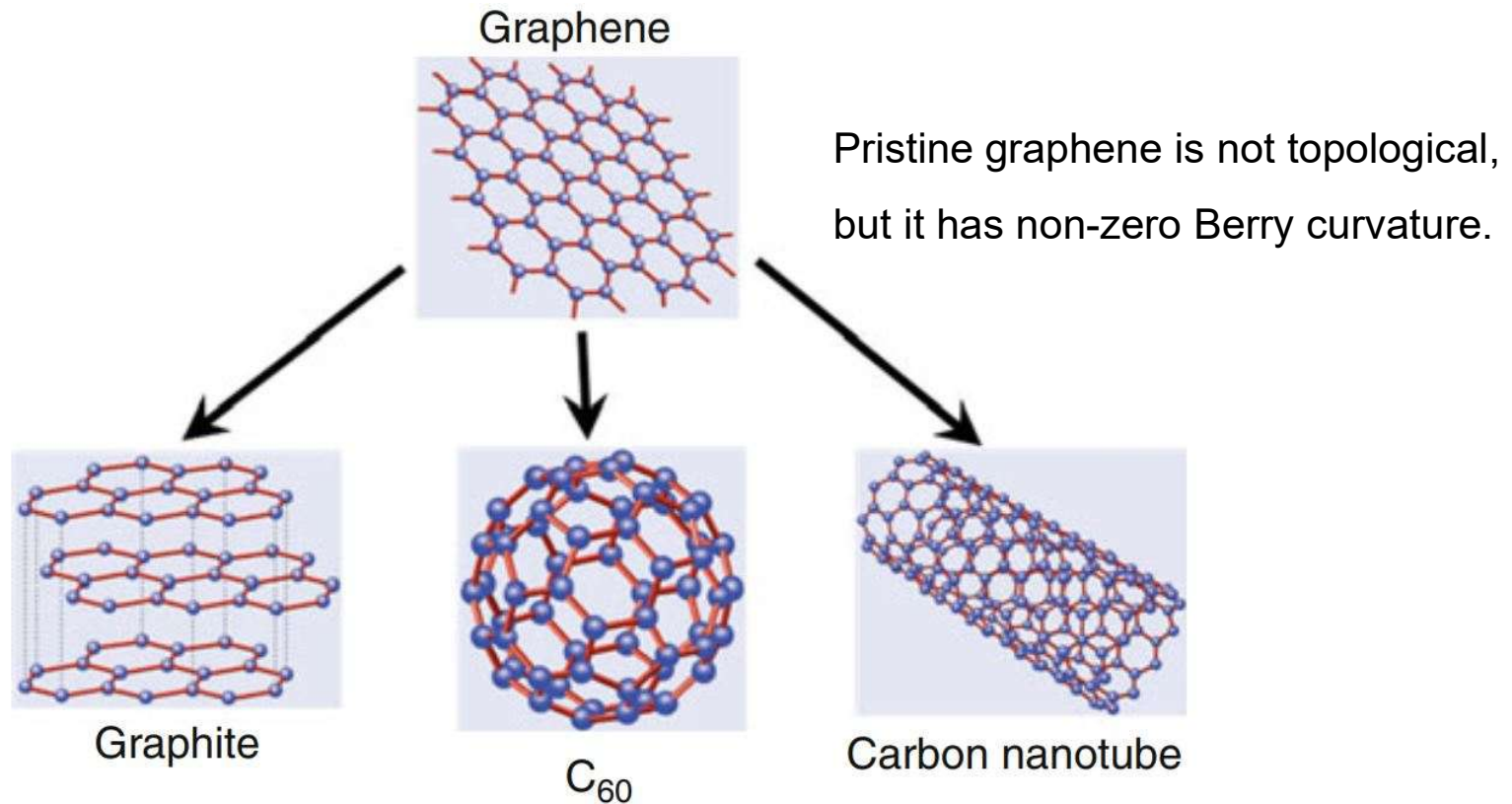


Two-dimensional material

- Graphene
 - symmetries
 - Effective Hamiltonian
- Transition metal dichalcogenide
 - Berry curvature
 - Optical transitions
- Haldane model
 - Haldane flux
 - Berry curvature

- 1947, [theory](#) of graphene by Wallace
- 1968, Mermin-Wagner theorem (no long-range order in 2D at finite T)
- 1985, discovery of [bucky ball](#) by Kroto, Smalley, and Curl (1996 Nobel prize)
- 1991, discovery of [carbon nanotube](#) by Iijima and Ichihashi.
- 2004, [first graphene produced](#) by Geim and Novoselov (2010 Nobel prize)



Extraordinary properties of graphene

- ❑ **Young's modulus of 1 TPa and intrinsic strength of 130 Gpa, the strongest materials ever tested.** (space elevator)

Cu: 0.117 TPa

Phys. Rev. B 76, 064120 (2007).

- ❑ **A prediction in 2015 suggested a melting point at least 5000 K.**
(in reality, sublimate near 3700 K)

- ❑ **Room-temperature electron mobility of $2.5 \times 10^5 \text{ cm}^2 \text{V}^{-1} \text{ s}^{-1}$**

Nano Lett. 11, 2396–2399 (2011).

- ❑ **The electrical resistivity of graphene $< 10^{-6} \Omega \cdot \text{cm}$, less than silver, the lowest known at RT.** (better than copper)

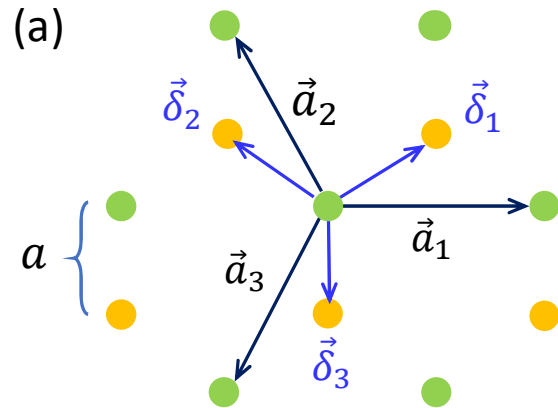
- ❑ **High thermal conductivity: above $3,000 \text{ Wm}^{-1} \text{K}^{-1}$**

Cu: $401 \text{ Wm}^{-1} \text{K}^{-1}$

Nature Mater. 10, 569–581 (2011).

- ❑ **Optical absorption of 2.3%** (related to fine structure constant)
Science 320, 1308 (2008).

1 Graphene lattice



- Lattice vectors

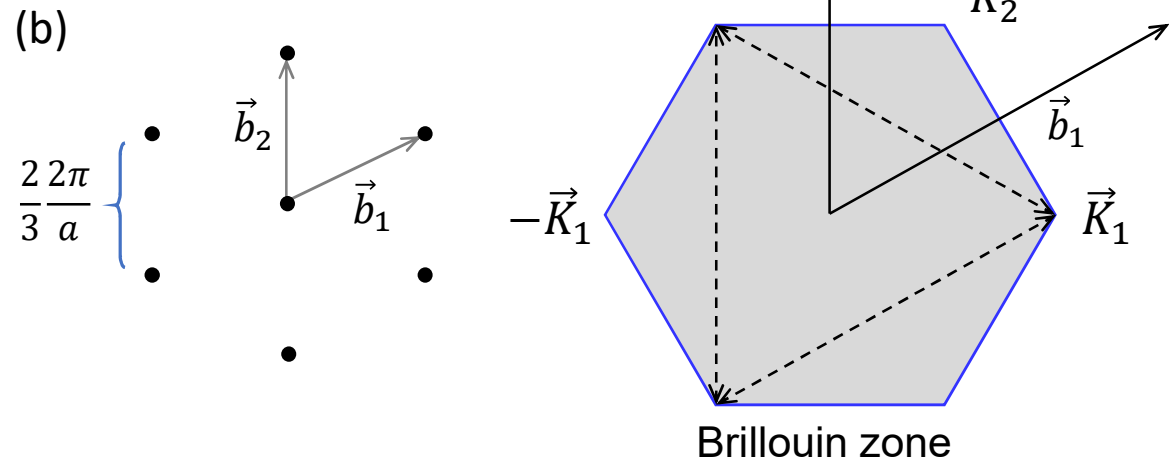
$$\mathbf{a}_1 = \sqrt{3}a\hat{x},$$

$$\mathbf{a}_2 = -\frac{\sqrt{3}}{2}a\hat{x} + \frac{3}{2}a\hat{y},$$

$$\mathbf{a}_3 = -\frac{\sqrt{3}}{2}a\hat{x} - \frac{3}{2}a\hat{y}.$$

$$a = 1.42 \text{ \AA}$$

$$a_0 = \sqrt{3}a \simeq 2.46 \text{ \AA}$$



- Reciprocal lattice vectors

$$\mathbf{b}_1 = \frac{2\pi}{a} \left(\frac{1}{\sqrt{3}}\hat{x} + \frac{1}{3}\hat{y} \right),$$

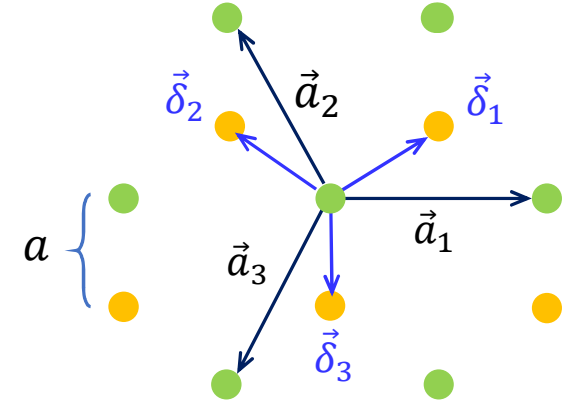
$$\mathbf{b}_2 = \frac{2\pi}{a} \frac{2}{3}\hat{y}.$$

Tight-binding model
(spin neglected)

