Nonlinear and Nonreciprocal Responses of Noncentrosymmetric Quantum Matters

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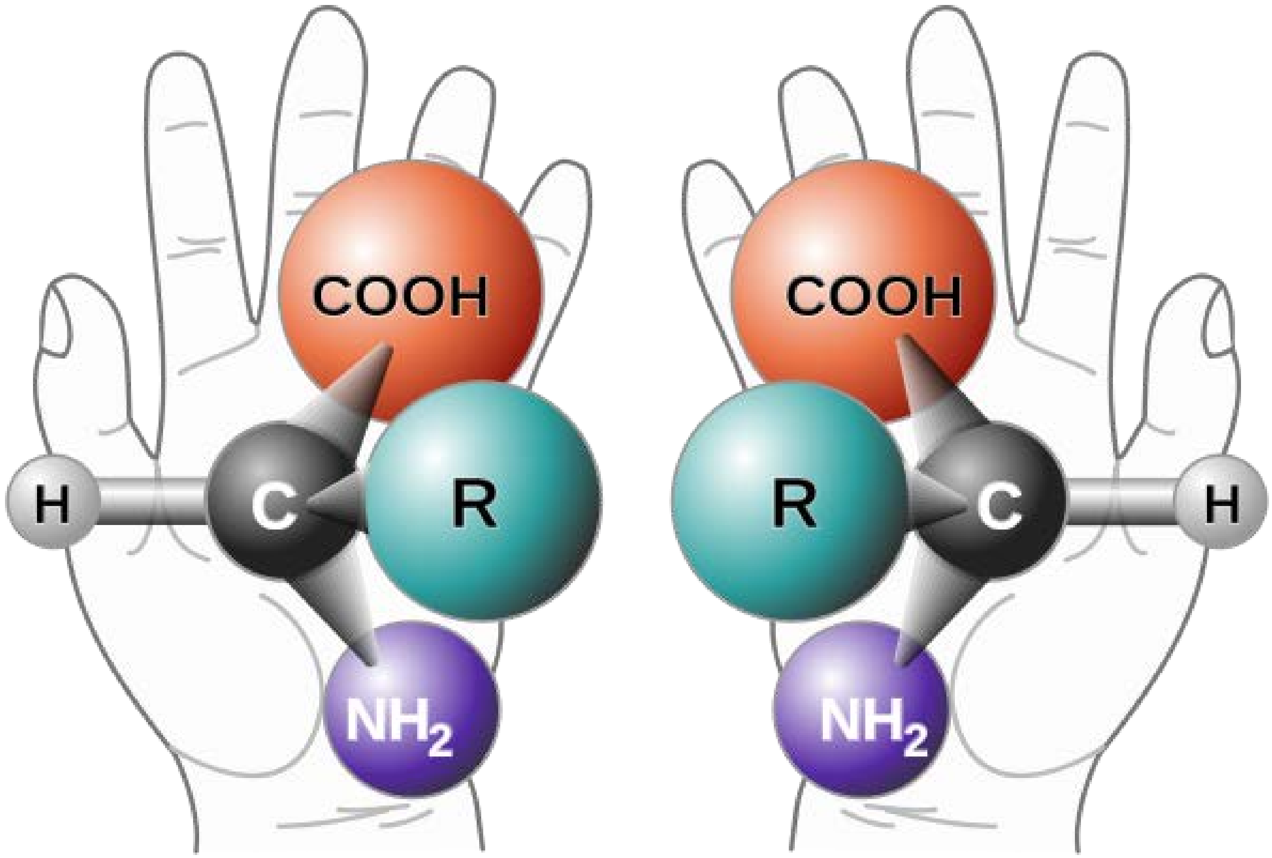
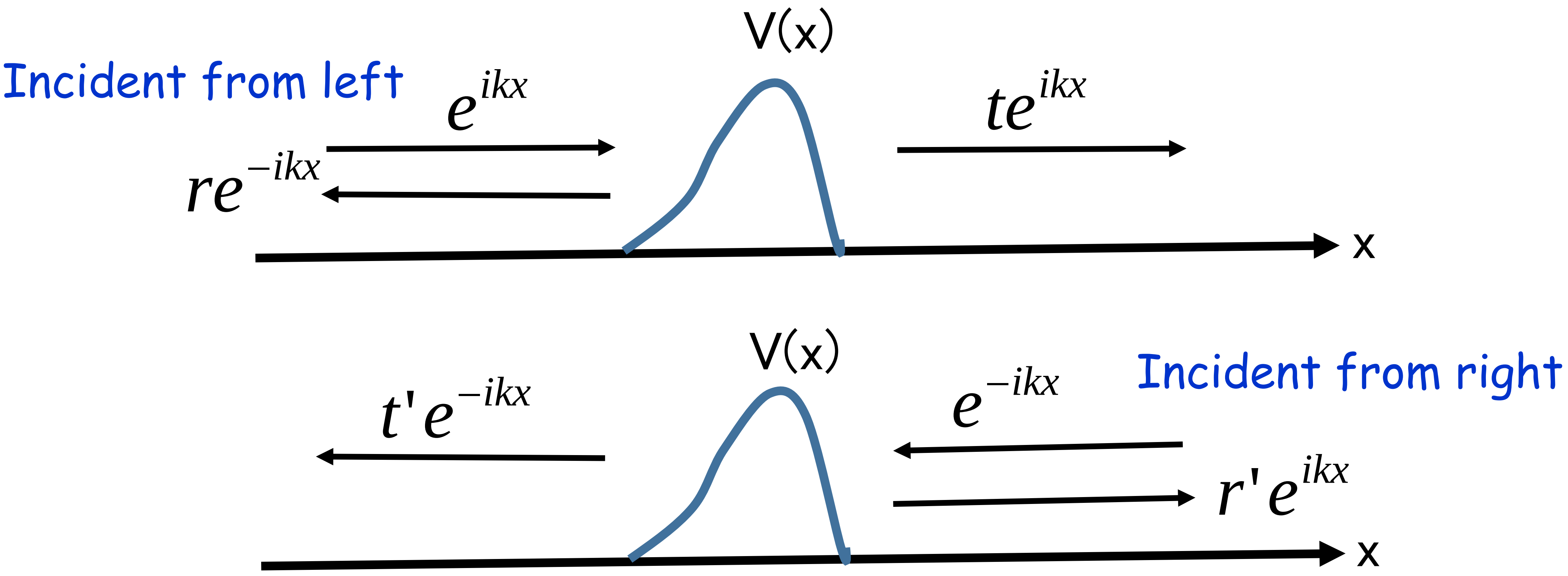
Chirality of structure



No Inversion I
No Mirror M

From Wikipedia

Right and Left directions of flow



$|t'|^2 = |t|^2 \quad |r'|^2 = |r|^2$ Unitary nature of S matrix: conservation of prob.

$t' = t$ Time-reversal symmetry T: S=S^Transpose

Asymmetry between t and -t

1. Microscopic time-reversal symmetry breaking

   external magnetic field   B
   magnetic ordering   M

2. Macroscopic irreversibility

   dissipation of energy
   diffusion

Non-reciprocal transport in non-centrosymmetric system

Time-reversal symmetry of microscopic dynamics vs irreversibility

$$\sigma_{\mu\nu}(k,\omega,B) = \sigma_{\nu\mu}(-k,\omega,-B)$$

Onsager's reciprocal relation
for linear response

Magnetochiral optical effect
directional dichroism

$$\varepsilon_{\mu\mu}(k,\omega,B) = \varepsilon_0 + \alpha k \cdot B$$

e.g. electromagnon in multiferroics

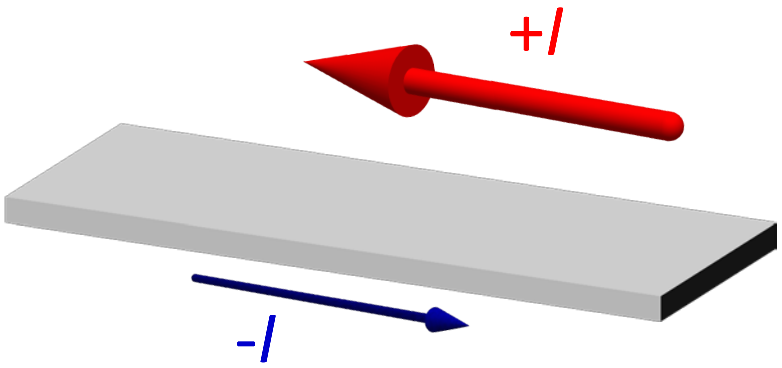
A. Loidl, Y.Tokura

$k \to I$ G. L. J. A. Rikken (2001)

"dichroism" of the electric current magnetochiral anisotropy

$$R\,(+I) \neq R\,(-I)$$

$$R = R_0\,(1 + \beta B^2 + \gamma B I)$$

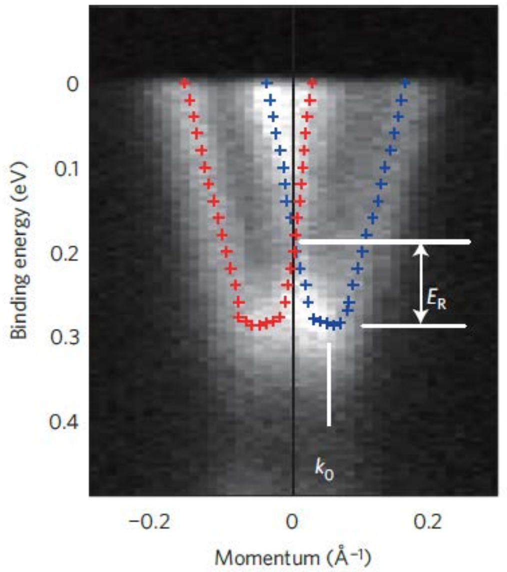


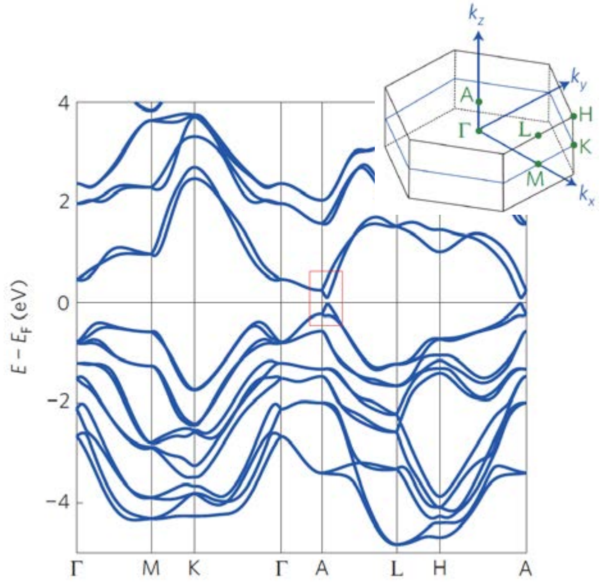
Broken inversion symmetry $\Leftrightarrow$ $\gamma \neq 0$

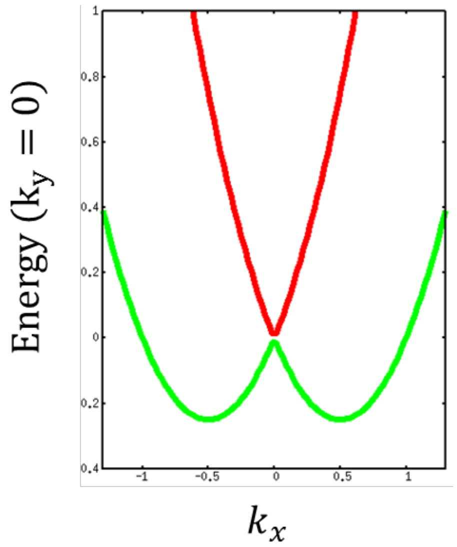
Nonlinear response $J = \sigma E + \alpha B E^2$

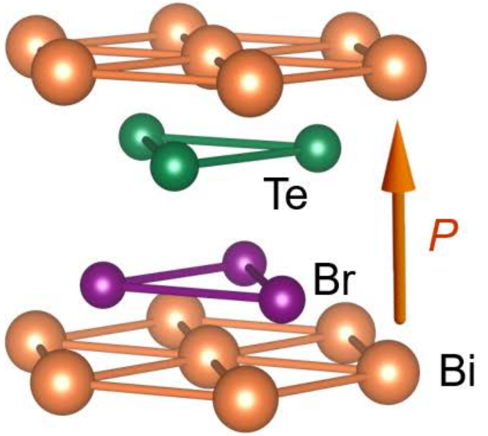
Band structure in noncentrosymmetric crystal

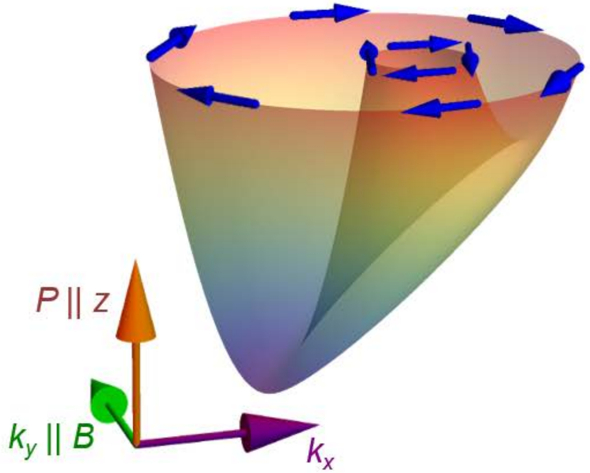
Time-reversal symmetry ➡ $\varepsilon_{\uparrow}(k) = \varepsilon_{\downarrow}(-k)$





