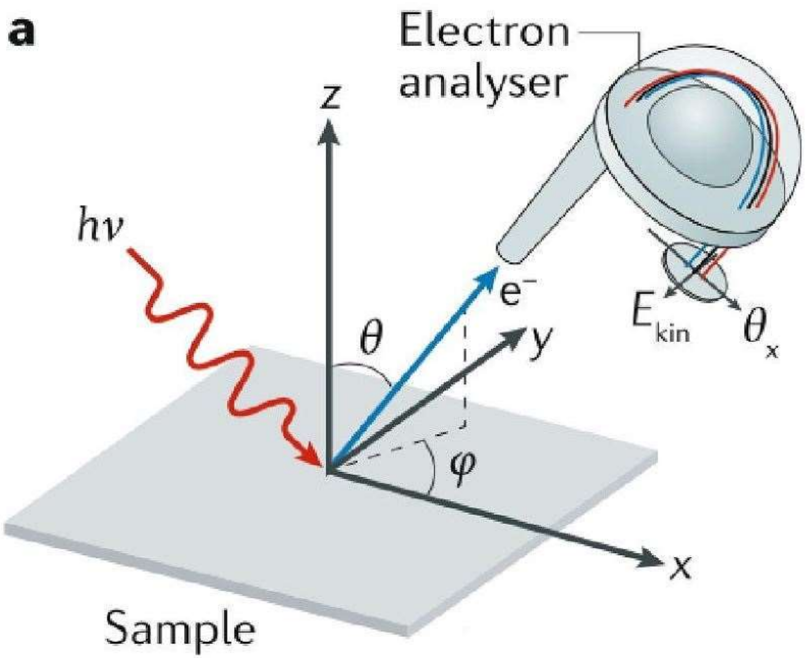
Berry curvature near degenerate point

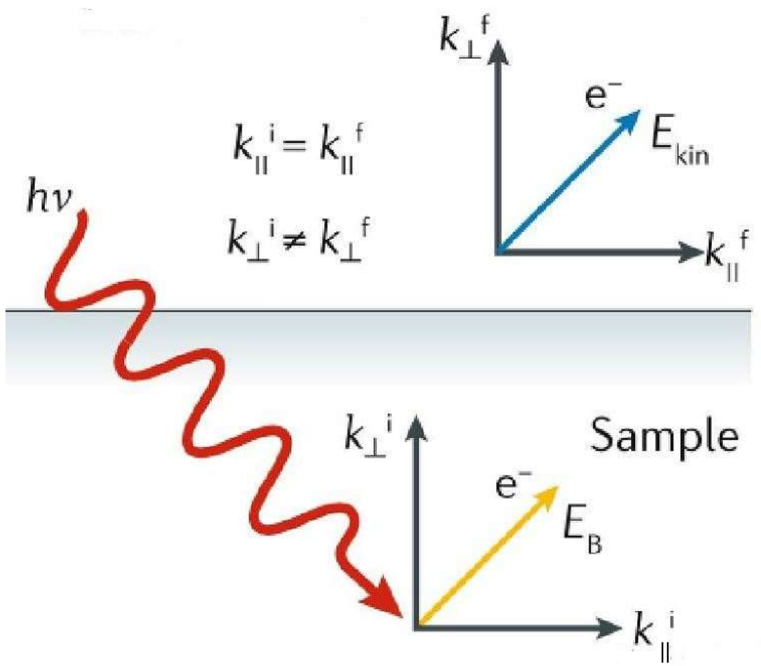
- 2D: SS of TI, Graphene
- 3D: Weyl semimetal (later)

How to verify the Dirac cone of surface states?

➡ Angle-Resolved Photo-Emission Spectroscopy (ARPES)

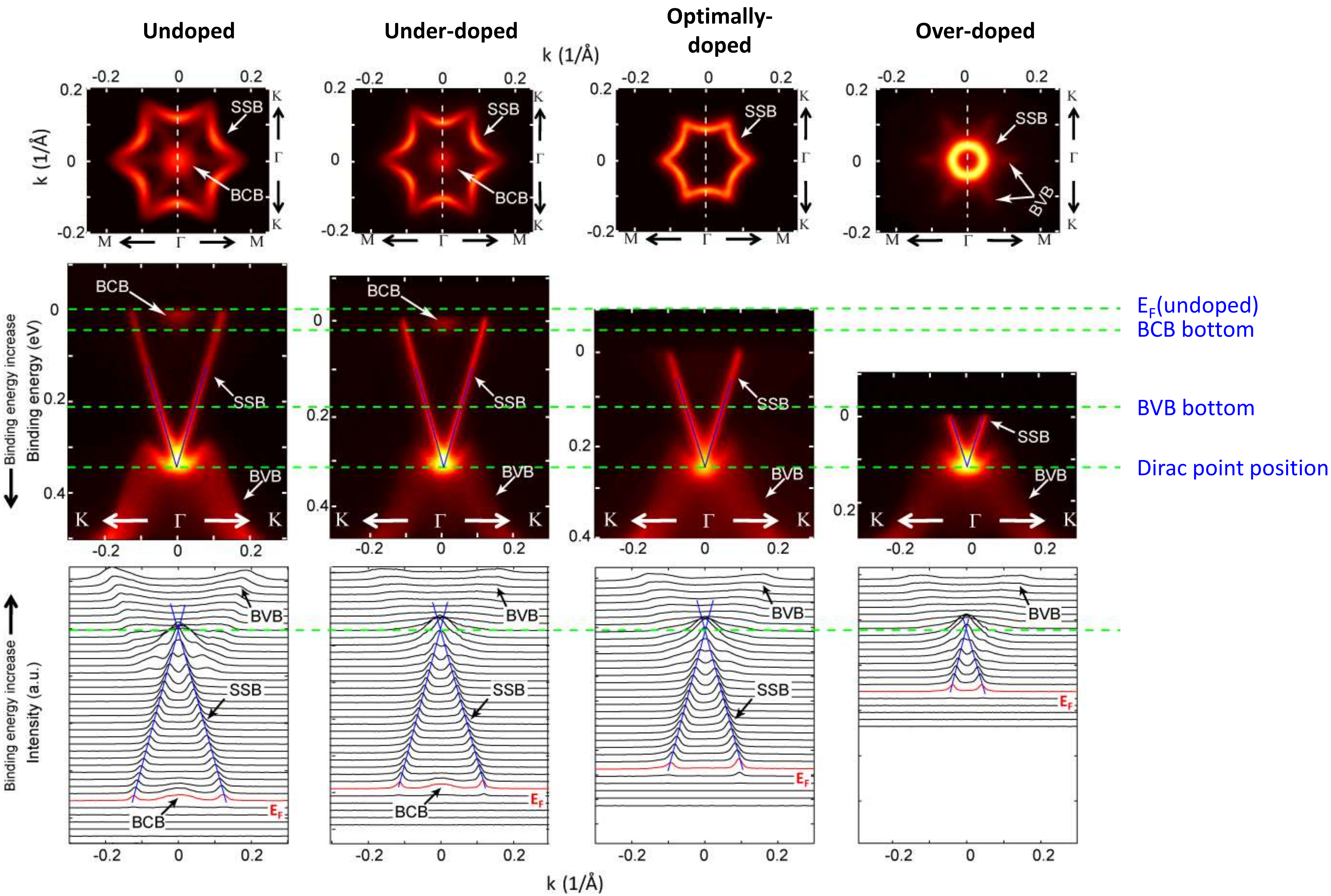
- Basically, it's photoelectric effect
- Can determine the energy dispersion of filled states
- Synchrotron radiation is used (20-100 eV)
- Sensitive to surface property (depth ~30 A), ideal for surface property and 2D material





Arpes experiment on Be_2Te_3 surface states, Shen group

Doping evolution of the FS and band structure



Effective Hamiltonian for the 2D surface state of 3D TI:

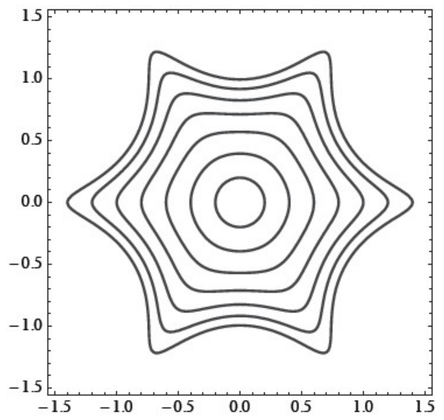
- Near the Dirac point.