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

$$(1) \quad \hat{H}_{NN} = t_1 \sum_{\mathbf{R}} \left(d_{\mathbf{R}+\delta_1}^\dagger c_{\mathbf{R}} + d_{\mathbf{R}+\delta_2}^\dagger c_{\mathbf{R}} + d_{\mathbf{R}+\delta_3}^\dagger c_{\mathbf{R}} \right) + h.c.$$

$$\begin{aligned} \delta_1 &= \frac{\sqrt{3}}{2} a \hat{x} + \frac{1}{2} a \hat{y}, \\ \delta_2 &= -\frac{\sqrt{3}}{2} a \hat{x} + \frac{1}{2} a \hat{y}, \\ \delta_3 &= -a \hat{y}. \end{aligned}$$



$$t_1 \approx 2.7 \text{ eV}$$

$$(2) \quad \begin{aligned} \hat{H}_{NNN} &= t_2 \sum_{\mathbf{R}} \left(c_{\mathbf{R}+\mathbf{a}_1}^\dagger c_{\mathbf{R}} + c_{\mathbf{R}+\mathbf{a}_2}^\dagger c_{\mathbf{R}} + c_{\mathbf{R}+\mathbf{a}_3}^\dagger c_{\mathbf{R}} \right) \\ &+ t_2 \sum_{\mathbf{R}} \left(d_{\mathbf{R}+\delta_1+\mathbf{a}_1}^\dagger d_{\mathbf{R}+\delta_1} + d_{\mathbf{R}+\delta_1+\mathbf{a}_2}^\dagger d_{\mathbf{R}+\delta_1} \right. \\ &\quad \left. + d_{\mathbf{R}+\delta_1+\mathbf{a}_3}^\dagger d_{\mathbf{R}+\delta_1} \right) + h.c., \end{aligned}$$

$$(3) \quad \hat{H}_{on-site} = \Delta \sum_{\mathbf{R}} c_{\mathbf{R}}^\dagger c_{\mathbf{R}} - \Delta \sum_{\mathbf{R}} d_{\mathbf{R}+\delta_1}^\dagger d_{\mathbf{R}+\delta_1}$$

Fourier
transform

$$c_{\mathbf{R}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}} c_{\mathbf{k}}$$

$$d_{\mathbf{R}+\delta_1} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{R}+\delta_1)} d_{\mathbf{k}}$$

$$\text{e.g., } \sum_{\mathbf{R}} d_{\mathbf{R}+\delta_1}^\dagger c_{\mathbf{R}} = \frac{1}{N} \sum_{\mathbf{k}, \mathbf{k}'} \sum_{\mathbf{R}} e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}} e^{-i\mathbf{k}'\cdot\delta_1} d_{\mathbf{k}'}^\dagger c_{\mathbf{k}}$$

$$= \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\delta_1} d_{\mathbf{k}}^\dagger c_{\mathbf{k}},$$

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

➔

$$\hat{H} = t_1 \sum_{\mathbf{k}} (e^{-i\mathbf{k}\cdot\delta_1} + e^{-i\mathbf{k}\cdot\delta_2} + e^{-i\mathbf{k}\cdot\delta_3}) d_{\mathbf{k}}^\dagger c_{\mathbf{k}}$$

$$+ t_2 \sum_{\mathbf{k}} (e^{-i\mathbf{k}\cdot\mathbf{a}_1} + e^{-i\mathbf{k}\cdot\mathbf{a}_2} + e^{-i\mathbf{k}\cdot\mathbf{a}_3}) c_{\mathbf{k}}^\dagger c_{\mathbf{k}}$$

$$+ t_2 \sum_{\mathbf{k}} (e^{-i\mathbf{k}\cdot\mathbf{a}_1} + e^{-i\mathbf{k}\cdot\mathbf{a}_2} + e^{-i\mathbf{k}\cdot\mathbf{a}_3}) d_{\mathbf{k}}^\dagger d_{\mathbf{k}} + h.c.$$

$$+ \Delta \sum_{\mathbf{k}} (c_{\mathbf{k}}^\dagger c_{\mathbf{k}} - d_{\mathbf{k}}^\dagger d_{\mathbf{k}})$$

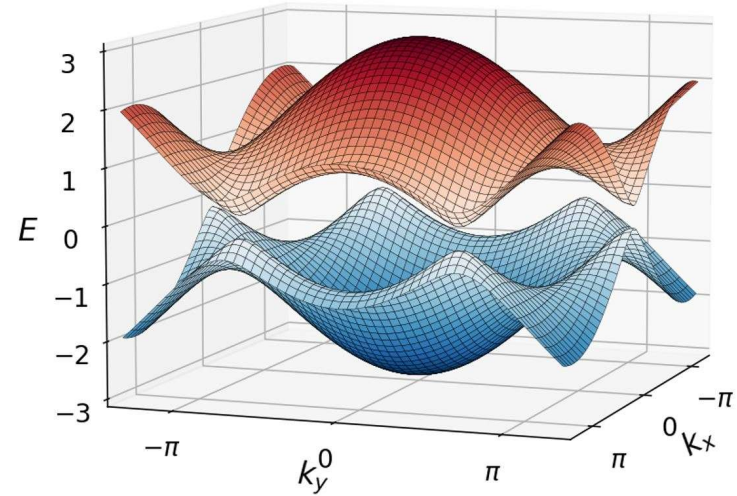
$$= \sum_{\mathbf{k}} \begin{pmatrix} c_{\mathbf{k}}^\dagger & d_{\mathbf{k}}^\dagger \end{pmatrix} H(\mathbf{k}) \begin{pmatrix} c_{\mathbf{k}} \\ d_{\mathbf{k}} \end{pmatrix}.$$

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

$$h_0(\mathbf{k}) = 2t_2 \sum_i \cos \mathbf{k} \cdot \mathbf{a}_i,$$

$$\mathbf{h}(\mathbf{k}) = \left(t_1 \sum_i \cos \mathbf{k} \cdot \boldsymbol{\delta}_i, -t_1 \sum_i \sin \mathbf{k} \cdot \boldsymbol{\delta}_i, \Delta \right)$$

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



$$\begin{aligned}
 |\mathbf{h}| &= \sqrt{3t_1^2 + 2t_1^2 (\cos \mathbf{k} \cdot \mathbf{a}_1 + \cos \mathbf{k} \cdot \mathbf{a}_2 + \cos \mathbf{k} \cdot \mathbf{a}_3) + \Delta^2} \\
 &= \sqrt{3t_1^2 + 2t_1^2 f(\mathbf{k}) + \Delta^2}, \quad t_1 \simeq 2.7 \text{ eV}
 \end{aligned}$$

$$\begin{aligned}
 f(\mathbf{k}) &\equiv \cos \mathbf{k} \cdot \mathbf{a}_1 + \cos \mathbf{k} \cdot \mathbf{a}_2 + \cos \mathbf{k} \cdot \mathbf{a}_3 \\
 &= \cos \sqrt{3}ak_x + 2 \cos \frac{\sqrt{3}}{2}ak_x \cos \frac{3}{2}ak_y.
 \end{aligned}$$

Stability of the nodal point in graphene

- TRS $H(\vec{k})^* = H(-\vec{k})$
 $\rightarrow h_x(\vec{k}), h_y(\vec{k}), h_z(\vec{k}) = \text{even, odd, even}$

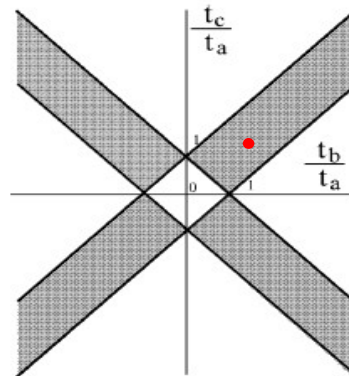
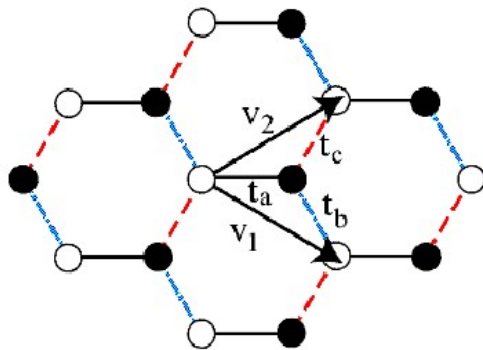
- SIS (for graphene, $\pi = \sigma_x$)

$$\sigma_x H(\vec{k}) \sigma_x = H(-\vec{k})$$

$$\rightarrow h_x(\vec{k}), h_y(\vec{k}), h_z(\vec{k}) = \text{even, odd, odd}$$

- TRS+SIS \rightarrow no σ_z term \leftarrow Co-dimension is 2
 (point degeneracy in 2D BZ)

- Global stability: point degeneracy is further protected by C_3 symmetry
 (Ch7, Bernevig)



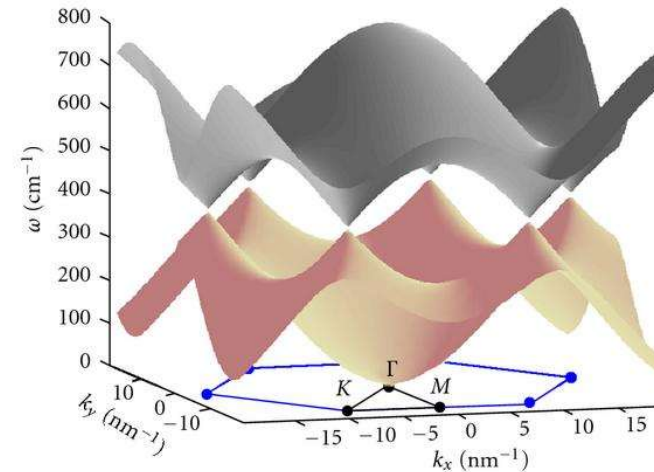
Hasegawa et al, PRB 2006

Low-energy effective Hamiltonian near Dirac point

$$\mathbf{K}_1 = \frac{2\pi}{a} \left(\frac{2}{3\sqrt{3}}, 0 \right),$$

$$\mathbf{K}_2 = \frac{2\pi}{a} \left(\frac{1}{3\sqrt{3}}, \frac{1}{3} \right)$$

Alternative:
 $\mathbf{K}_2 = -\mathbf{K}_1$



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

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

(rewrite $k_{1,2}$ simply as k) \rightarrow

$$H_{12}(\mathbf{k}) \simeq it_1 a \mathbf{k} \cdot \left(\pm \frac{3}{2} i, -\frac{3}{2} \right)$$

$$= t_1 a \left(\mp \frac{3}{2} k_x - \frac{3}{2} i k_y \right)$$

$$\mathbf{H}(\mathbf{k}) \simeq \begin{pmatrix} \Delta & \frac{3}{2} t_1 a (\mp k_x - i k_y) \\ \frac{3}{2} t_1 a (\mp k_x + i k_y) & -\Delta \end{pmatrix}$$

$$= \hbar v_F (\tau k_x \sigma_x + k_y \sigma_y) + \Delta \sigma_z,$$

$$v_F = \frac{3}{2} \frac{a t_1}{\hbar} \simeq \frac{c}{300}$$

\uparrow
Valley $\tau = \pm$

In Chap 3, we learned that

Time reversal symmetry: $\vec{F}_n(\vec{k}) = -\vec{F}_n(-\vec{k})$

Space inversion symmetry: $\vec{F}_n(\vec{k}) = +\vec{F}_n(-\vec{k})$

- With both symmetries, (for non-degenerate state) the Berry curvature is zero. So we need to break either TRS or SIS.
- If we break only SIS, then

$$\vec{F}_n(K_2) = -\vec{F}_n(K_1) \quad \text{valley Hall effect}$$

- If we break only TRS, then

$$\vec{F}_n(K_2) = +\vec{F}_n(K_1) \quad \text{Haldane model}$$

e.g. $H \rightarrow H' = \hbar v_F \vec{\sigma}^* \cdot (-\vec{k} - \vec{K}_2) + \Delta \sigma_z$
with
TRS $= -\hbar v_F \vec{\sigma}^* \cdot (\vec{k} - \vec{K}_1) + \Delta \sigma_z$

$$(h_x, h_y, h_z) \rightarrow (-h_x, h_y, h_z)$$

So the Berry curvature at opposite valleys have opposite signs.

