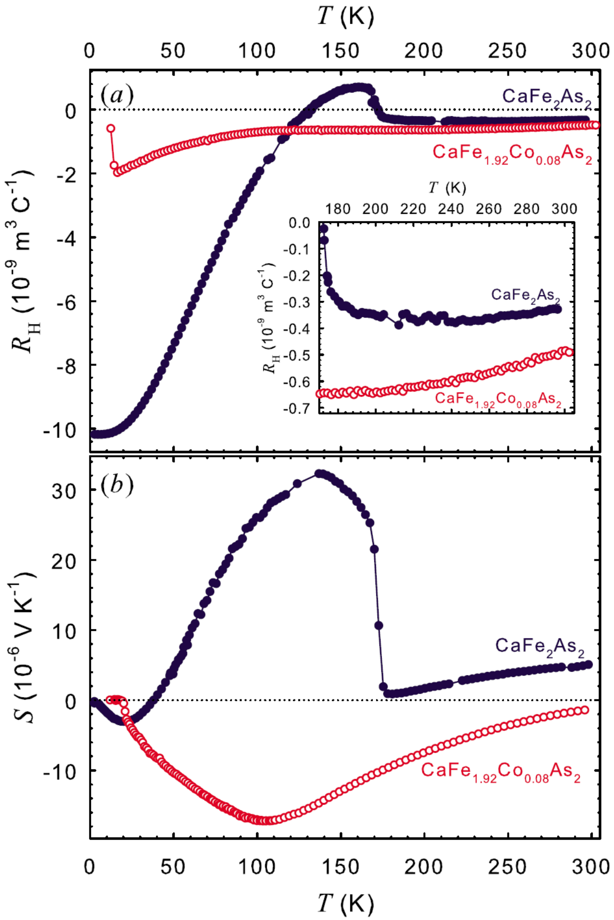


実験？

M. Matusiak et al., PRB **81**, 020510(R) (2010)

ホール係数

熱起電力



⭐低温でどちらも負

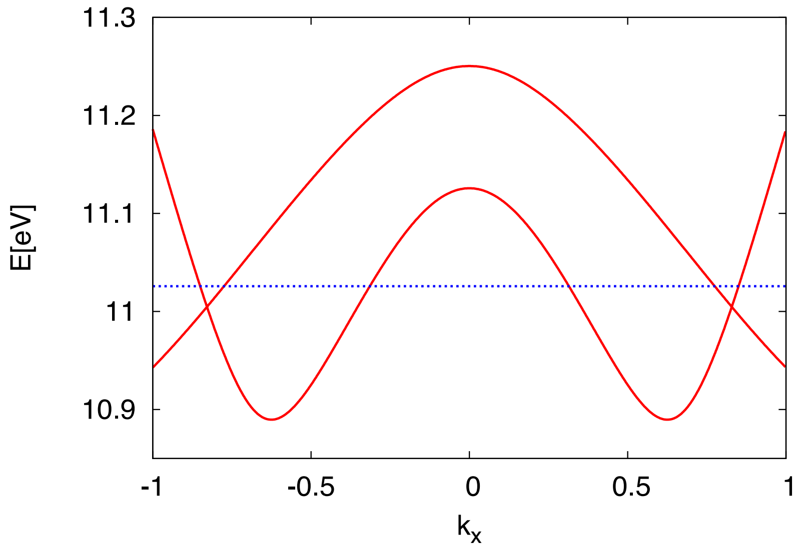
⭐異なる温度で符号反転

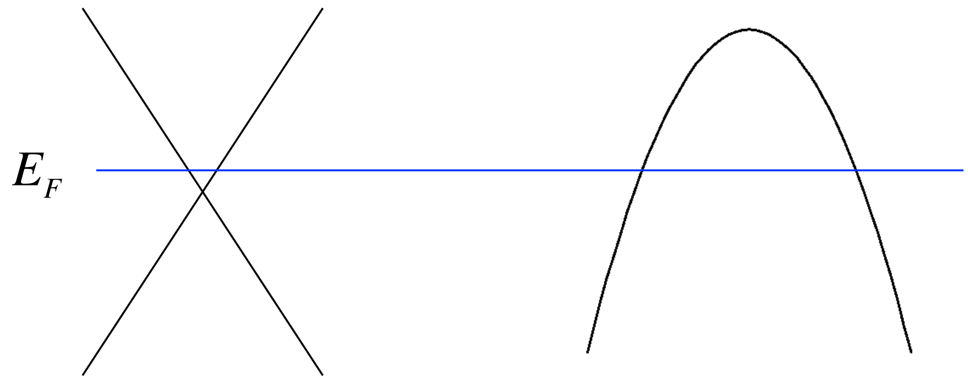
⭐少数、電子キャリア

量子振動の解析

N.Harrison and S.E. Sebastian,
PRB 80, 224512 (2009).