Constraint from symmetry (T, M, and C_3)

Fu PRL 2010

$$H(\vec{k}) = \varepsilon_0(\vec{k}) I_{2\times 2} + v_k \left(k_x\sigma_y - k_y\sigma_x\right) + \frac{\lambda}{2}\left(k_+^3 + k_-^3\right)\sigma_z$$

Warped Dirac cone

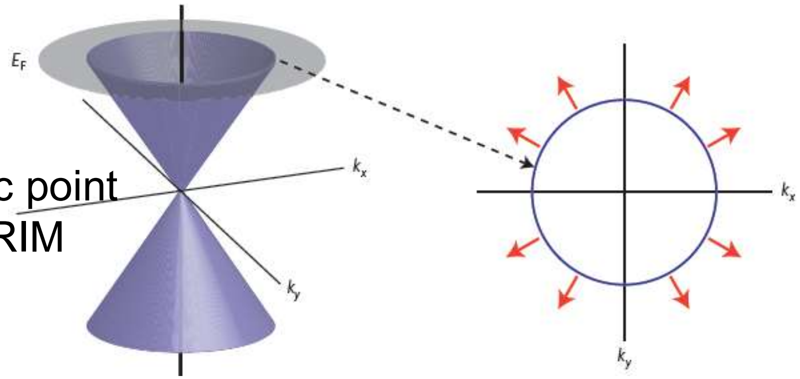


- To lowest order in k,

$$H_{SS} = \alpha(\vec{k}\times\vec{\sigma})_z, \quad \langle\vec{\sigma}\rangle \perp \vec{k}$$

or

$$H_{SS} = \alpha(\vec{k}\cdot\vec{\sigma})_z, \quad \langle\vec{\sigma}\rangle // \vec{k}$$

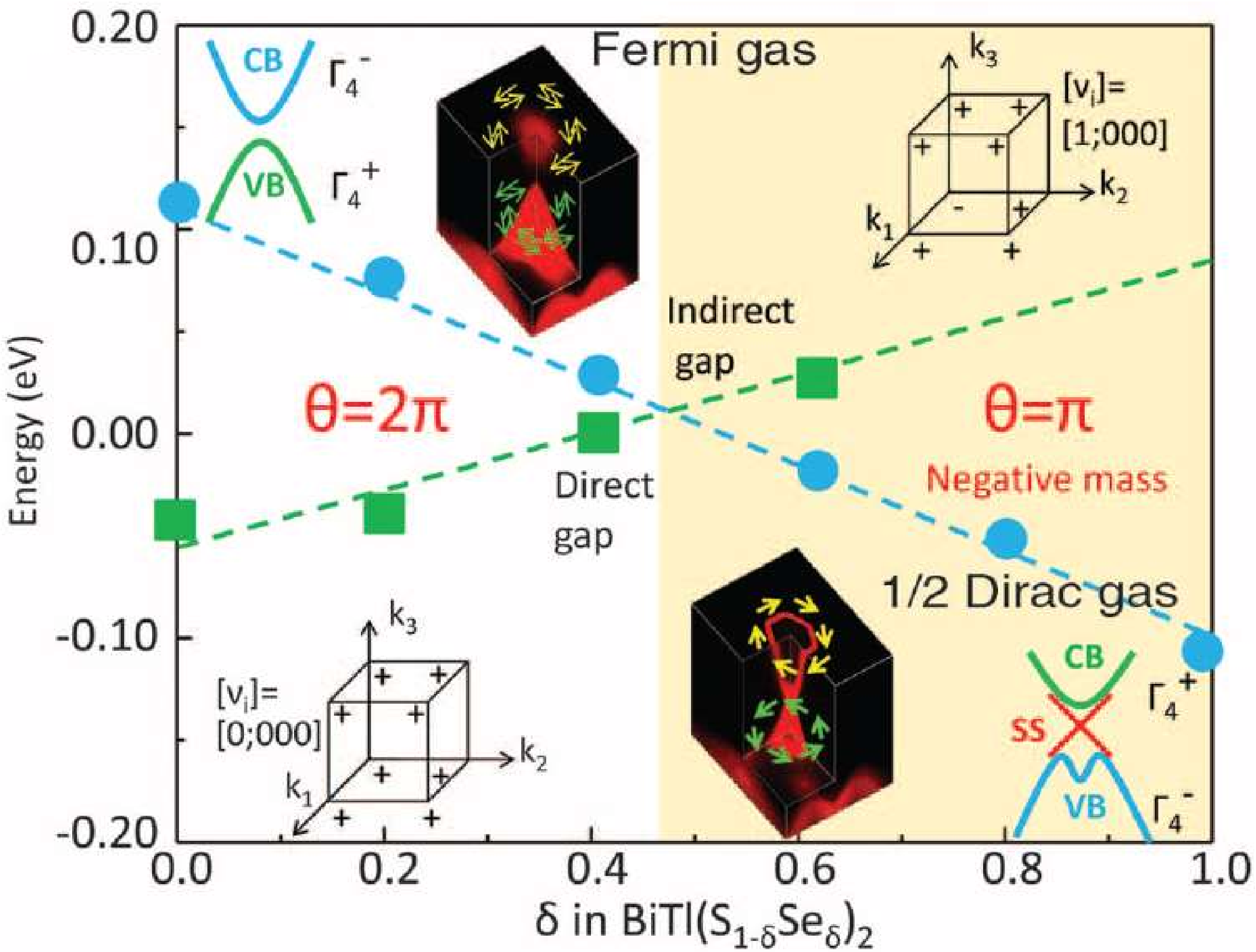


spin-momentum locking (Dirac cone with spin texture)