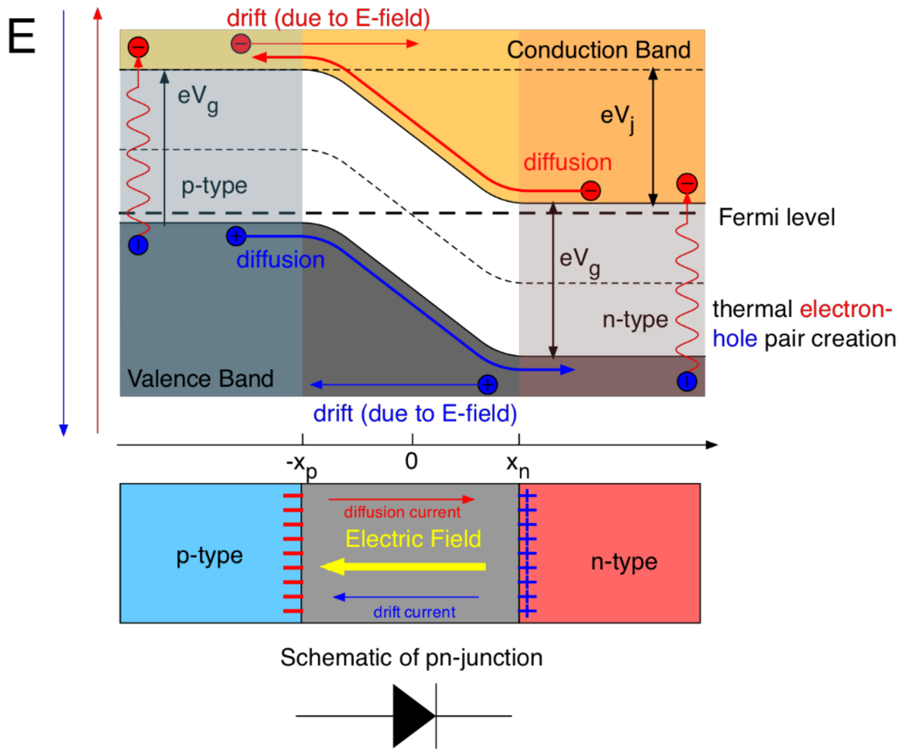




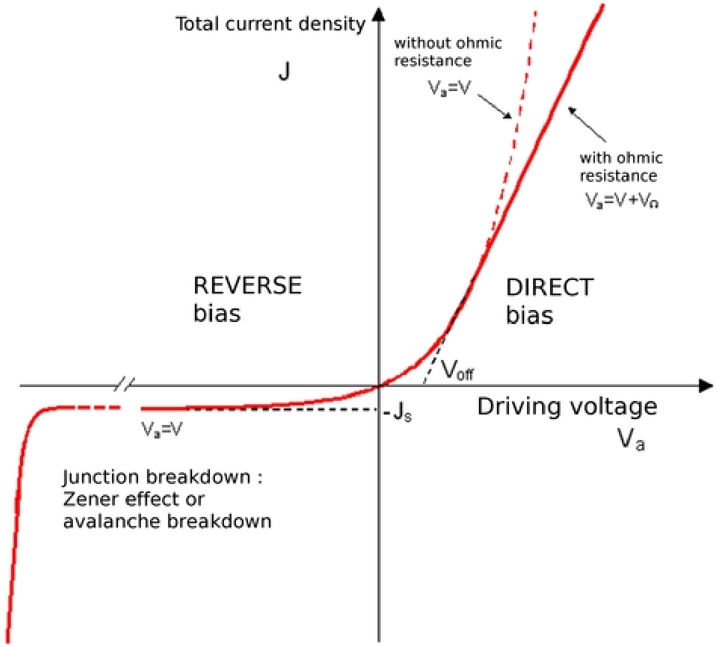


K. Ishizaka *et al. Nat. Mater.* **10**, 521 (2011).

pn junction



Schematic of pn-junction



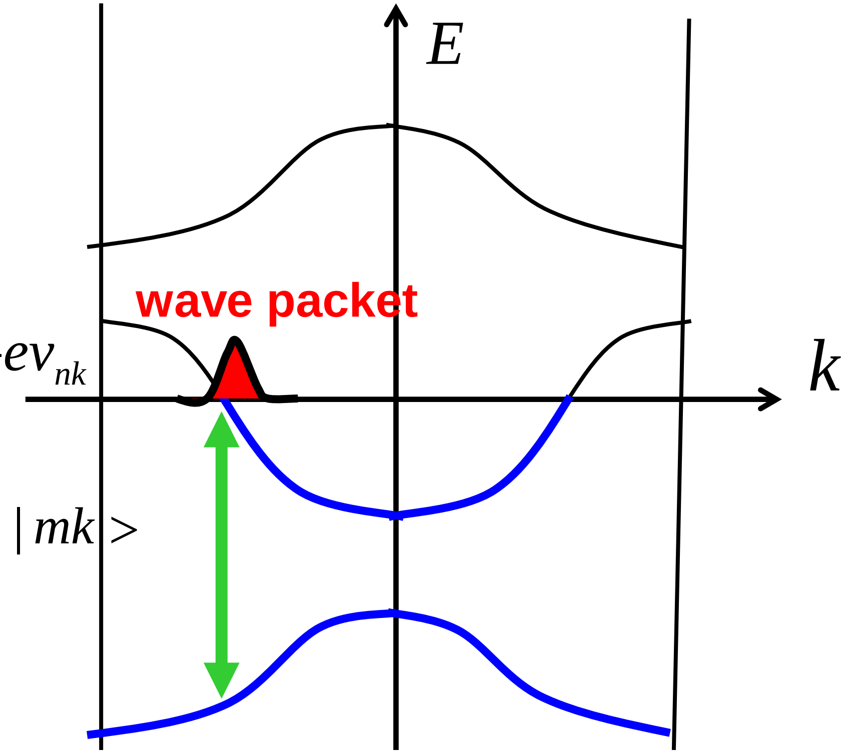
http://quantumwise.com/publications/tutorials/item/828-silicon-p-n-junction

http://www.optique-ingenieur.org/en/courses/OPI_ang_M05_C02/co/Contenu_09.html

Nonreciprocal Response	Linear Response	Nonlinear Response
Time-reversal Unbroken	Forbidden	Shift current Nonlinear Hall effect pn junction
Time-reversal Broken	Optical ME effect Magnetochiral effect Nonreciprocal magnon	Nonreciprocal nonlinear optical effect Electric magnetochiral effect Inverse Edelstein effect Magnetochiral anisotropy

Table 1

Intra- and Inter-band matrix elements of current



Wavefunction matters !!

Of-diagonal matrix elements

- Distort the band structure by E
- Additional current

Even a filled band can
support current
e.g., polarization current
quantum Hall current

$$< nk | J | nk >= -e < nk | \frac{\partial H(k)}{\partial k} | nk >= -e \frac{\partial \varepsilon_n(k)}{\partial k}$$

$$< nk | J | mk >= -e < nk | \frac{\partial H(k)}{\partial k} | mk >= -e(\varepsilon_{nk} - \varepsilon_{mk}) < nk | \frac{\partial}{\partial k} | mk >$$

Time-reversal	$b(k) = -b(-k)$
Inversion	$b(k) = b(-k)$
➡	$b(k) = 0$

Berry Phase Curvature in k-space

$$\psi_{nk}(r) = e^{ikr} u_{nk}(r)$$

Bloch wavefucntion

$$a_n(k) = -i < u_{nk} | \nabla_k | u_{nk} >$$

Berry phase connection in k-space

$$x_i = r_i + a_n(k) = i\partial_{k_i} + a_n(k)$$

covariant derivative

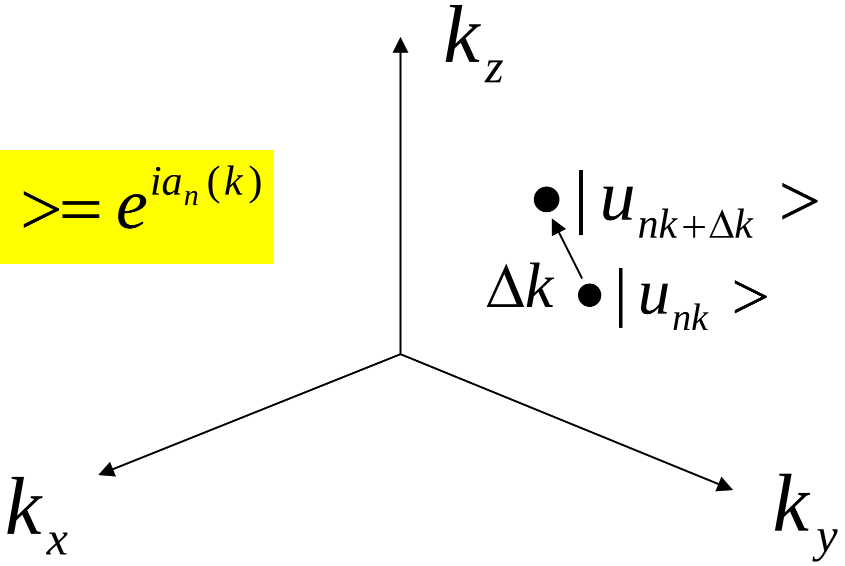
$$[x, y] = i(\partial_{k_x} a_{ny}(k) - \partial_{k_y} a_{nx}(k)) = i b_{nz}(k)$$

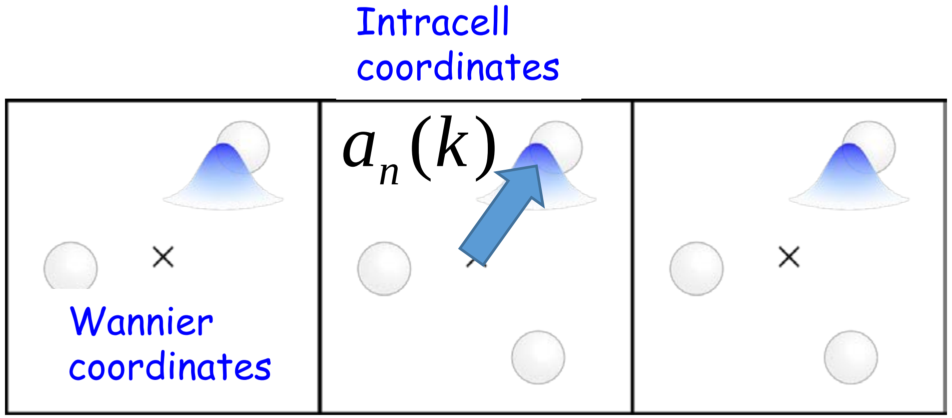
Curvature in k-space

$$\frac{dx(t)}{dt} = -i[x, H] = \frac{k_x}{m} - i[x, y]\frac{\partial V}{\partial y} = \frac{k_x}{m} + b_{nz}(k)\frac{\partial V}{\partial y}$$

Anomalous Velocity and
Anomalous Hall Effect

$$< u_{nk} | u_{nk+\Delta k} > = e^{i a_n(k)}$$





DC nonreciprocal responses

$$\underline{\hat{G}}(\pi) = \underline{\hat{G}}_0(\pi)\left[1 + \left(\underline{\hat{\Sigma}}(\pi) - \underline{\hat{\Sigma}}_0(\pi)\right)\underline{\hat{G}}(\pi) - \sum_{n=1}^{\infty}\frac{1}{n!}\left(\pi^0 - \hat{H}_0(\boldsymbol{\pi}) - \underline{\hat{\Sigma}}(\pi)\right)\left(\prod_{i=1}^{n}\frac{i\hbar q F^{\mu_i\nu_i}}{2}\overleftarrow{\partial}_{\pi^{\mu_i}}\overrightarrow{\partial}_{\pi^{\nu_i}}\right)\underline{\hat{G}}(\pi)\right]$$

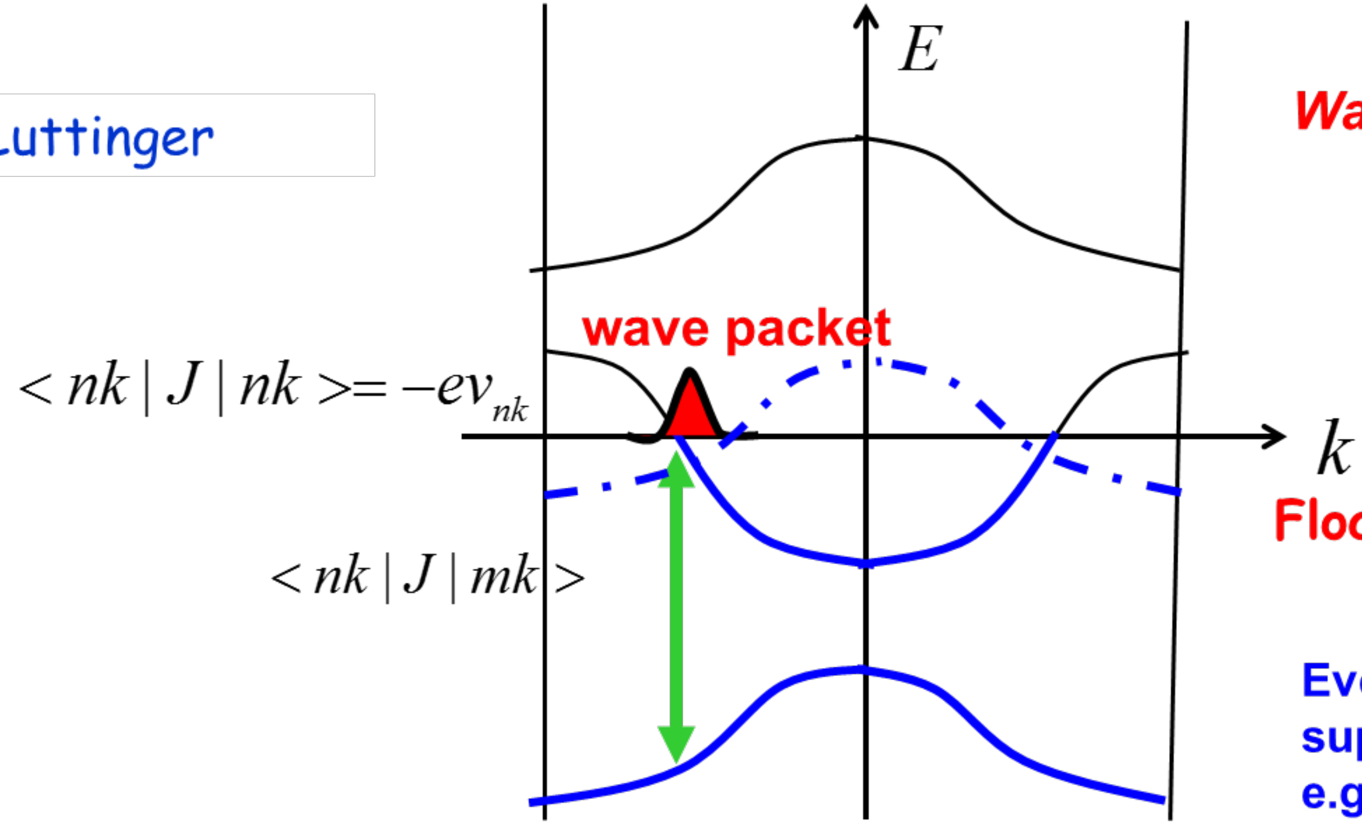
$$\pi = p + eA$$ ➡ Expansion of Keldysh Green's function in constant E and B.
Multiband effect fully taken into account.