Simplified model





$$\varepsilon_k^{(e)} = vk - \varepsilon_0 \qquad \varepsilon_k^{(h)} = -\frac{k^2}{2m} + \varepsilon_h$$

Formula

ホール係数

$$R_H = \frac{1}{B_z}\frac{\sigma_{xy}}{\sigma_{xx}^2} \qquad \sigma_{xy}^{(e)} + \sigma_{xy}^{(h)}$$

Jones-Zener formula

$$\sigma_{xy} = \frac{e^3 B_z}{\hbar\Omega}\sum_{\mathbf{k}}\left(-\frac{\partial f_{\mathbf{k}}^{(0)}}{\partial \varepsilon_k}\right)\tau_{\mathbf{k}}^2 v_{kx}\left(v_{kx}\frac{\partial v_{ky}}{\partial k_y} - v_{ky}\frac{\partial v_{ky}}{\partial k_x}\right) \qquad \tau^2$$

熱起電力

$$S = \frac{1}{eT}\frac{\frac{1}{\Omega}\sum_{\mathbf{k}}\left(-\frac{\partial f_k}{\partial \varepsilon_k}\right)(\varepsilon_k - \mu)\tau_k v_{kx}^2}{\frac{1}{\Omega}\sum_{\mathbf{k}}\left(-\frac{\partial f_k}{\partial \varepsilon_k}\right)\tau_k v_{kx}^2} \qquad \tau$$