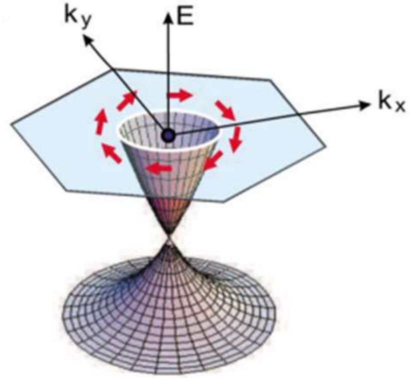
Spin-resolved ARPES

Band inversion, parity change, emergence of SS, and

spin-momentum locking



$$H_{SS} = \alpha(\vec{k} \times \vec{\sigma})_z$$

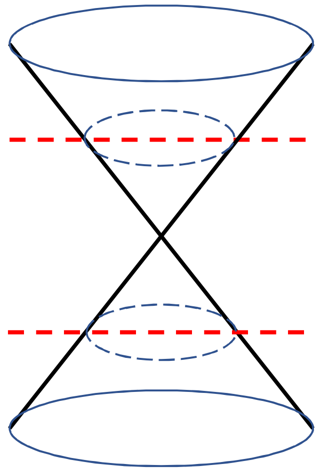


S.Y. Xu et al Science 2011

Berry curvature in surface state

Near a Dirac point

$$\mathrm{H}_{SS} = \alpha(\boldsymbol{\sigma} \times \mathbf{k})_z + O(k^2)$$

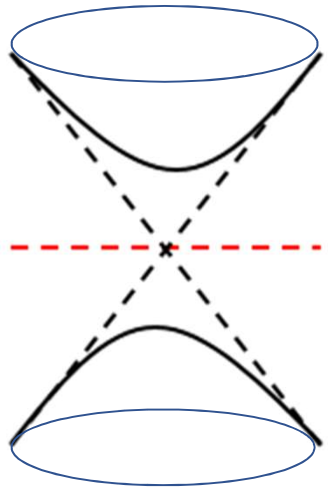


$$\gamma_C = \mp\frac{\Omega_C}{2} = \mp\pi$$ For a circle C around a DP

$$\Rightarrow \quad F_z^{\pm} = \mp\pi\delta^2(\mathbf{k})$$

$$\Rightarrow \quad \sigma_H = 0$$

- Open a gap by magnetization



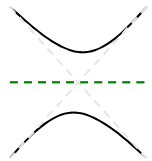
HW 1 $$\mathrm{H}_{SS} = \alpha(\boldsymbol{\sigma} \times \mathbf{k})_z + m\sigma_z$$

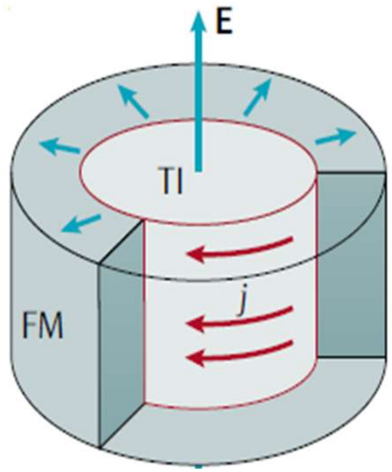
(a) $$F_z^{\pm} = \mp\frac{\alpha^2 m}{2(m^2+\alpha^2k^2)^{3/2}}$$

(b) $$\sigma_H = \frac{e^2}{h}\frac{1}{2\pi}\int d^2k F_z^- = \frac{1}{2}\frac{e^2}{h}$$

Half-integer QHE

Electromagnetic response of TI surface state





Surface state ∼2 DEG

- Hall current $J_H = \boxed{\frac{e^2}{2h}} E$

➡ • Induced magnetization

$$M = \frac{e^2}{2h} E$$

Magnetoelectric (ME) coupling

➡ Effective Lagrangian for EM wave

$$L_{EM} = L_0 + L_{axion}$$

$$L_0 = \frac{\varepsilon_0}{2}\left(E^2 - c^2 B^2\right) - \rho\phi + \vec{J}\cdot\vec{A}$$

$$L_{axion} = \boxed{\frac{e^2}{2h}} \vec{E}\cdot\vec{B} = \sqrt{\frac{\varepsilon_0}{\mu_0}}\,\alpha\,\frac{\Theta}{\pi}\,\vec{E}\cdot\vec{B}$$

fine structure constant

$$\alpha = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{\hbar c} \approx \frac{1}{137}$$

"axion" angle
軸子

$$\Theta = \begin{cases} \pi & \text{for TI} \\ 0 & \text{for trivial} \end{cases}$$

Cr_2O_3: θ∼π/24
(TRS is broken)

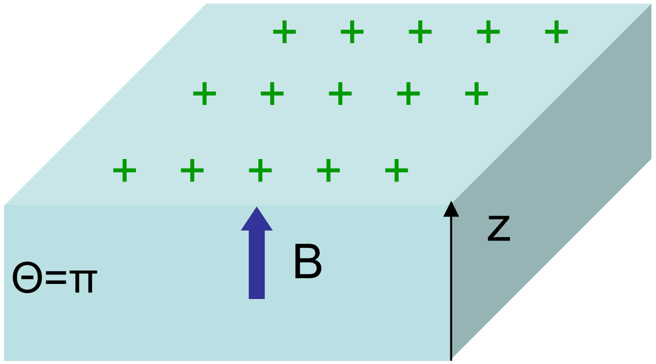
A particle proposed by Wilczek *et al* to fix the strong CP problem

Z. Wang et al, New J. Phys. 2010

Maxwell eqs with axion coupling (suppose ε, μ are constants)

$$\begin{cases} \nabla\cdot\left(\vec{E}+\alpha\frac{\Theta}{\pi}c\vec{B}\right)=\frac{\rho}{\varepsilon} \\ \nabla\times\left(\vec{B}-\alpha\frac{\Theta}{\pi c}\vec{E}\right)=\mu\vec{J}+\frac{\partial}{c^2\partial t}\left(\vec{E}+\alpha\frac{\Theta}{\pi}c\vec{B}\right) \\ \nabla\cdot\vec{B}=0 \\ \nabla\times\vec{E}=-\frac{\partial}{\partial t}\vec{B} \end{cases}$$

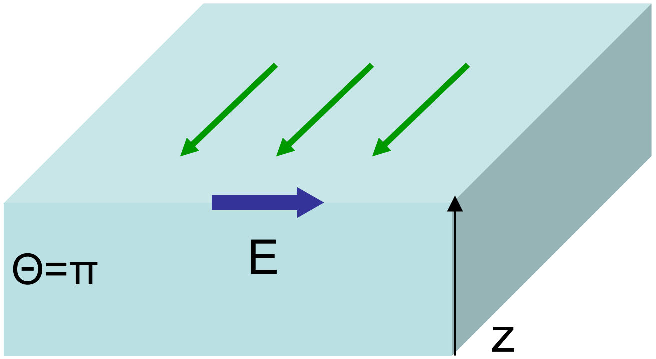
e.g., $\Theta(\vec{r})=\pi h(-z)$



$$\rho_\Theta=c\alpha\varepsilon\delta(z)B_z$$

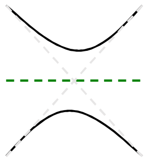
Effective charge and effective current

$$\begin{cases} \nabla\cdot\vec{E}=\frac{\rho+\rho_\Theta}{\varepsilon} \\ \rho_\Theta=-\frac{c\alpha\varepsilon}{\pi}\nabla\cdot\left(\Theta\vec{B}\right) \\ \nabla\times\vec{B}=\mu\left(\vec{J}+\vec{J}_\Theta\right)+\frac{1}{c^2}\frac{\partial\vec{E}}{\partial t} \\ \vec{J}_\Theta=\frac{\alpha}{\pi c\mu}\nabla\times\left(\Theta\vec{E}\right)+\frac{\alpha}{\pi c\mu}\frac{\partial}{\partial t}\left(\Theta\vec{B}\right) \end{cases}$$



$$\vec{J}_\Theta=-\frac{\alpha}{c\mu}\delta(z)\hat{z}\times\vec{E}\rightarrow\sigma_{xy}=\frac{1}{2}\frac{e^2}{h}$$

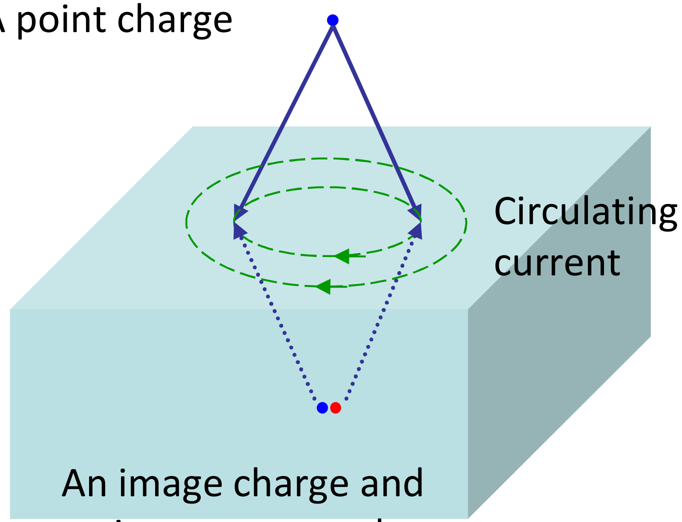
Axion effect



Static:

- Half-integer QHE
- Magnetic monopole in TI
- …

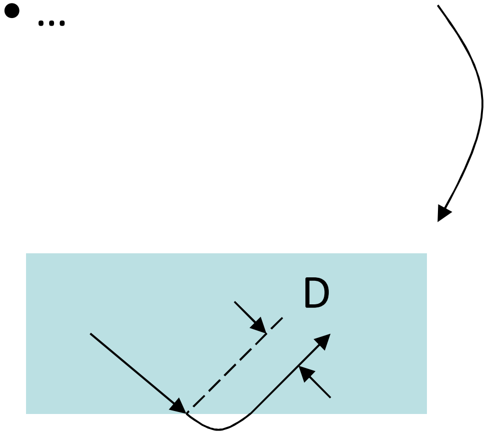
A point charge



Qi, Hughes, and Zhang, Science 2009

Dynamic:

- Snell's law
- Fresnel formulas
- Brewster angle
- Goos-Hänchen effect
- …



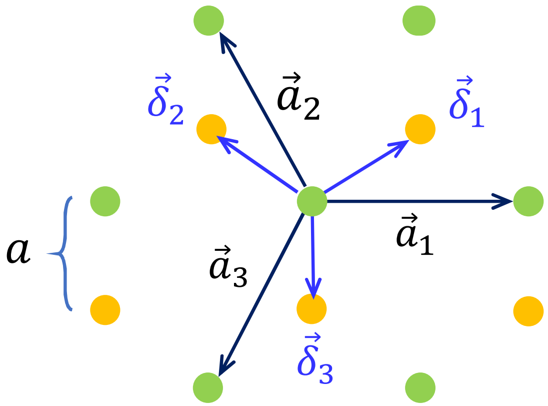
Longitudinal shift of reflected beam (total reflection)

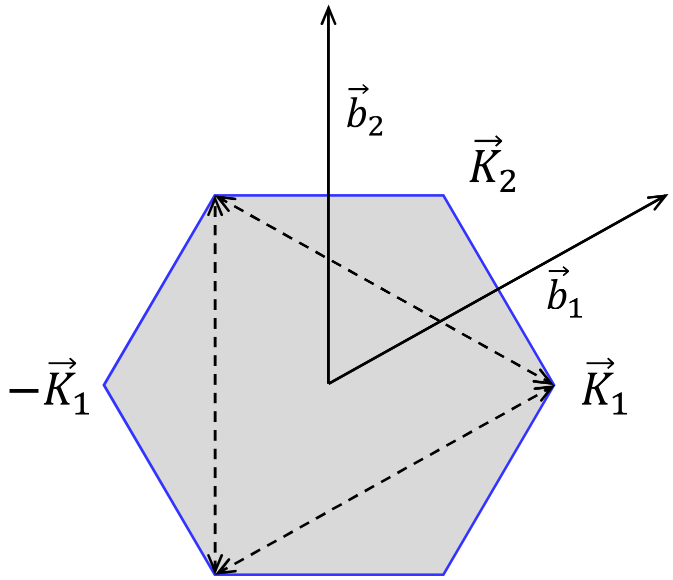
Chang and Yang, PRB 2009

Berry curvature near degenerate point

- 2D: SS of TI, Graphene
- 3D: Weyl semimetal (later)

Graphene without spin





Brillouin zone

$$\hat{H} = \hat{H}_{NN} + \hat{H}_{NNN} + \hat{H}_{on-site}.$$

(1)
$$\hat{H}_{NN} = t_1 \sum_{\mathbf{R}} \left(d^{\dagger}_{\mathbf{R}+\boldsymbol{\delta}_1} c_{\mathbf{R}} + d^{\dagger}_{\mathbf{R}+\boldsymbol{\delta}_2} c_{\mathbf{R}} + d^{\dagger}_{\mathbf{R}+\boldsymbol{\delta}_3} c_{\mathbf{R}} \right) + h.c.$$

(2)
$$\begin{aligned} \hat{H}_{NNN} &= t_2 \sum_{\mathbf{R}} \left(c^{\dagger}_{\mathbf{R}+\mathbf{a}_1} c_{\mathbf{R}} + c^{\dagger}_{\mathbf{R}+\mathbf{a}_2} c_{\mathbf{R}} + c^{\dagger}_{\mathbf{R}+\mathbf{a}_3} c_{\mathbf{R}} \right) \\ &+ t_2 \sum_{\mathbf{R}} \left(d^{\dagger}_{\mathbf{R}+\boldsymbol{\delta}_1+\mathbf{a}_1} d_{\mathbf{R}+\boldsymbol{\delta}_1} + d^{\dagger}_{\mathbf{R}+\boldsymbol{\delta}_1+\mathbf{a}_2} d_{\mathbf{R}+\boldsymbol{\delta}_1} \right. \\ &\qquad \left. + d^{\dagger}_{\mathbf{R}+\boldsymbol{\delta}_1+\mathbf{a}_3} d_{\mathbf{R}+\boldsymbol{\delta}_1} \right) + h.c., \end{aligned}$$

(3)
$$\hat{H}_{on-site} = \Delta \sum_{\mathbf{R}} c^{\dagger}_{\mathbf{R}} c_{\mathbf{R}} - \Delta \sum_{\mathbf{R}} d^{\dagger}_{\mathbf{R}+\boldsymbol{\delta}_1} d_{\mathbf{R}+\boldsymbol{\delta}_1}$$

Fourier transform

$$\boxed{\begin{aligned} c_{\mathbf{R}} &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}} c_{\mathbf{k}} \\ d_{\mathbf{R}+\boldsymbol{\delta}_1} &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{R}+\boldsymbol{\delta}_1)} d_{\mathbf{k}} \end{aligned}}$$

Orthogonal relation

$$\sum_{\mathbf{R}} e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}} = N\delta_{\mathbf{k}'\mathbf{k}}.$$

e.g.,

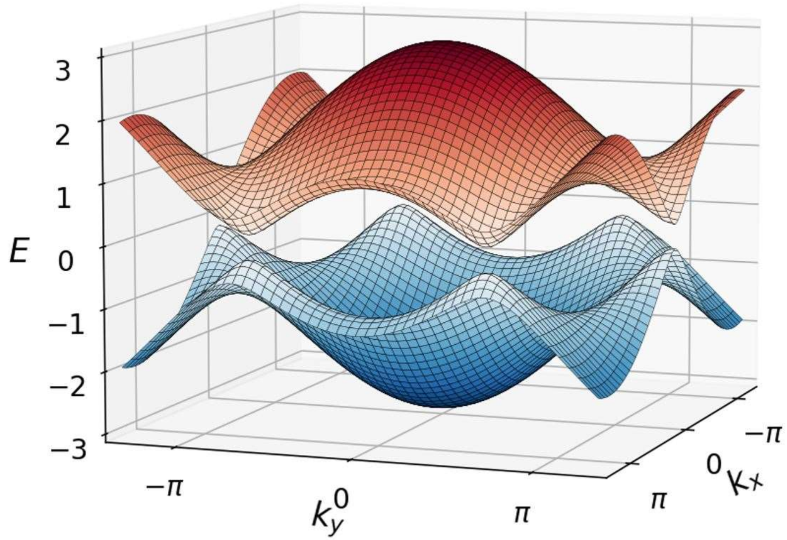
$$\begin{aligned} \sum_{\mathbf{R}} d^{\dagger}_{\mathbf{R}+\boldsymbol{\delta}_1} c_{\mathbf{R}} &= \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}'} \sum_{\mathbf{R}} e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}} e^{-i\mathbf{k}'\cdot\boldsymbol{\delta}_1} d^{\dagger}_{\mathbf{k}'} c_{\mathbf{k}} \\ &= \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\boldsymbol{\delta}_1} d^{\dagger}_{\mathbf{k}} c_{\mathbf{k}}, \end{aligned}$$

