

# POEM: Physics of Emergent Materials

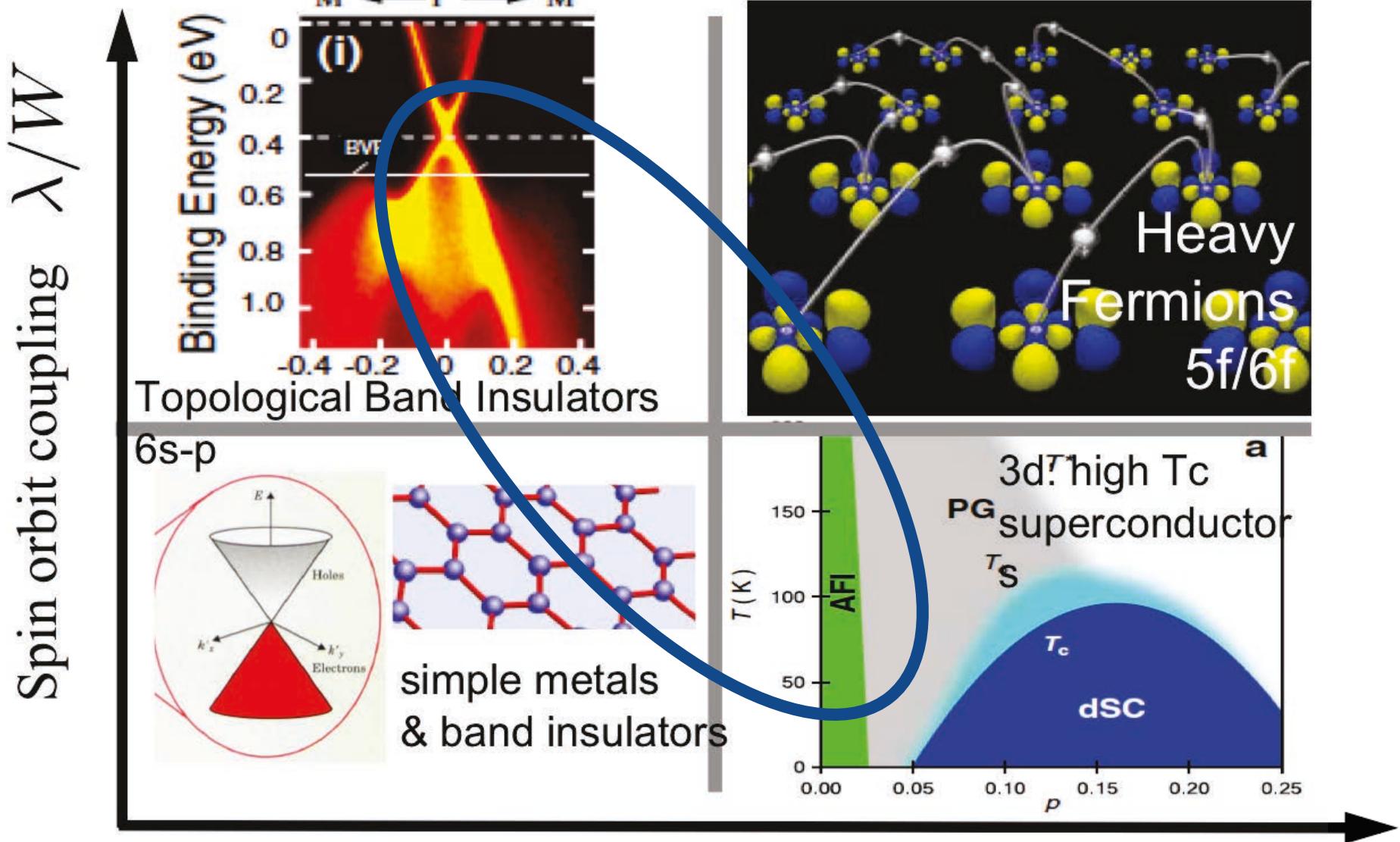
Nandini Trivedi

L1: Spin Orbit Coupling

L2: Topology and Topological Insulators

Reference: Bernevig Topological Insulators and Topological Superconductors

Tutorials: May 24, 25 (2017)



# Scope of Lectures and Anchor Points:

## 1. Spin-Orbit Interaction

- atomic SOC
- band SOC: dresselhaus and rashba
- symmetries: time reversal, inversion, mirror

## 2. Berry Phase and Topological Invariant

- two level system
- “graphene” + different mass terms + spin

## 3. The many Hall effects

- integer qhe and chern #

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DAY1

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- two level system
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DAY2

## 3. The many Hall effects

- integer qhe and chern #

*My philosophy....*  
choose simplicity and insight over completeness

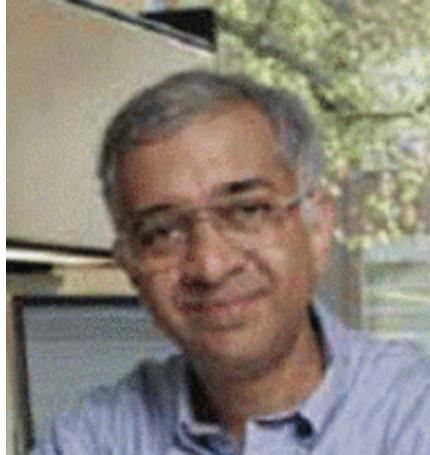
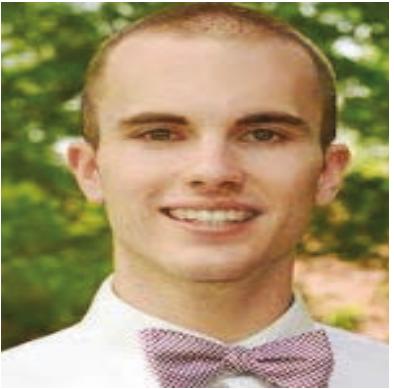
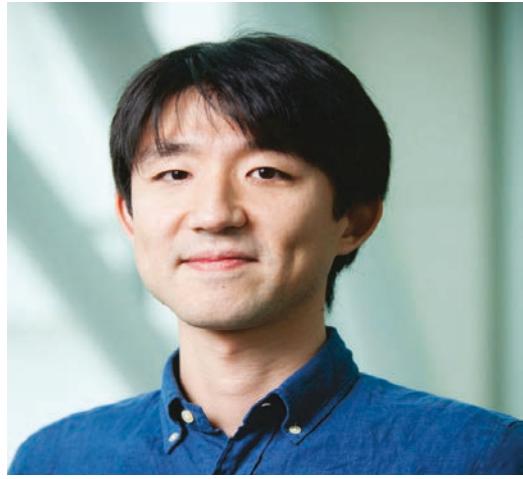
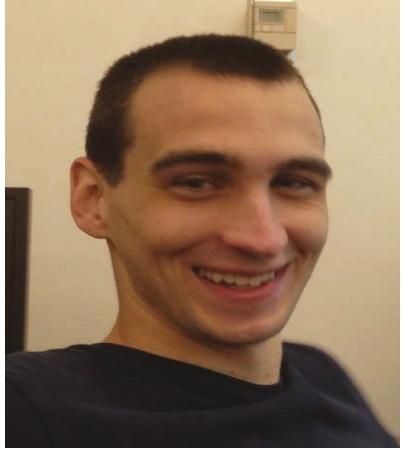
### Toy Problems:

#### Day 1:

- 1) 1d SOC: spin-momentum locking
- 2) Two level system (Spin  $\frac{1}{2}$  in a magnetic field) and Berry Phase
- 3) Graphene: dirac points protected by inversion and TR

#### Day 2:

- 4) 1d SSH [polyacetylene] model and topological invariant
- 5) Graphene continued:
  - Break inversion: sublattice potential
  - Break TR: Haldane mass



*...with a  
little  
help  
from my  
friends*

...

## Basics/Repository

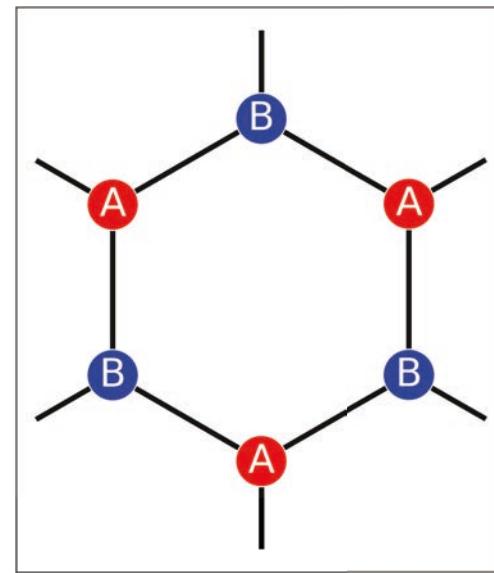
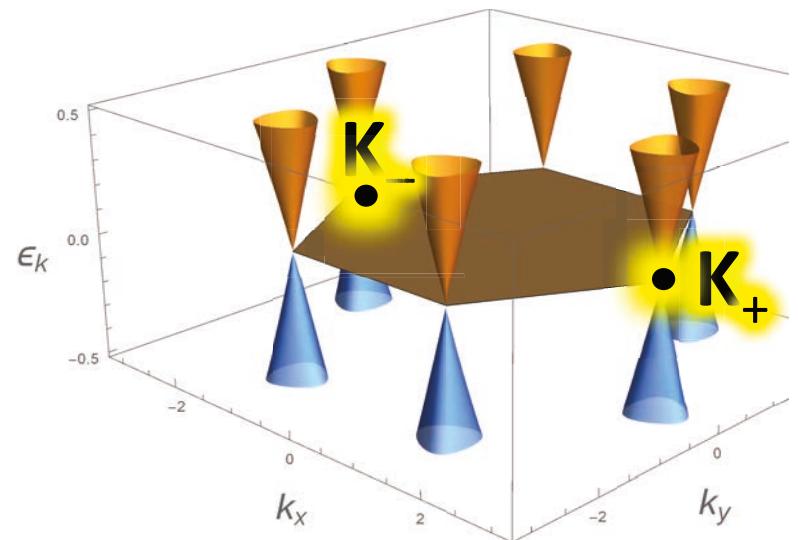
- Pauli Matrices
- Symmetries: Inversion, Mirror, Time Reversal
- Polar vs Axial (pseudo) vector

Pauli spin matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$\sigma$  Spin  
 $\tau$  Sublattice  
 $\chi$  Valley



## Symmetries:

- Time Reversal
- Inversion
- Mirror

# Time Reversal (without spin)

Definition:

$$T : t \rightarrow -t \quad TR \Rightarrow [H, T] = 0$$

Transformation of various operators under T

$T\hat{x}T^{-1} = \hat{x}$	$T\hat{p}T^{-1} = -\hat{p}$	$TiT^{-1} = -i$	$T\hat{L}T^{-1} = -\hat{L}$
$T[\hat{x}, \hat{p}]T^{-1} = Ti\hbar T^{-1} = -[\hat{x}, \hat{p}] = -i\hbar$			

$$Tc_j T^{-1} = c_j \quad Tc_k T^{-1} = c_{-k} \quad Th(k) T^{-1} = h(-k)$$

$T = K$        $T^2 = 1$

K:Complex conjugate

# Definition: Time Reversal (with half integer spin)

$$T : t \rightarrow -t \quad TR \Rightarrow [H, T] = 0 \quad \Rightarrow T|\Psi\rangle \quad \text{and} \quad |\Psi\rangle$$

are both eigenvectors with eigenvalue E

$$T = e^{-i\pi S_y} K$$

$$T^2 = -1$$

$$T^2 = -i\sigma_y i\sigma_y K K = -\sigma_y^2 = -1$$

Kramer's degeneracy: every energy level is at least doubly degenerate

$$\vec{S} = (\hbar/2)\vec{\sigma}$$

$$e^{-i\pi\sigma_y/2} = -i\sigma_y = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

$$T c_{j\uparrow} T^{-1} = -c_{j\downarrow}$$

$$T c_{j\downarrow} T^{-1} = c_{j\uparrow}$$

Same for dagger operators

$$Th(k)T^{-1} = h(-k)$$

# Polar vs Axial vectors

Saturday, May 20, 2017 7:43 PM

Polar  $\equiv$  "usual" vector

e.g.  $\vec{r}$ ,  $\vec{p}$ ,  $\vec{\nabla}$ ,  $\vec{E}$  etc

under a transformation A

$$\begin{matrix} \vec{v}_p \\ \uparrow \\ \text{polar} \end{matrix} \rightarrow A \begin{matrix} \vec{v}_p \\ \uparrow \\ \text{polar} \end{matrix}$$

Axial  $\equiv$  pseudo vector

$$\text{e.g. } \vec{L} = \vec{r} \times \vec{p}, \vec{s}$$

$$\vec{v}_a \rightarrow (\det A) A \vec{v}_a$$

## Inversion

$$A = I = \begin{pmatrix} -1 & & \\ & -1 & \\ & & -1 \end{pmatrix}$$

$$\vec{r} \rightarrow -\vec{r} \quad \text{etc}$$

$$\vec{L} \rightarrow \vec{L}$$

$$\vec{s} \rightarrow \vec{s}$$

$$\vec{B} \rightarrow \vec{B}$$

$$\det I = -1$$

$$\vec{L} = \vec{r} \times \vec{p}$$

- polar  $\times$  polar = axial

$$\vec{\nabla} \times \vec{B} = \dots \vec{J}$$

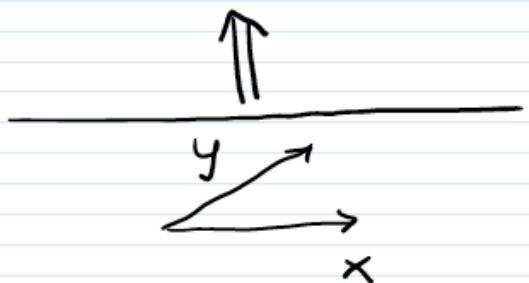
- polar  $\times$  axial = polar

$$\vec{M} \times \vec{H} = \vec{\tau}$$

- axial  $\times$  axial = axial

Mirror:

$z$ - Mirror  $\sigma_h(xy)$



$$x \rightarrow x$$

$$y \rightarrow y$$

$$z \rightarrow -z$$

$$L_x \rightarrow -L_x$$

$$L_y \rightarrow -L_y$$

$$L_z \rightarrow L_z$$

$\sigma_v(xz)$   
Y-mirror

$x \rightarrow x$
$y \rightarrow -y$
$z \rightarrow z$

$L_x \rightarrow -L_x$
$L_y \rightarrow L_y$
$L_z \rightarrow -L_z$

$\sigma_v(yz)$   
X-mirror

$x \rightarrow -x$
$y \rightarrow y$
$z \rightarrow z$

$L_x \rightarrow L_x$
$L_y \rightarrow -L_y$
$L_z \rightarrow -L_z$

$$\vec{L} = \vec{r} \times \vec{p}$$

$$L_x = y p_z - z p_y$$

$$L_y = z p_x - x p_z$$

$$L_z = x p_y - y p_x$$

# Scope of Lectures and Anchor Points:

## 1. Spin-Orbit Interaction

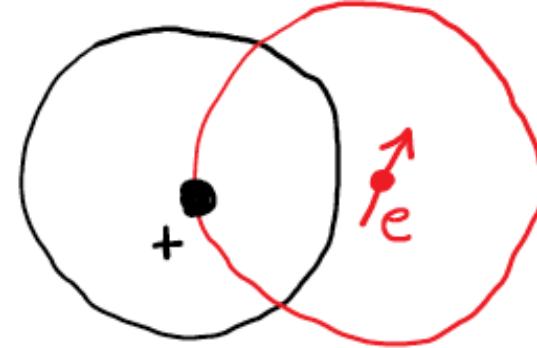
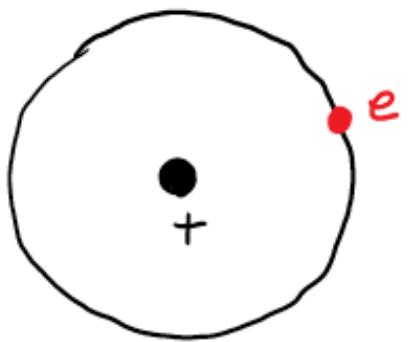
- atomic SOC
- band SOC: dresselhaus and rashba
- symmetries: time reversal, inversion, mirror

## 2. Berry Phase and Topological Invariant

- two level system
- graphene

## 3. Hall effects

- integer qhe and chern #



$$\vec{B} = \vec{v} \times \vec{E}$$

$$\propto \vec{L}$$

$$\vec{E} = E \hat{r}$$

$$= \frac{E}{r} \vec{r}$$

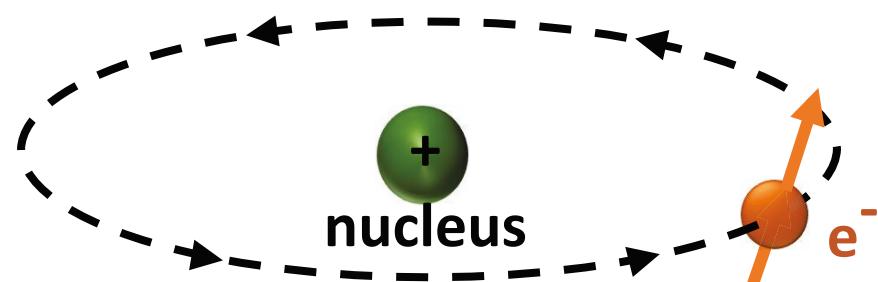
$$\vec{L} = \vec{r} \times m\vec{v}$$

$$H = \vec{\sigma} \cdot \vec{B} = \lambda \vec{\sigma} \cdot \vec{L}$$

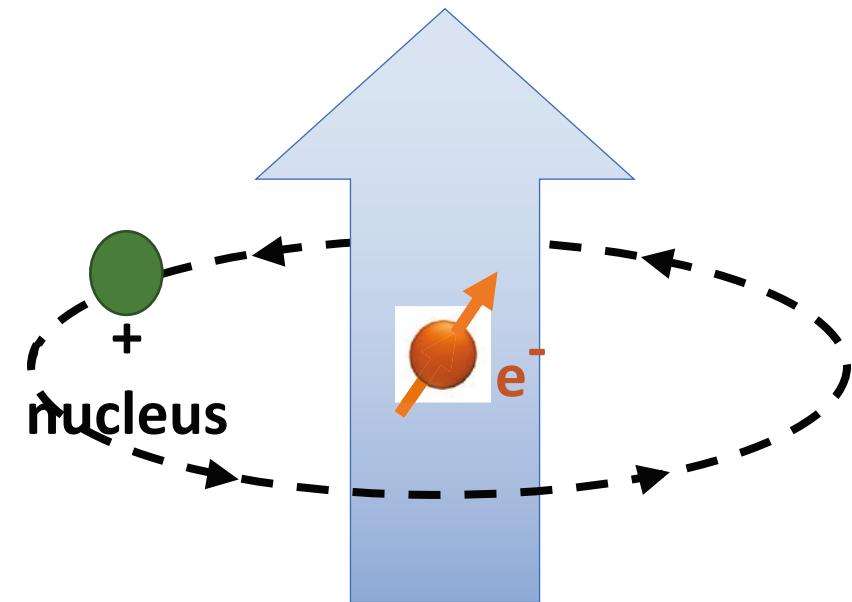
Zeeman Effect

spin orbit coupling

# Spin-Orbit Coupling



magnetic field seen by electron



$$H_{\text{SO}} = \frac{1}{m_e^2 c^2} \frac{1}{r} \frac{dV}{dr} \vec{S} \cdot \vec{L} \quad \rightarrow \quad \lambda \vec{L} \cdot \vec{S}$$

When is Spin Orbit coupling large?  
What materials?

# Transition Metals

valence electrons in the d shell

1 IA 1A																				18 VIIIA 8A
1 H Hydrogen $[1s^1]$	2 IIA 2A																		2 He Helium $[1s^2]$	
3 Li Lithium $[He]2s^1$	4 Be Beryllium $[He]2s^2$																		10 Ne Neon $[He]2s^22p^6$	
11 Na Sodium $[Ne]3s^1$	12 Mg Magnesium $[Ne]3s^2$	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIIB	8	9	10	11 IB	12 IIB								18 VIIIA 8A	
19 K Potassium $[Ar]4s^1$	20 Ca Calcium $[Ar]4s^2$	21 Sc Scandium $[Ar]3d^14s^2$	22 Ti Titanium $[Ar]3d^24s^2$	23 V Vanadium $[Ar]3d^34s^2$	24 Cr Chromium $[Ar]3d^54s^1$	25 Mn Manganese $[Ar]3d^54s^2$	26 Fe Iron $[Ar]3d^64s^2$	27 Co Cobalt $[Ar]3d^74s^2$	28 Ni Nickel $[Ar]3d^84s^1$	29 Cu Copper $[Ar]3d^{10}4s^1$	30 Zn Zinc $[Ar]3d^{10}4s^2$									2 He Helium $[1s^2]$
37 Rb Rubidium $[Kr]5s^1$	38 Sr Strontium $[Kr]4d^25s^2$	39 Y Yttrium $[Kr]4d^15s^2$	40 Zr Zirconium $[Kr]4d^25s^2$	41 Nb Niobium $[Kr]4d^35s^1$	42 Mo Molybdenum $[Kr]4d^55s^2$	43 Tc Technetium $[Kr]4d^55s^1$	44 Ru Ruthenium $[Kr]4d^75s^1$	45 Rh Rhodium $[Kr]4d^{10}$	46 Pd Palladium $[Kr]4d^{10}5s^1$	47 Ag Silver $[Kr]4d^{10}5s^2$	48 Cd Cadmium $[Kr]4d^{10}5s^2$									18 VIIIA 8A
55 Cs Cesium $[Xe]6s^1$	56 Ba Barium $[Xe]6s^2$	57-71	72 Hf Hafnium $[Xe]4f^145d^6s^2$	73 Ta Tantalum $[Xe]4f^145d^36s^2$	74 W Tungsten $[Xe]4f^145d^6s^2$	75 Re Rhenium $[Xe]4f^145d^6s^2$	76 Os Osmium $[Xe]4f^145d^6s^2$	77 Ir Iridium $[Xe]4f^145d^6s^2$	78 Pt Platinum $[Xe]4f^145d^6s^1$	79 Au Gold $[Xe]4f^145d^{10}6s^1$	80 Hg Mercury $[Xe]4f^145d^{10}6s^2$								18 VIIIA 8A	
87 Fr Francium $[Rn]7s^1$	88 Ra Radium $[Rn]7s^2$	89-103	104 Rf Rutherfordium $[Rn]5f^146d^77s^2$	105 Db Dubnium $[Rn]5f^146d^77s^2$	106 Sg Seaborgium $[Rn]5f^146d^77s^2$	107 Bh Bohrium $[Rn]5f^146d^77s^2$	108 Hs Hassium $[Rn]5f^146d^77s^2$	109 Mt Meitnerium $[Rn]5f^146d^77s^2$	110 Ds Darmstadium $[Rn]5f^146d^77s^2$	111 Rg Roentgenium $[Rn]5f^146d^77s^2$	112 Cn Copernicium $[Rn]5f^146d^77s^2$								18 VIIIA 8A	
			[261]	[262]	[266]	[264]	[269]	[268]	[269]	[272]	[277]								18 VIIIA 8A	
Lanthanide Series	57 La Lanthanum $[Xe]5d^16s^2$	58 Ce Cerium $[Xe]4f^15d^16s^2$	59 Pr Praseodymium $[Xe]4f^36s^2$	60 Nd Neodymium $[Xe]4f^46s^2$	61 Pm Promethium $[Xe]4f^56s^2$	62 Sm Samarium $[Xe]4f^66s^2$	63 Eu Europium $[Xe]4f^76s^2$	64 Gd Gadolinium $[Xe]4f^76s^2$	65 Tb Terbium $[Xe]4f^96s^2$	66 Dy Dysprosium $[Xe]4f^{10}6s^2$	67 Ho Holmium $[Xe]4f^{11}6s^2$	68 Er Erbium $[Xe]4f^{12}6s^2$	69 Tm Thulium $[Xe]4f^{13}6s^2$	70 Yb Ytterbium $[Xe]4f^{14}6s^2$	71 Lu Lutetium $[Xe]4f^{14}5d^16s^2$					18 VIIIA 8A
Actinide Series	89 Ac Actinium $[Rn]6d^17s^2$	90 Th Thorium $[Rn]6d^27s^2$	91 Pa Protactinium $[Rn]5f^26d^17s^2$	92 U Uranium $[Rn]5f^36d^17s^2$	93 Np Neptunium $[Rn]5f^46d^17s^2$	94 Pu Plutonium $[Rn]5f^56d^17s^2$	95 Am Americium $[Rn]5f^77s^2$	96 Cm Curium $[Rn]5f^76d^17s^2$	97 Bk Berkelium $[Rn]5f^96d^17s^2$	98 Cf Californium $[Rn]5f^96d^17s^2$	99 Es Einsteinium $[Rn]5f^116d^17s^2$	100 Fm Fermium $[Rn]5f^116d^17s^2$	101 Md Mendelevium $[Rn]5f^137s^2$	102 No Nobelium $[Rn]5f^146d^17s^2$	103 Lr Lawrencium $[Rn]5f^146d^17s^2$					18 VIIIA 8A

Configurations denoted with a \* are unknown and the listed values are predicted.