- Effective Hamiltonian near degenerate point

$$H_0 = \hbar v_F (\mp k_x \sigma_x + k_y \sigma_y) + \Delta \sigma_z \text{ at } \pm K, \quad \hbar v_F \equiv \frac{3}{2} t_1 a$$

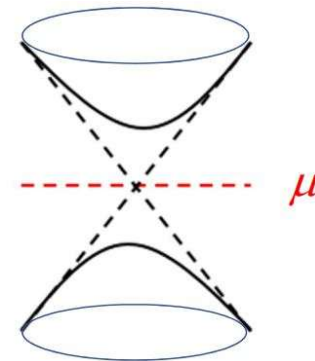
- Berry curvature

$$F_{z\tau}^{\pm}(\mathbf{k}) = \pm \tau \frac{1}{2} \frac{\hbar^2 v_F^2 \Delta}{\hbar^3}$$

$$\int_{all} d^2k F_{\tau}^{\pm} = \pm \tau \pi \quad (\text{Drop sub } z)$$

$$\rightarrow \sigma_H = \frac{e^2}{h} \frac{1}{2\pi} \int d^2k F_{\tau}^{-} = -\frac{\tau e^2}{2h}$$

Total Hall conductivity is zero due to the cancellation between 2 valleys.

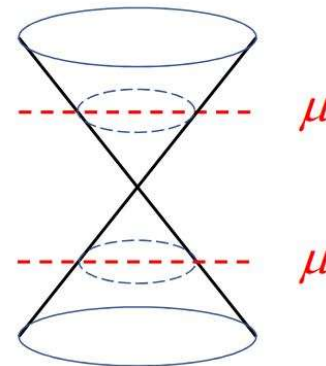


- Gapless limit (at $+K$):

$$\rightarrow \text{Berry phase (surrounding } +K): \quad \gamma_C = \pm \pi$$

Berry phase remains the same as long as C encircles the origin

$$\rightarrow F^{\pm}(\vec{k}) = \pm \pi \delta^2(\vec{k})$$

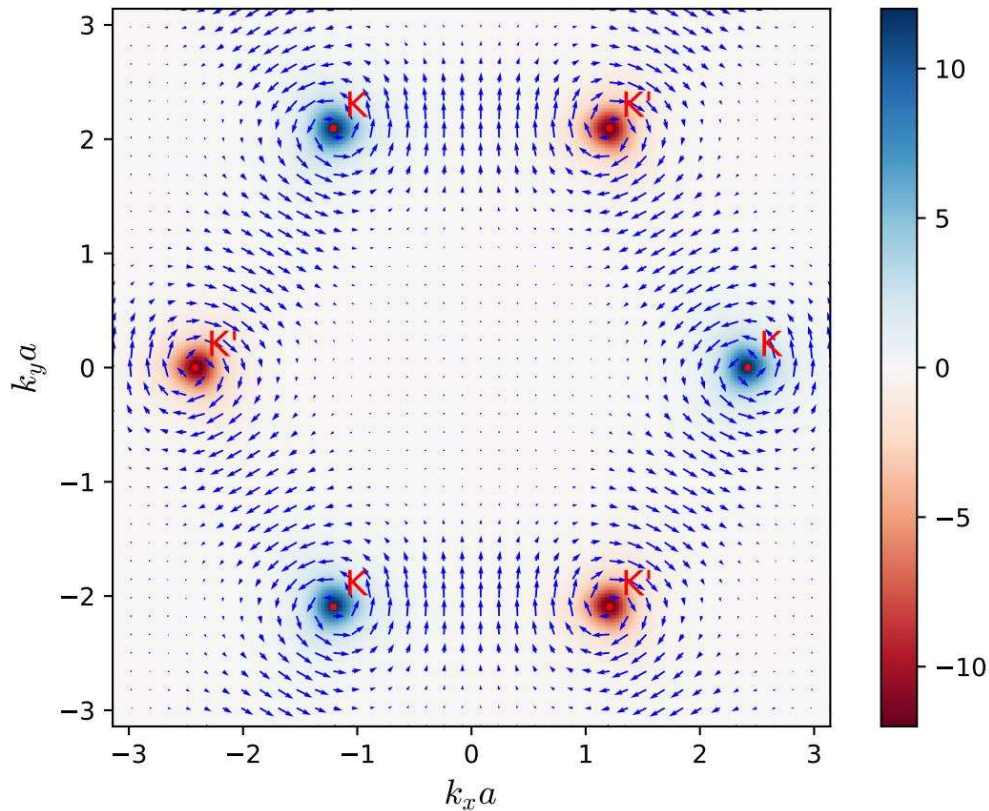


Berry curvature over the whole BZ

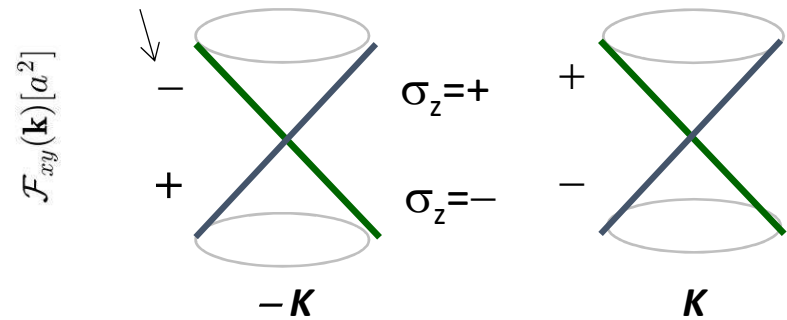
$$F_z^\pm(\mathbf{k}) = \mp \frac{1}{2h^3} \mathbf{h} \cdot \frac{\partial \mathbf{h}}{\partial k_x} \times \frac{\partial \mathbf{h}}{\partial k_y}$$

➔
$$F_z^\pm(\mathbf{k}) = \mp \frac{\sqrt{3}/2}{2h^3} a^2 t_1^2 \Delta (\sin \mathbf{k} \cdot \mathbf{a}_1 + \sin \mathbf{k} \cdot \mathbf{a}_2 + \sin \mathbf{k} \cdot \mathbf{a}_3)$$

Berry connection and Berry curvature



Sign of F



Cayssol and Fuchs, 2021

Cf:
$$F_{xy}^\pm(\mathbf{k}) = \pm a^2 \frac{\sqrt{3} t^2 M}{|E(\mathbf{k})|^3} \sin\left(\mathbf{k} \cdot \frac{\boldsymbol{\delta}_2 - \boldsymbol{\delta}_3}{2}\right) \sin\left(\mathbf{k} \cdot \frac{\boldsymbol{\delta}_3 - \boldsymbol{\delta}_1}{2}\right) \sin\left(\mathbf{k} \cdot \frac{\boldsymbol{\delta}_1 - \boldsymbol{\delta}_2}{2}\right)$$

Graphene in magnetic field

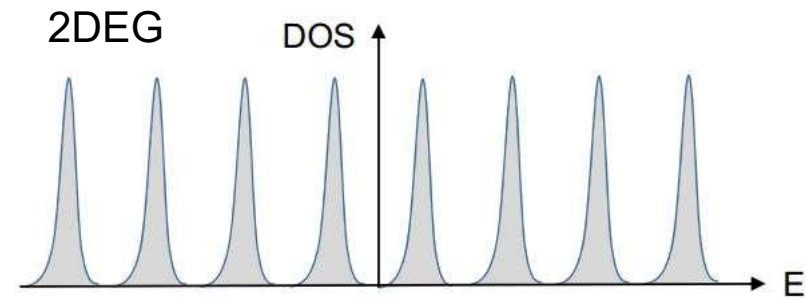
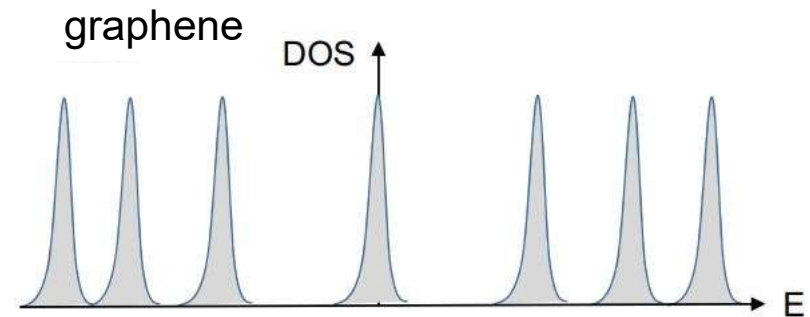
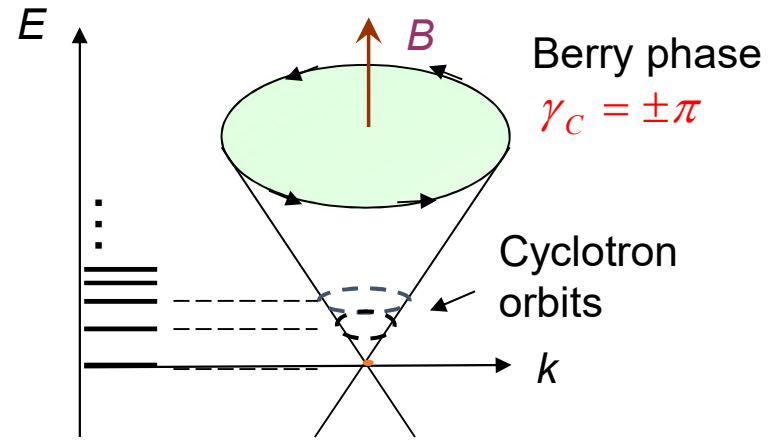
Bohr-Sommerfeld quantization (Kittel)

$$\underbrace{\frac{1}{2} \oint_C (\vec{k} \times d\vec{k}) \cdot \hat{z}}_{\text{Orbital area}} = 2\pi \left(n + \frac{1}{2} - \underbrace{\frac{\gamma_C}{2\pi}}_{\text{Correction from Berry phase}} \right) \frac{eB}{\hbar}$$