Non-interacting case
No E-dependence of Σ ➡

$$G^{<}_{E^2} = -\frac{i}{2}G_0[\partial_\omega G_0^{-1}\partial_k G_E - \partial_k G_0^{-1}\partial_\omega G_E]^< + \frac{1}{4}G_0[\partial_\omega^2 G_0^{-1}\partial_k^2 G_0 + \partial_k^2 G_0^{-1}\partial_\omega^2 G_0]^<.$$

AC nonreciprocal response – Shift current

Kurplus-Luttinger



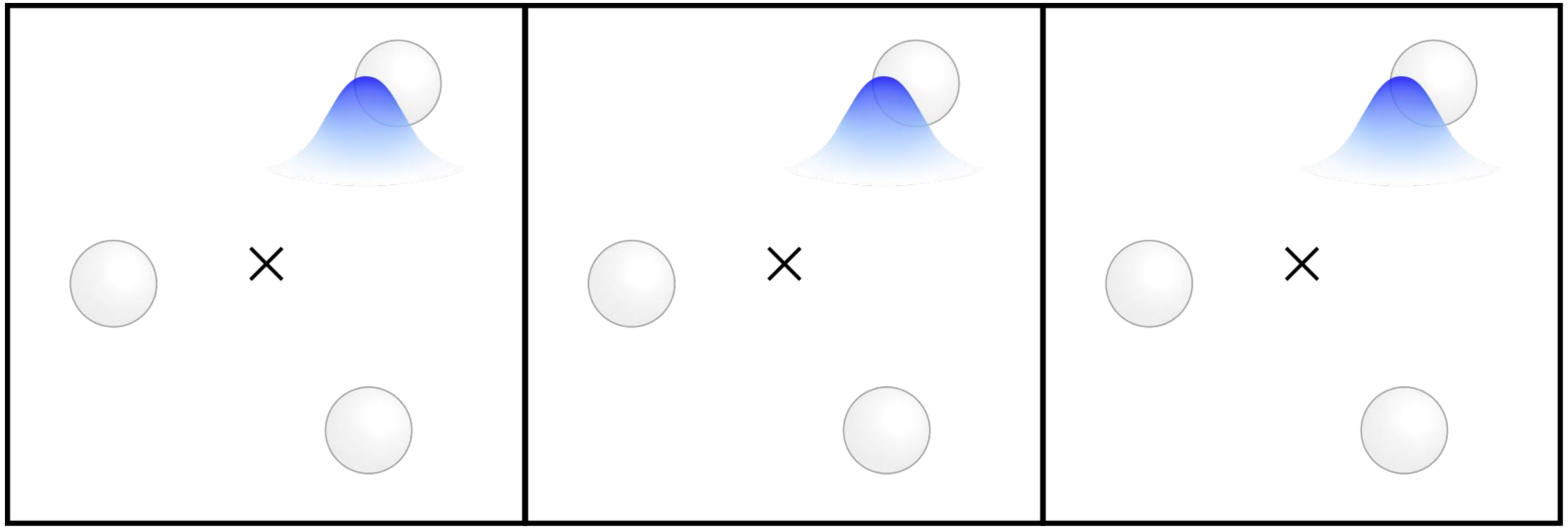
Wavefunction matters !!

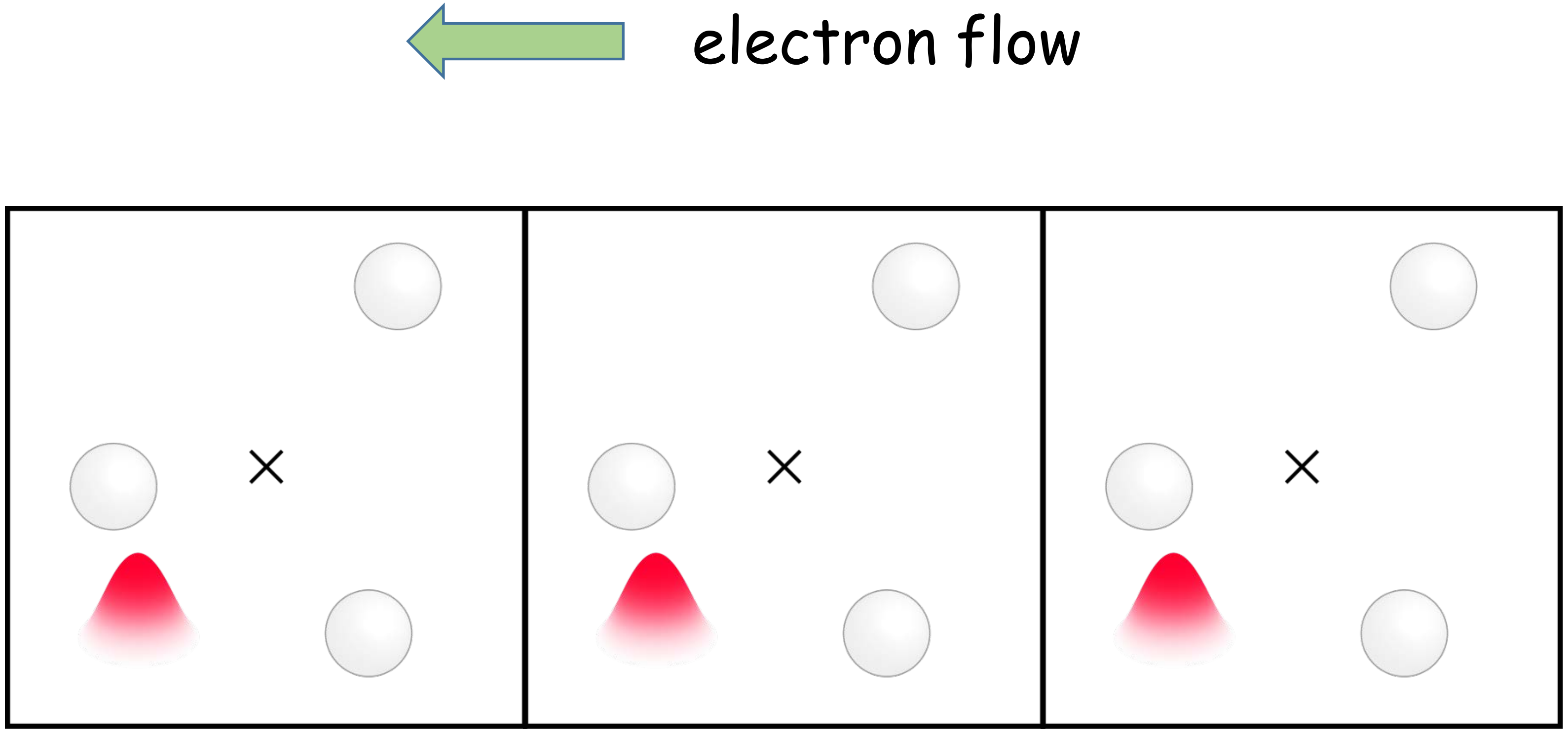
Floquet band with anti-crossings

Even a filled band can support current
e.g., polarization current
quantum Hall current Q. Niu et al.

$$<nk|J|nk>=-e<nk|\frac{\partial H(k)}{\partial k}|nk>=-e\frac{\partial \varepsilon_n(k)}{\partial k}$$

$$<nk|J|mk>=-e<nk|\frac{\partial H(k)}{\partial k}|mk>=-e(\varepsilon_{nk}-\varepsilon_{mk})<nk|\frac{\partial}{\partial k}|mk>$$




electron flow

First-principles calculation of shift current

Steve M. Young and Andrew M. Rappe, Phys. Rev. Lett. 109, 116601 (2012)

$$J_q = \sigma_q^{rs} E_r E_s$$

$$\sigma_q^{rs}(\omega) = \pi e \left(\frac{e}{m\hbar\omega}\right)^2 \sum_{n',n''} \int d\mathbf{k} \, (f[n''\mathbf{k}] - f[n'\mathbf{k}])$$

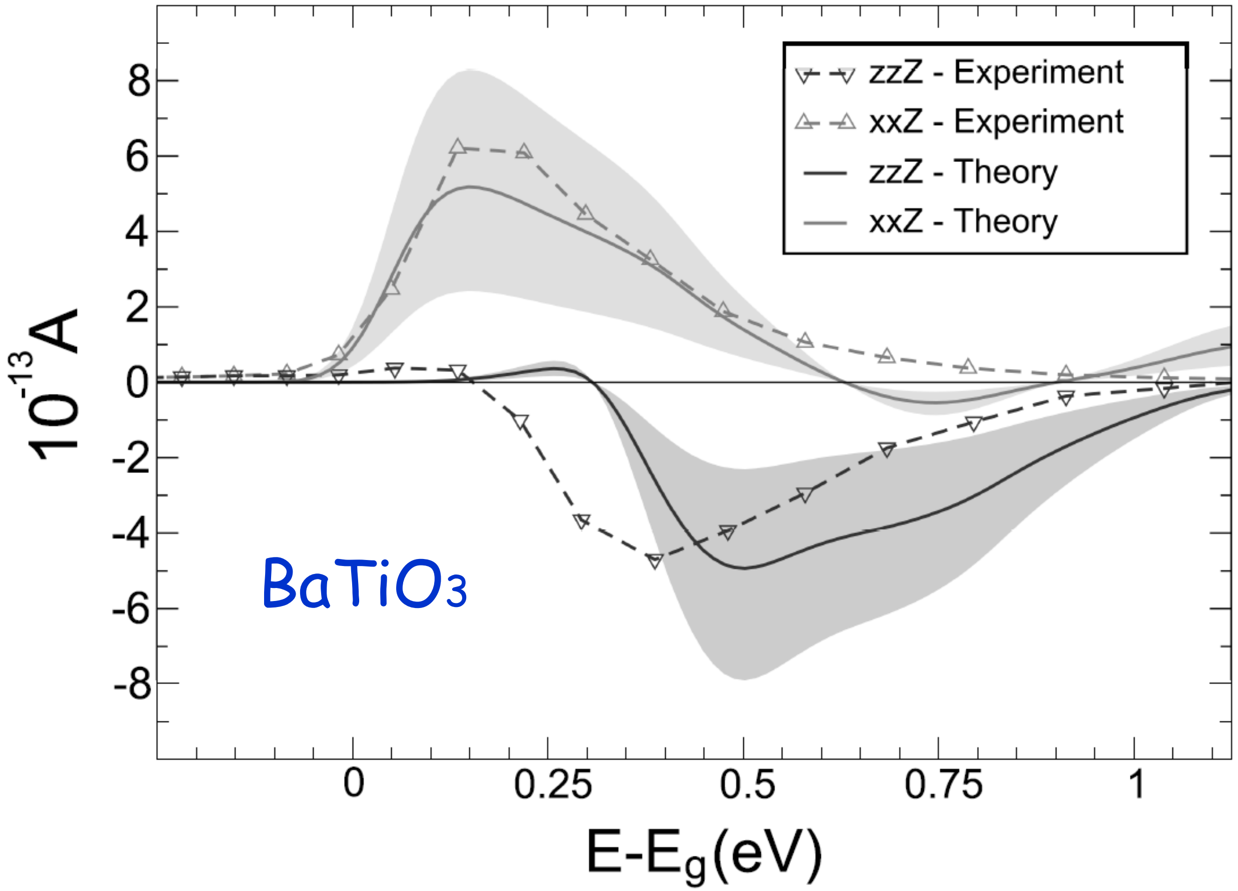
$$\times \langle n'\mathbf{k}| \hat{P}_r |n''\mathbf{k}\rangle \langle n''\mathbf{k}| \hat{P}_s |n'\mathbf{k}\rangle$$

$$\times \left(-\frac{\partial \phi_{n'n''}(\mathbf{k},\mathbf{k})}{\partial k_q} - [\chi_{n''q}(\mathbf{k}) - \chi_{n'q}(\mathbf{k})]\right)$$

$$\times \delta\left(\omega_{n''}(\mathbf{k}) - \omega_{n'}(\mathbf{k}) \pm \omega\right)$$

$\phi_{nn'}$ phase of the transition matrix element

χ_n Berry connection (vector potential)



R. von Baltz & W. Kraut, PRB1981 J.E. Sipe & A.I. Shkrebtii, PRB2000

Topological nature of Floquet bands in Keldysh formalism

T. Morimoto, NN Science Adv. 2016

$$h = \begin{pmatrix} \epsilon_1^0 & iFv_{12}^0 \\ -iFv_{21}^0 & \epsilon_2^0 \end{pmatrix} \equiv \epsilon + \boldsymbol{d} \cdot \boldsymbol{\sigma}$$