**s shell****L = 0**

1 IA 1A	1.008 <b>H</b> Hydrogen $1s^1$	2 IIA 2A
3 6.941 <b>Li</b> Lithium $[He]2s^1$	4 9.012 <b>Be</b> Beryllium $[He]2s^2$	
11 22.990 <b>Na</b> Sodium $[Ne]3s^1$	12 24.305 <b>Mg</b> Magnesium $[Ne]3s^2$	
19 39.098 <b>K</b> Potassium $[Ar]4s^1$	20 40.078 <b>Ca</b> Calcium $[Ar]4s^2$	
37 84.468 <b>Rb</b> Rubidium $[Kr]5s^1$	38 87.62 <b>Sr</b> Strontium $[Kr]5s^2$	
55 132.905 <b>Cs</b> Cesium $[Xe]6s^1$	56 137.327 <b>Ba</b> Barium $[Xe]6s^2$	
87 223.020 <b>Fr</b> Francium $[Rn]7s^1$	88 226.025 <b>Ra</b> Radium $[Rn]7s^2$	
89-103 <b>Rf</b> Rutherfordium $[Rn]5f^{14}6d^27s^2$	104 <b>Dubnium</b> Dubnium $[Rn]5f^{14}6d^37s^2$	105 <b>Sg</b> Seaborgium $[Rn]5f^{14}6d^47s^2$

# Transition Metals

**d shell****L = 2**

13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	18 VIIIA 8A
5 10.811 <b>B</b> Boron $[He]2s^22p^1$	6 12.011 <b>C</b> Carbon $[He]2s^22p^2$	7 14.007 <b>N</b> Nitrogen $[He]2s^22p^3$	8 15.999 <b>O</b> Oxygen $[He]2s^22p^4$	9 18.998 <b>F</b> Fluorine $[He]2s^22p^5$	2 4.003 <b>He</b> Helium $1s^2$
13 26.982 <b>Al</b> Aluminum $[Ne]3s^23p^1$	14 28.086 <b>Si</b> Silicon $[Ne]3s^23p^2$	15 30.974 <b>P</b> Phosphorus $[Ne]3s^23p^3$	16 32.066 <b>S</b> Sulfur $[Ne]3s^23p^4$	17 35.453 <b>Cl</b> Chlorine $[Ne]3s^23p^5$	18 39.948 <b>Ar</b> Argon $[Ne]3s^23p^6$
31 69.732 <b>Ga</b> Gallium $[Ar]3d^{10}4s^24p^1$	32 72.61 <b>Ge</b> Germanium $[Ar]3d^{10}4s^24p^2$	33 74.922 <b>As</b> Arsenic $[Ar]3d^{10}4s^24p^3$	34 78.972 <b>Se</b> Selenium $[Ar]3d^{10}4s^24p^4$	35 79.904 <b>Br</b> Bromine $[Ar]3d^{10}4s^24p^5$	36 84.80 <b>Kr</b> Krypton $[Ar]3d^{10}4s^24p^6$
49 114.818 <b>In</b> Indium $[Kr]4d^{10}5s^1$	50 118.71 <b>Sn</b> Tin $[Kr]4d^{10}5s^2$	51 121.760 <b>Sb</b> Antimony $[Kr]4d^{10}5s^25p^3$	52 127.6 <b>Te</b> Tellurium $[Kr]4d^{10}5s^25p^4$	53 126.904 <b>I</b> Iodine $[Kr]4d^{10}5s^25p^5$	54 131.29 <b>Xe</b> Xenon $[Kr]4d^{10}5s^25p^6$
81 204.383 <b>Tl</b> Thallium $[Xe]4f^{10}6s^2$	82 207.2 <b>Pb</b> Lead $[Xe]4f^{10}6s^26p^2$	83 208.980 <b>Bi</b> Bismuth $[Xe]4f^{10}6s^26p^3$	84 [208.982] <b>Po</b> Polonium $[Xe]4f^{10}6s^26p^4$	85 209.987 <b>At</b> Astatine $[Xe]4f^{10}6s^26p^5$	86 222.018 <b>Rn</b> Radon $[Xe]4f^{10}6s^26p^6$

Configurations denoted with \* are unknown and the listed values are predicted.

**f shell**  
**L = 3**

<b>Lanthanide Series</b>	57 138.906 <b>La</b> Lanthanum $[Xe]5d^16s^2$	58 140.115 <b>Ce</b> Cerium $[Xe]4f^15d^16s^2$	59 140.908 <b>Pr</b> Praseodymium $[Xe]4f^36s^2$	60 144.24 <b>Nd</b> Neodymium $[Xe]4f^96s^2$	61 144.913 <b>Pm</b> Promethium $[Xe]4f^16s^2$	62 150.36 <b>Sm</b> Samarium $[Xe]4f^56s^2$	63 151.966 <b>Eu</b> Europium $[Xe]4f^76s^2$	64 157.25 <b>Gd</b> Gadolinium $[Xe]4f^96s^2$	65 158.925 <b>Tb</b> Terbium $[Xe]4f^{10}6s^2$	66 162.50 <b>Dy</b> Dysprosium $[Xe]4f^{10}6s^2$	67 164.930 <b>Ho</b> Holmium $[Xe]4f^{11}6s^2$	68 167.26 <b>Er</b> Erbium $[Xe]4f^{12}6s^2$	69 168.934 <b>Tm</b> Thulium $[Xe]4f^{13}6s^2$	70 173.04 <b>Yb</b> Ytterbium $[Xe]4f^{14}6s^2$	
<b>Actinide Series</b>	89 227.028 <b>Ac</b> Actinium $[Rn]6d^17s^2$	90 232.038 <b>Th</b> Thorium $[Rn]6d^27s^2$	91 231.036 <b>Pa</b> Protactinium $[Rn]5f^26d^17s^2$	92 238.029 <b>U</b> Uranium $[Rn]5f^36d^17s^2$	93 237.048 <b>Np</b> Neptunium $[Rn]5f^46d^17s^2$	94 244.064 <b>Pu</b> Plutonium $[Rn]5f^56d^17s^2$	95 243.061 <b>Am</b> Americium $[Rn]5f^76d^17s^2$	96 247.070 <b>Cm</b> Curium $[Rn]5f^76d^17s^2$	97 247.070 <b>Bk</b> Berkelium $[Rn]5f^96d^17s^2$	98 [251.080] <b>Cf</b> Flerovium $[Rn]5f^{10}6d^17s^2$	99 [254] <b>Es</b> Einsteinium $[Rn]5f^{10}7s^2$	100 257.095 <b>Fm</b> Fermium $[Rn]5f^{10}7s^2$	101 258.1 <b>Md</b> Mendelevium $[Rn]5f^{11}7s^2$	102 259.101 <b>No</b> Nobelium $[Rn]5f^{14}6d^17s^2$	103 [262] <b>Lr</b> Lawrencium $[Rn]5f^{14}6d^17s^2$

# Spherical Symmetry

- Wavefunction for atomic orbitals

$$\psi(\vec{r}) = R(r) \Omega(\theta, \phi)$$

↑                      ↑  
radial part            angular part  
(spherical Harmonics)

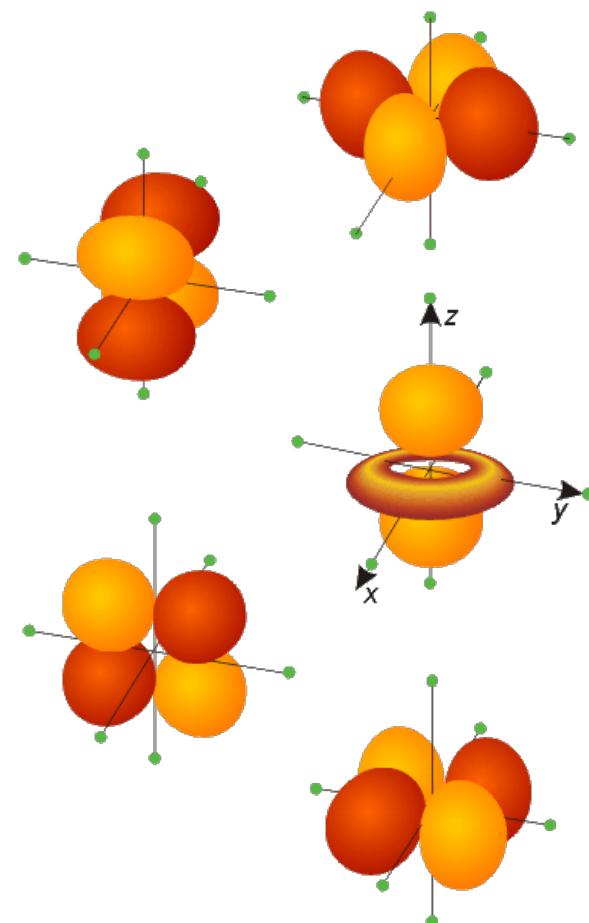
- For the **d** shell:

$$\Omega(\theta, \phi) = Y_l^m(\theta, \phi) \quad \text{with} \quad l = 2$$

$m = +2$   
 $m = +1$   
 $m = 0$   
 $m = -1$   
 $m = -2$

# d Orbitals

- Atomic orbitals are linear combinations of spherical harmonics



$$d_{x^2-y^2} = \frac{1}{\sqrt{2}} (Y_2^{-2} + Y_2^{+2})$$

$$d_{zx} = \frac{1}{\sqrt{2}} (Y_2^{-1} - Y_2^{+1})$$

$$d_{z^2} = Y_2^0$$

$$d_{yz} = \frac{i}{\sqrt{2}} (Y_2^{-1} + Y_2^{+1})$$

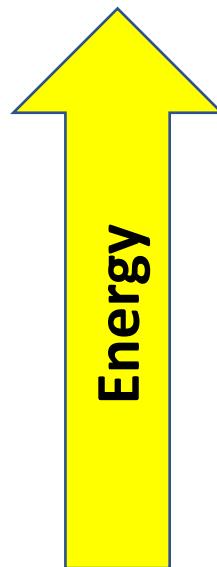
$$d_{xy} = \frac{i}{\sqrt{2}} (Y_2^{-2} - Y_2^{+2})$$

# Crystal Field Splitting

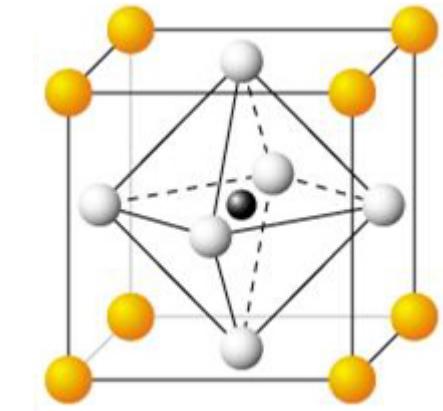
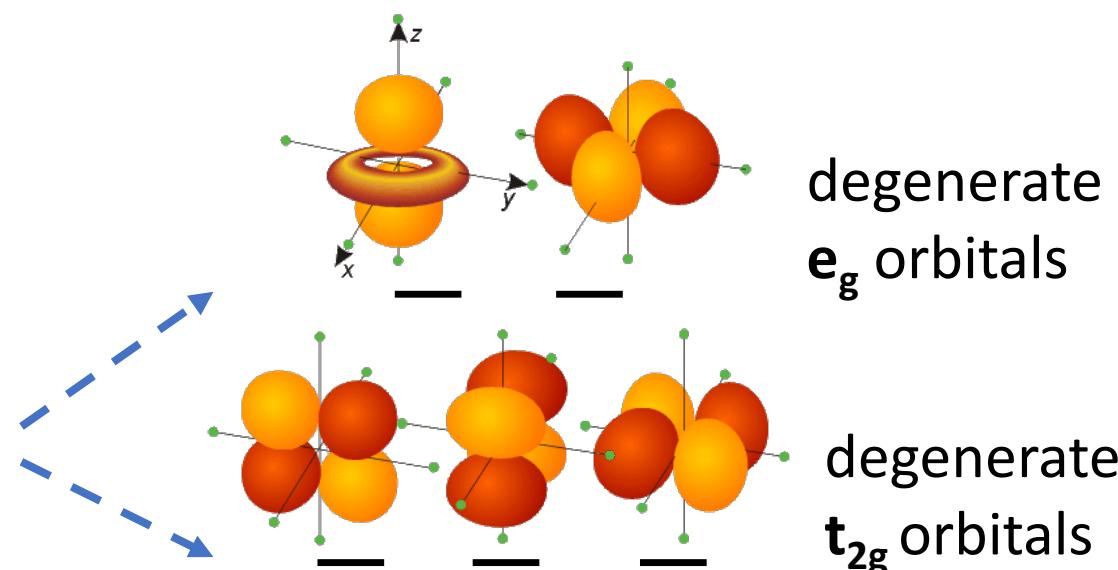
Spherical Symmetry

... reduced to ...

Octahedral Symmetry



degenerate d orbitals



\*\* Omitting the  $\hbar$  factor from  $L$ .

# $L = 2$ Angular Momentum

$$L_x = \frac{1}{2} (L_+ + L_-)$$

$$L_y = \frac{1}{2i} (L_+ - L_-)$$

$$L_x = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 \\ 0 & \sqrt{\frac{3}{2}} & 0 & \sqrt{\frac{3}{2}} & 0 \\ 0 & 0 & \sqrt{\frac{3}{2}} & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

$$L_y = \begin{pmatrix} 0 & -i & 0 & 0 & 0 \\ i & 0 & -i\sqrt{\frac{3}{2}} & 0 & 0 \\ 0 & i\sqrt{\frac{3}{2}} & 0 & -i\sqrt{\frac{3}{2}} & 0 \\ 0 & 0 & i\sqrt{\frac{3}{2}} & 0 & -i \\ 0 & 0 & 0 & i & 0 \end{pmatrix}$$

**Eigenbasis of  $L_z$** 

$$L_z = \begin{pmatrix} +2 & 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -2 \end{pmatrix}$$

↔       $|L = 2, m = +2\rangle$   
           ↔       $|L = 2, m = +1\rangle$   
           ↔       $|L = 2, m = 0\rangle$   
           ↔       $|L = 2, m = -1\rangle$   
           ↔       $|L = 2, m = -2\rangle$

# $L = 2$ Angular Momentum

$$L_x = \left( \begin{array}{ccc|cc} 0 & 0 & 0 & -i\sqrt{3} & -i \\ 0 & 0 & +i & 0 & 0 \\ 0 & -i & 0 & 0 & 0 \\ \hline +i\sqrt{3} & 0 & 0 & 0 & 0 \\ +i & 0 & 0 & 0 & 0 \end{array} \right) \quad L_y = \left( \begin{array}{ccc|cc} 0 & 0 & -i & 0 & 0 \\ 0 & 0 & 0 & +i\sqrt{3} & -i \\ +i & 0 & 0 & 0 & 0 \\ \hline 0 & -i\sqrt{3} & 0 & 0 & 0 \\ 0 & +i & 0 & 0 & 0 \end{array} \right)$$

**Orbital basis**

$$L_z = \left( \begin{array}{ccc|cc} 0 & +i & 0 & 0 & 0 \\ -i & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & +2i \\ \hline 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -2i & 0 & 0 \end{array} \right)$$

←  $|d_{yz}\rangle$   
 ←  $|d_{zx}\rangle$   
 ←  $|d_{xy}\rangle$   
 ←  $|d_{z^2}\rangle$   
 ←  $|d_{x^2-y^2}\rangle$

\*\* Omitting the  $\hbar$  factor from  $L$ .