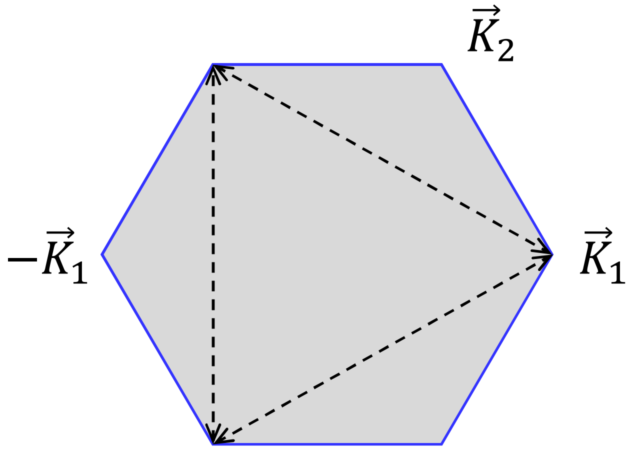
$$\begin{aligned} \hat{H} &= t_1 \sum_{\mathbf{k}} \left(e^{-i\mathbf{k}\cdot\boldsymbol{\delta}_1} + e^{-i\mathbf{k}\cdot\boldsymbol{\delta}_2} + e^{-i\mathbf{k}\cdot\boldsymbol{\delta}_3}\right) d^{\dagger}_{\mathbf{k}} c_{\mathbf{k}} \\ &+ t_2 \sum_{\mathbf{k}} \left(e^{-i\mathbf{k}\cdot\mathbf{a}_1} + e^{-i\mathbf{k}\cdot\mathbf{a}_2} + e^{-i\mathbf{k}\cdot\mathbf{a}_3}\right) c^{\dagger}_{\mathbf{k}} c_{\mathbf{k}} \\ &+ t_2 \sum_{\mathbf{k}} \left(e^{-i\mathbf{k}\cdot\mathbf{a}_1} + e^{-i\mathbf{k}\cdot\mathbf{a}_2} + e^{-i\mathbf{k}\cdot\mathbf{a}_3}\right) d^{\dagger}_{\mathbf{k}} d_{\mathbf{k}} + h.c. \\ &+ \Delta \sum_{\mathbf{k}} \left(c^{\dagger}_{\mathbf{k}} c_{\mathbf{k}} - d^{\dagger}_{\mathbf{k}} d_{\mathbf{k}}\right) \\ &= \sum_{\mathbf{k}} \left(c^{\dagger}_{\mathbf{k}}, d^{\dagger}_{\mathbf{k}}\right) \mathsf{H}(\mathbf{k}) \begin{pmatrix} c_{\mathbf{k}} \\ d_{\mathbf{k}} \end{pmatrix}. \end{aligned}$$

$$
\begin{aligned}
\mathrm{H}(\mathbf{k}) &= \begin{pmatrix} 2t_2\sum_i \cos\mathbf{k}\cdot\mathbf{a}_i + \Delta & t_1\sum_i e^{i\mathbf{k}\cdot\boldsymbol{\delta}_i} \\ t_1\sum_i e^{-i\mathbf{k}\cdot\boldsymbol{\delta}_i} & 2t_2\sum_i \cos\mathbf{k}\cdot\mathbf{a}_i - \Delta \end{pmatrix} \\
&= h_0(\mathbf{k}) + \mathbf{h}(\mathbf{k})\cdot\boldsymbol{\sigma},
\end{aligned}
$$

$$
\Rightarrow \quad \varepsilon_\pm(\mathbf{k}) = h_0(\mathbf{k}) \pm |\mathbf{h}(\mathbf{k})|
$$

$$
|\mathbf{h}| = \sqrt{3t_1^2 + 2t_1^2(\cos\mathbf{k}\cdot\mathbf{a}_1 + \cos\mathbf{k}\cdot\mathbf{a}_2 + \cos\mathbf{k}\cdot\mathbf{a}_3) + \Delta^2}
$$





Gapless (Dirac point) at
$$
\begin{cases}
\mathbf{K}_1 = \dfrac{2\pi}{a}\left(\dfrac{2}{3\sqrt{3}}, 0\right), \\
\mathbf{K}_2 = \dfrac{2\pi}{a}\left(\dfrac{1}{3\sqrt{3}}, \dfrac{1}{3}\right) \quad \text{or } -\mathbf{K}_1
\end{cases}
$$

Effective Hamiltonian near Dirac point

$$\mathbf{k} = \mathbf{K}_i + \mathbf{k}_i, \quad |\mathbf{k}_i| \ll |\mathbf{K}_i|; \; i = 1, 2.$$

$$H_{12}(\mathbf{k}) = t_1 \left(e^{i\mathbf{K}_i \cdot \boldsymbol{\delta}_1} e^{i\mathbf{k}_i \cdot \boldsymbol{\delta}_1} + e^{i\mathbf{K}_i \cdot \boldsymbol{\delta}_2} e^{i\mathbf{k}_i \cdot \boldsymbol{\delta}_2} + e^{i\mathbf{K}_i \cdot \boldsymbol{\delta}_3} e^{i\mathbf{k}_i \cdot \boldsymbol{\delta}_3} \right)$$

	$i = 1$	2	3
$\mathbf{K}_1 \cdot \boldsymbol{\delta}_i =$	$+\frac{2\pi}{3}$	$-\frac{2\pi}{3}$	0
$\mathbf{K}_2 \cdot \boldsymbol{\delta}_i =$	$-\frac{2\pi}{3}$	$+\frac{2\pi}{3}$	0
$e^{i\mathbf{K}_{1/2} \cdot \boldsymbol{\delta}_i} =$	$-\frac{1}{2} \mp \frac{\sqrt{3}}{2} i$	$-\frac{1}{2} \pm \frac{\sqrt{3}}{2} i$	1

$$\mathrm{H}(\mathbf{k}) \simeq \begin{pmatrix} \Delta & \frac{3}{2} t_1 a (\pm k_x - i k_y) \\ \frac{3}{2} t_1 a (\pm k_x + i k_y) & -\Delta \end{pmatrix}$$
$$= \boxed{\hbar v_F (\tau k_x \sigma_x + k_y \sigma_y) + \Delta \sigma_z,}$$

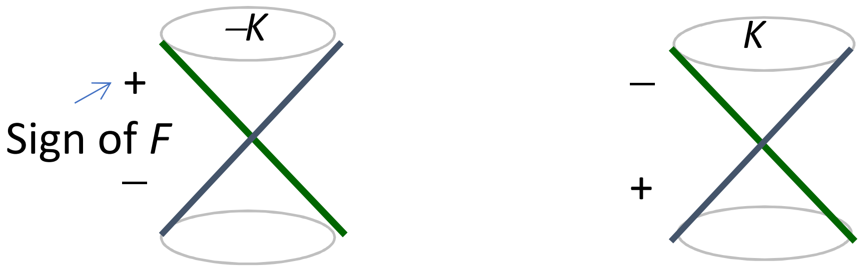
$\tau \equiv \pm$ for $\pm K_1$ 2 inequivalent Dirac “valleys”