→ $\pi k^2 = 2\pi \left(n + \frac{1}{2} - \frac{\gamma_C}{2\pi} \right) \frac{eB}{\hbar}$

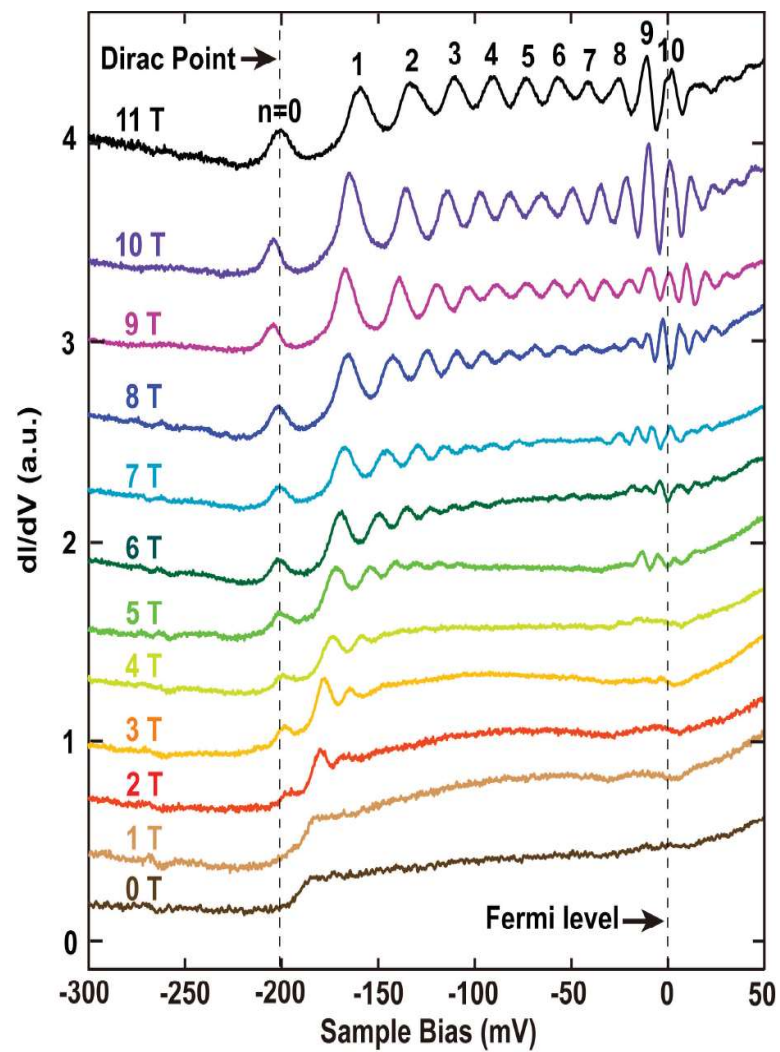
$E(k) = \hbar v_F k$

→ $E_n = v_F \sqrt{2eB\hbar n}$ Landau levels in graphene

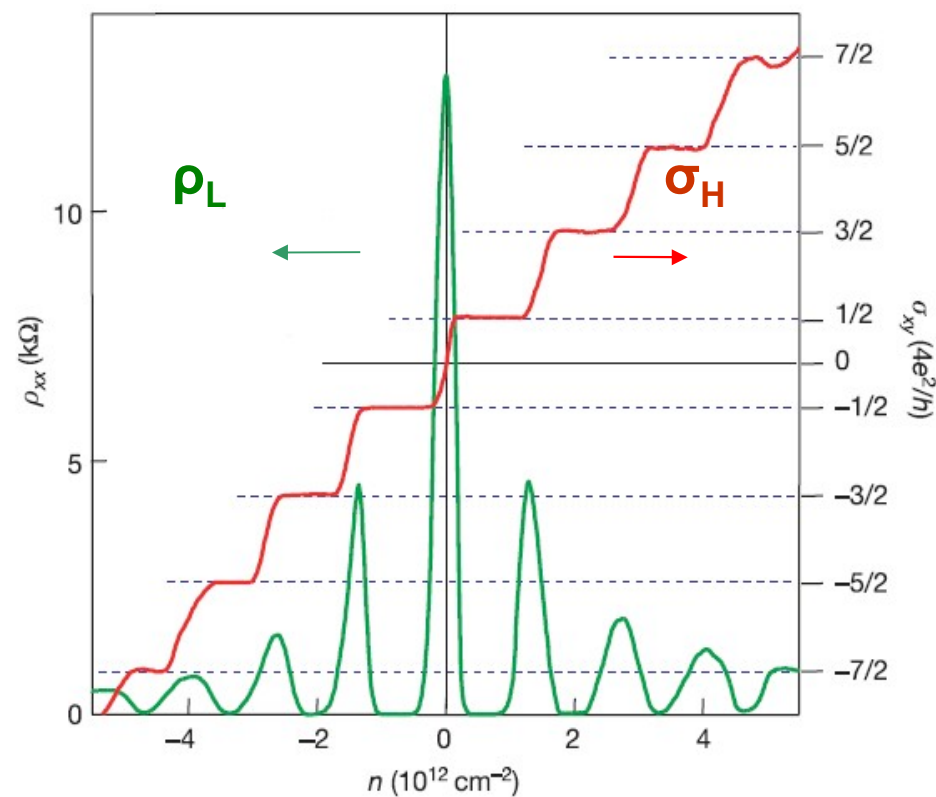


STM experiment

(Cheng et al, PRL 2010)



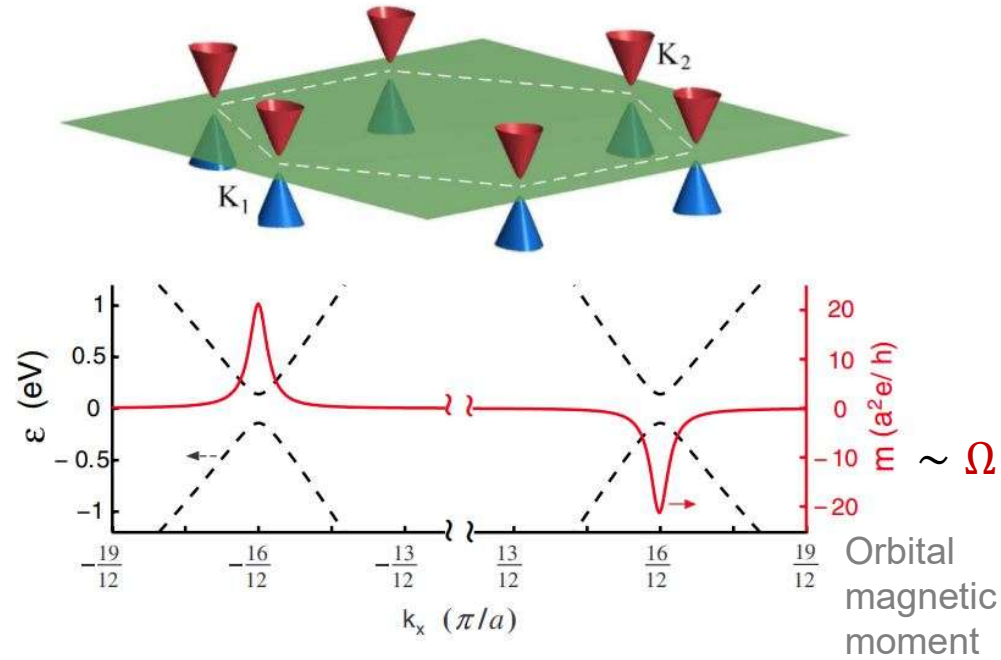
Quantum Hall effect in graphene



Novoselov et al, Nature 2005

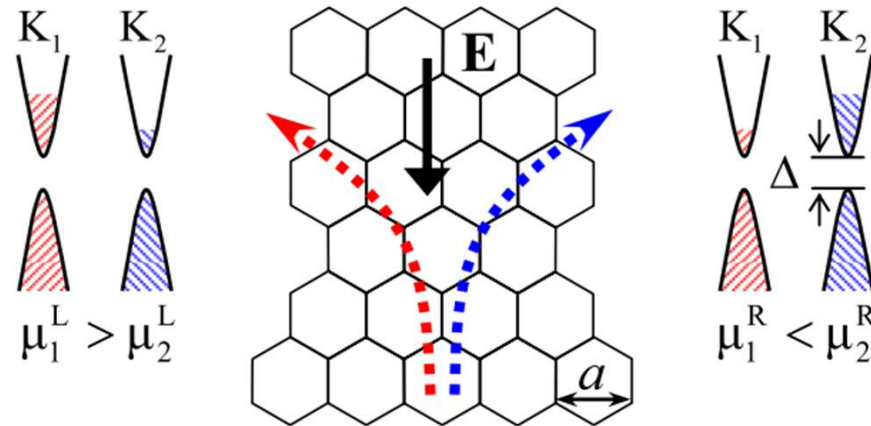
Valley Hall effect (Xiao et al, PRL 2007)

$B = 0$



Opposite anomalous velocities
from two valleys

$$\mathbf{v}_n(\mathbf{k}) = \frac{1}{\hbar} \frac{\partial \epsilon_{n\mathbf{k}}}{\partial \mathbf{k}} + \frac{e}{\hbar} \mathbf{E} \times \mathbf{F}_n(\mathbf{k})$$