Conduction and valence bands are coupled to particle bath Independently

$$G^< = \frac{(\omega - \epsilon - i\Gamma + \boldsymbol{d} \cdot \boldsymbol{\sigma})\Sigma^<(\omega - \epsilon + i\Gamma + \boldsymbol{d} \cdot \boldsymbol{\sigma})}{[(\omega - \epsilon - i\Gamma)^2 - d^2][(\omega - \epsilon + i\Gamma)^2 - d^2]}$$

$$J = \frac{\Gamma(d_x b_y - d_y b_x)}{2(d^2 + \Gamma^2)} + \frac{d_z^2 b_z}{4(d^2 + \Gamma^2)} + \frac{b_z}{4} \equiv J_1 + J_2 + J_3.$$

$$b = \partial d / \partial k$$

Current

$$J_1 = F^2 \frac{\Gamma}{2(d_z^2 + F^2|v_{12}^0|^2 + \Gamma^2)} |v_{12}^0|^2 R_k.$$

$$= \frac{\pi E^2}{2\Omega^2} \frac{\Gamma}{\sqrt{\frac{E^2}{\Omega^2} + \Gamma^2}} \delta(d_z)|v_{12}^0|^2 R_k.$$

$$R_k = \left[\frac{\partial}{\partial k} \mathrm{Im}(\log v_{21}^0) + a_{22} - a_{11}\right]$$

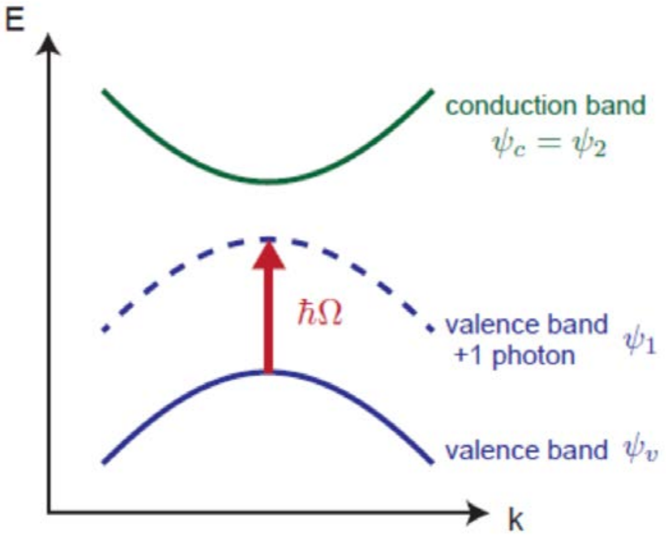
Shift-current
Even order response to E

See also A.M. Cook et al., Nature Commun. 2017

Exciton formation

T. Morimoto, NN PRB 2016

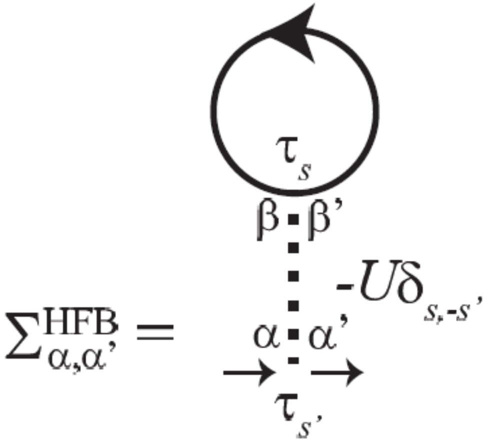
$$Av'(\boldsymbol{k}) = -\int dk' V_{\boldsymbol{k}\boldsymbol{k}'}\Delta(\boldsymbol{k}') \qquad \Delta(\boldsymbol{k}) = \langle \psi^{\dagger}_{2,\boldsymbol{k}}\psi_{1,\boldsymbol{k}}\rangle$$



Bethe-Salpeter equation for exciton formation

$$\Delta(\boldsymbol{k}) = Av_{12}\frac{d_z - i\frac{\Gamma}{2}}{2(d^2+\frac{\Gamma^2}{4})} - \frac{d_z - i\frac{\Gamma}{2}}{2(d^2+\frac{\Gamma^2}{4})}\int dk' V_{\boldsymbol{k}\boldsymbol{k}'}\Delta(\boldsymbol{k}')$$

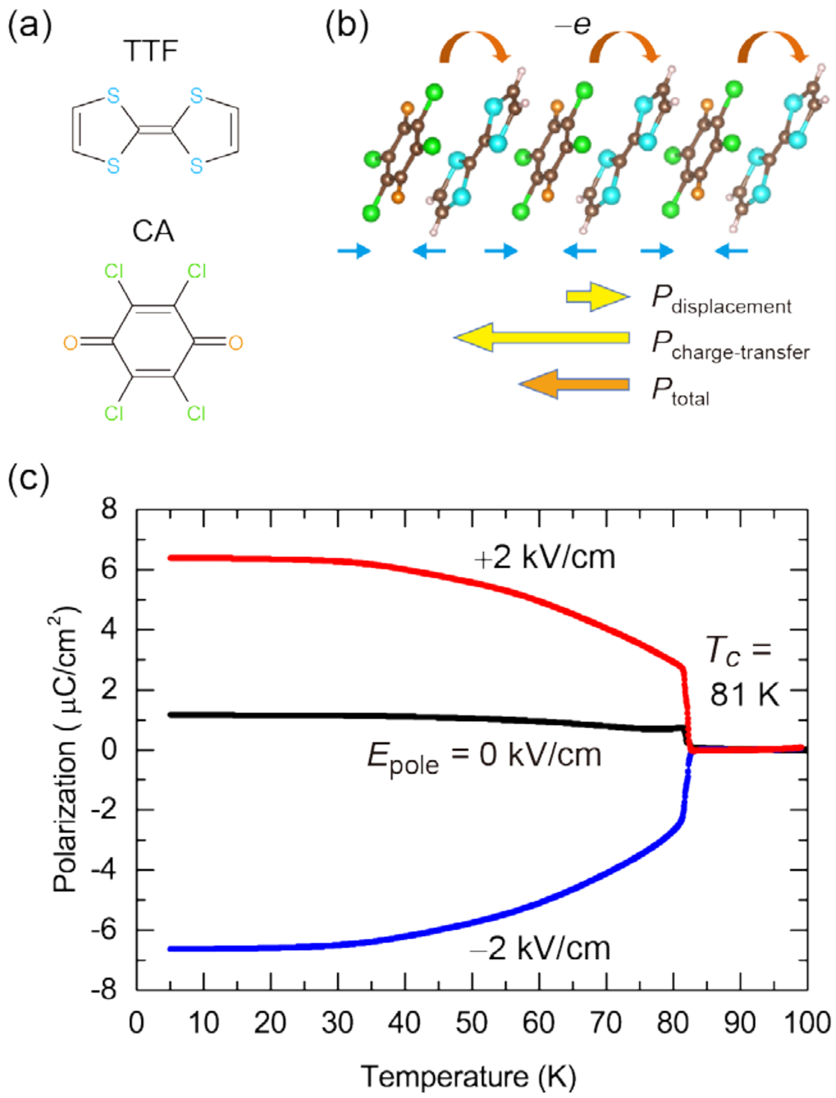
$$J \cong A^2 \frac{V'}{2|d_z(0)|}\frac{\Gamma}{[2d_z(0)+V']^2+\Gamma^2}|v_{12}(0)|^2 R_2(0)$$