# $t_{2g}$ Angular Momentum

- When the  $t_{2g}$  and  $e_g$  energy levels are **sufficiently split** and the filling is  $d^6$  or less, we may only consider operators acting in the  $t_{2g}$  subspace and can project all operators into this subspace.

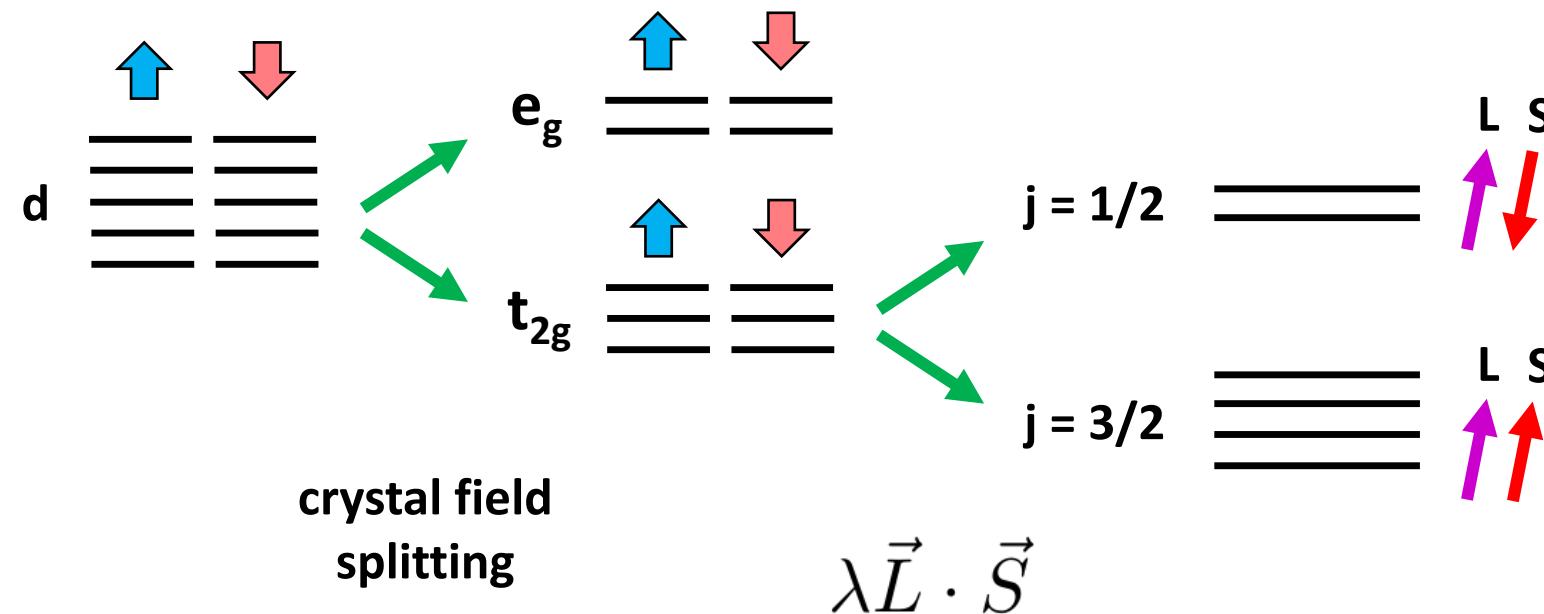
$$L_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & +i \\ 0 & -i & 0 \end{pmatrix} \quad L_y = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ +i & 0 & 0 \end{pmatrix} \quad L_z = \begin{pmatrix} 0 & +i & 0 \\ -i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

- Effective  $L = 1$  angular momentum
- The components satisfy the **negative** of the usual commutation relations.

$$\vec{L} \times \vec{L} = -i\vec{L}$$

# Spin-Orbit Coupling

- For  $t_{2g}$  orbitals, the effective  $L = 1$  and  $S = 1/2$  combine to total  $j = 1/2$  and  $j = 3/2$ .



# Spin-Orbit Assisted Mott Insulators

Similar...

Co, Rh, Ir: 5 valence electrons in the d shell

$\text{Sr}_2\text{XO}_4$  tetragonal  
BCC crystal structure

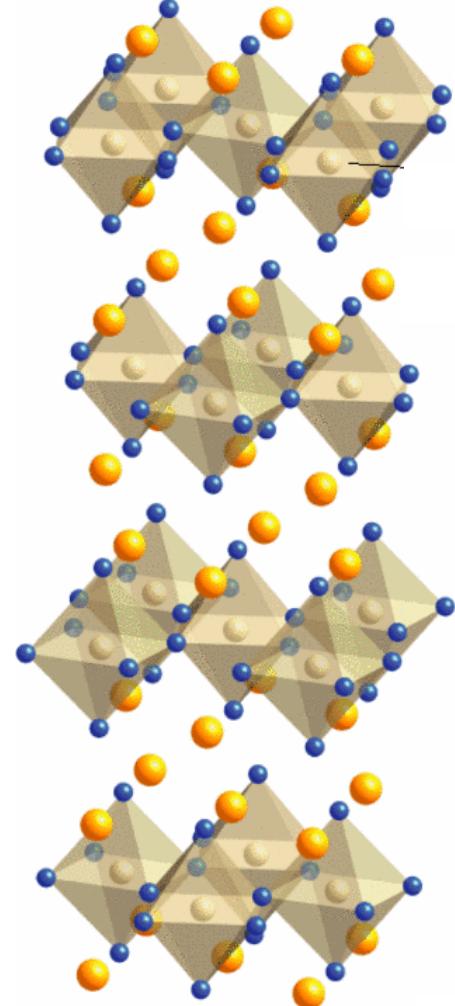
$\uparrow$ <b>U</b>	<b>26</b> 55.933 <b>Fe</b> Iron $[\text{Ar}]3d^64s^2$	<b>27</b> 58.933 <b>Co</b> Cobalt $[\text{Ar}]3d^74s^2$	<b>28</b> 58.693 <b>Ni</b> Nickel $[\text{Ar}]3d^84s^2$
$\downarrow$ <b><math>\lambda</math></b>	<b>44</b> 101.07 <b>Ru</b> Ruthenium $[\text{Kr}]4d^75s^1$	<b>45</b> 102.906 <b>Rh</b> Rhodium $[\text{Kr}]4d^85s^1$	<b>46</b> 106.42 <b>Pd</b> Palladium $[\text{Kr}]4d^{10}$
$\downarrow$	<b>76</b> 190.23 <b>Os</b> Osmium $[\text{Xe}]4f^{14}5d^66s^2$	<b>77</b> 192.22 <b>Ir</b> Iridium $[\text{Xe}]4f^{14}5d^76s^2$	<b>78</b> 195.08 <b>Pt</b> Platinum $[\text{Xe}]4f^{14}5d^96s^1$

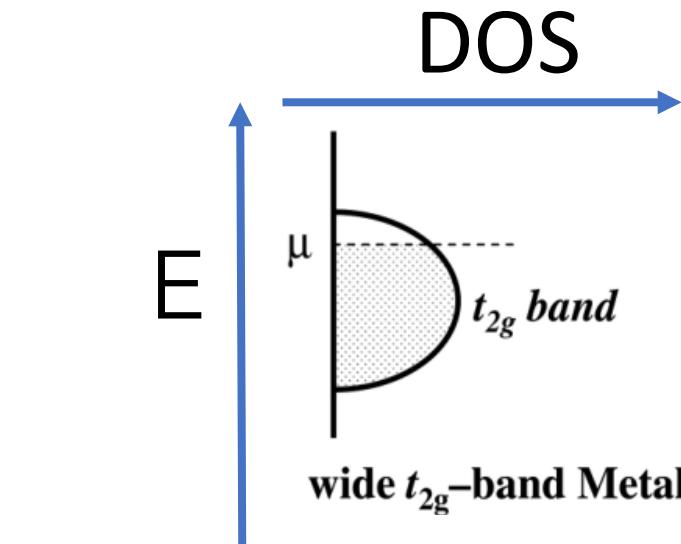
Yet....

$\text{Sr}_2\text{CoO}_4$  (Mott Insulator)

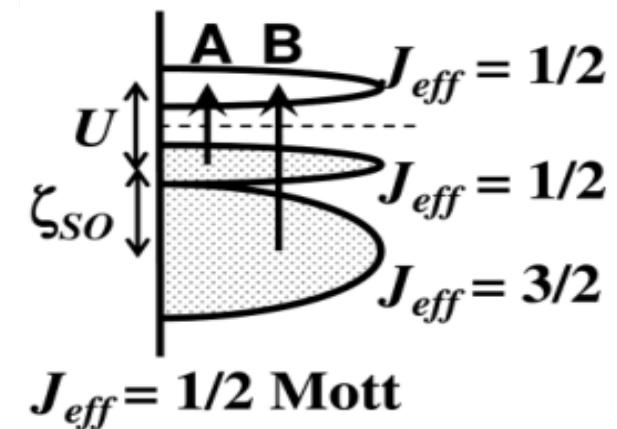
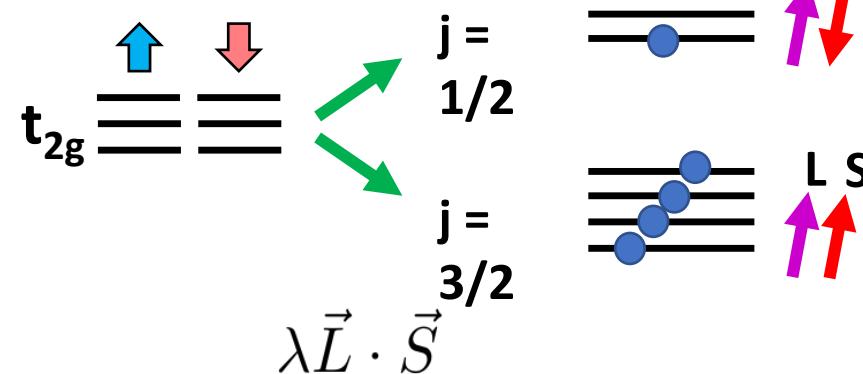
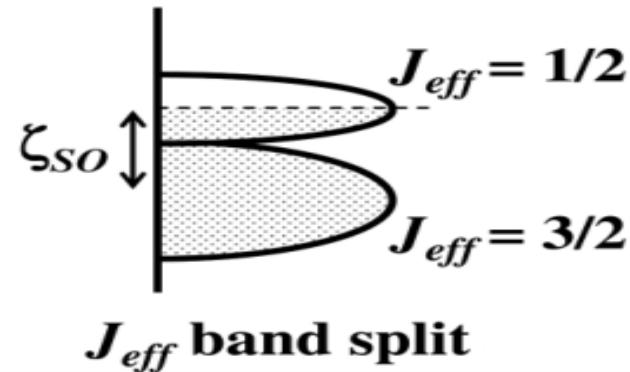
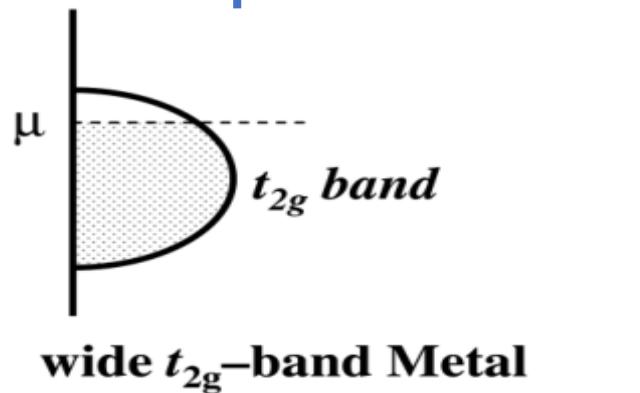
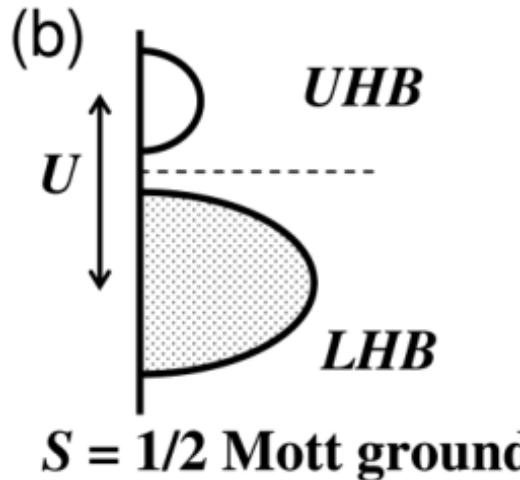
$\text{Sr}_2\text{RhO}_4$  (metal)

$\text{Sr}_2\text{IrO}_4$  (insulator)





$E$



SOC assisted  
Mott Insulator:  
 $Sr_2IrO_4$

Mott  
Insulator:  
 $Sr_2CoO_4$

# Scope of Lectures and Anchor Points:

## 1. Spin-Orbit Interaction

- atomic SOC
- band SOC: dresselhaus and rashba
- symmetries: time reversal, inversion, mirror

## 2. Berry Phase and Topological Invariant

- two level system
- graphene

## 3. Hall effects

- integer qhe and chern #

*My philosophy....*  
choose simplicity and insight over completeness

## Toy Problems:

### Day 1:

- 1) 1d SOC: spin-momentum locking
- 2) Two level system (Spin  $\frac{1}{2}$  in a magnetic field) and Berry Phase
- 3) Graphene: dirac points protected by inversion and TR