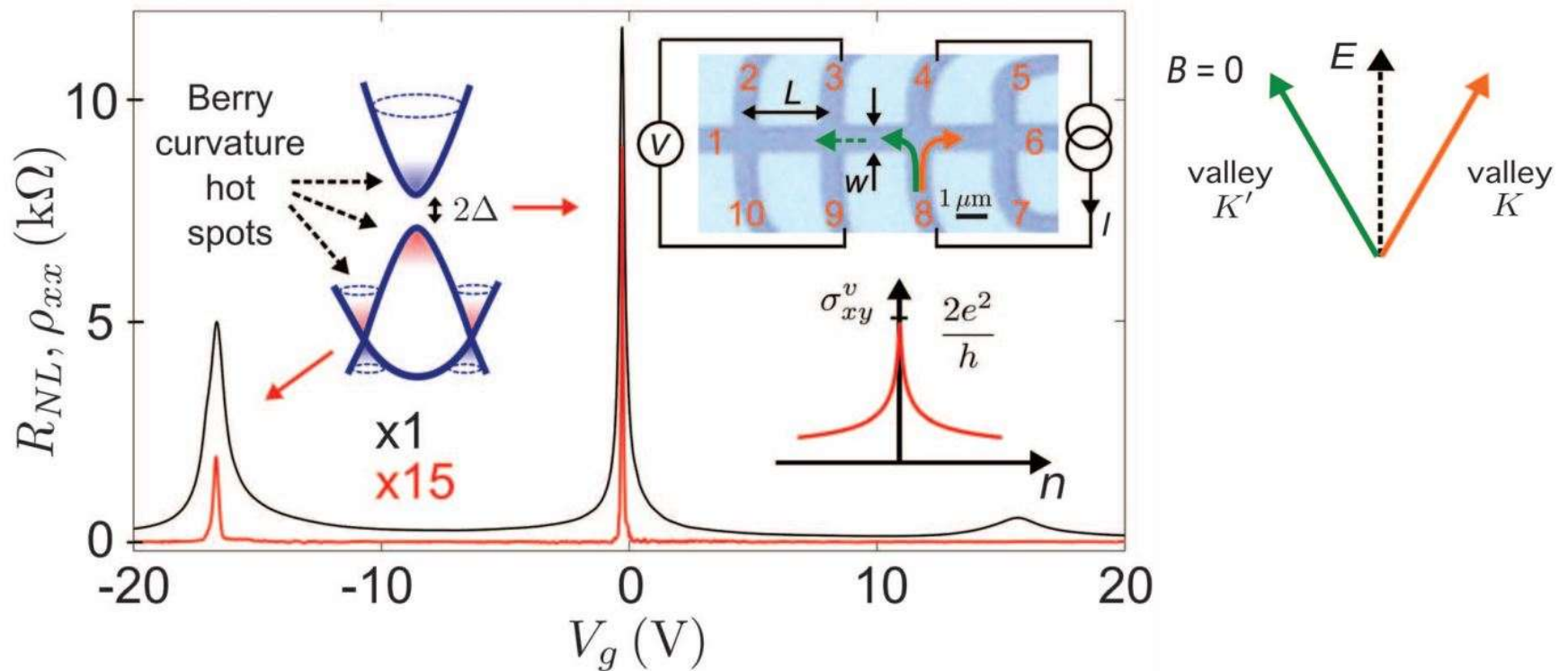
VALLEYTRONICS

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 $\rightarrow 2\Delta = 30$ meV)

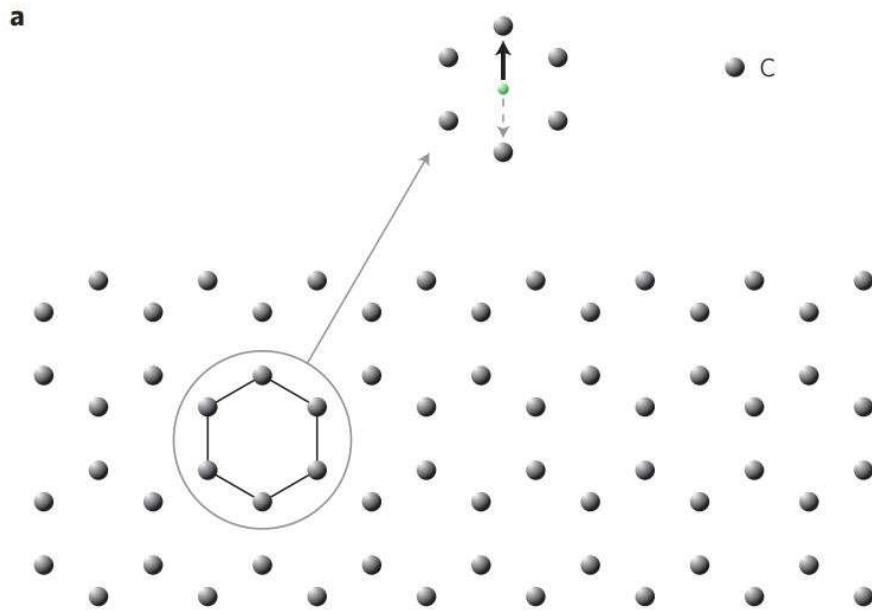


矽烯

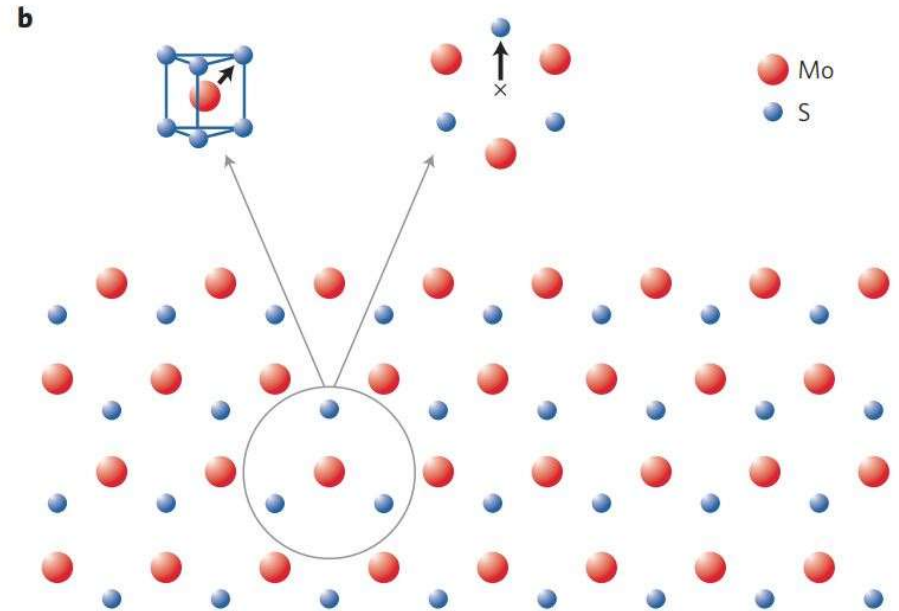
2D material: graphene, silicene, hBN, TMD ...e6c

Graphene (with SIS)

monolayer MoS₂ (without SIS)



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



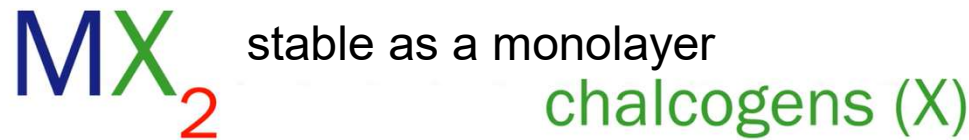
An energy gap ~ 1.9 eV
(easier for optical and electrical control)

2 Transition Metal Dichalcogenide (TMD) 過渡金屬二硫屬化合物

硫族化物 **chalcogens (X)**

hydrogen 1 H 1.0079																	helium 2 He 4.0026						
lithium 3 Li 6.941	beryllium 4 Be 9.0122																	boron 5 B 10.811	carbon 6 C 12.011	nitrogen 7 N 14.007	oxygen 8 O 15.999	fluorine 9 F 18.998	neon 10 Ne 20.180
sodium 11 Na 22.990	magnesium 12 Mg 24.305																	aluminum 13 Al 26.982	silicon 14 Si 28.086	phosphorus 15 P 30.974	sulfur 16 S 32.065	chlorine 17 Cl 35.453	argon 18 Ar 39.948
potassium 19 K 39.098	calcium 20 Ca 40.078	scandium 21 Sc 44.956	titanium 22 Ti 47.887	vanadium 23 V 50.942	chromium 24 Cr 51.996	manganese 25 Mn 54.938	iron 26 Fe 55.845	cobalt 27 Co 58.933	nickel 28 Ni 58.693	copper 29 Cu 63.546	zinc 30 Zn 65.39	gallium 31 Ga 69.723	germanium 32 Ge 72.61	arsenic 33 As 74.922	selenium 34 Se 78.96	bromine 35 Br 79.904	krypton 36 Kr 83.80						
rubidium 37 Rb 85.468	strontium 38 Sr 87.62	yttrium 39 Y 88.906	zirconium 40 Zr 91.224	niobium 41 Nb 92.906	molybdenum 42 Mo 95.94	technetium 43 Tc 98	ruthenium 44 Ru 101.07	rhodium 45 Rh 102.91	palladium 46 Pd 106.42	silver 47 Ag 107.87	cadmium 48 Cd 112.41	indium 49 In 114.82	tin 50 Sn 118.71	antimony 51 Sb 121.76	tellurium 52 Te 127.6	iodine 53 I 126.90	xenon 54 Xe 131.29						
cesium 55 Cs 132.91	barium 56 Ba 137.33	* 57-70	lanthanum 57 Lu 174.97	hafnium 72 Hf 178.49	tantalum 73 Ta 180.95	wolfram 74 W 183.84	reuterium 75 Re 186.21	osmium 76 Os 190.23	iridium 77 Ir 192.22	platinum 78 Pt 195.08	gold 79 Au 196.97	mercury 80 Hg 200.59	thallium 81 Tl 203.38	lead 82 Pb 207.2	bismuth 83 Bi 208.98	polonium 84 Po 209	astatine 85 At 210	radon 86 Rn 222					
francium 87 Fr [223]	radium 88 Ra [226]	* * 89-102	actinium 89 Ac [227]	thorium 90 Th [232]	protactinium 91 Pa [231]	uranium 92 U [238]	neptunium 93 Np [237]	plutonium 94 Pu [244]	americium 95 Am [243]	curium 96 Cm [247]	berkelium 97 Bk [247]	californium 98 Cf [251]	lawrencium 99 Lr [260]	unbinilium 100 Uub [285]	untrium 101 Uu [288]	unquadrium 102 Uuq [293]							

transition metals (M)