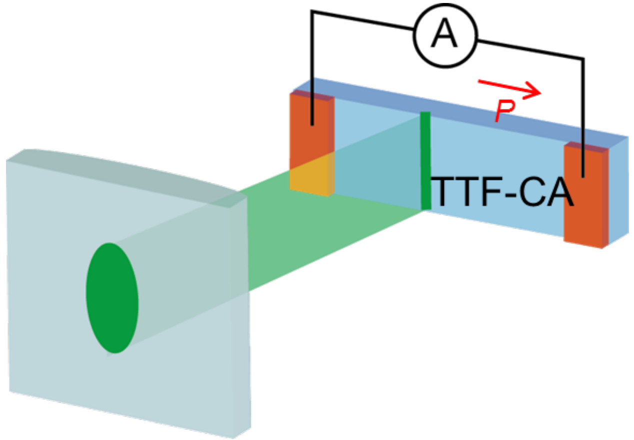
Hanai-Littilewood-Ohashi

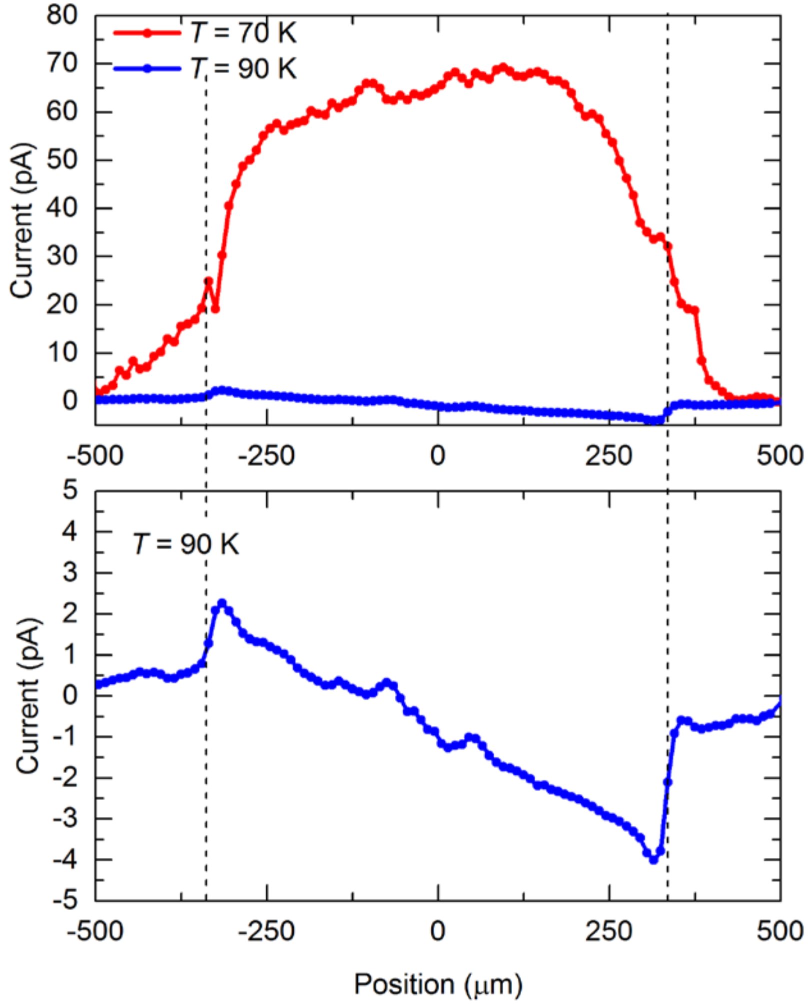
Nonlocal nature of shift current

Y. Nakamura et al.

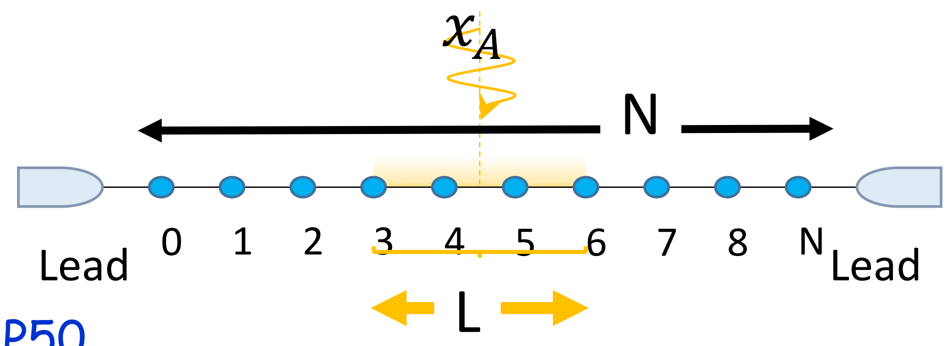


Position dependence
Nakamura *et al.*



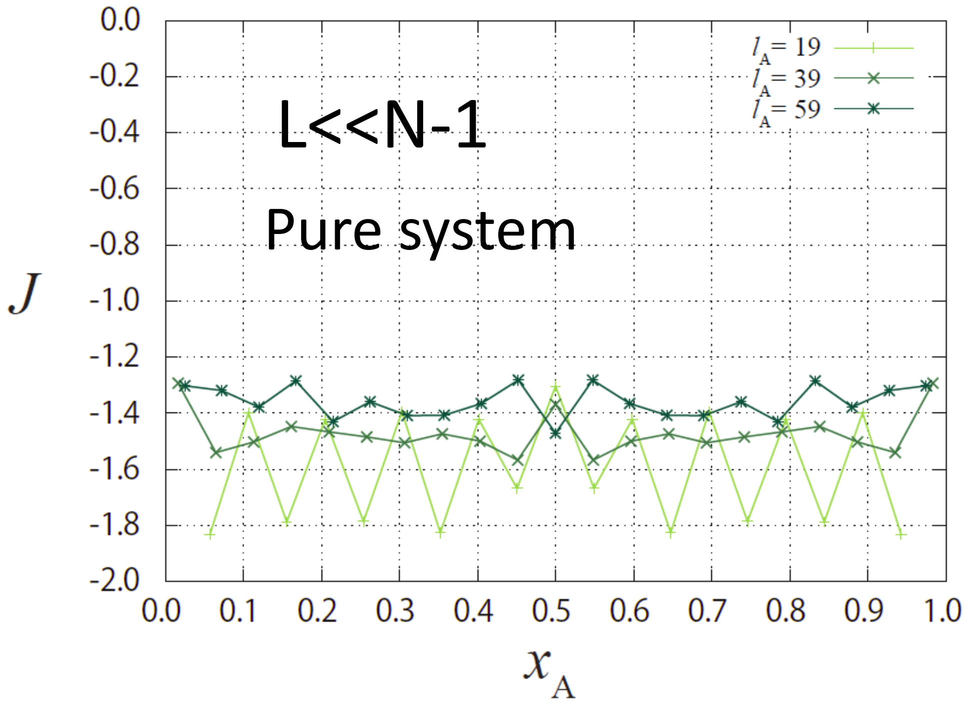


Localization and shift current

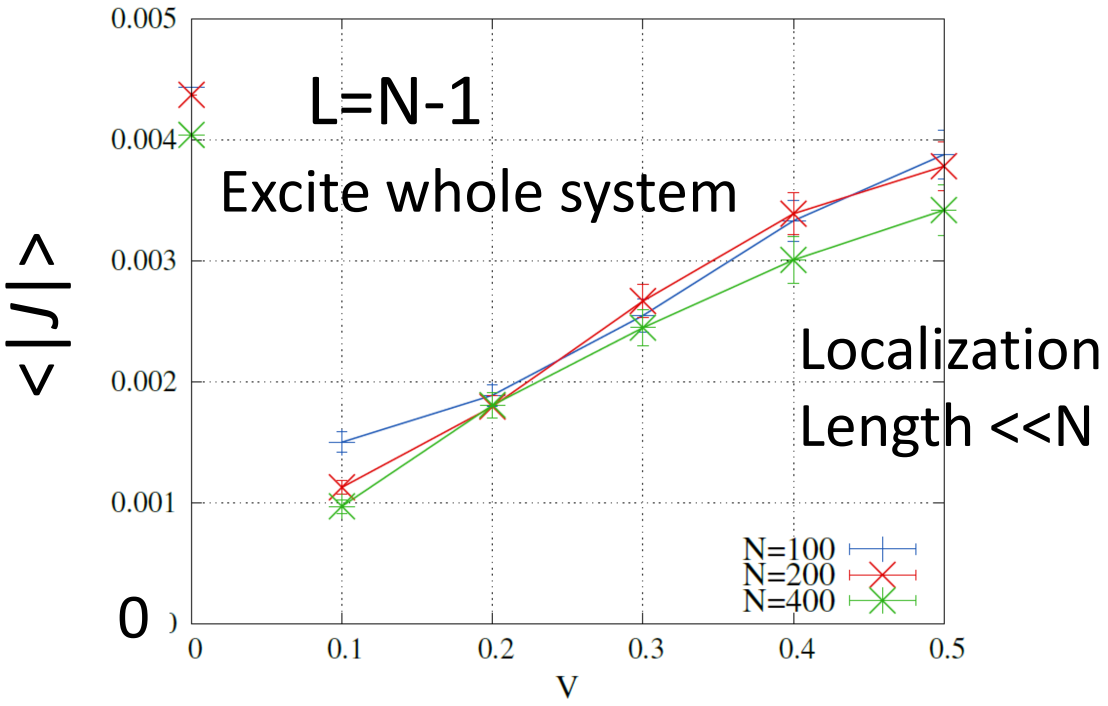


H. Ishizuka, NN NJP 2017 P50

preliminary



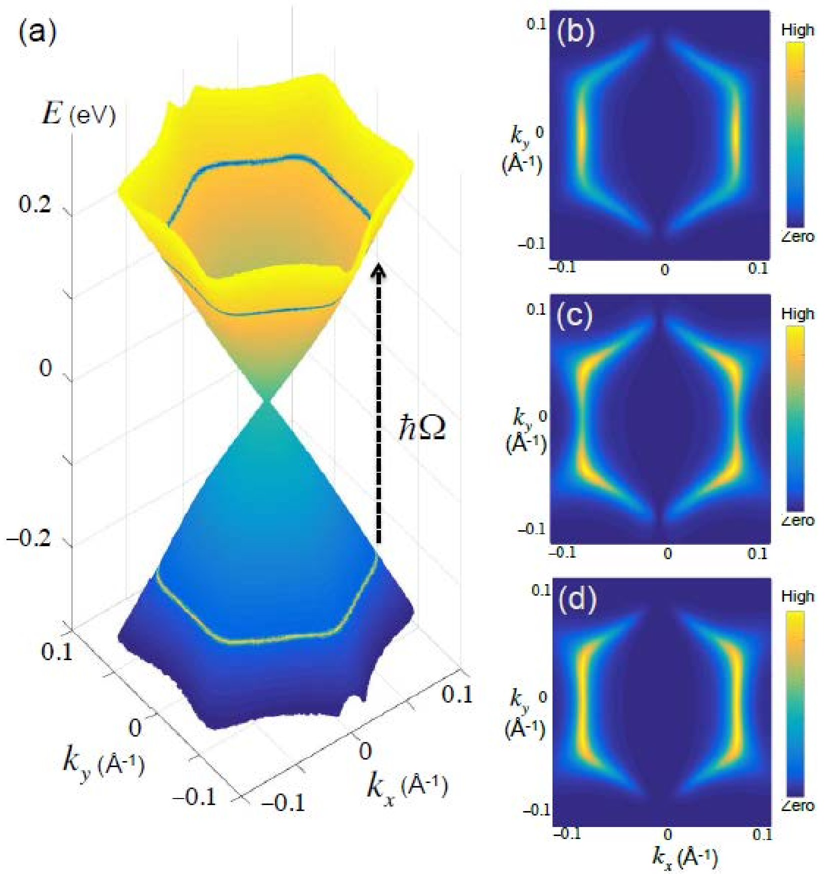
Positon of local excitation



Disorder strength

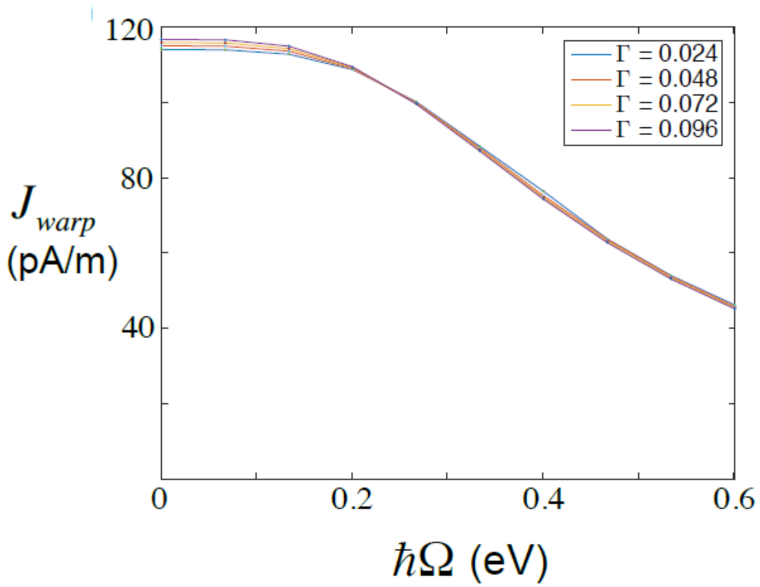
Shift current on the surface of TI

K.W.Kim, T.Morimoto, NN arXiv:1607.03888, PRB 2017



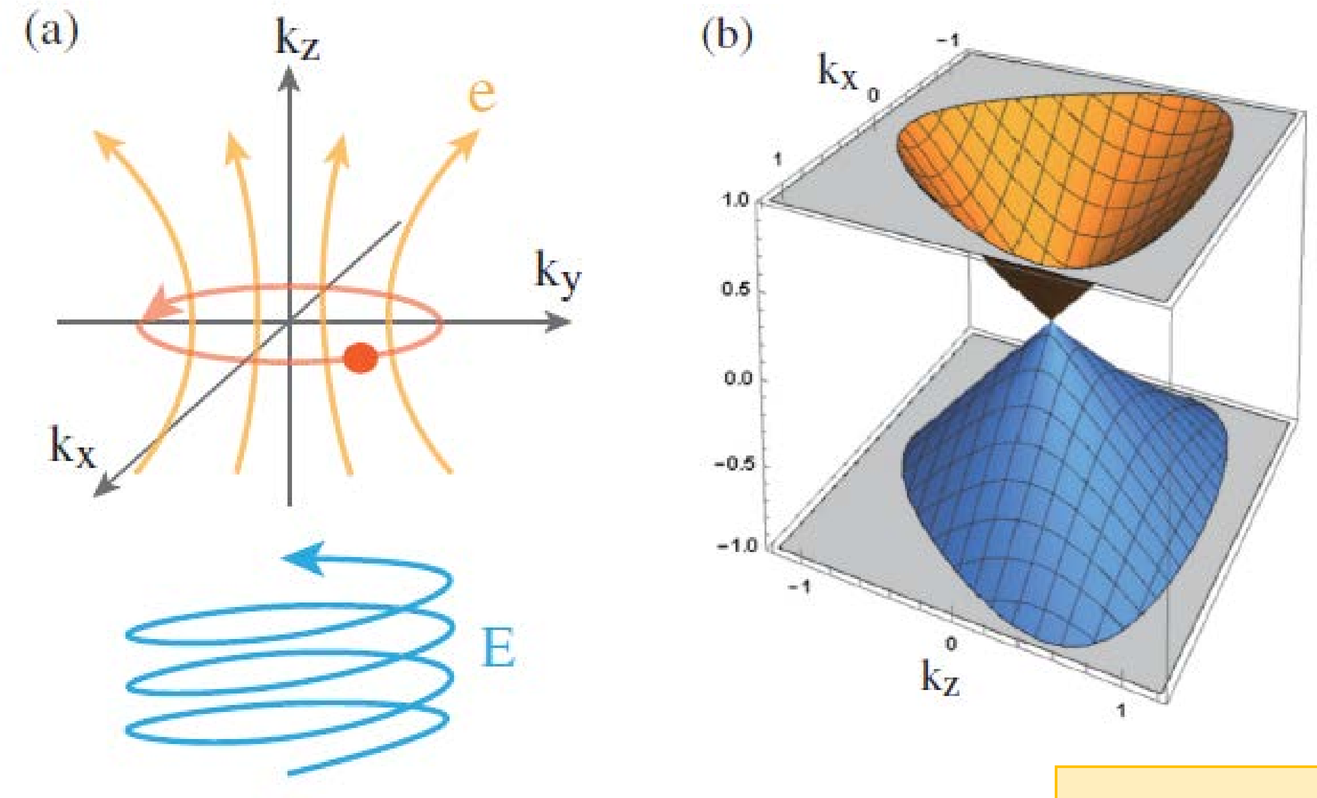
$$J_{warp} = -\frac{3\lambda}{16 v_F^2}\left[E_y^2\hat{y} - E_x^2\hat{y} - E_x E_y \hat{x} - E_y E_x \hat{x}\right]$$

$$= \frac{3\lambda E_0^2}{16 v_F^2}\left[\sin 2\phi \hat{x} + \cos 2\phi \hat{y}\right]$$



Emergent electric field of 3d Weyl fermion in momentum space

H. Ishizuka et al., PRL 2016



$$H(\vec{k},t) = \sum_{\nu} \sigma_\nu R_\nu(\vec{k},t)$$

$$R_x(\vec{k}) = vk_x + gD_y + \frac{\alpha_2}{2}k_xk_z,$$

$$R_y(\vec{k}) = vk_y - gD_x + \frac{\alpha_2}{2}k_yk_z,$$

$$R_z(\vec{k}) = v_zk_z + \frac{\alpha_1}{2}(k_x^2 + k_y^2 - 2k_z^2),$$

c.f. Moore-Orenstein PRL 2010
Sodeman-Fu PRL 2015

$$\bar{e}^z_{R,L} = \bar{e}^z_{+R,L} = \pm\pi \frac{4(v^2 - 2v_z^2)\alpha_1 - 3vv_z\alpha_2}{30v^5v_z^3} \times \alpha_1(\mu g D)^2\omega\cos(\chi).$$

Theorems

Nonreciprocal dc transport with time-reversal symmetry

in noncentrosymmetric systems:

dc E-field: requires both irreversibility and electron correlation

virtual excitation by interband matrix element of J

ac E-field: the quantum geometry of the multiband structure even

in noninteracting systems

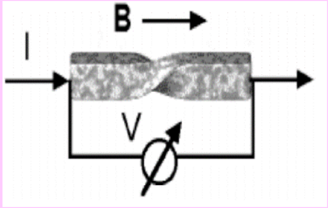
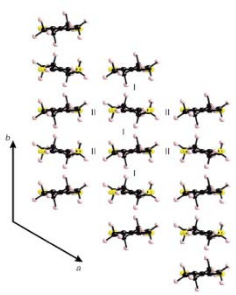
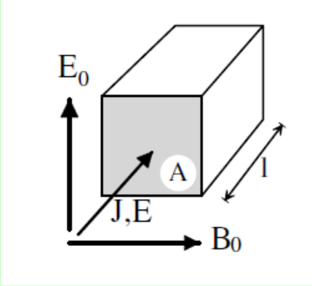
robust against the exciton formation and localization

real excitation by interband matrix element of J

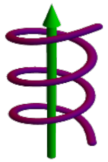
Nonreciprocal Response	Linear Response	Nonlinear Response
Time-reversal Unbroken	Forbidden	Shift current Nonlinear Hall effect pn junction
Time-reversal Broken	Optical ME effect Magnetochiral effect Nonreciprocal magnon	Nonreciprocal nonlinear optical effect Electric magnetochiral effect Inverse Edelstein effect Magnetochiral anisotropy