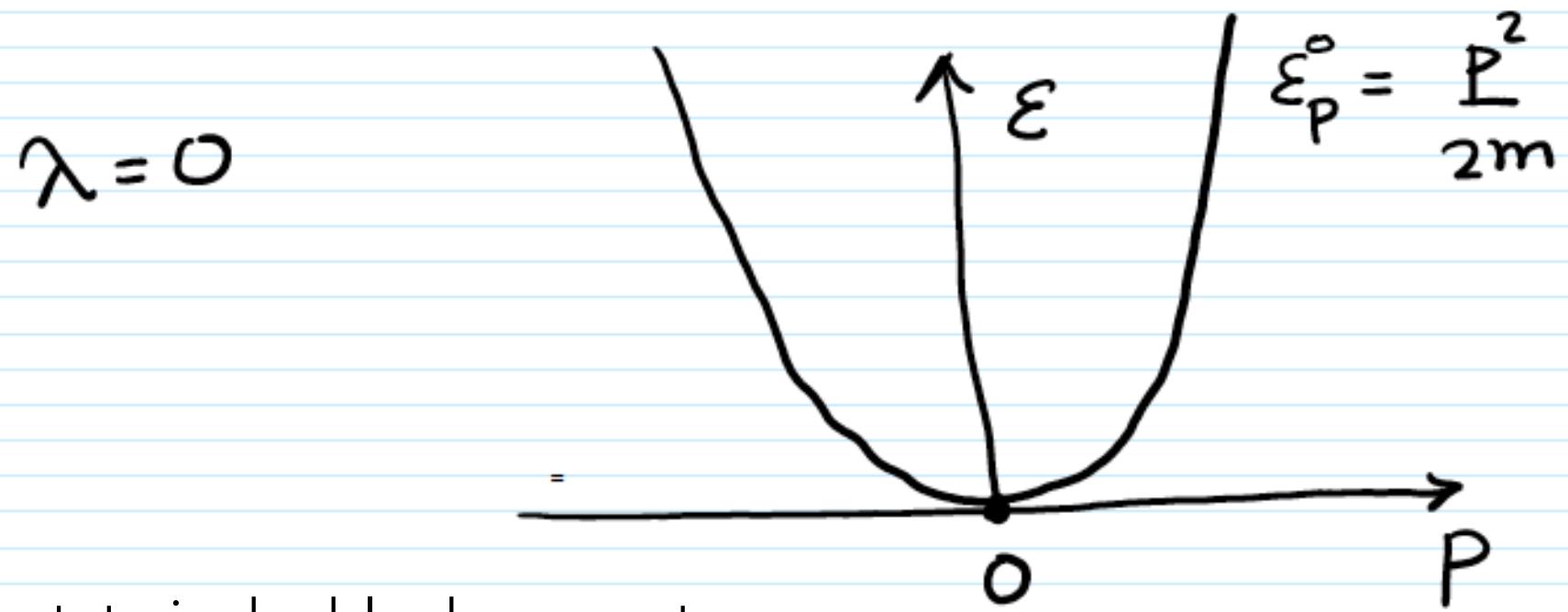
### Day 2:

- 4) 1d SSH [polyacetylene] model and topological invariant
- 5) Graphene continued:
  - Break inversion: sublattice potential
  - Break TR: Haldane mass

Spin-orbit coupling in bands  
Example in 1d: spin-momentum locking

$$\mathcal{H} = \frac{\underline{p}^2}{2m} \mathbf{1} - \lambda \sigma_z \underline{p}$$

Spin – momentum coupling

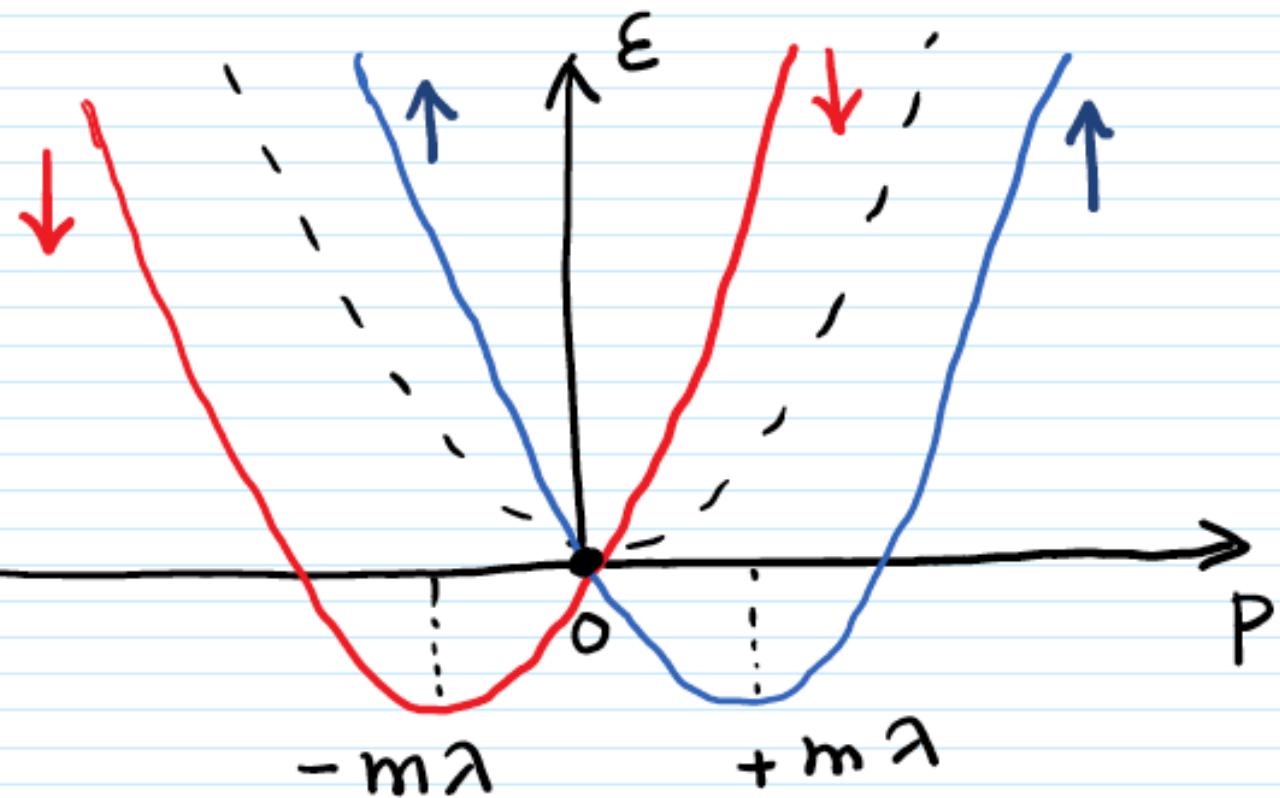


Each eigenstate is doubly degenerate:  
Kramer's degeneracy

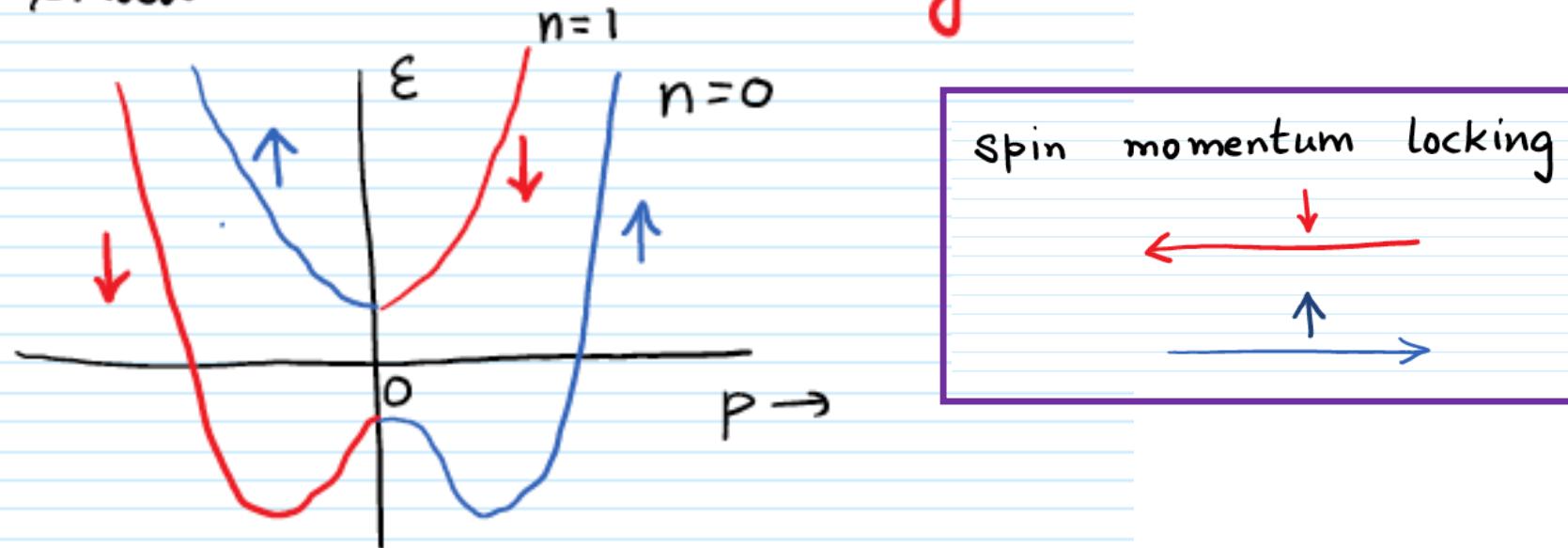
$$\lambda \neq 0 \quad \mathcal{H} = \begin{pmatrix} \uparrow & \epsilon_p^0 - \lambda p & 0 \\ \downarrow & 0 & \epsilon_p^0 + \lambda p \end{pmatrix}$$

Degeneracy  
between up and  
down spins is lifted  
by SOC

Except at specific  
TRIM: time reversal  
invariant momenta  
e.g.  $p=0$



Apply small Zeeman field along  $\hat{z}^c$



Gap opens up at the degenerate point.

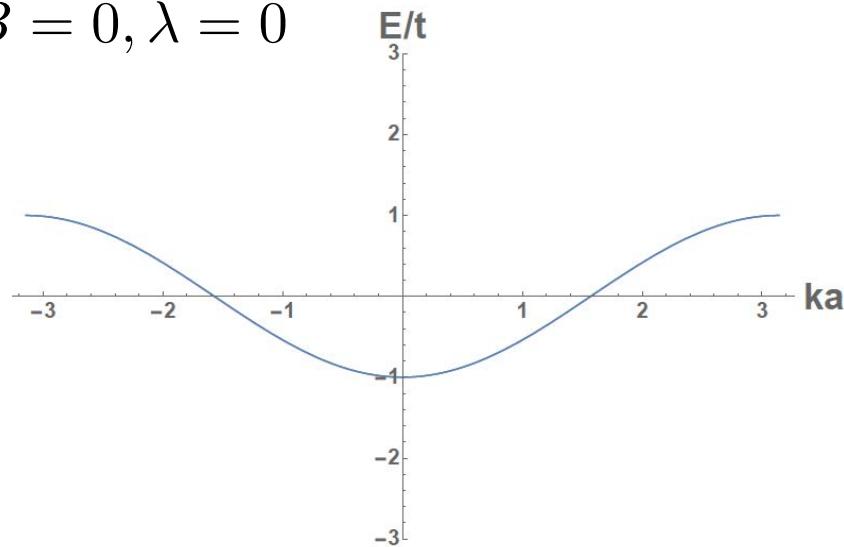
Traverse the BZ always remaining in the lowest band. (adiabatic evolution).