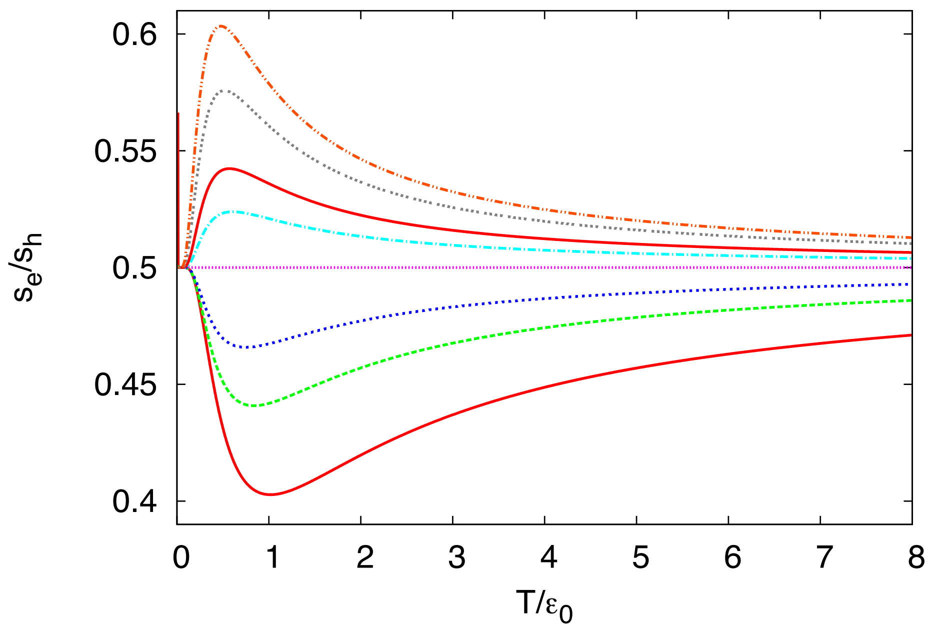
Sign change condition

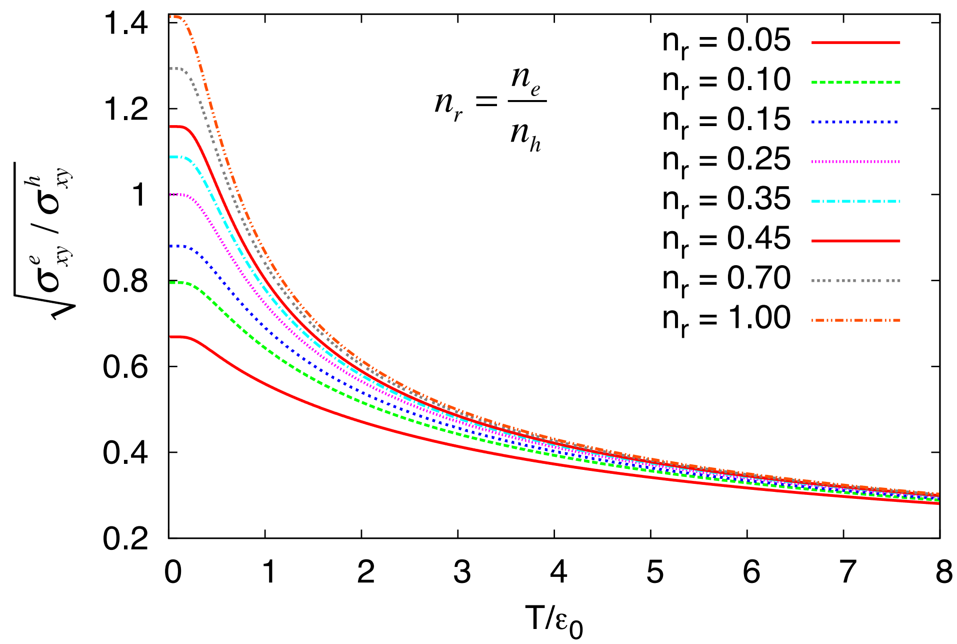
$$S = \frac{-s_e + s_h}{(den.)}$$

$$\sigma_{xy} = \frac{-\sigma_{xy}^e + \sigma_{xy}^h}{(den.)}$$

$$\frac{s_e}{s_h} \propto \frac{\tau_e}{\tau_h}$$

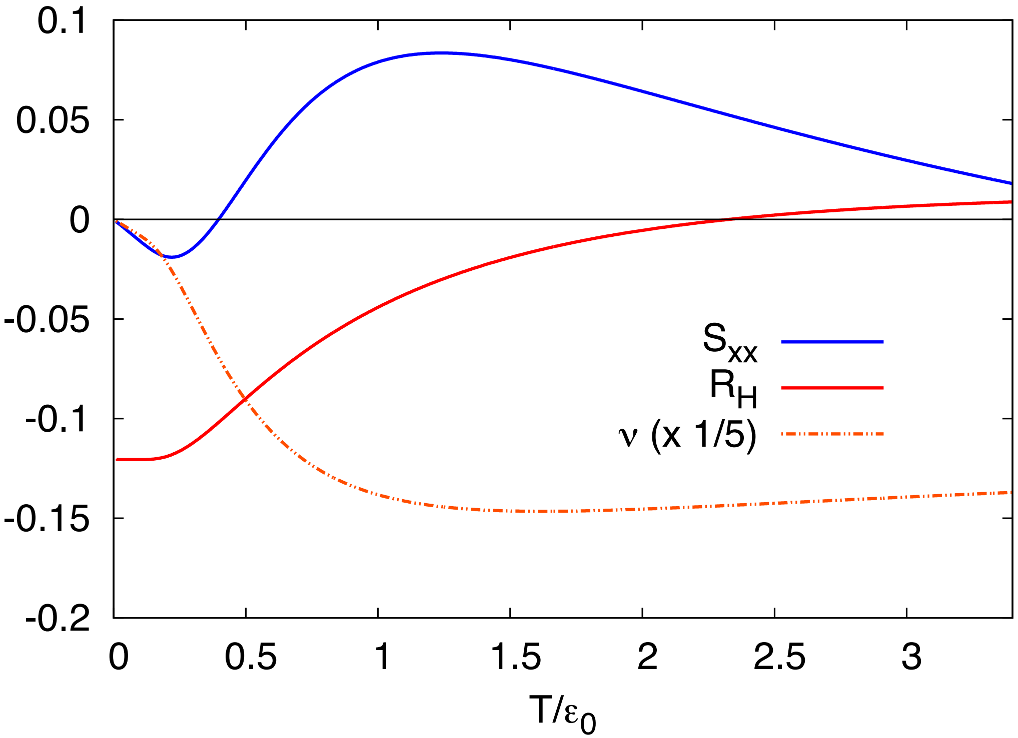
$$\frac{\sigma_{xy}^e}{\sigma_{xy}^h} \propto \left(\frac{\tau_e}{\tau_h}\right)^2$$

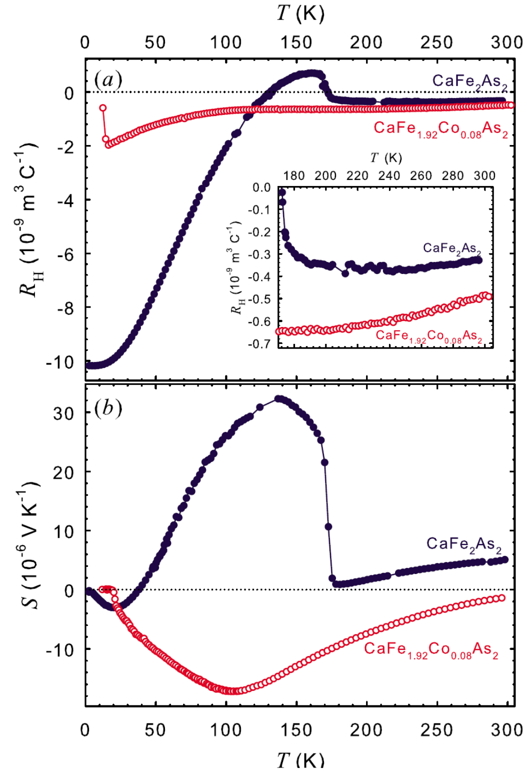


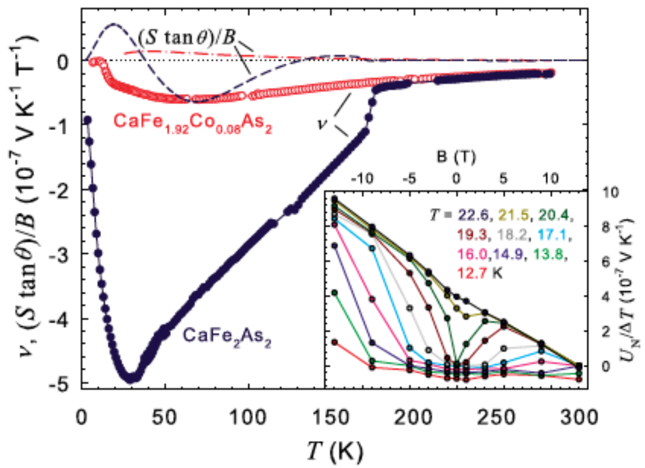


結果

TM, E. Kaneshita, and T. Tohyama, PRL 105, 037203 (2010).