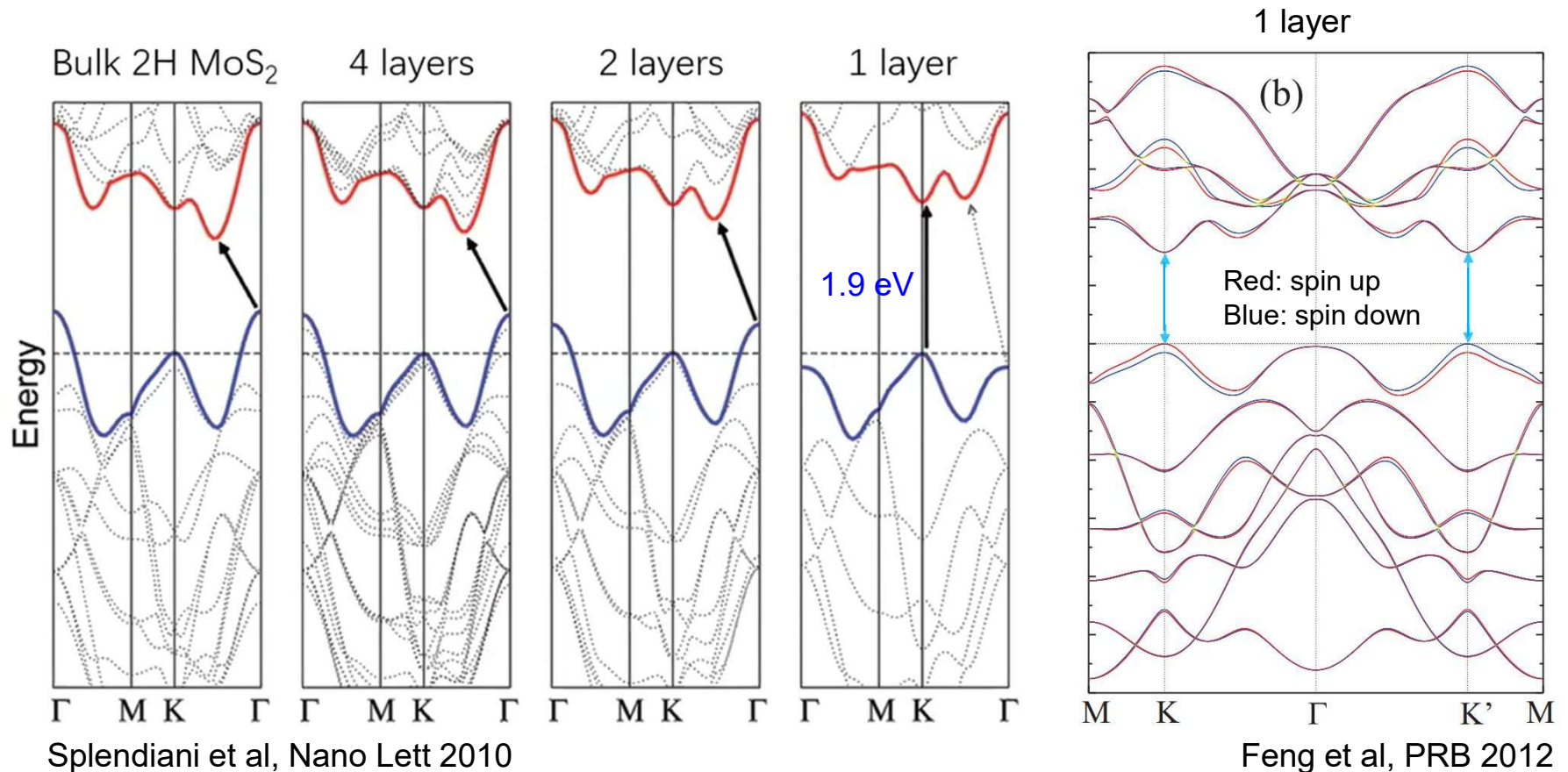


hydrogen 1 H 1.0079																	helium 2 He 4.0026						
lithium 3 Li 6.941	beryllium 4 Be 9.0122																	boron 5 B 10.811	carbon 6 C 12.011	nitrogen 7 N 14.007	oxygen 8 O 15.999	fluorine 9 F 18.998	neon 10 Ne 20.180
sodium 11 Na 22.990	magnesium 12 Mg 24.305																	aluminum 13 Al 26.982	silicon 14 Si 28.086	phosphorus 15 P 30.974	sulfur 16 S 32.065	chlorine 17 Cl 35.453	argon 18 Ar 39.948
potassium 19 K 39.098	calcium 20 Ca 40.078	scandium 21 Sc 44.956	titanium 22 Ti 47.887	vanadium 23 V 50.942	chromium 24 Cr 51.996	manganese 25 Mn 54.938	iron 26 Fe 55.845	cobalt 27 Co 58.933	nickel 28 Ni 58.693	copper 29 Cu 63.546	zinc 30 Zn 65.39	gallium 31 Ga 69.723	germanium 32 Ge 72.61	arsenic 33 As 74.922	selenium 34 Se 78.96	bromine 35 Br 79.904	krypton 36 Kr 83.80						
rubidium 37 Rb 85.468	strontium 38 Sr 87.62	yttrium 39 Y 88.906	zirconium 40 Zr 91.224	niobium 41 Nb 92.906	molybdenum 42 Mo 95.94	technetium 43 Tc 98	ruthenium 44 Ru 101.07	rhodium 45 Rh 102.91	palladium 46 Pd 106.42	silver 47 Ag 107.87	cadmium 48 Cd 112.41	indium 49 In 114.82	tin 50 Sn 118.71	antimony 51 Sb 121.76	tellurium 52 Te 127.6	iodine 53 I 126.90	xenon 54 Xe 131.29						
cesium 55 Cs 132.91	barium 56 Ba 137.33	* 57-70	lanthanum 57 Lu 174.97	hafnium 72 Hf 178.49	tantalum 73 Ta 180.95	wolfram 74 W 183.84	reuterium 75 Re 186.21	osmium 76 Os 190.23	iridium 77 Ir 192.22	platinum 78 Pt 195.08	gold 79 Au 196.97	mercury 80 Hg 200.59	thallium 81 Tl 203.38	lead 82 Pb 207.2	bismuth 83 Bi 208.98	polonium 84 Po 209	astatine 85 At 210	radon 86 Rn 222					
francium 87 Fr [223]	radium 88 Ra [226]	* * 89-102	actinium 89 Ac [227]	thorium 90 Th [232]	protactinium 91 Pa [231]	uranium 92 U [238]	neptunium 93 Np [237]	plutonium 94 Pu [244]	americium 95 Am [243]	curium 96 Cm [247]	berkelium 97 Bk [247]	californium 98 Cf [251]	lawrencium 99 Lr [260]	unbinilium 100 Uub [285]	untrium 101 Uu [288]	unquadrium 102 Uuq [293]							

transition metals (M)

Transition Metal Dichalcogenide: MoS₂

- Bulk material indirect band gap (with SIS)
Single layer **direct band gap** (without SIS) → Massive Dirac fermion
- **Large SO coupling, spin-valley locking** (due to Kramer degeneracy)
- Room temperature mobility 3-4 order of magnitude lower than in graphene
- Strong Coulomb interaction, excitons ... etc.



Valley Hall effect in a MoS₂ monolayer

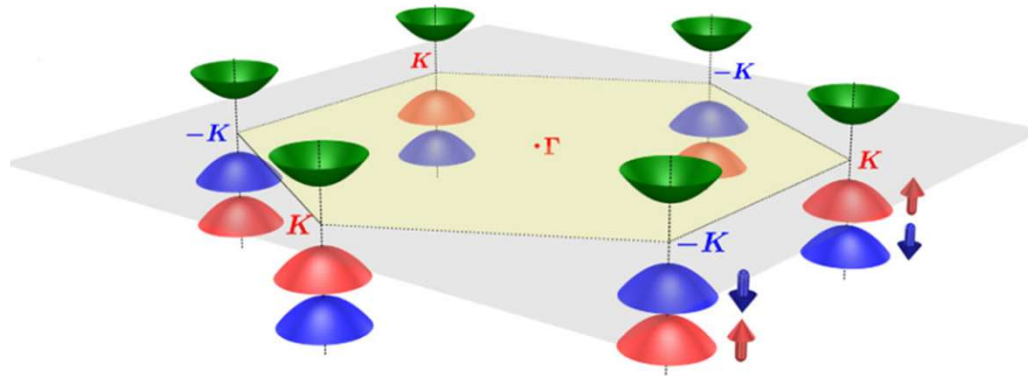


Fig from Xiao et al, PRL 2012

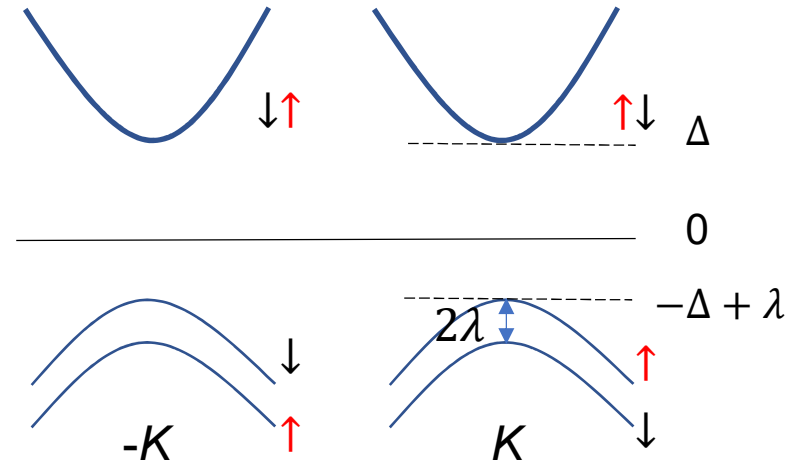
- 2-band model near massive Dirac points:

$$H = \alpha(\tau k_x \sigma_x + k_y \sigma_y) + \Delta' \sigma_z + \frac{\lambda}{2}$$

$$\Delta' \equiv \Delta - \lambda/2$$

$$\varepsilon_k^{c/v} = \pm \sqrt{\alpha^2 k^2 + \Delta'^2} + \frac{\lambda}{2}$$