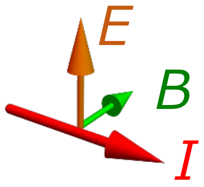
Table 1

Magnetochiral anisotropy - tiny effect

	Bi helices	Organics	Si FET
			
	G. L. J. A. Rikken *et al.* *PRL* **87**, 236602 (2001).	F. Pop *et al.* *Nat. Commun*. **5**, 3757 (2014).	G. L. J. A. Rikken *et al.* *PRL* **94**, 016601 (2005).
$\gamma\,(\mathrm{T}^{-1}\mathrm{A}^{-1})$	10^{-3}	10^{-2}	10^{-1}

$$\gamma \sim 10^4 T^{-1} A^{-1}$$



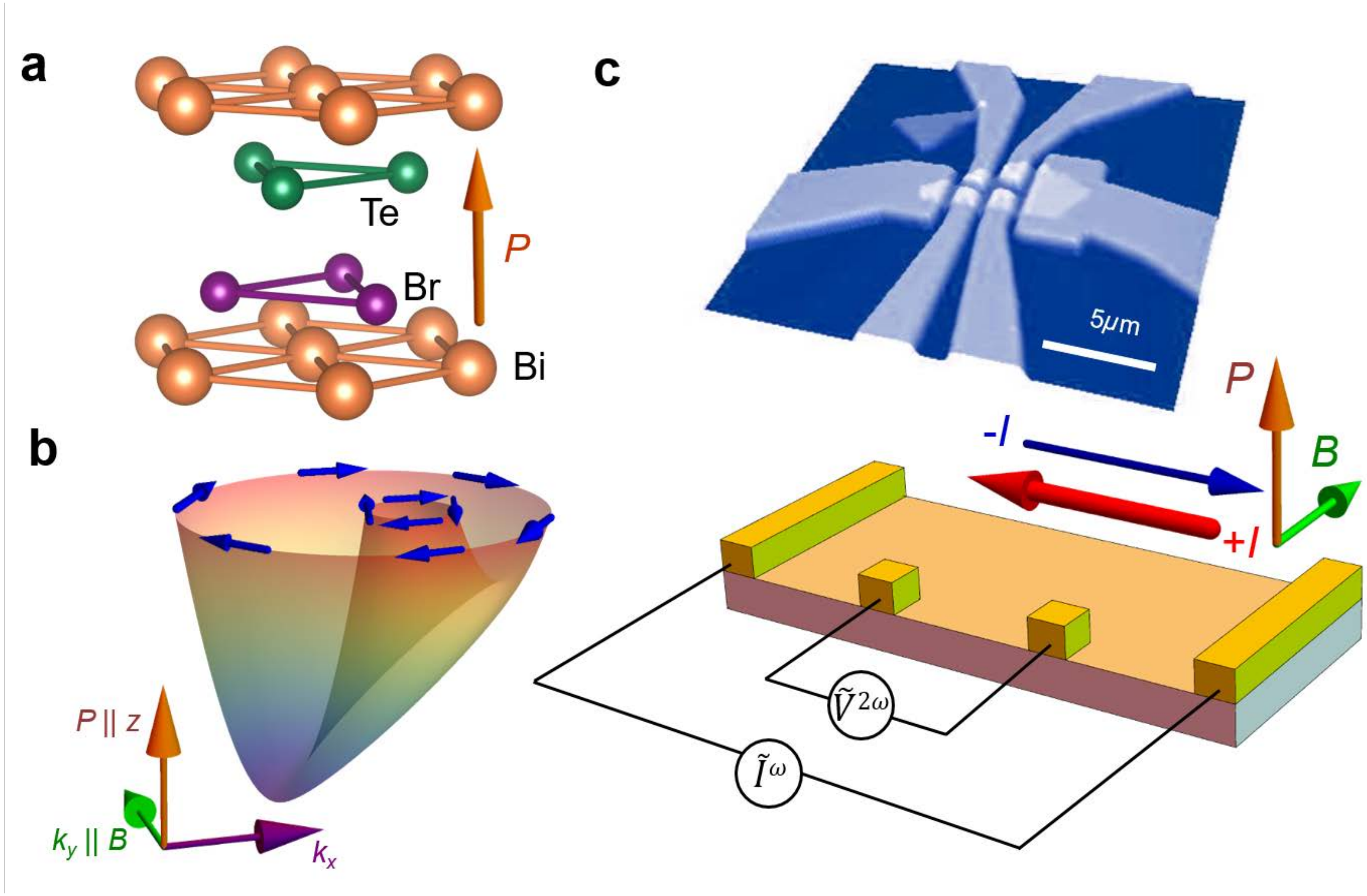


$$R = R_0\,(1 + \beta B^2 + \gamma B I)$$

$$\mu_B B,\ \varepsilon_{SOI} << \varepsilon_F$$

Enhanced magnetochiral anisotropy in BiTeBr

Y.Iwasa G, Y.Tokura G, NN G   Nature Phys. 2017



Magnetochiral anisotropy in Rashba model

K. Hamamoto

$$H = \frac{k_z^2}{2m_\parallel} + \frac{k_x^2 + k_y^2}{2m_\perp} + \lambda(k_x\sigma_y - k_y\sigma_x) - B_y\sigma_y$$

Boltzmann equation

$$-e\boldsymbol{E}\cdot\frac{\partial f}{\partial \boldsymbol{k}} = -\frac{1}{\tau}(f - f_0)$$

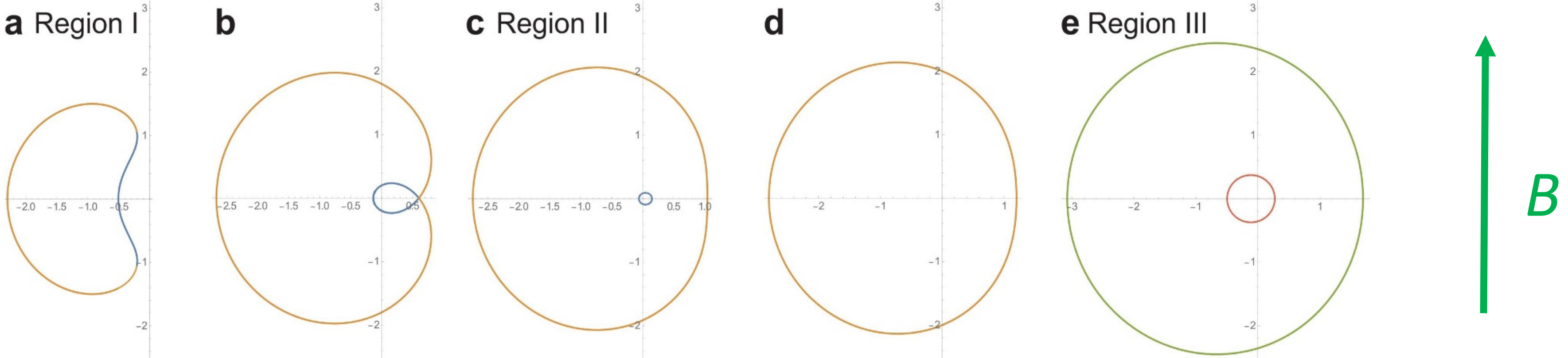
Expand in E

$$f = f_0 + f_1 + f_2 + \cdots,$$

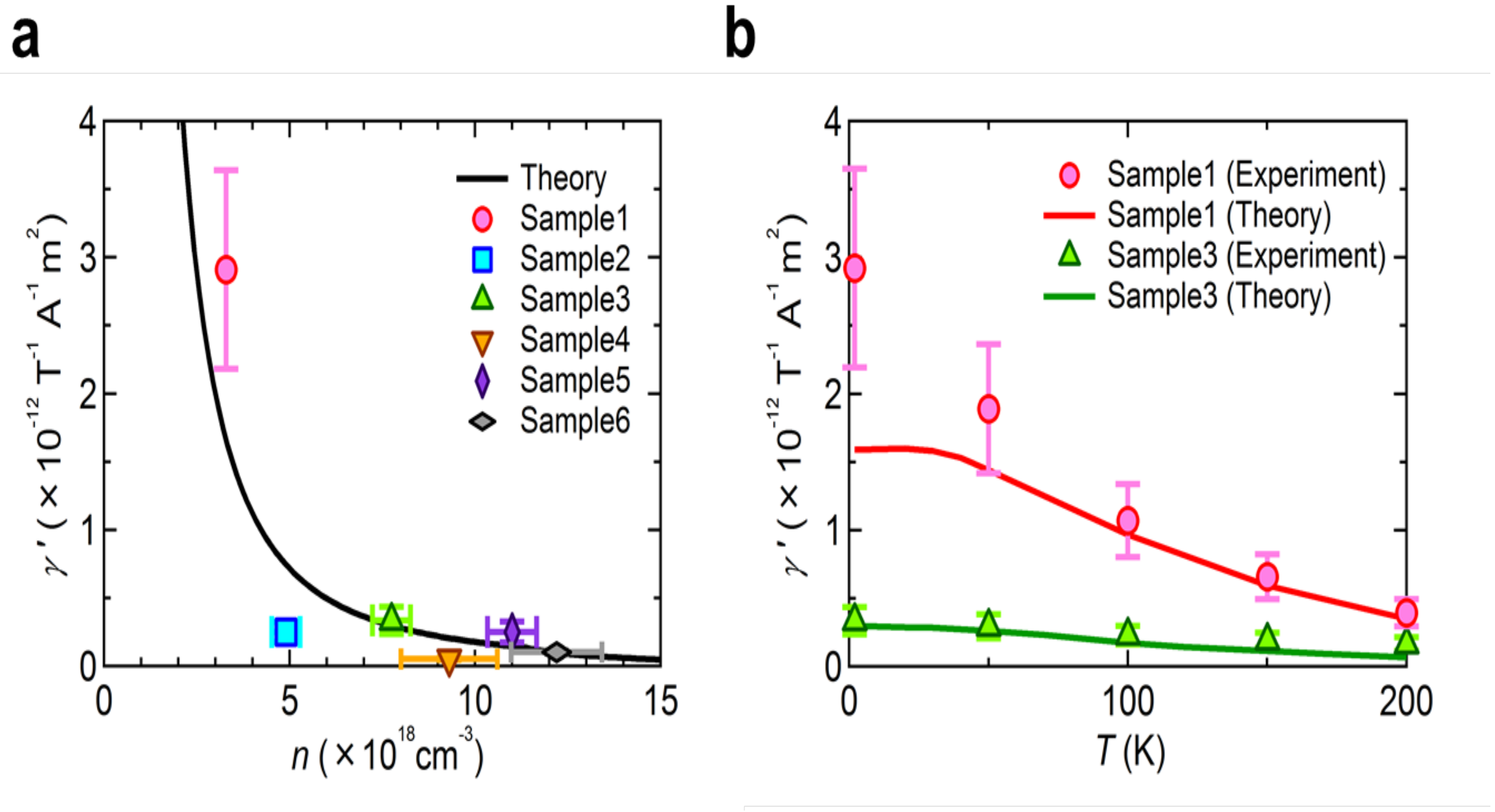
$$J_x = J_x^{(1)} + J_x^{(2)} = \sigma_1 E_x + \sigma_2 E_x^2$$

γ is independent of τ in the single relaxation time approx. like Hall coefficient

γ diverges as n → 0   increasing Fermi energy   γ is zero when two FSs coexist



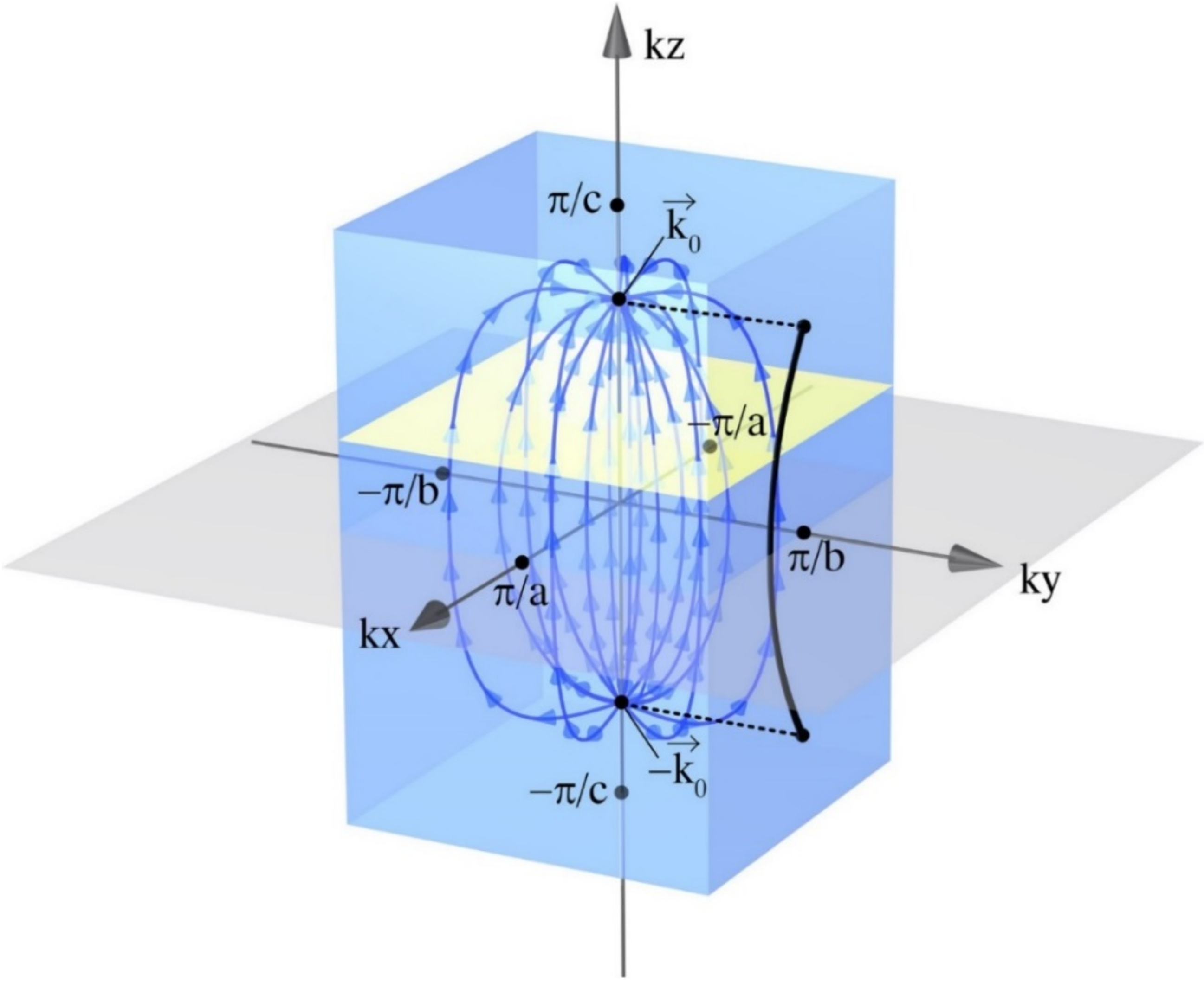
No fitting parameters !