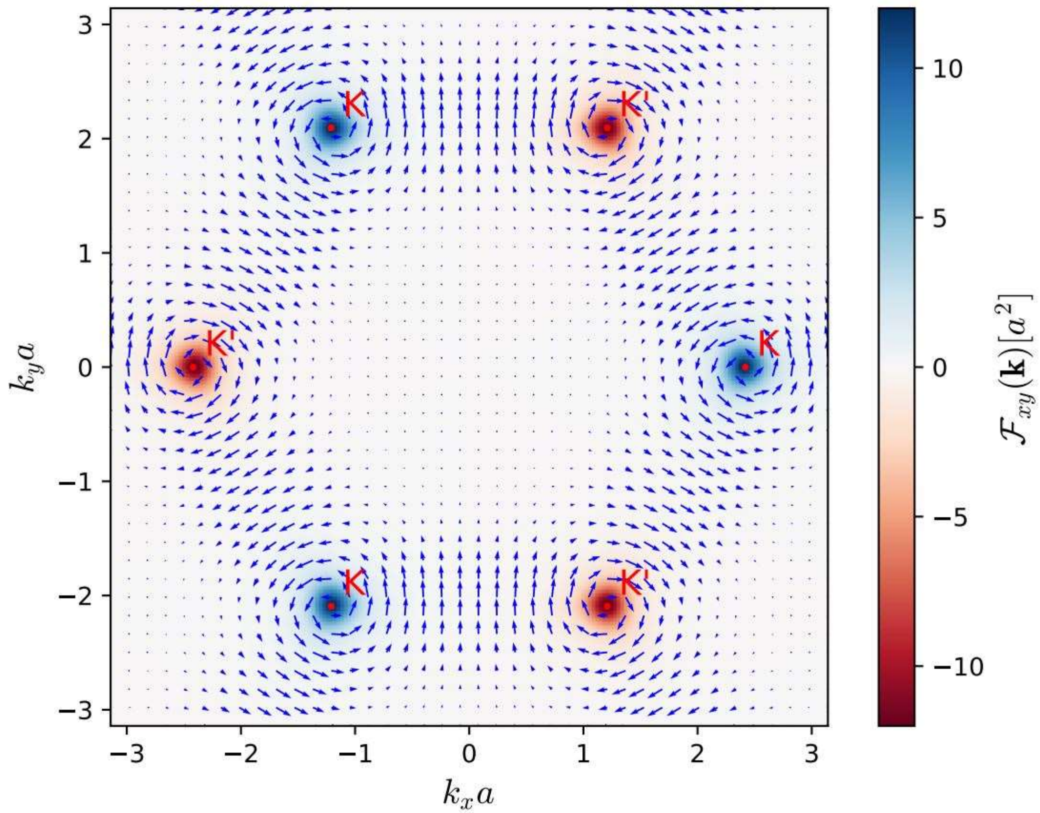
Berry curvature $$F_z^{\pm}(\mathbf{k}) = \mp \frac{1}{2h^3} \mathbf{h} \cdot \frac{\partial \mathbf{h}}{\partial k_x} \times \frac{\partial \mathbf{h}}{\partial k_y}.$$

Berry curvature

Near Dirac point $$F^{\pm}_{z\tau}(\mathbf{K}_1) = \pm\tau\frac{9}{8}\frac{a^2t_1^2\Delta}{h^3} = \pm\tau\frac{1}{2}\frac{\hbar^2v_F^2\Delta}{h^3}$$

Conduction band and valence band have opposite Berry curvatures

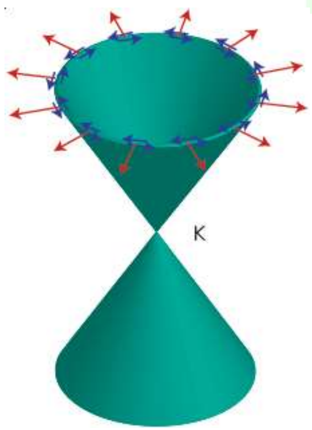


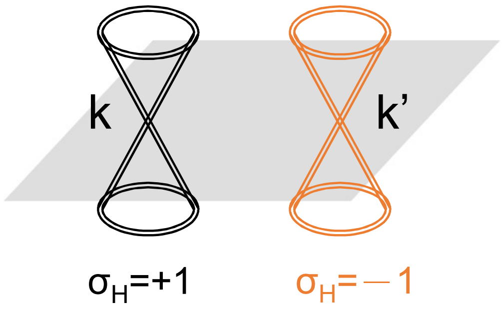


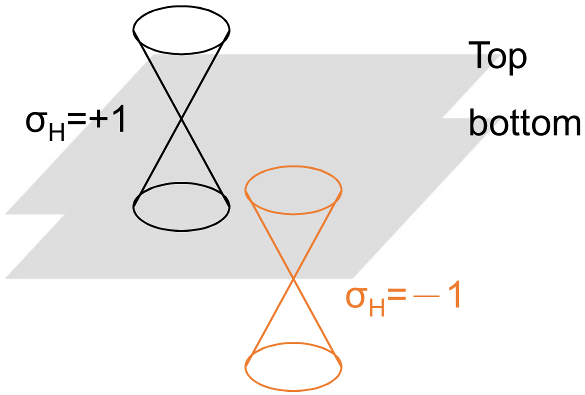
Dirac point:

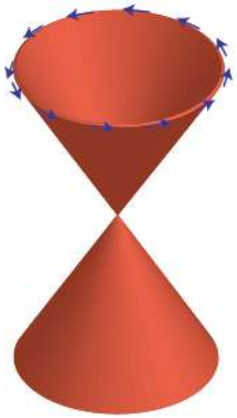
Graphene vs. Topological insulator

even number	odd number (on one side)
located at Fermi energy	not located at E_F
half integer QHE (×4)	half integer QHE (if E_F is located at DP)
spin is not locked with k	spin is locked with k
can be opened by substrate (DP protected by TRS + SIS)	*cannot* be opened if there is TRS