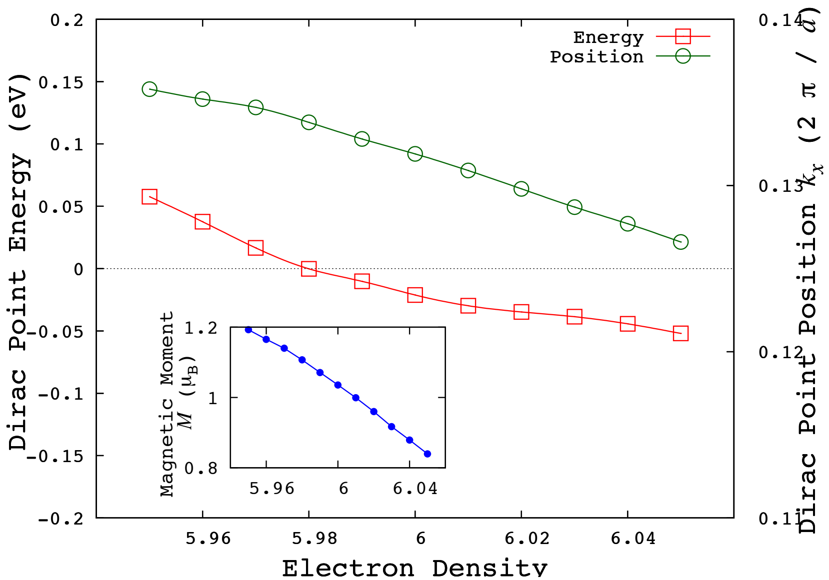


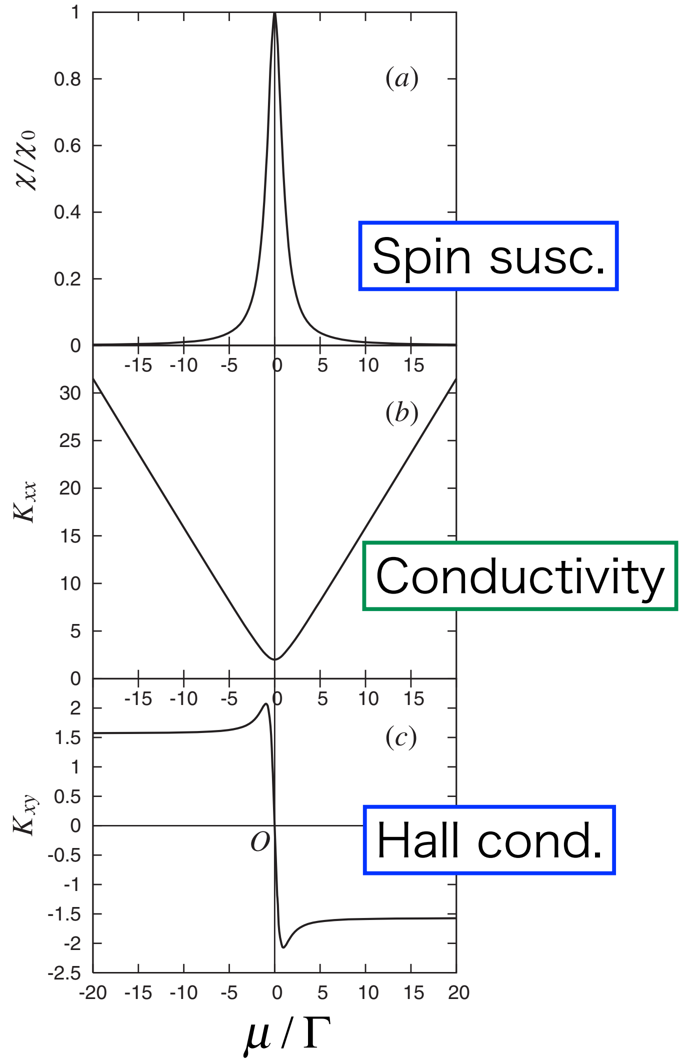




$$n_r = \frac{n_e}{n_h} = 0.05 \qquad \tau_r = \frac{\tau_h}{\tau_e} = 0.45$$

Doping依存性？





H. Fukuyama, JPSJ **76**, 043711 (2007).

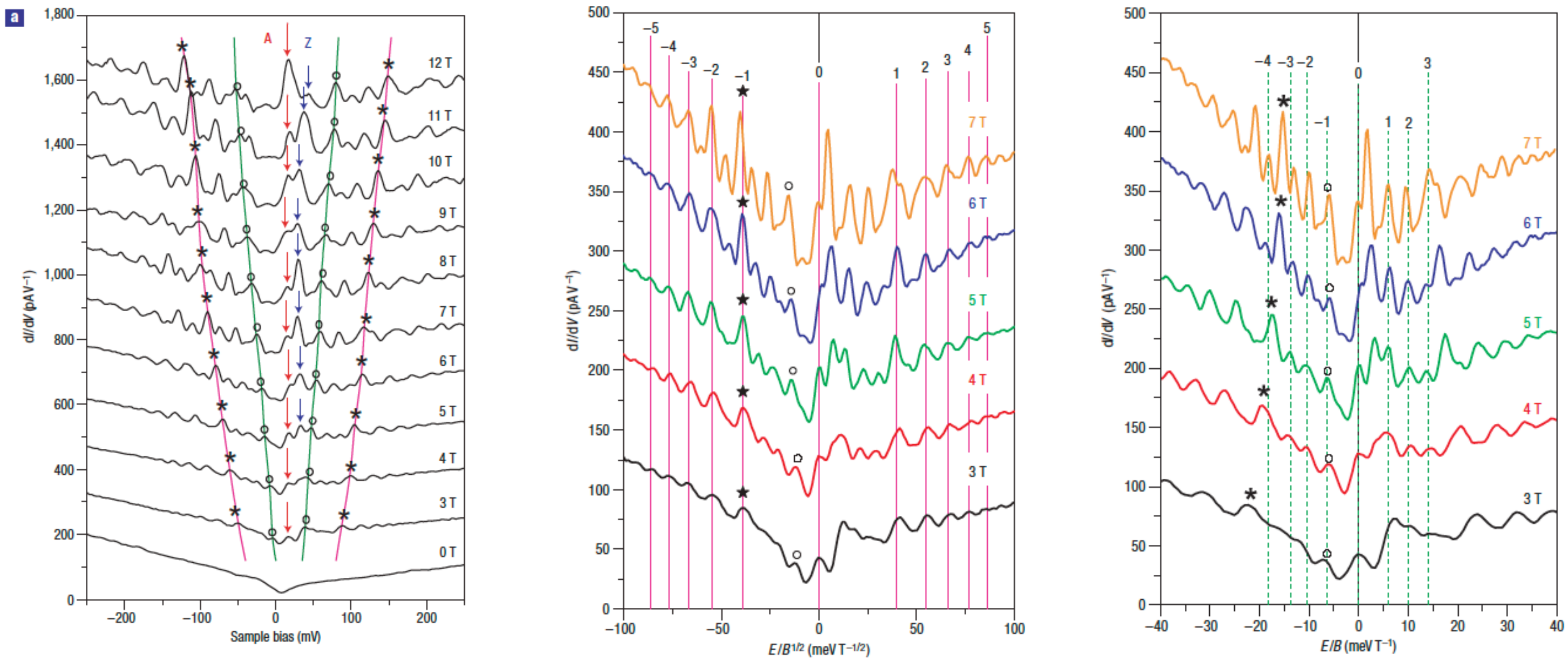
Landau levels?