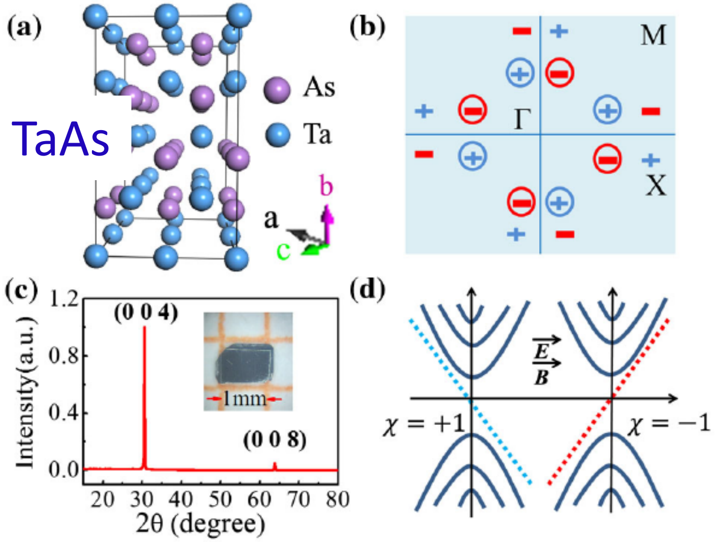
$\gamma \sim 1 T^{-1} A^{-1}$

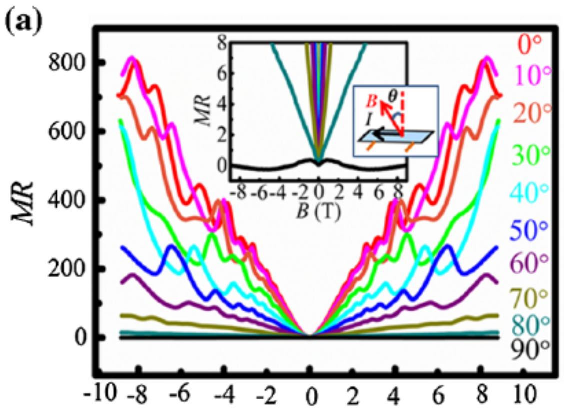
$\gamma' = \gamma A$ $\quad A$ cross section of the sample

Weyl semimetals



X. Huang et al., PRX 2015





negative magnetoresistance
due to chiral anomaly

Chiral anomaly in Weyl semimetals

$$\frac{dQ^5}{dt} = \frac{2\nu}{(2\pi)^2}\frac{e^2}{\hbar^2}\boldsymbol{E}\cdot\boldsymbol{B}$$

$$Q^5 = \frac{\nu e^2 \tau}{4\pi^2\hbar^2}\boldsymbol{E}\cdot\boldsymbol{B}$$

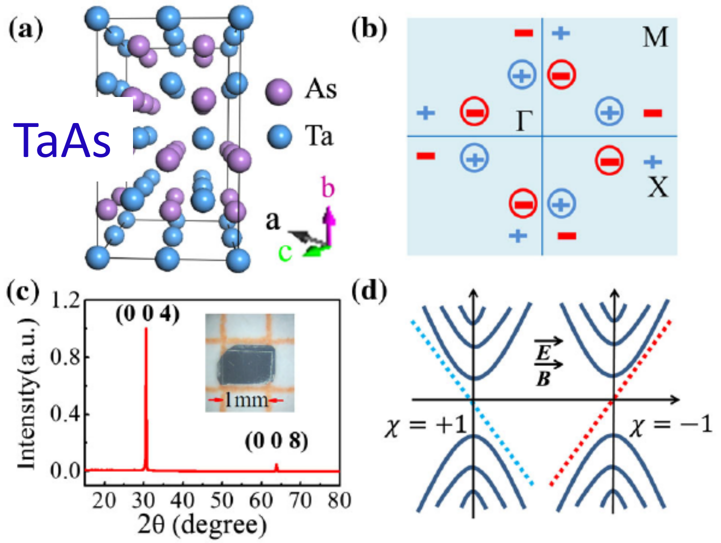
$$\boldsymbol{J} = -(e^2/h^2)\mu^5\boldsymbol{B}$$

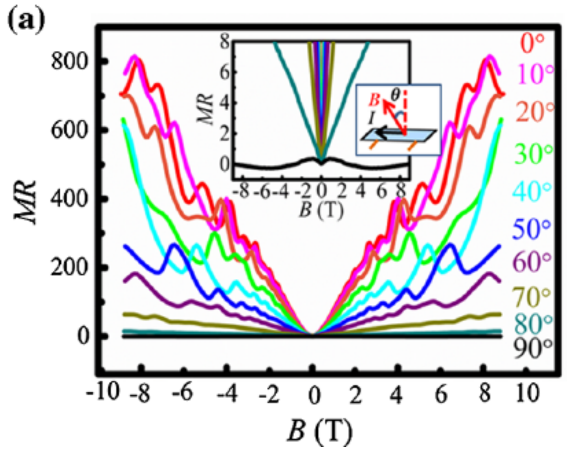
μ_5 chemical potential difference
in non-equilibrium steady state

$$\Delta J \propto \tau(B\cdot E)B$$

K. Fukushima, D. Kharzeev

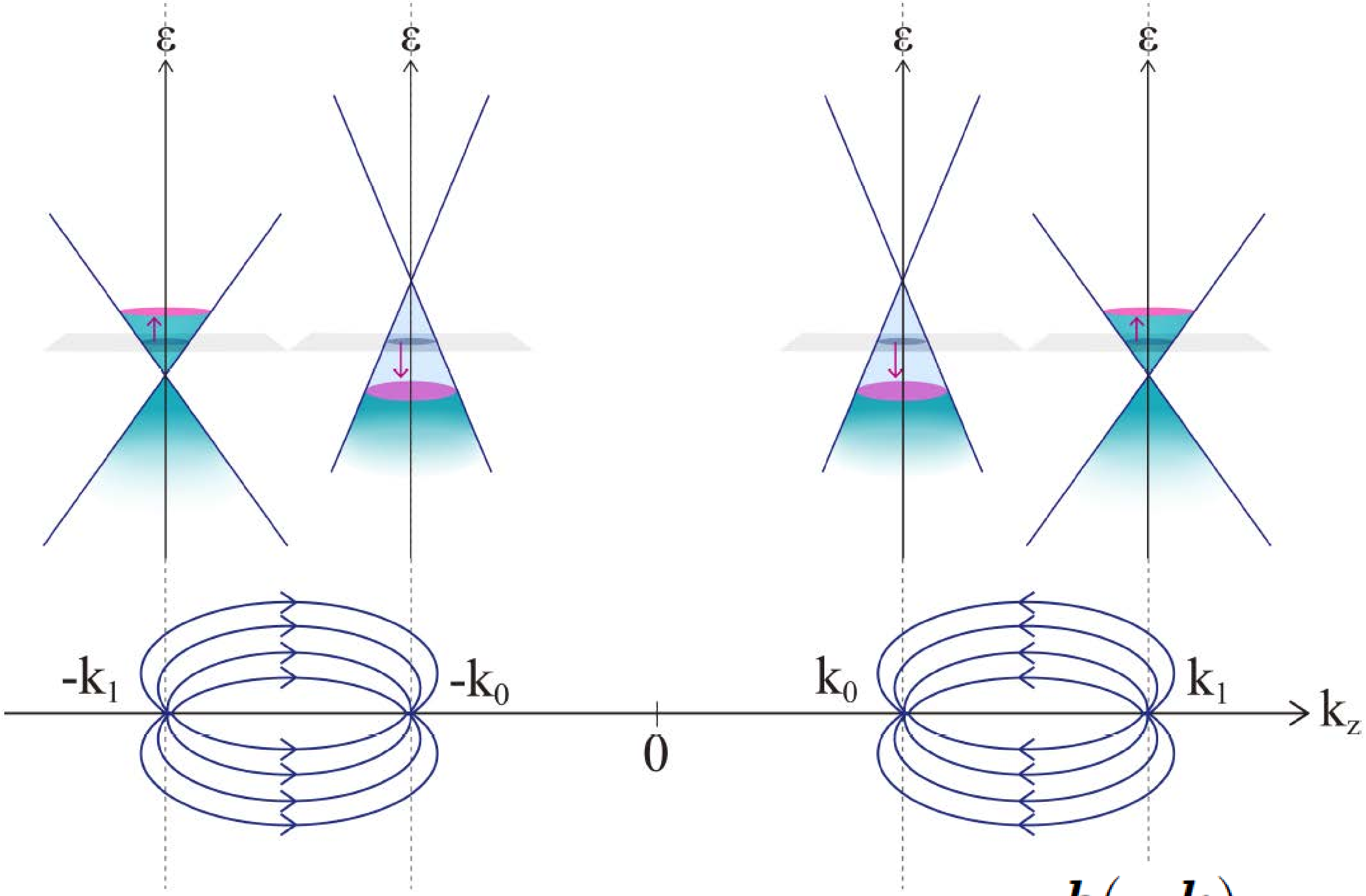
X. Huang et al., PRX 2015





negative magnetoresistance
due to chiral anomaly

Weyl fermions in noncentrosymemtric semimetals



$$\boldsymbol{b}(-\boldsymbol{k}) = -\boldsymbol{b}(\boldsymbol{k})$$

Magnetochial anisotropy in noncentrosymemtric Weyl semimetals

T. Morimoto, NN PRL2016

$$\Delta\sigma_\pm = \frac{1}{3}e^2 v_\pm^2 \tau \frac{dD_\pm(\epsilon)}{d\epsilon}\Delta\epsilon_\pm$$

$$\Delta\sigma_\pm = \pm\nu \frac{e^4}{6\pi^2\hbar^2}\frac{v_\pm^2\tau^2}{\epsilon_\pm}\boldsymbol{E}\cdot\boldsymbol{B}.$$

$$\rho = \rho_0(1 + \gamma \boldsymbol{I}\cdot\boldsymbol{B})$$

$$\gamma' = \gamma A$$

$$\gamma' = -\frac{2\delta\sigma/(\boldsymbol{E}\cdot\boldsymbol{B})}{\sigma^2} = -\frac{12\pi^2\hbar^4}{\nu}\left(\frac{v_+^2}{\epsilon_+} - \frac{v_-^2}{\epsilon_-}\right)\left(\frac{\epsilon_+^2}{v_+} + \frac{\epsilon_-^2}{v_-}\right)^{-2}$$

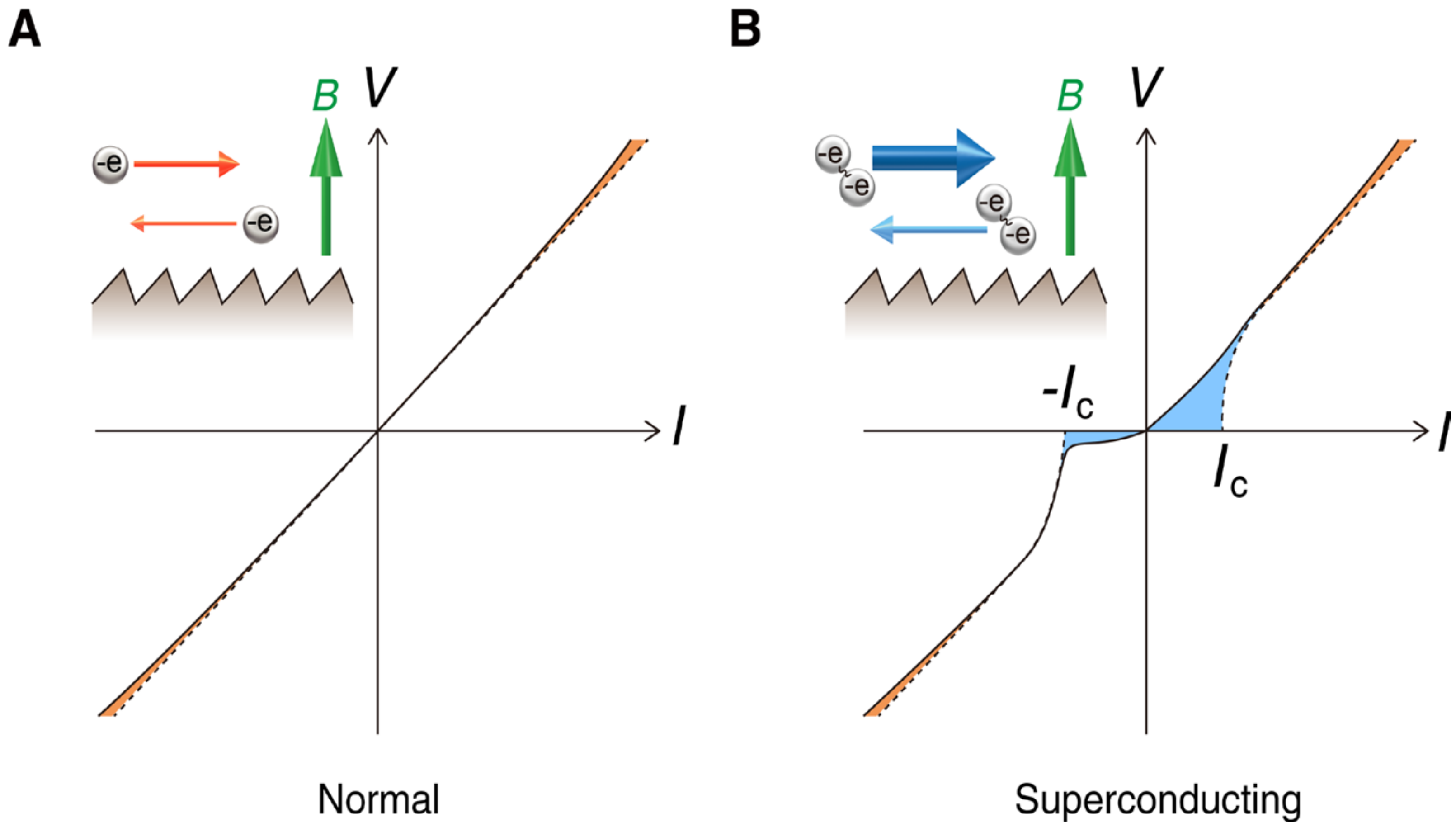
$v \sim 4\times 10^5 m/\sec$ $|\varepsilon_\pm| \sim 10meV$ ⇒ $\gamma' \simeq 3\times 10^{-8}\times \mathrm{m^2T^{-1}A^{-1}}$