→ The electron spin will twist from  $\downarrow$  for  $-p$  to  $\uparrow$  for  $+p$

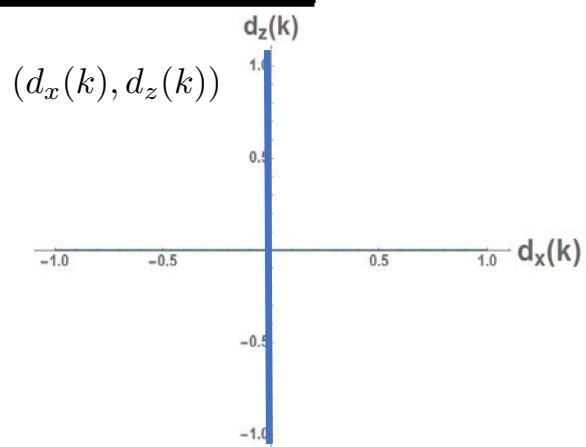
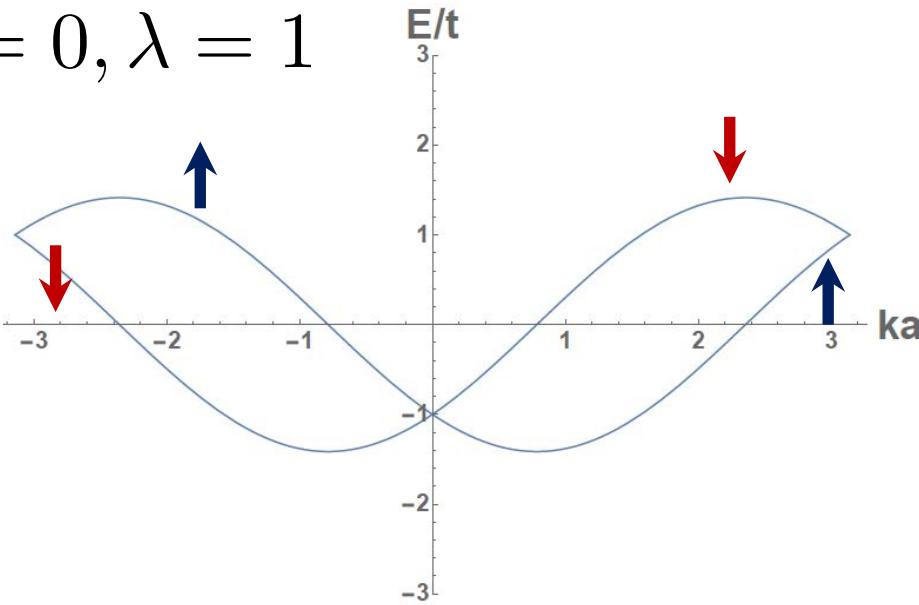
$$h(k) = -\cos(k)\sigma_0 - \lambda \sin(k)\sigma_z - B\sigma_x = -\cos(k)\sigma_0 + \vec{d}(k) \cdot \vec{\sigma}$$

$$d_x(k) = -B \quad d_z(k) = -\lambda \sin(k)$$

$$B = 0, \lambda = 0$$



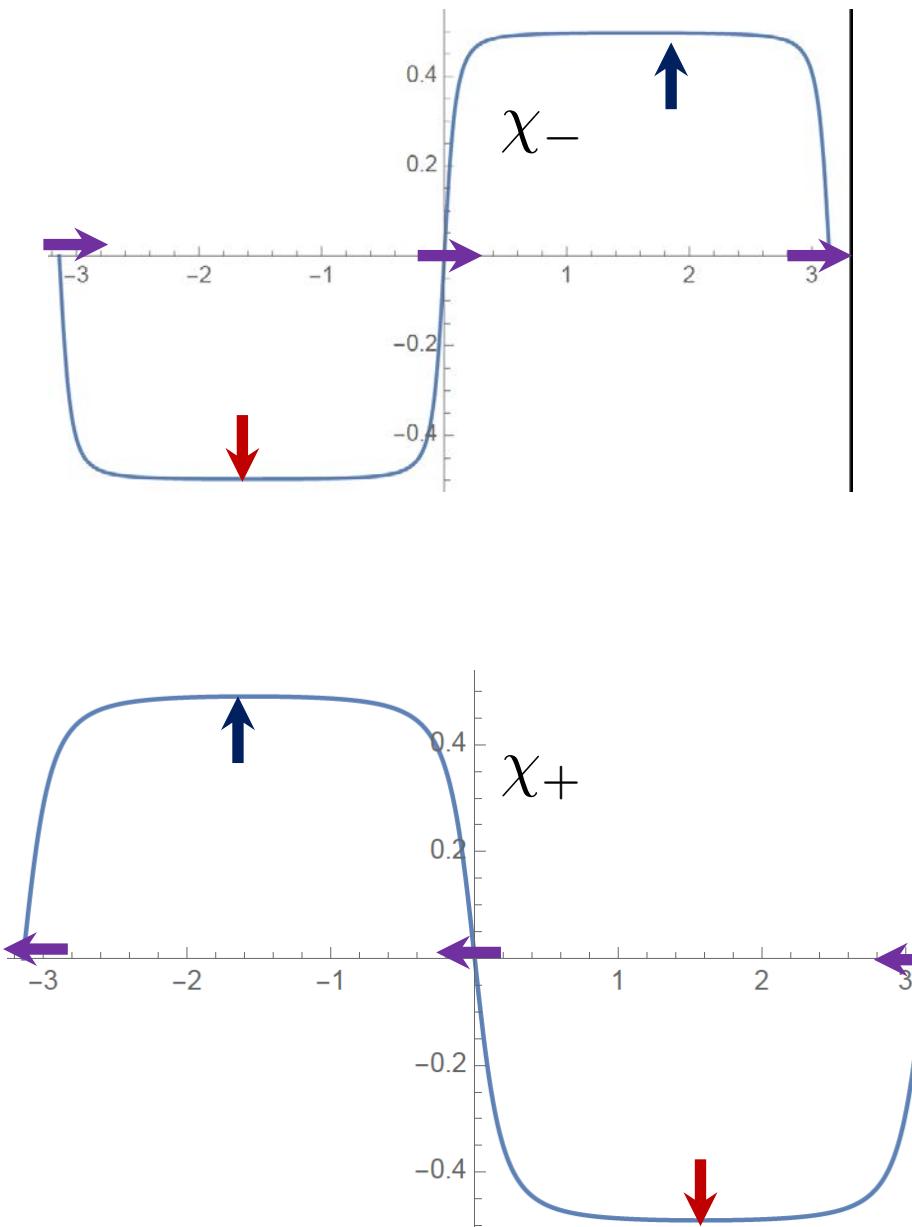
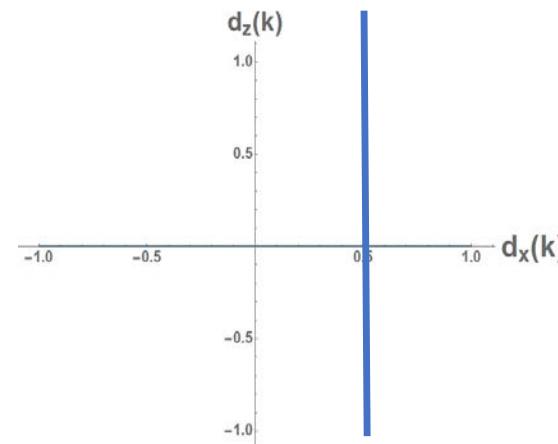
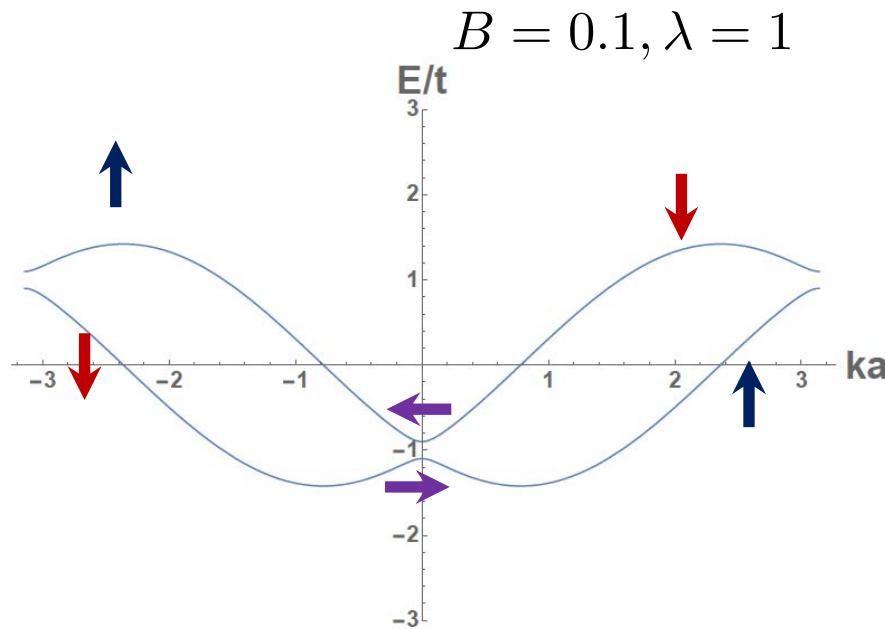
$$B = 0, \lambda = 1$$


 $\chi_-$ 

Eigenvector corresponding  
to lower energy

 $\chi_+$ 

Eigenvector corresponding  
to upper energy



No Winding: hence topologically trivial

# Scope of Lectures and Anchor Points:

## 1. Spin-Orbit Interaction

- atomic SOC
- band SOC: dresselhaus and rashba
- symmetries: time reversal, inversion, mirror

## 2. Berry Phase and Topological Invariant

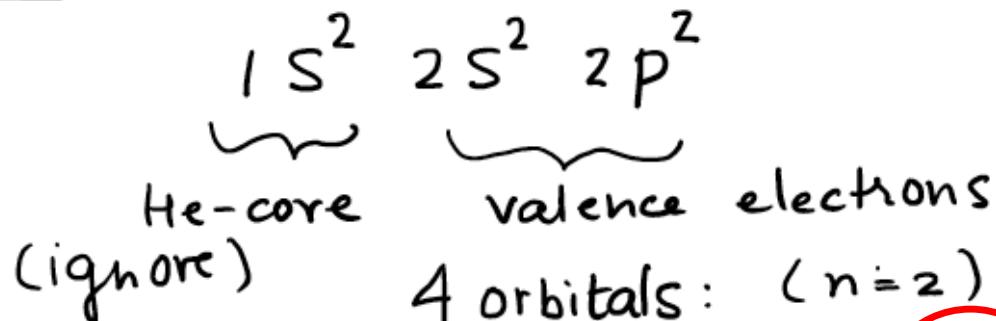
- two level system
- graphene + mass terms

## 3. Hall effects

- integer qhe and chern #

## Graphene

- topological quantum matter
- quantum criticality at Dirac point

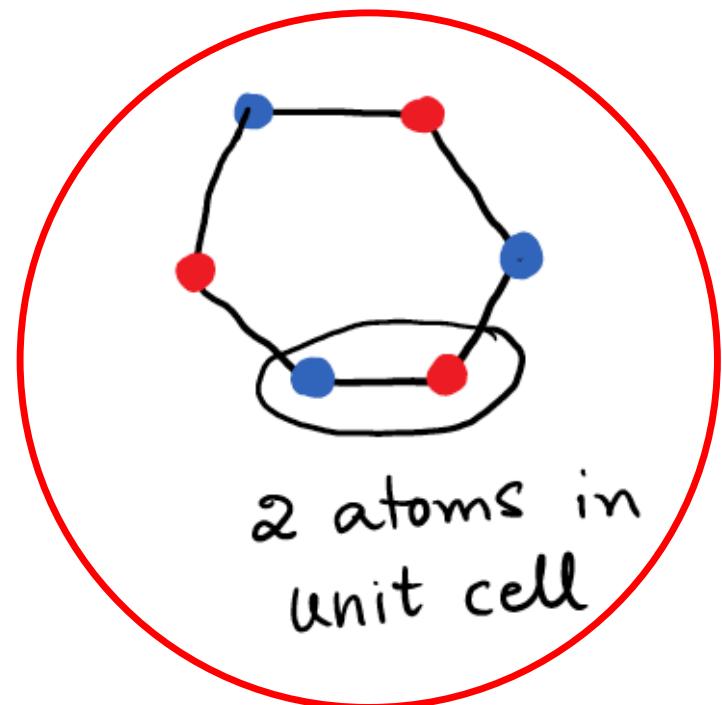
Electronic structureCarbon :  $Z = 6$ 4 orbitals: ( $n=2$ ) $[S, P_x, P_y, P_z]$  $sp^2$  bonding

planar structure

Honeycomb lattice



not a Bravais lattice

(environment as viewed from  
each lattice site is  
not identical)

Aside:

 $2S^2$   $2P^2$  $\rightarrow$  total spin  $S=1$ total orbital  $L=1$ total g.s.  $J=0$

Bands at the chemical potential are derived from  $p_z$  orbitals

Within unit cell:

$$\# \text{ atoms} = 2$$

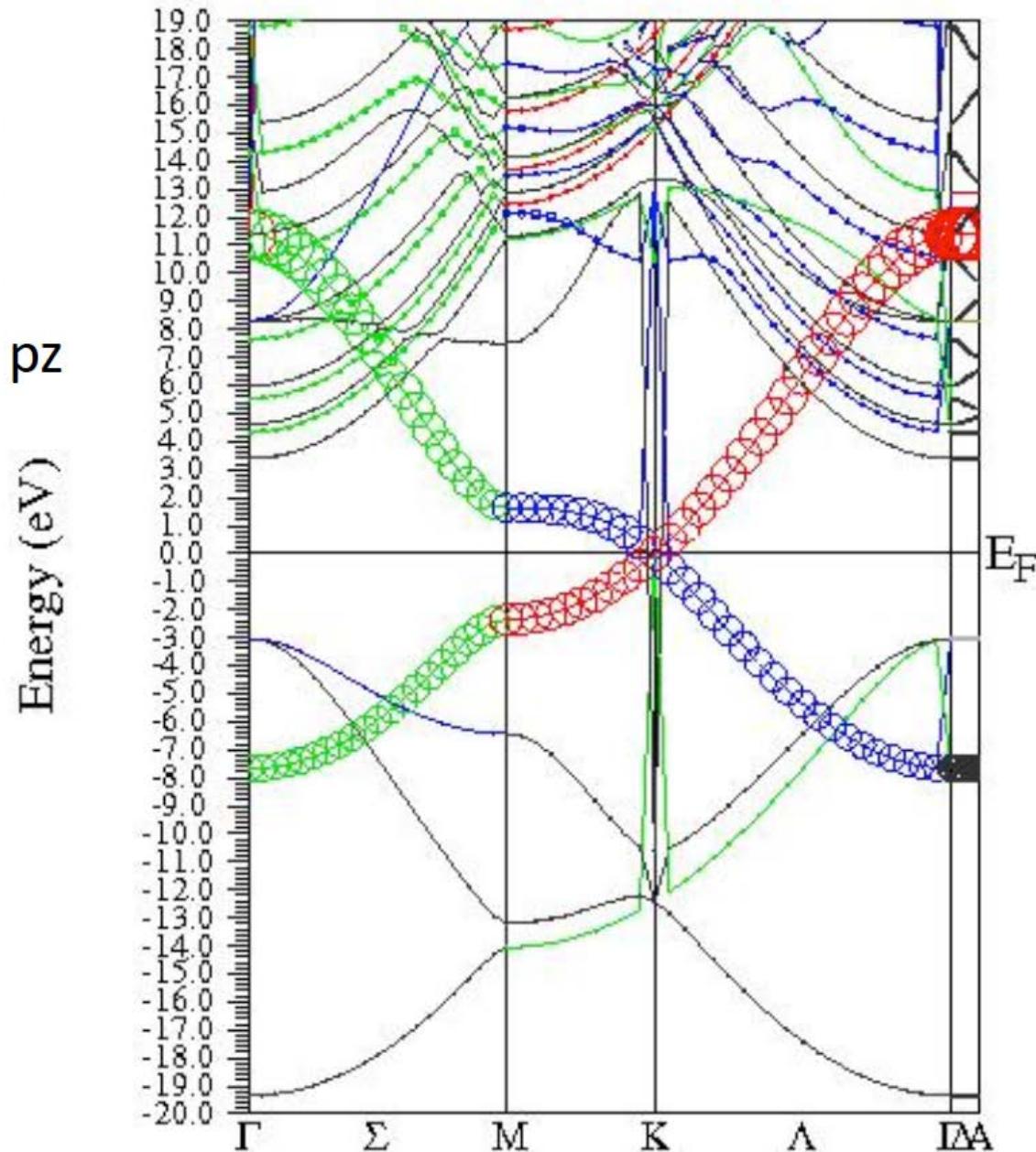
$$\# \text{ orbitals} (4 \times 2) = 8$$