$$E_n = C\sqrt{|n|B}$$

$$C = \mathrm{sgn}(n)\sqrt{2e\hbar v_z^x v_x^y\left(1-\left(\frac{v_0^x}{v_z^x}\right)^2\right)^{3/2}}$$

STS of graphite

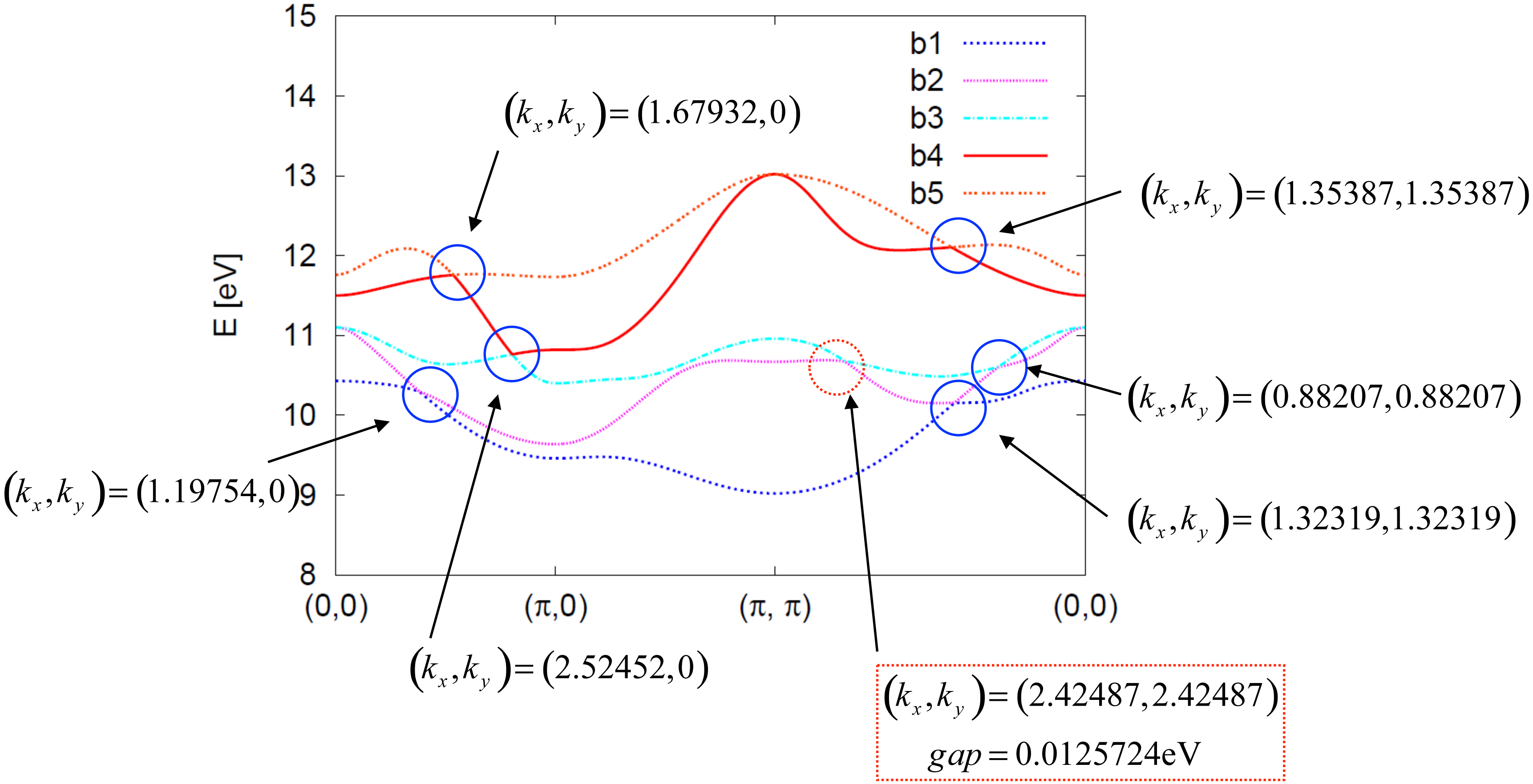
G. Li and E. Y. Andrei, Nature Phys. **3**, 623 (2007).