- Berry curvature



$$F_c^\tau(\mathbf{k}) = \frac{\tau}{2} \frac{\alpha^2 \Delta'}{[\alpha^2 k^2 + \Delta'^2]^{3/2}}$$

Opposite valleys have opposite BCs

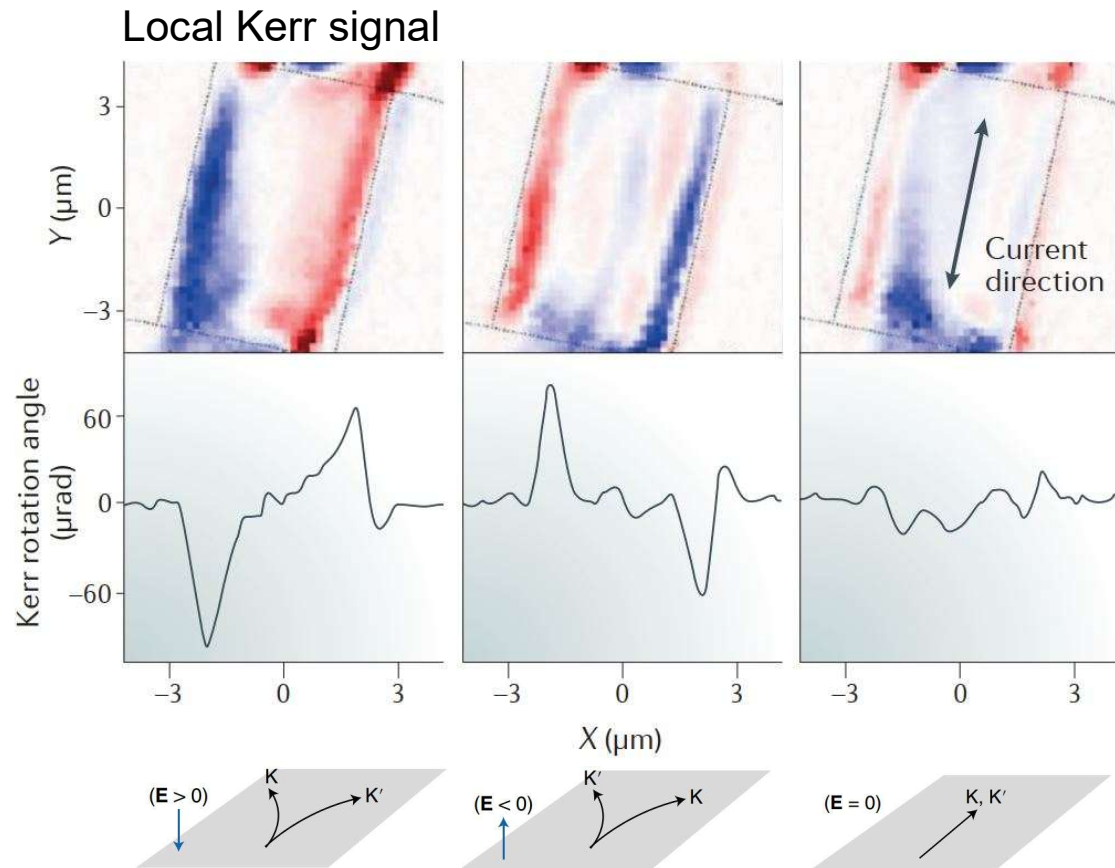
- For partially-filled valence band,

$$\begin{aligned} \sigma_H^\tau &= \frac{1}{2\pi} \int d^2 k F_c^\tau(\mathbf{k}) \\ &= \frac{\tau}{2} \left[1 - \frac{\Delta'}{\sqrt{\alpha^2 k_F^2 + \Delta'^2}} \right] \end{aligned}$$

The valley Hall effect in MoS₂ 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
Bilayer MoS₂ with SIS (broken by E field)



- Graphene
 - symmetries
 - Effective Hamiltonian
- Transition metal dichalcogenide
 - Berry curvature
 - Optical transitions
- Haldane model
 - Haldane flux
 - Berry curvature

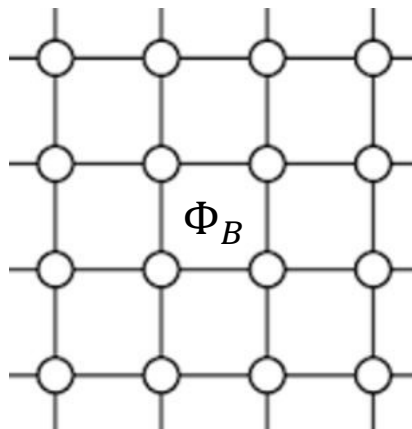
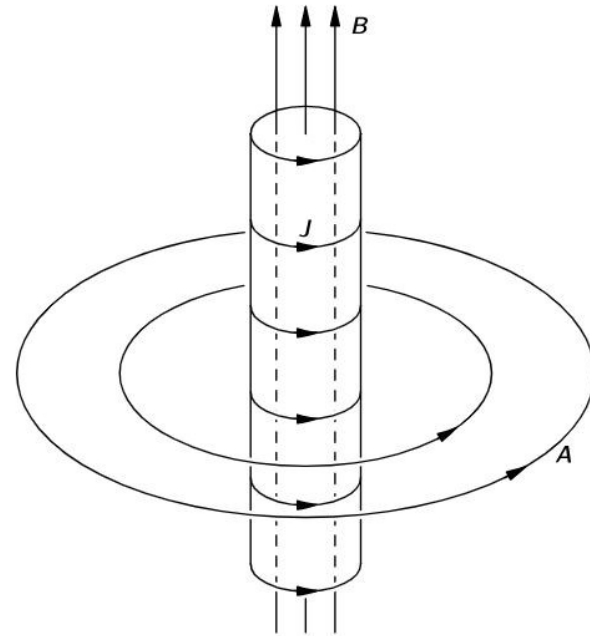
First, electron hopping in a magnetic field

- Aharonov-Bohm (AB) phase

For a closed loop C,

$$\psi' = e^{i\frac{e}{\hbar} \oint_C d\vec{r} \cdot \vec{A}} \psi = e^{2\pi i \frac{\Phi_B}{\Phi_0}}, \quad \Phi_0 \equiv h/e$$

- AB phase and electron hopping



3 Haldane's graphene model, PRL 1989
(no net magnetic field, but TRS is broken)

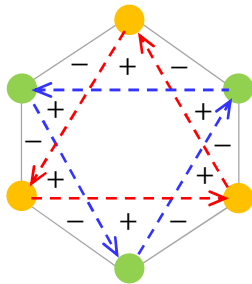
$$H = -t_1 \sum_{\langle i,j \rangle} c_i^\dagger c_j + \Delta \sum_i \xi_i c_i^\dagger c_i + t_2 \sum_{\langle\langle i,j \rangle\rangle} e^{i v_{ij} \phi} c_i^\dagger c_j \quad \text{NNN}$$

\wedge break SIS \wedge break TRS

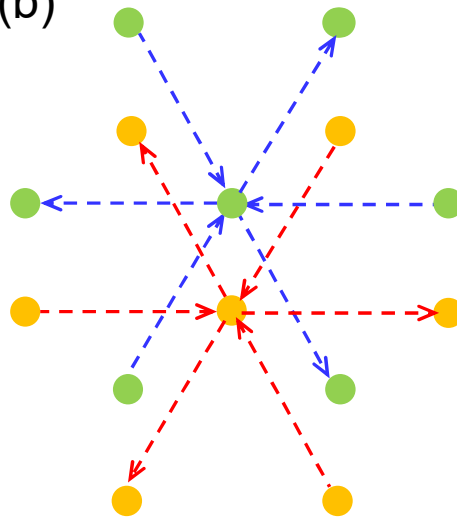
As a result of
Haldane flux

$$\begin{aligned} \mathbf{R}_A &\rightarrow \mathbf{R}_A + \mathbf{a}_i \text{ get } e^{-i\phi}, \quad i = 1, 2, 3 \\ \mathbf{R}_A &\rightarrow \mathbf{R}_A - \mathbf{a}_i \text{ get } e^{+i\phi}, \\ \mathbf{R}_B &\rightarrow \mathbf{R}_A + \mathbf{a}_i \text{ get } e^{+i\phi}, \\ \mathbf{R}_B &\rightarrow \mathbf{R}_A - \mathbf{a}_i \text{ get } e^{-i\phi}. \end{aligned}$$

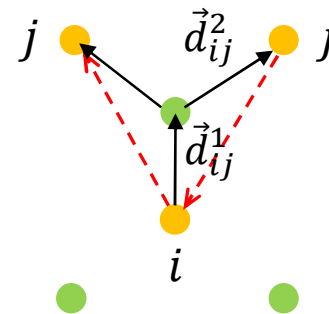
(a)



(b)



(c)



$$v_{ij} \equiv \text{sign}(\hat{d}_{ij}^1 \times \hat{d}_{ij}^2)_z$$

NNN coupling

$$\hat{H}_{NNN} = t_2 \sum_{\mathbf{R}} \sum_{i=1}^3 \left(c_{\mathbf{R}+\mathbf{a}_i}^\dagger c_{\mathbf{R}} e^{-i\phi} + h.c. \right) \\ + t_2 \sum_{\mathbf{R}} \sum_{i=1}^3 \left(d_{\mathbf{R}+\mathbf{a}_i}^\dagger d_{\mathbf{R}} e^{+i\phi} + h.c. \right).$$

$$= 2t_2 \sum_{\mathbf{k}} \sum_i \left[\cos(\mathbf{k} \cdot \mathbf{a}_i + \phi) c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + \cos(\mathbf{k} \cdot \mathbf{a}_i - \phi) d_{\mathbf{k}}^\dagger d_{\mathbf{k}} \right]$$

$$= \sum_{\mathbf{k}} \left(c_{\mathbf{k}}^\dagger, d_{\mathbf{k}}^\dagger \right) \mathbf{H}_{NNN}(\mathbf{k}) \begin{pmatrix} c_{\mathbf{k}} \\ d_{\mathbf{k}} \end{pmatrix}$$

$$\mathbf{H}_{NNN}(\mathbf{k}) = 2t_2 \begin{pmatrix} \sum_i \cos(\mathbf{k} \cdot \mathbf{a}_i + \phi) & 0 \\ 0 & \sum_i \cos(\mathbf{k} \cdot \mathbf{a}_i - \phi) \end{pmatrix}$$