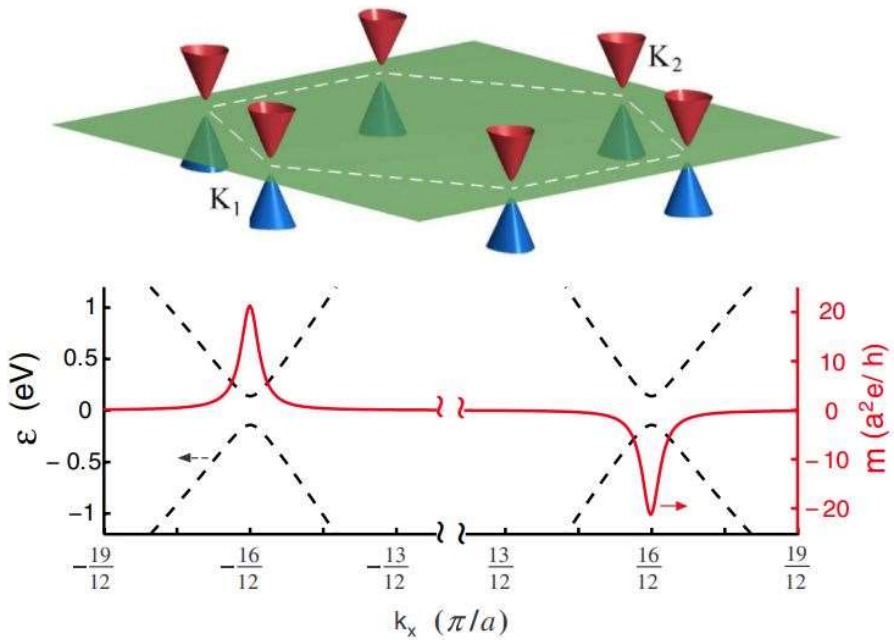








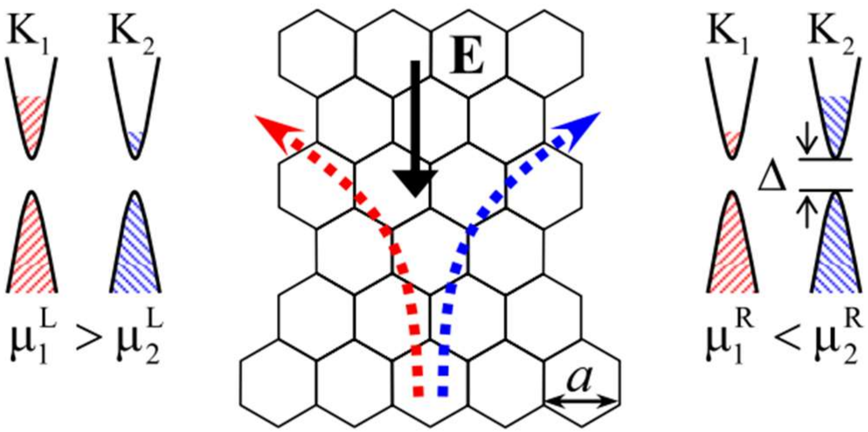
Valley Hall effect (Xiao et al, PRL 2007)



B=0 !

$\leftarrow \Omega \sim m$

Orbital magnetic moment



Opposite Lorentz-like forces

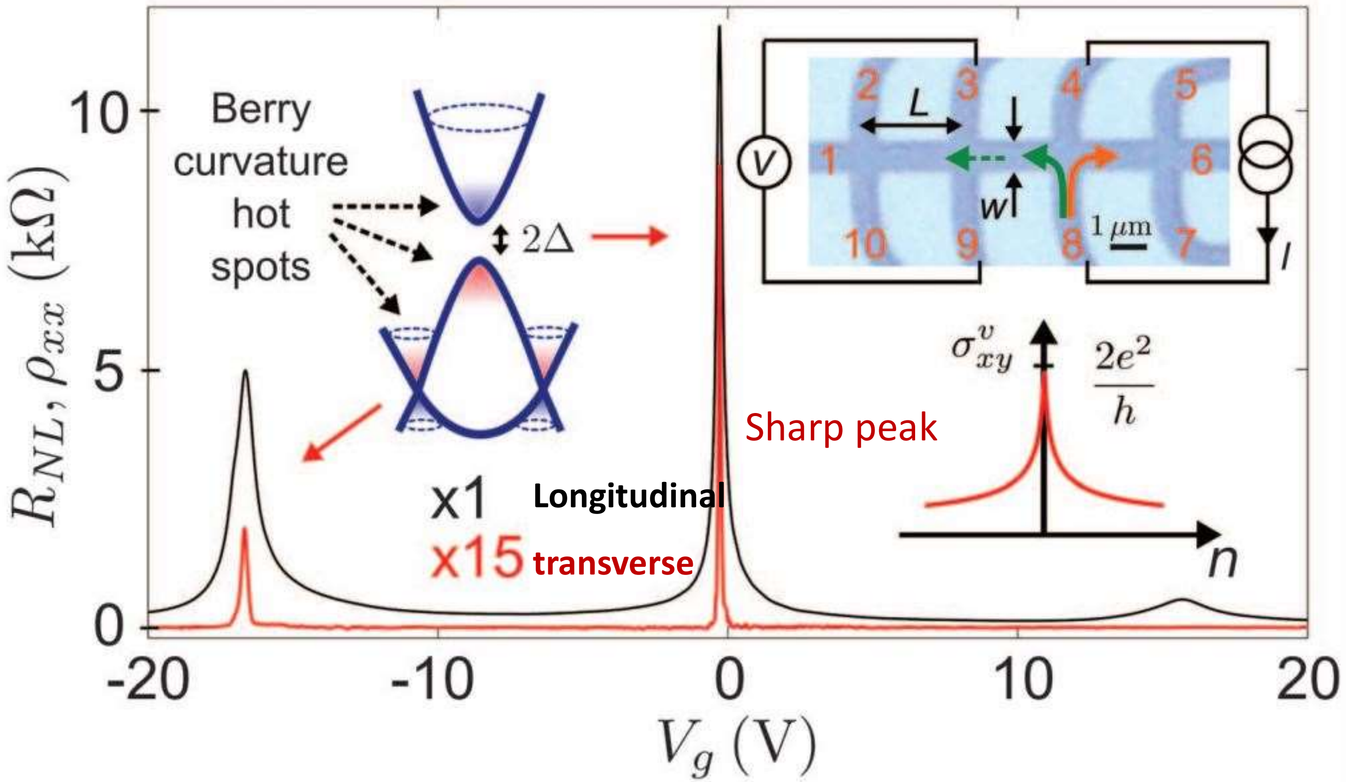
VALLEYTRONICS

Detecting topological currents in graphene superlattices

Science, 2014

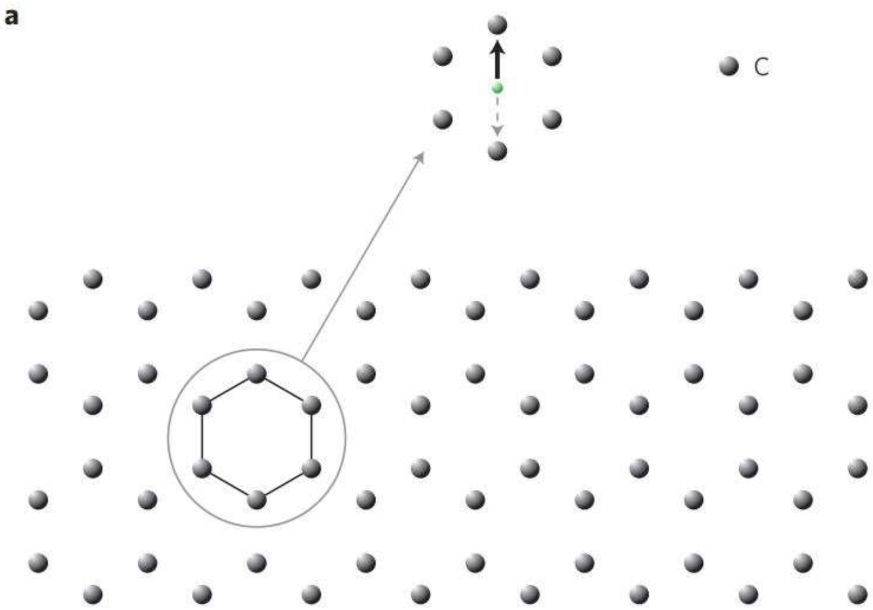
R. V. Gorbachev,[1,2*] J. C. W. Song,[3,4*] G. L. Yu,[1] A. V. Kretinin,[2] F. Withers,[2] Y. Cao,[1] A. Mishchenko,[1] I. V. Grigorieva,[2] K. S. Novoselov,[2] L. S. Levitov,[3*] A. K. Geim[1,2]†