$E/\sqrt{B}$

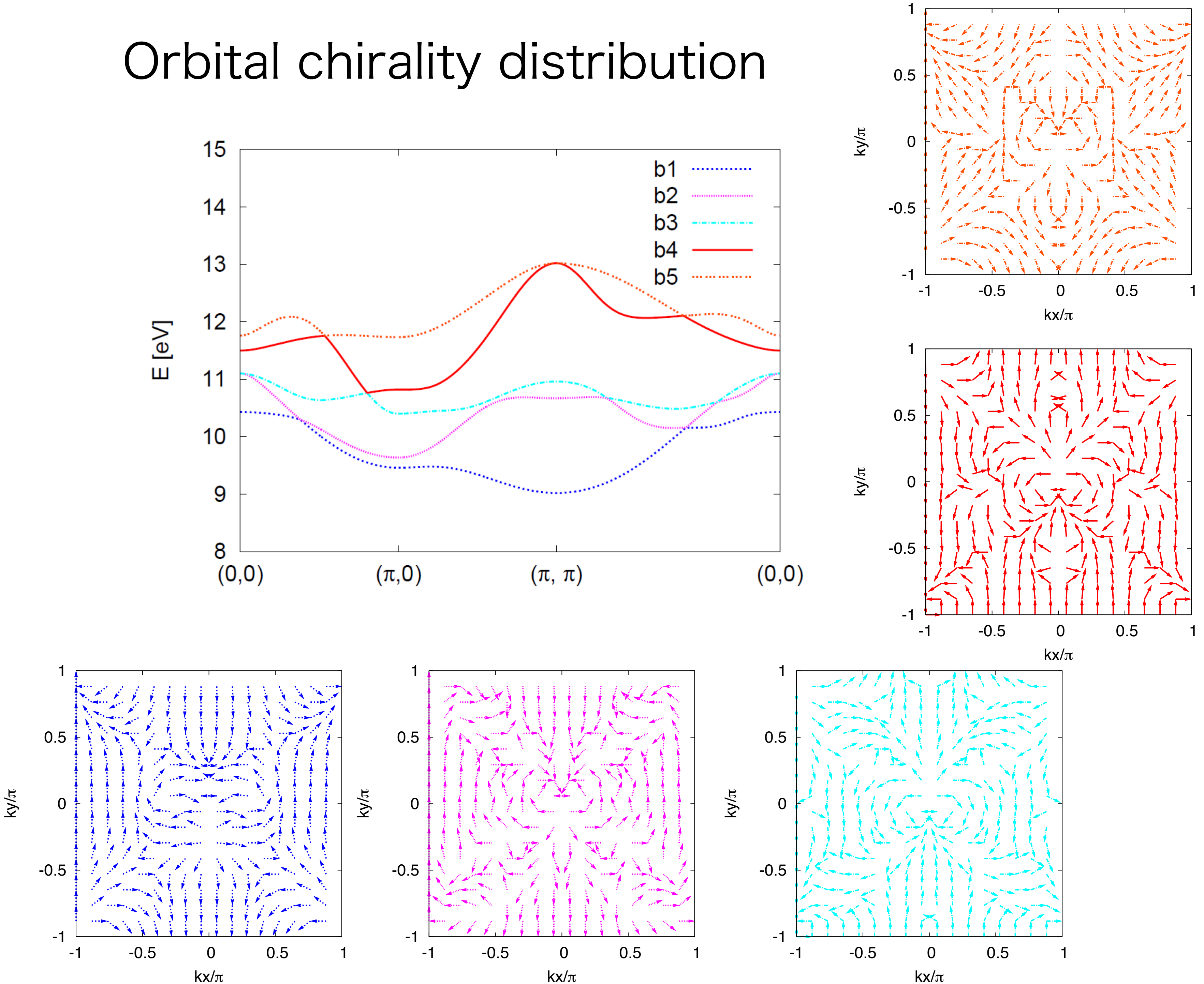
E/B

常磁性相？



15
14
13
12
11
10
9
8
E [eV]
b1
b2
b3
b4
b5
(0,0)
(π,0)
(π, π)
(0,0)
$(k_x, k_y) = (1.67932, 0)$
$(k_x, k_y) = (1.35387, 1.35387)$
$(k_x, k_y) = (0.88207, 0.88207)$
$(k_x, k_y) = (1.32319, 1.32319)$
$(k_x, k_y) = (1.19754, 0)$
$(k_x, k_y) = (2.52452, 0)$
$(k_x, k_y) = (2.42487, 2.42487)$
$gap = 0.0125724\text{eV}$