➔ $\mathbf{H}(\mathbf{k}) = \frac{h_{11} + h_{22}}{2} + \mathbf{h} \cdot \boldsymbol{\sigma}$

$$\mathbf{h} = \left(t_1 \sum_i \cos \mathbf{k} \cdot \boldsymbol{\delta}_i, -t_1 \sum_i \sin \mathbf{k} \cdot \boldsymbol{\delta}_i, \frac{h_{11} - h_{22}}{2} + \Delta \right)$$

$$= \underline{-2t_2 \sum_i \sin \mathbf{k} \cdot \mathbf{a}_i \sin \phi} + \Delta$$

Near Dirac point

$$h_3(\mathbf{k}) = \pm 3\sqrt{3}t_2 \sin \phi + \Delta + O(k^2).$$

let $h_3 = m_\tau(\phi, \Delta)$ a ϕ -dependent effective mass

$$\rightarrow \mathbf{H}_\tau(\mathbf{k}) = \frac{h_{11} + h_{22}}{2} + \begin{pmatrix} m_\tau & \hbar v_F(\tau k_x - ik_y) \\ \hbar v_F(\tau k_x + ik_y) & -m_\tau \end{pmatrix}$$

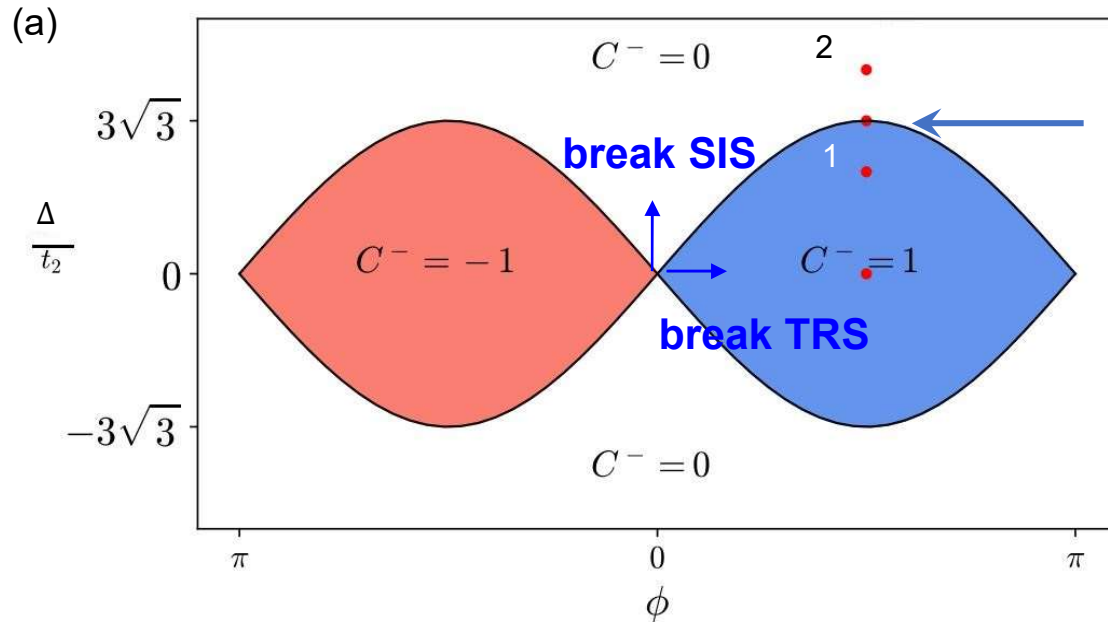
$$F_{z\tau}^+(\mathbf{k}) = \frac{\tau}{2} \frac{\hbar^2 v_F^2 m_\tau}{(\hbar^2 v_F^2 k^2 + m_\tau^2)^{3/2}}$$

The Dirac gap is closed when

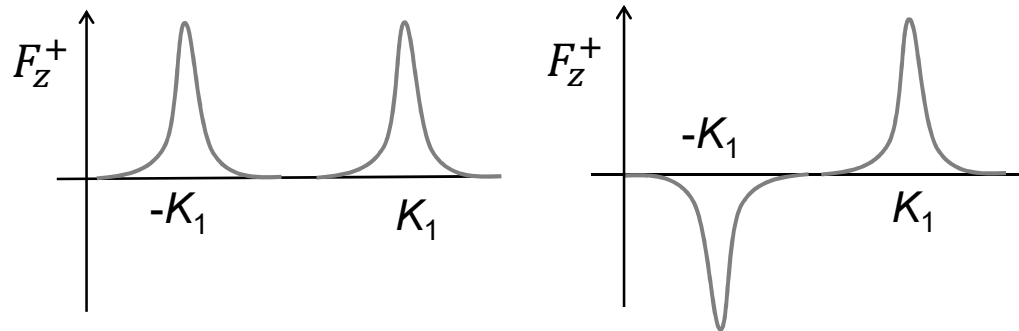
$$m_\pm(\phi, \Delta) = \pm 3\sqrt{3}t_2 \sin \phi + \Delta = 0$$

Phase diagram Zero-field quantum Hall effect phases ($\nu = \pm 1$, where $\sigma^{xy} = \nu e^2/h$) occur if $|M/t_2| < 3\sqrt{3}|\sin\phi|$.

Fig from Atteia's thesis, 2018

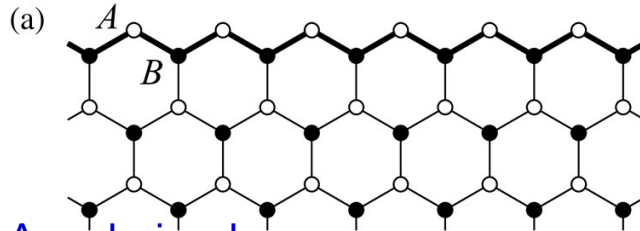


(b) Berry curvatures of point 1 (left) and 2 (right)

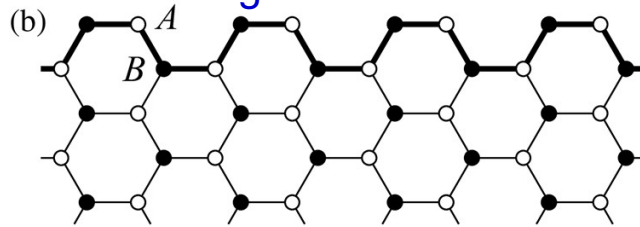


Edge state in different graphene models (for zigzag edge)

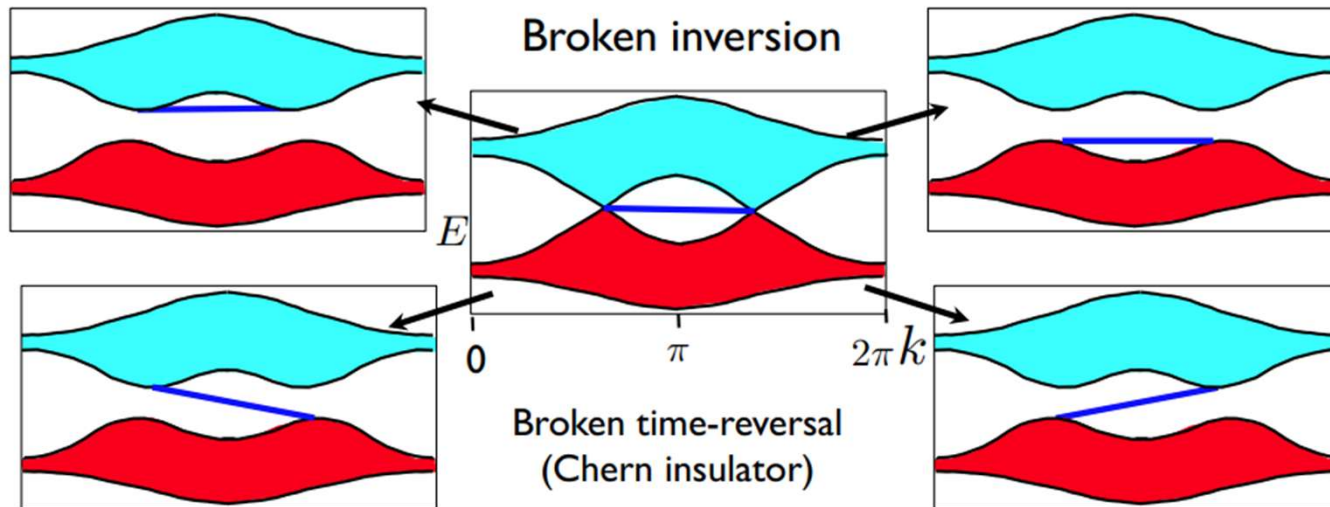
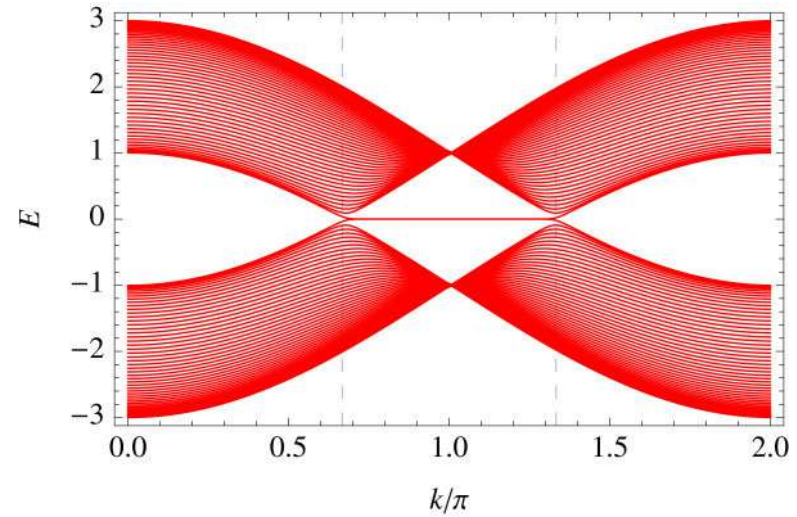
Zigzag edge



Armchair edge



Edge states for zigzag edge (Fujita, 1996)



Haldane, Nobel lecture