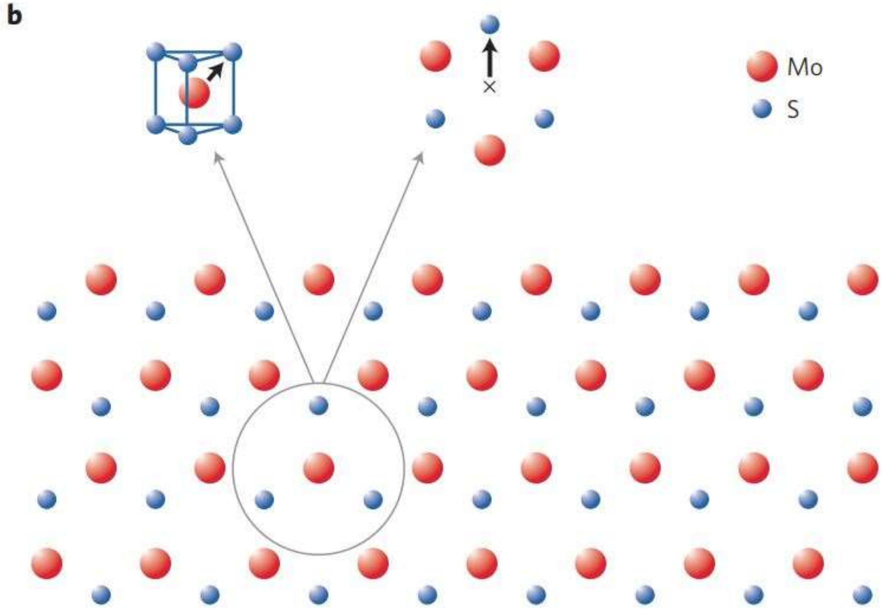
Graphene on hBN (breaking inversion symm, E_g=30 meV)



Graphene (with SIS)

monolayer MoS_2 (without SIS)

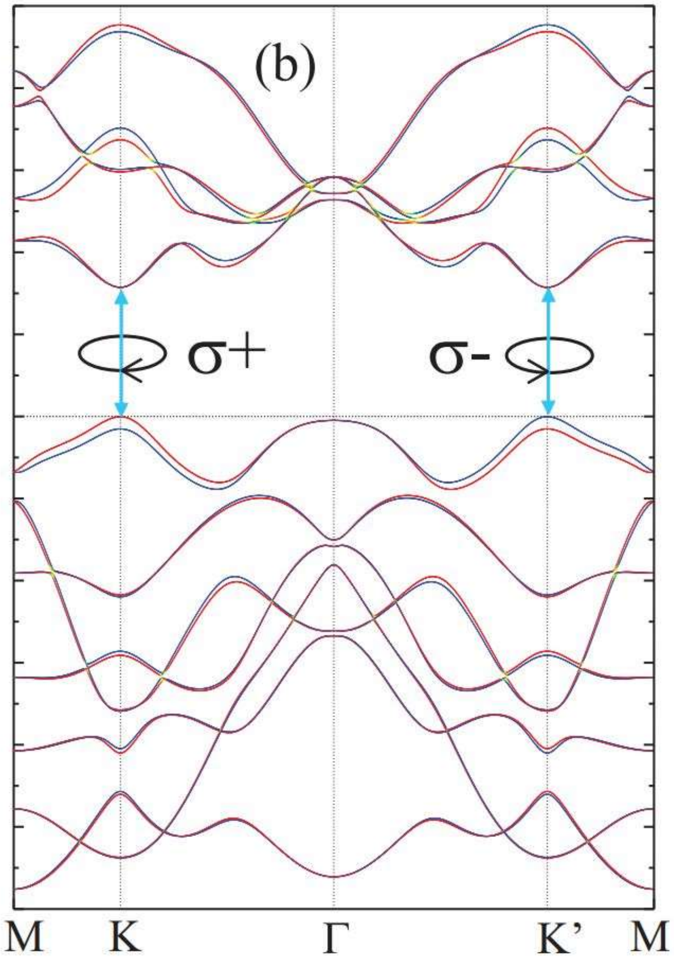




Graphene on hBN breaks SIS,
opens a gap ~ 30 mV

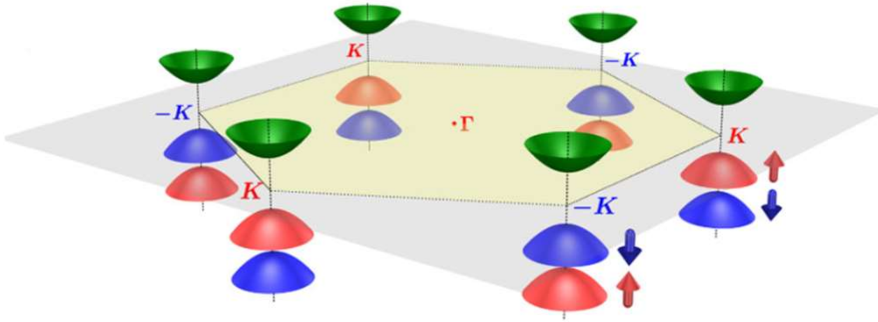
An energy gap ~ 1.9 eV
(easier for optical and electrical control)

Band structure for MoS_2



Opposite valleys have opposite BC and opposite magnetic moment

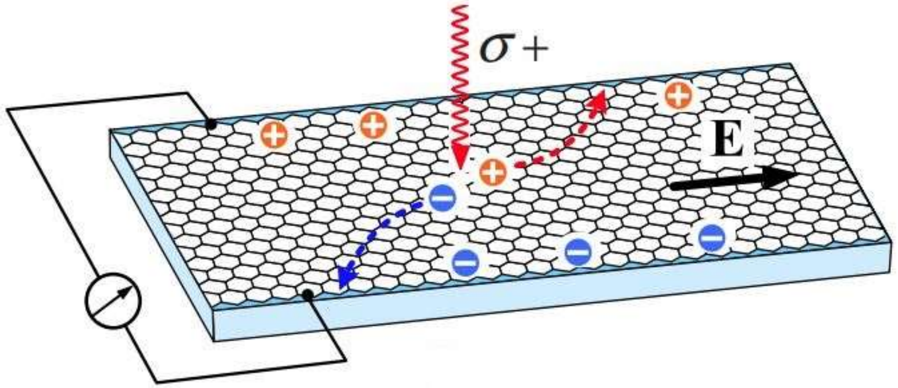
Feng et al, PRB 2012



- *K*, *K'* population imbalance induced by optical pumping

→ net Hall current

photo-induced AHE



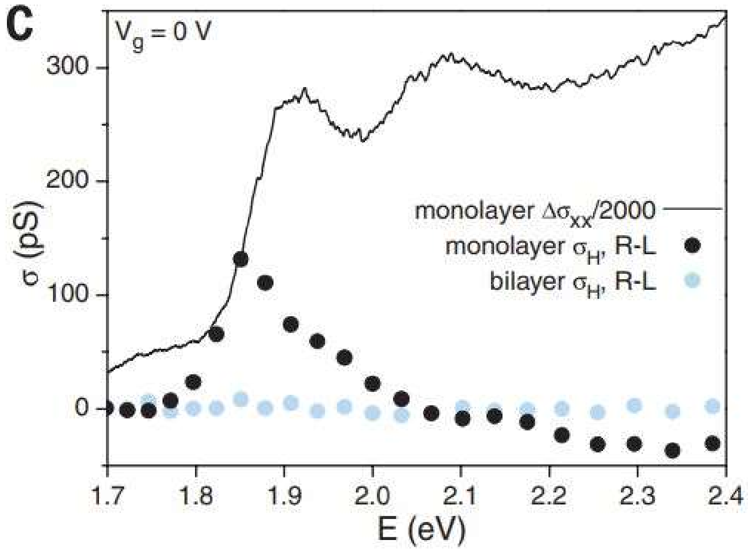
Electron and hole (in the same valley) contribute to the same current

Fig from Yao et al, PRB 2008

VALLEYTRONICS Science, 2014

The valley Hall effect in MoS_2 transistors

K. F. Mak,[1,2*] K. L. McGill,[2] J. Park,[1,3] P. L. McEuen[1,2*]



Lee et al, Nature Nano Tech, 2016

Local Kerr signal