$\gamma \sim 10T^{-1}A^{-1}$ TaAs

$$\gamma' \boldsymbol{J}\cdot\boldsymbol{B} \simeq 3\times 10^{-4}\times (J/(1\mathrm{A/cm^2}))(B/1\ \mathrm{T})$$

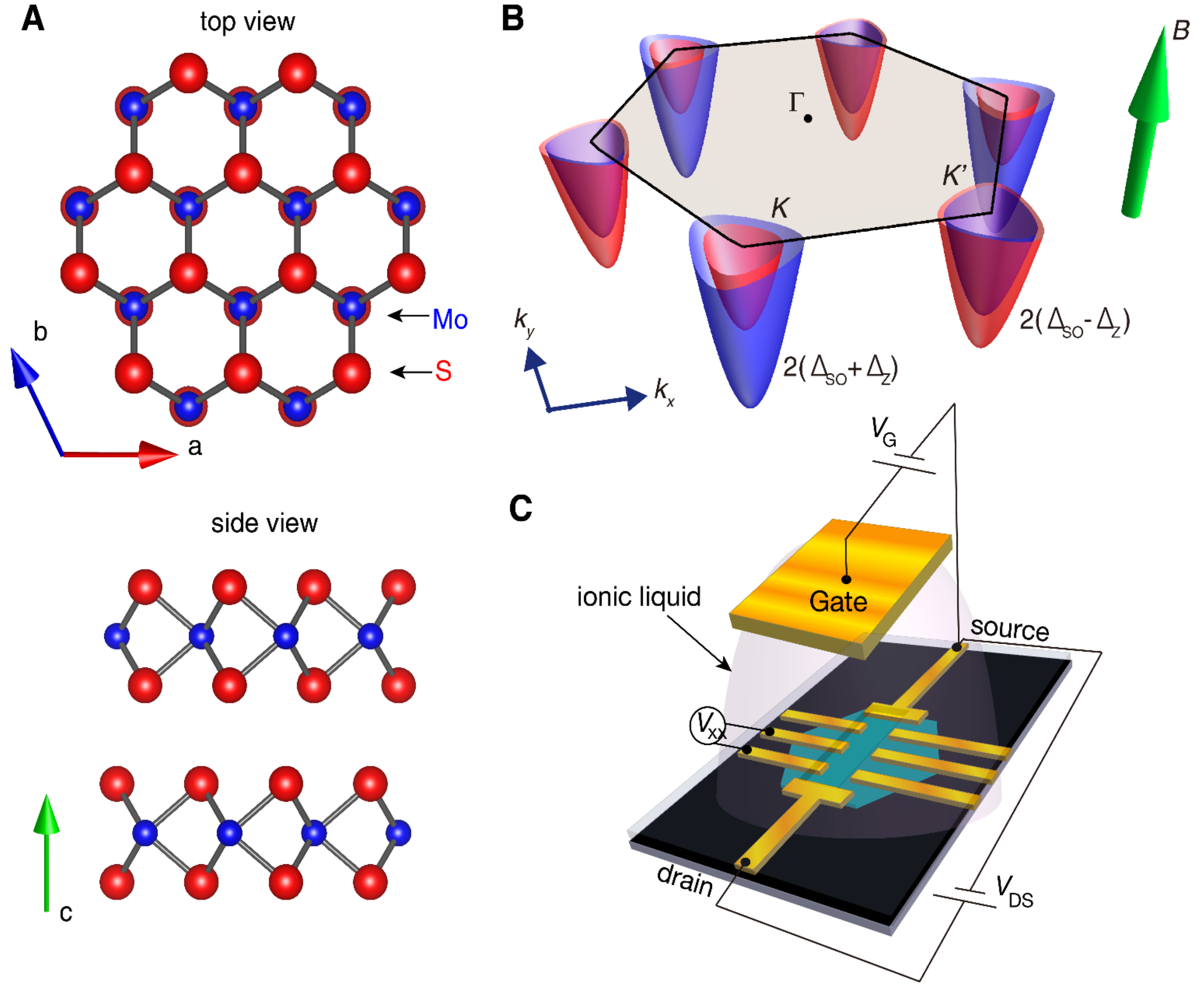
Giant enhancement of non-reciprocal response in superconductor

Wakatsuki, Saito et al. Science Adv. 2017



$$\Delta_{SC} \sim \mu_B B,\ \varepsilon_{SOI} << \varepsilon_F$$

Band structure and spin splitting in MoS2



Paraconductivity due to SC fluctuation in noncentrosymmetric MoS2

$$H_{k\sigma\tau} = \frac{\hbar^2 k^2}{2m} + \tau_z \lambda k_x (k_x^2 - 3k_y^2) - \Delta_Z \sigma_z - \Delta_{SO} \sigma_z \tau_z,$$

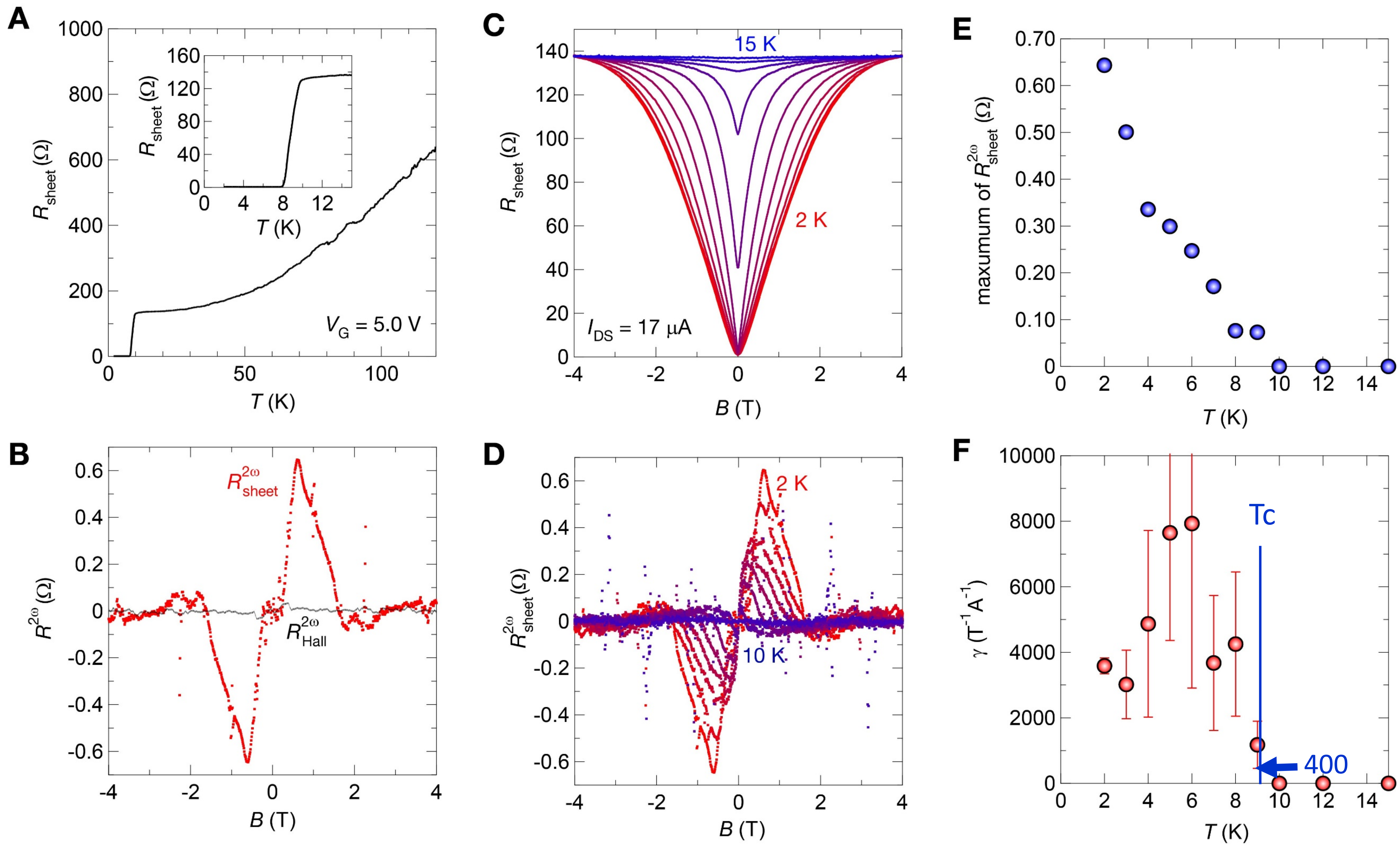
$$F = \int \mathrm{d}\boldsymbol{r} \Psi^* \left[a + \frac{\boldsymbol{p}^2}{4m} + \frac{\Lambda B}{\hbar^3} (p_x^3 - 3p_x p_y^2) \right] \Psi + \frac{b}{2} \int d\,\boldsymbol{r} |\Psi(\boldsymbol{r})|^4,$$

$$\Lambda = \frac{93\zeta(5)}{28\zeta(3)} \frac{g\mu_\mathrm{B} \Delta_\mathrm{SO} \lambda}{(\pi k_\mathrm{B} T_\mathrm{c})^2}$$

$$\boldsymbol{j} = \frac{e^2}{16\hbar} \epsilon^{-1} \boldsymbol{E} - \frac{\pi e^3 m \Lambda B}{64 \hbar^3 k_\mathrm{B} T_\mathrm{c}} \epsilon^{-2} \boldsymbol{F}(\boldsymbol{E})$$

$$\frac{\gamma_S}{\gamma_N} \sim \left(\frac{\varepsilon_F}{k_B T_c} \right)^3$$

$$\epsilon = \frac{T - T_c}{T_c} \qquad \boldsymbol{F}(\boldsymbol{E}) = (E_x^2 - E_y^2, -2E_x E_y)$$



A
B
C
D
E
F
V_G = 5.0 V
I_DS = 17 μA
15 K
2 K
10 K
Tc
400
T (K)
B (T)
R_sheet (Ω)
R^2ω (Ω)
R^2ω_sheet
R^2ω_Hall
maxumum of R^2ω_sheet (Ω)
γ (T^-1 A^-1)

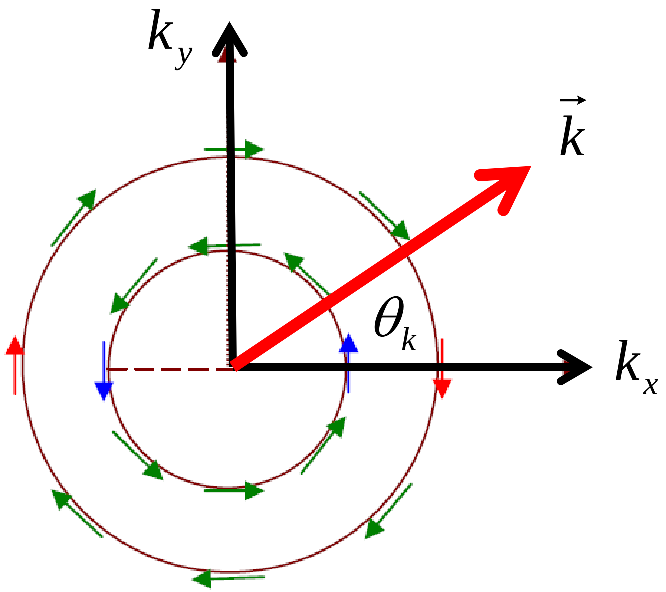
Rashba superconductor

$$H=\sum_k \psi_k^+(\xi_k+\lambda\vec{k}_{2D}\cdot\vec{\sigma})\psi_k+\Delta_s\psi_k^+ i\sigma_y\psi_{-k}^+ +\Delta_p\psi_k^+ i(\vec{d}(\vec{k})\cdot\vec{\sigma})\sigma_y\psi_{-k}^+ + h.c.$$

Chiral base $\psi_{k\uparrow}=\frac{1}{\sqrt{2}}(c_{k+}+e^{-i\theta_k}c_{k-}),\quad \psi_{k\downarrow}=\frac{1}{\sqrt{2}}(e^{i\theta_k}c_{k+}-c_{k-})$

$$H=\sum_k(\xi_k\pm\lambda|\vec{k}|)c_{k\pm}^+c_{k\pm}+(-\Delta_s+\Delta_p)e^{-i\theta_k}c_{k+}^+c_{-k+}^+ +(\Delta_s+\Delta_p)e^{i\theta_k}c_{k-}^+c_{-k-}^+ + h.c.$$

+ and – bands are p+ip superconductor



Frigeri et al. 2004

Fu-Kane, 2008
Proximity effect of 3D topological insulator and s-wave SC

Z2 classification of DIII in 2D

$|\Delta_s|>|\Delta_p|$ Non-topological

$|\Delta_s|<|\Delta_p|$ Topological→ helical Majorana

Y.Yanaka-Yokoyama-Balatsky-N.N.
Fujimoto-Sato

Summary

- Non-linear and non-reciprocal responses in nontrosymmetric systems contain rich physics

- Time-reversal symmetry plays an important role

- Nonreciprocal response without T-breaking is related to "interband current" and "quantum geometry"
  - Electron correlation gives the dc nonreciprocal response
  - Shift current in photovoltaic effect from Berry phase

- Enhancement of Magnetochiral anisotropy
  - Polar Rashba semiconductor
  - Weyl semimetals due to chiral anomaly
  - Bosonic transport due to Cooper pairing

Symmetry   Quantum Geometry   Electron Correlation   Irreversibility