Orbital chirality distribution



Summary

α-(BEDT-TTF)$_2$I$_3$

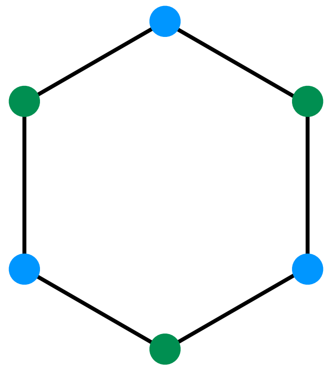
- bulkのDirac電子系
- Dirac電子系に特徴的な輸送現象

Iron-based superconductors

- 軌道に関連したDirac電子系
- 輸送現象に関与
  - Doping依存性？
  - Landau準位の観測？
  - 超伝導との関係？

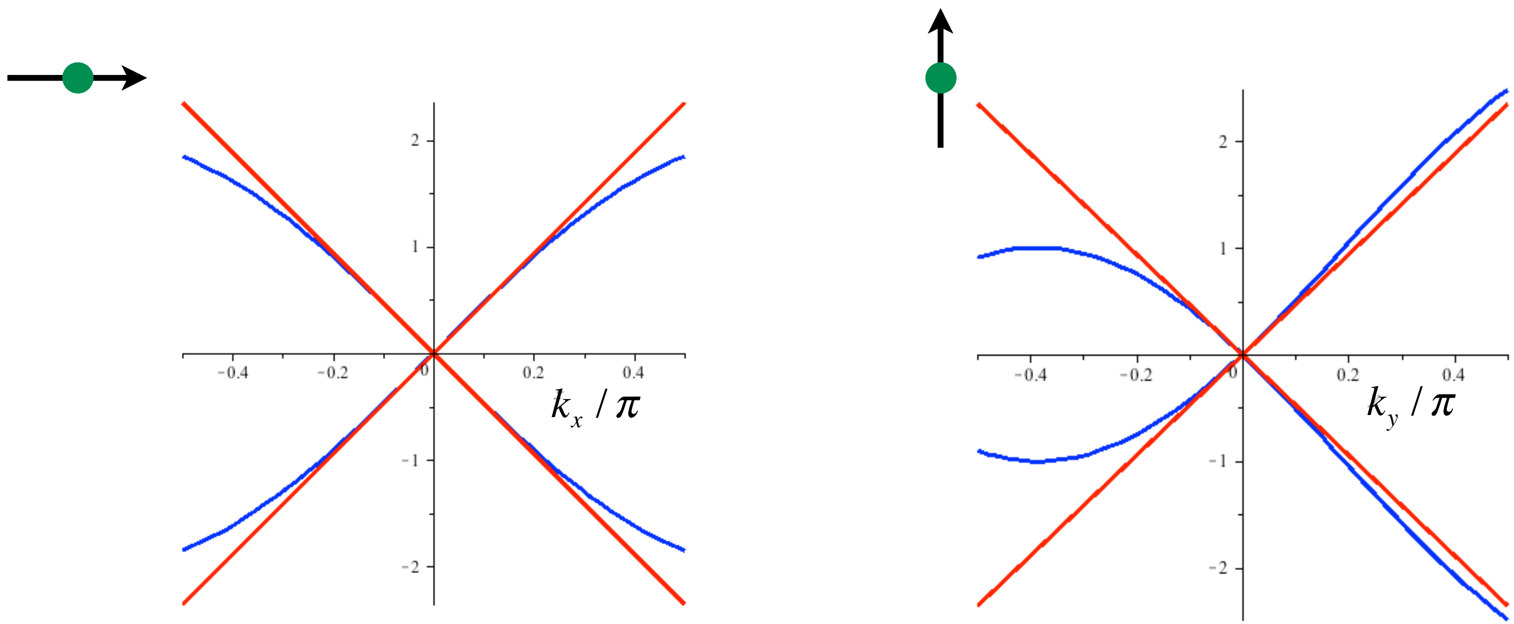
Appendix

Linear dispersion in graphene



$$K = \frac{2\pi}{3a}\left(1, \frac{1}{\sqrt{3}}\right)$$

$$K' = \frac{2\pi}{3a}\left(1, -\frac{1}{\sqrt{3}}\right)$$



Derivation of Dirac Hamiltonian in graphene

$$\kappa_k = -t\left[e^{ik_x a} + e^{i\left(-\frac{1}{2}k_x a + \frac{\sqrt{3}}{2}k_y a\right)} + e^{-i\left(\frac{1}{2}k_x a + \frac{\sqrt{3}}{2}k_y a\right)} \right]$$

$$\kappa_{K+k_x} = \frac{3}{4}\left(\sqrt{3}+i\right)k_x + O\left(k_x^2\right) \qquad \kappa_{K'+k_x} = \frac{3}{4}\left(\sqrt{3}+i\right)k_x + O\left(k_x^2\right)$$

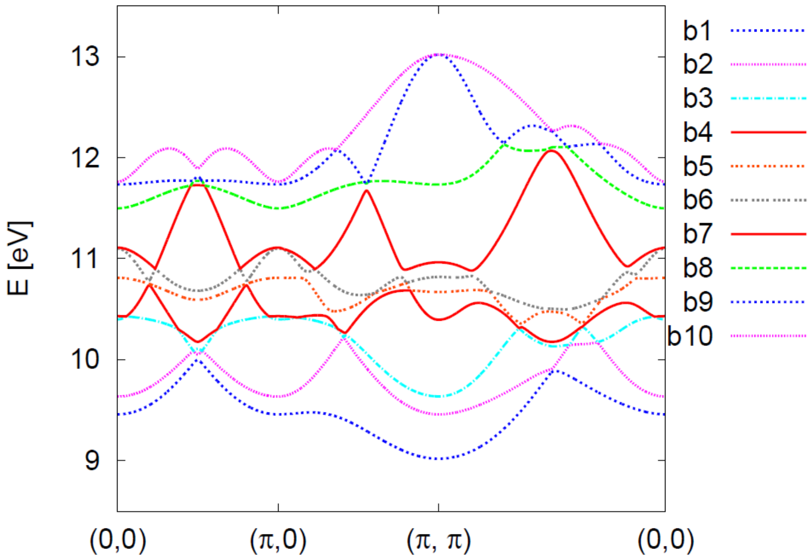
$$\kappa_{K+k_y} = \frac{3}{4}\left(-i\sqrt{3}+1\right)k_y + O\left(k_y^2\right) \qquad \kappa_{K'+k_y} = \frac{3}{4}\left(i\sqrt{3}-1\right)k_y + O\left(k_y^2\right)$$

$$H_{K+k} = \frac{3}{2}t\begin{pmatrix} 0 & e^{\pi i/6}\left(k_x - ik_y\right) \\ e^{-\pi i/6}\left(k_x + ik_y\right) & 0 \end{pmatrix} \qquad H_{K'+k} = \frac{3}{2}t\begin{pmatrix} 0 & e^{\pi i/6}\left(k_x + ik_y\right) \\ e^{-\pi i/6}\left(k_x - ik_y\right) & 0 \end{pmatrix}$$

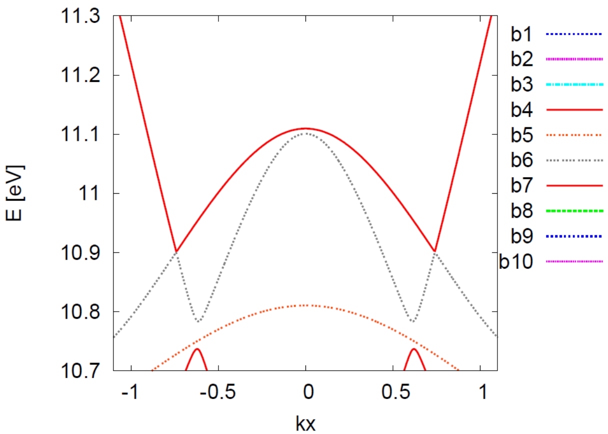
$$U = \begin{pmatrix} e^{\pi i/12} & 0 \\ 0 & e^{-\pi i/12} \end{pmatrix}$$

$$U^\dagger H_{K+k} U = \frac{3}{2}t\begin{pmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{pmatrix} \qquad U^\dagger H_{K'+k} U = \frac{3}{2}t\begin{pmatrix} 0 & k_x + ik_y \\ k_x - ik_y & 0 \end{pmatrix}$$

Dirac point



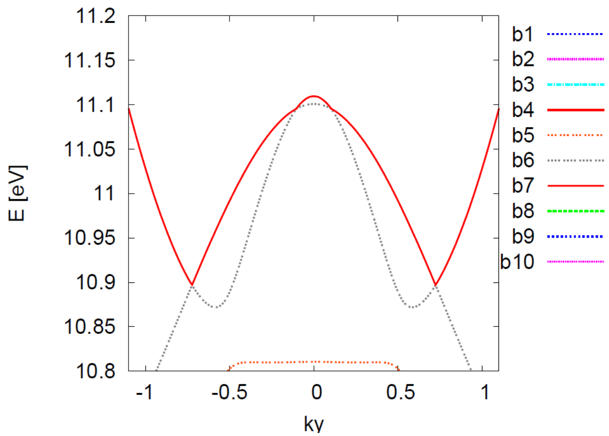
kx-axis



$$\left(k_x, k_y\right) = \left(0.7446, 0.\right)$$

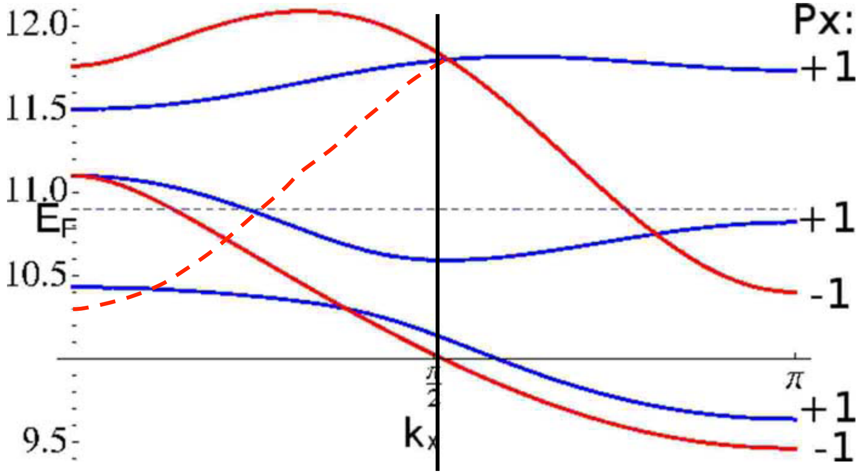
$$E = 10.908\text{eV}$$

ky-axis

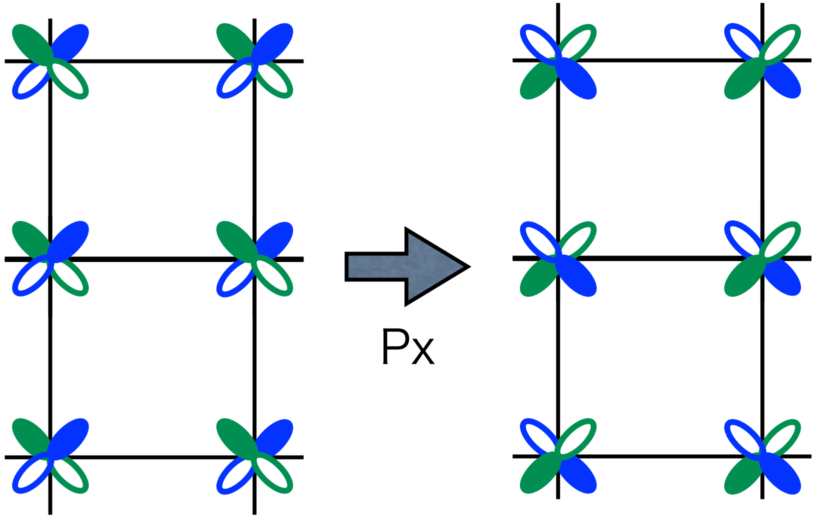


Mass gap?

Y. Ran *et al.*, PRB **79**, 014505 (2009)



Q=(p,0) folding of the band



$$M^{SDW}_{(+1,+1)} \neq 0$$

$$M^{SDW}_{(+1,-1)} = 0$$