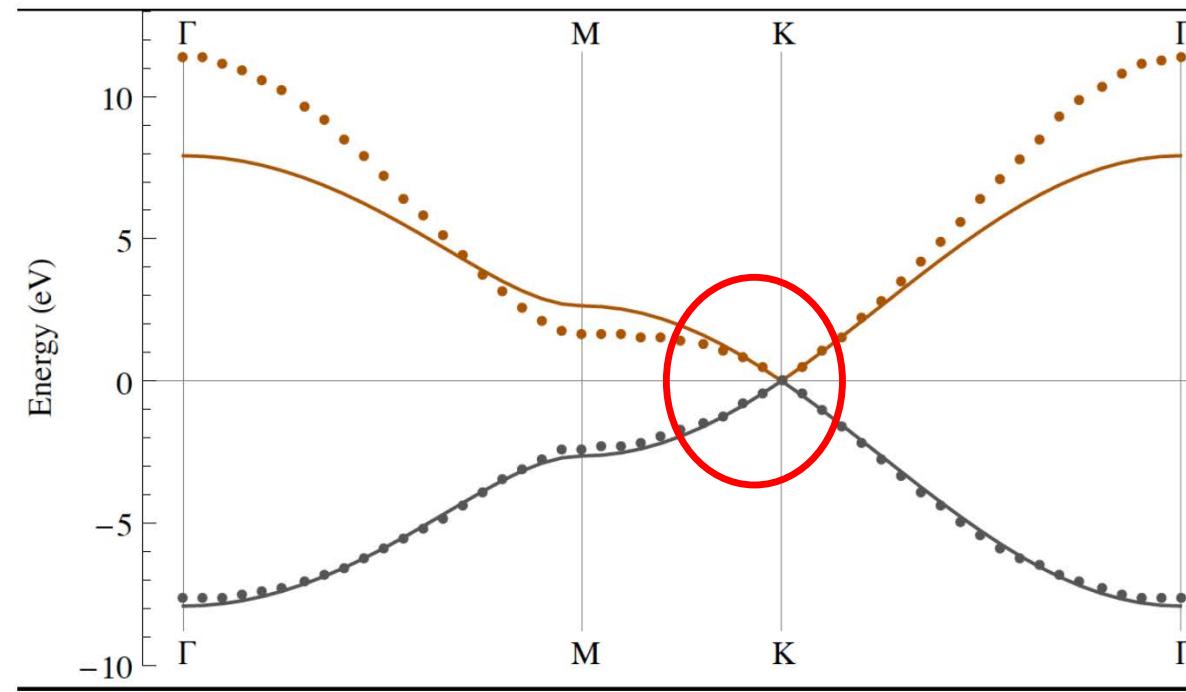
$$\# \text{ electrons} (4 \times 2) = 8$$

$\Rightarrow \frac{1}{2}$  filled

: each orbital can hold 2 electrons (spin up & down)

When the atoms come together they form bands.





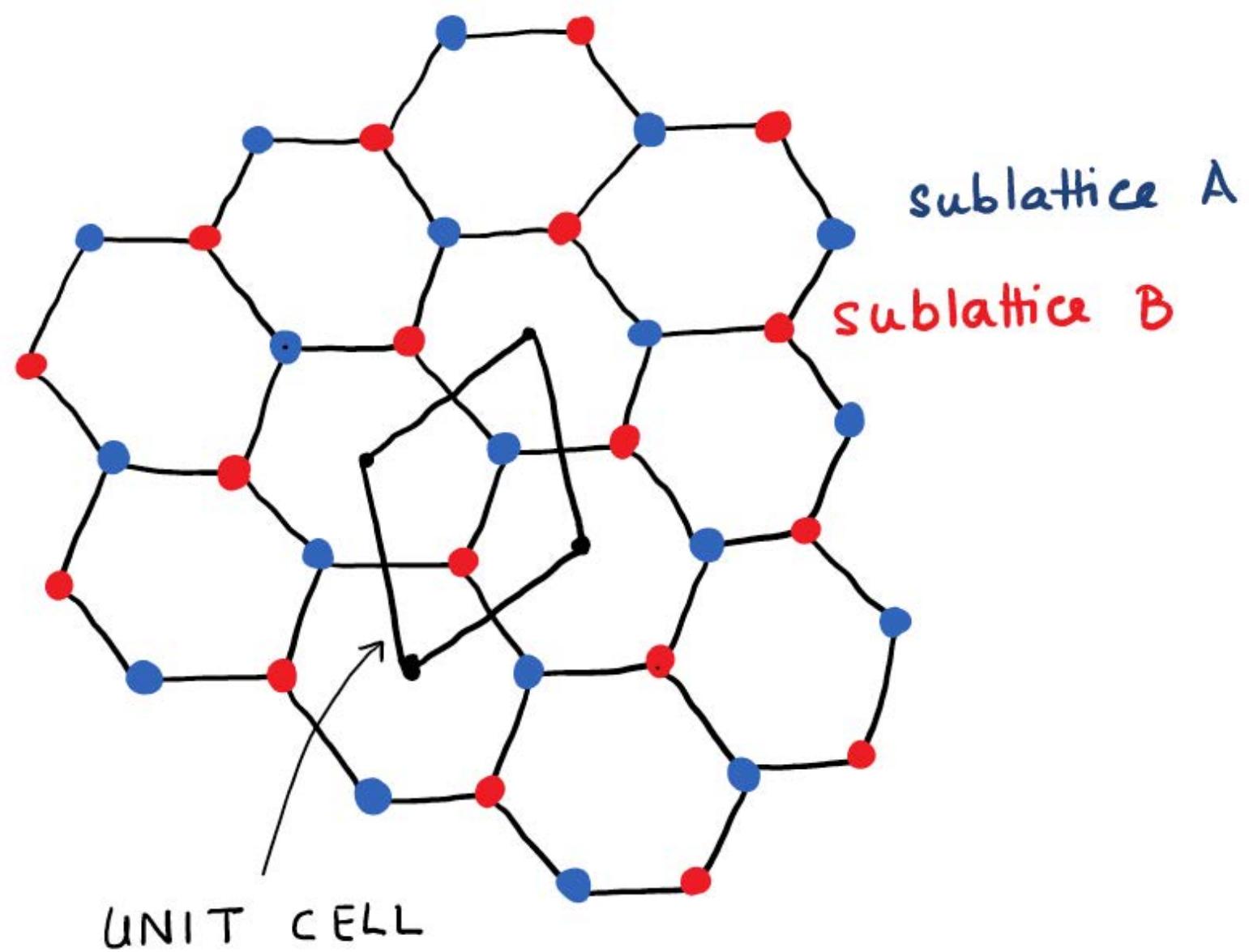
Tightbinding Fits:  $t=2.64$  eV

$$v_F \approx c/350$$

$$\hbar v_F = \frac{3}{2} t a$$

$$\epsilon = \pm t \sqrt{1 + 4 \cos(k_x a) \cos(k_y b) + 4 \cos^2(k_y b)^2}$$

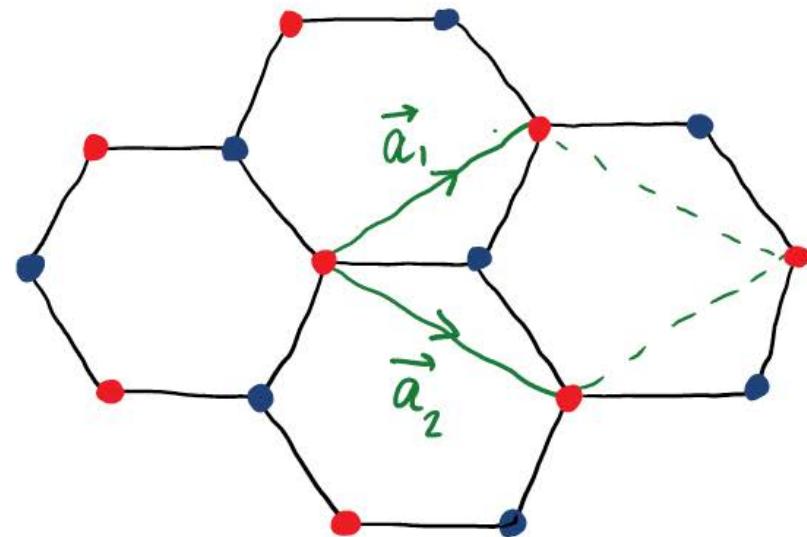
Graphene Material → Honeycomb



When the atoms come together they form bands.

# Real Space Structure

Sunday, April 30, 2017 8:45 PM



$a_0 \equiv a_{c-c} = 1.42 \text{ \AA}^0$   
nearest neighbor  
carbon-carbon

2 atoms in unit cell.

$$\left. \begin{aligned} \vec{a}_1 &= \left( \frac{3}{2} \hat{x} + \frac{\sqrt{3}}{2} \hat{y} \right) a_0 \\ \vec{a}_2 &= \left( \frac{3}{2} \hat{x} - \frac{\sqrt{3}}{2} \hat{y} \right) a_0 \end{aligned} \right\} \begin{aligned} &= a \hat{x} + b \hat{y} \\ &\text{basis vectors} \\ &= a \hat{x} - b \hat{y} \end{aligned}$$

$$a = \frac{3}{2} a_0 \quad b = \frac{\sqrt{3}}{2} a_0$$

Lattice spanned by

$$\vec{R}_{nm} = n \vec{a}_1 + m \vec{a}_2 \quad (n, m \in \mathbb{Z})$$

Momentum Space Structure

Sunday, April 30, 2017 8:55 PM

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_1 = \frac{\pi}{a} \hat{x} + \frac{\pi}{b} \hat{y}$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$= \frac{\pi}{a} \hat{x} - \frac{\pi}{b} \hat{y}$$

For a 2D structure

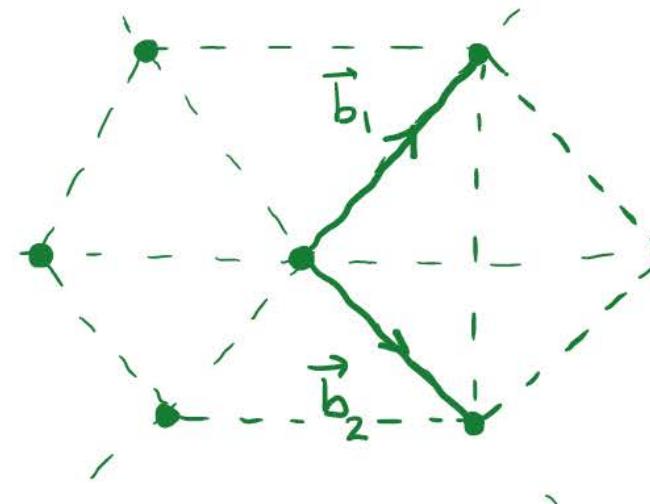
$$\vec{a}_3 = a_3 \hat{z}$$

 $a_3 \rightarrow a_0 \leftarrow c-c$  distance

The magnitude of  $a_3$  cancels in the evaluation of the  $b_i$

Reciprocal lattice  
in momentum space

$$\vec{G} = n\vec{b}_1 + m\vec{b}_2 \quad (n, m \in \mathbb{Z})$$



BRILLOUIN ZONE: UNIT CELL IN MOMENTUM SPACE  
Find region enclosed by bisectors of vectors  
to nearest neighbor points in reciprocal space

Definitions:

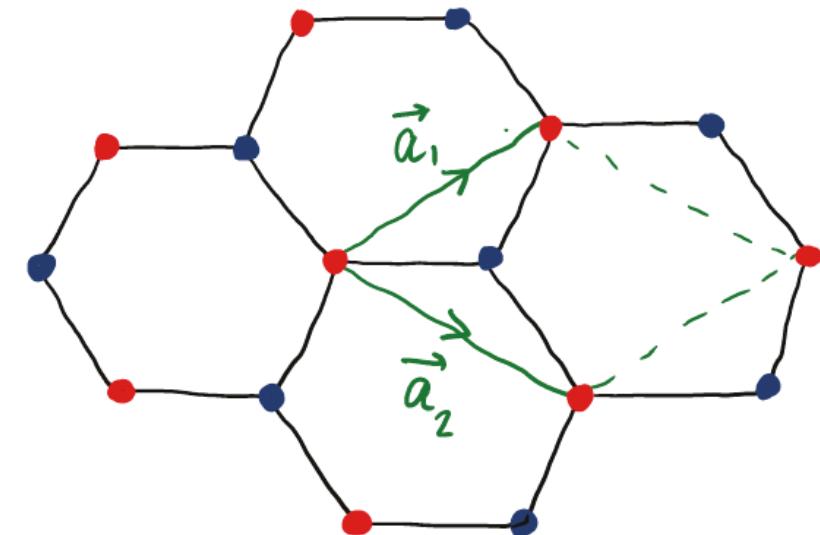
$$a = \frac{3}{2} a_0$$

$$b = \frac{\sqrt{3}}{2} a_0$$

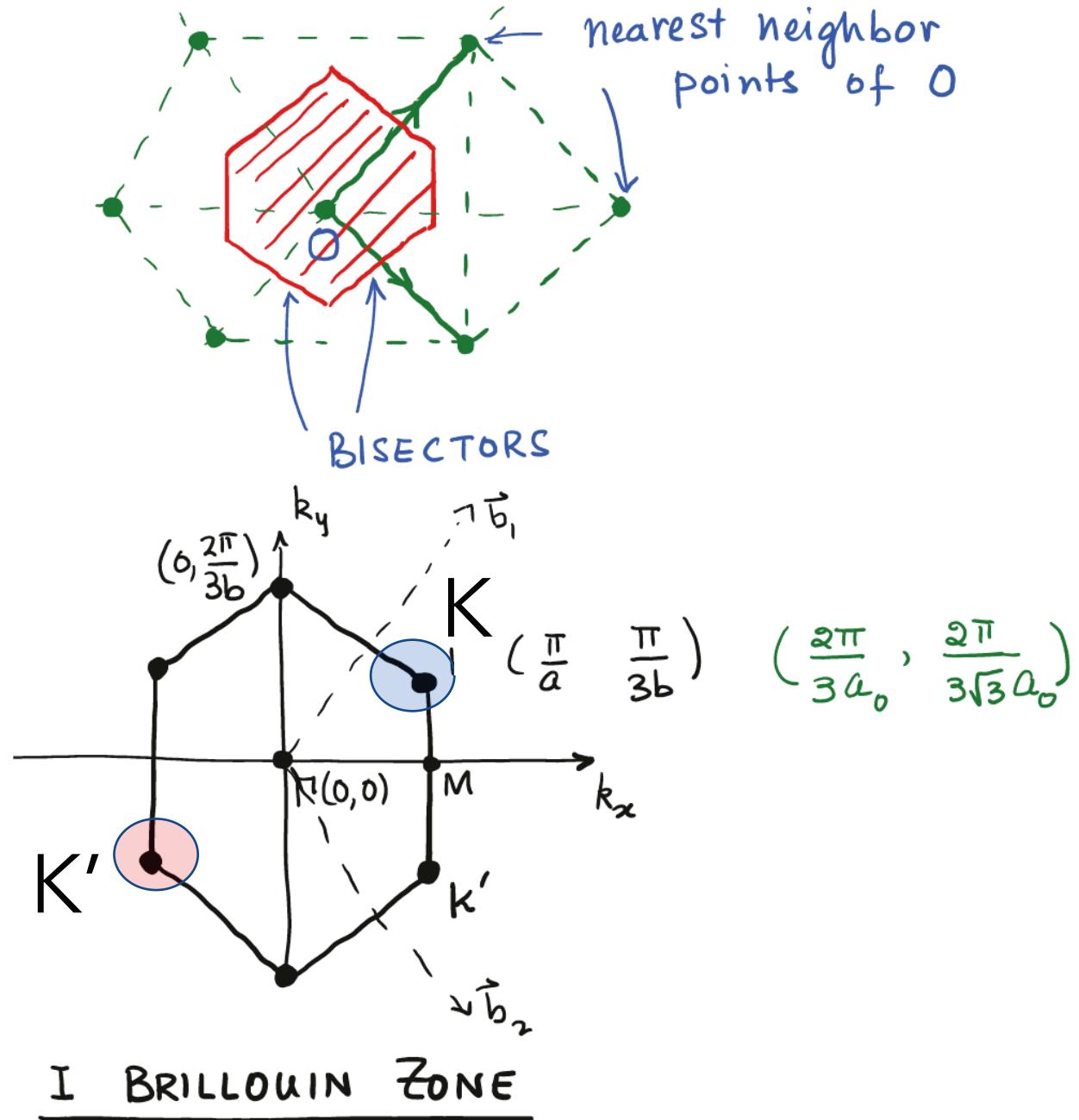
# Real Space Structure

Sunday, April 30, 2017

8:45 PM



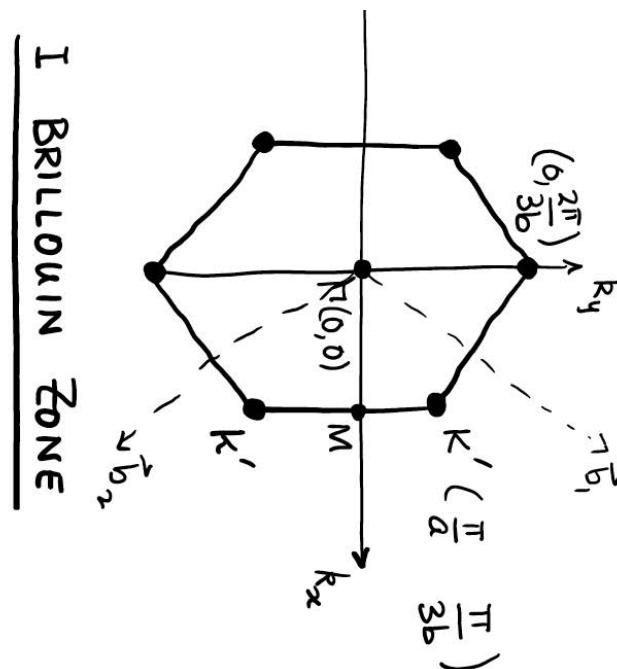
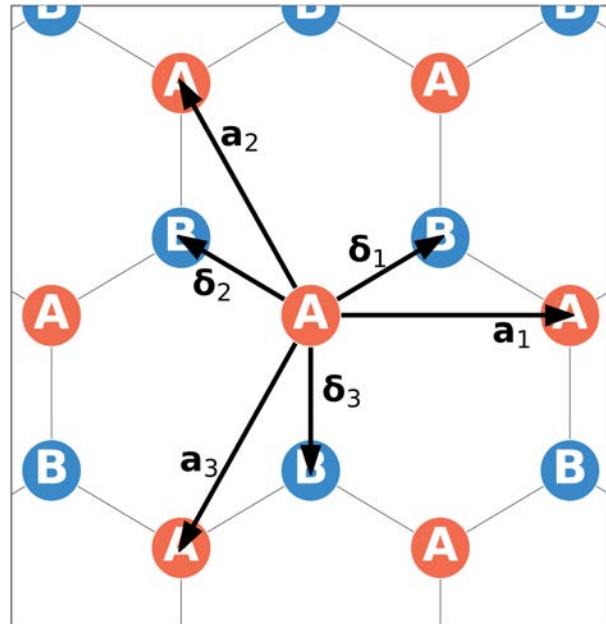
$$\begin{aligned}\vec{a}_1 &= \left( \frac{3}{2} \hat{x} + \frac{\sqrt{3}}{2} \hat{y} \right) a_0 \\ \vec{a}_2 &= \left( \frac{3}{2} \hat{x} - \frac{\sqrt{3}}{2} \hat{y} \right) a_0\end{aligned}$$



# Tight-binding model with nearest neighbor hopping on a honeycomb lattice

$$\mathcal{H} = -t \sum_{\langle i_A, j_B \rangle} \left( c_{i_A \sigma}^\dagger c_{j_B \sigma} + \text{H.c.} \right)$$

$i_A, j_B$  are nearest-neighbor sites, respectively in sublattice A and B (colored red and blue) and  $\sigma$  is a spin index that we suppress



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

Here  $\alpha$  is a sublattice index

$$\mathcal{H} = -t \sum_{\mathbf{k}} \begin{pmatrix} c_{\mathbf{k}A}^\dagger & c_{\mathbf{k}B}^\dagger \end{pmatrix} \underbrace{\begin{pmatrix} 0 & h_{\mathbf{k}} \\ h_{\mathbf{k}}^* & 0 \end{pmatrix}}_{H_{\mathbf{k}}} \begin{pmatrix} c_{\mathbf{k}A} \\ c_{\mathbf{k}B} \end{pmatrix}$$

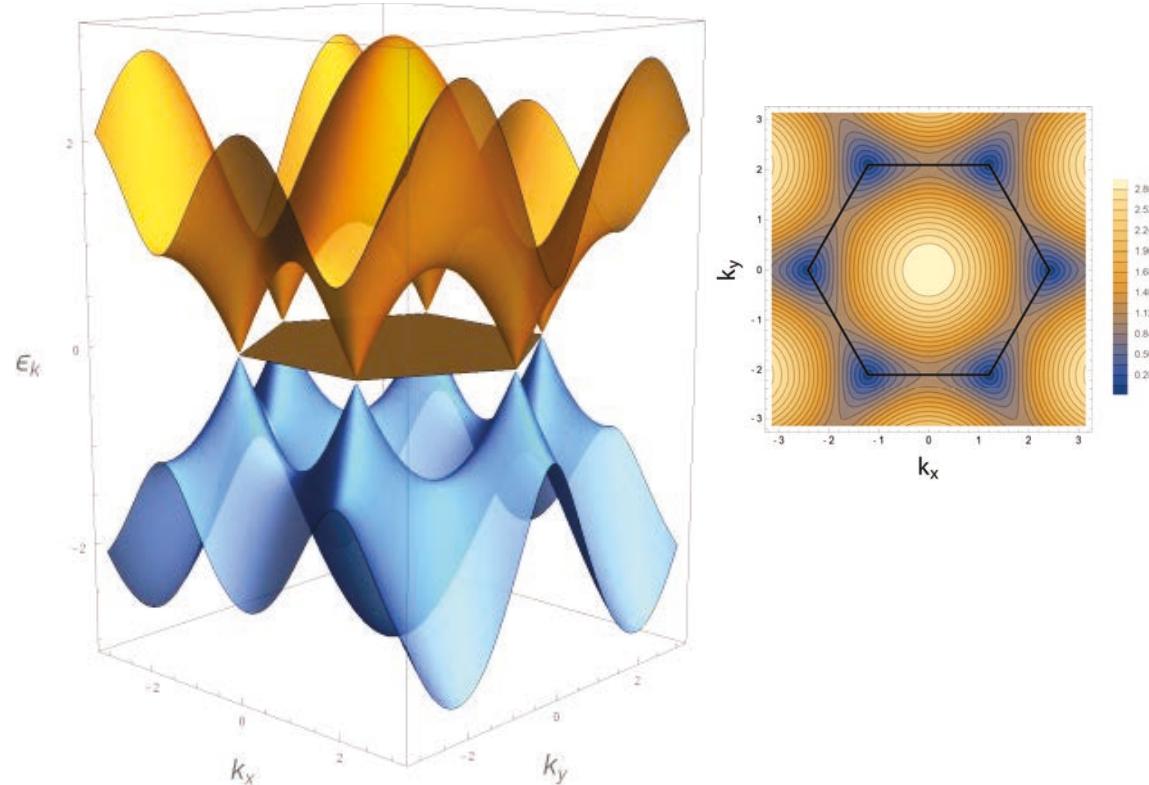
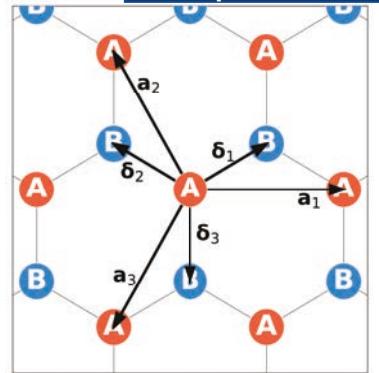
Eigenenergies at momentum  $\mathbf{k}$

$$E_{\pm} = \pm \sqrt{3 + 2 \cos(\sqrt{3}k_y a) + 4 \cos\left(\frac{\sqrt{3}}{2}k_y a\right) \cos\left(\frac{3}{2}k_x a\right)}$$

Dirac nodes at  $\mathbf{K}_{\pm} = \left( \pm \frac{4\pi}{3\sqrt{3}a}, 0 \right)$

$$H_{\mathbf{k}} = \begin{pmatrix} 0 & h_{\mathbf{k}} \\ h_{\mathbf{k}}^* & 0 \end{pmatrix} = \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\tau}$$

$$h_{\mathbf{k}} = -t \sum_j e^{i\mathbf{k} \cdot \delta_j}$$



*My philosophy....*  
choose simplicity and insight over completeness

### Toy Problems:

#### Day 1:

- 1) 1d SOC: spin-momentum locking
- 2) Two level system (Spin  $\frac{1}{2}$  in a magnetic field) and Berry Phase
- 3) Graphene: dirac points protected by inversion and TR

#### Day 2:

- 4) 1d SSH [polyacetylene] model and topological invariant
- 5) Graphene continued:
  - Break inversion: sublattice potential
  - Break TR: Haldane mass

## 2 level system

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e in a magnetic field

$$\mathcal{H} = \vec{\sigma} \cdot \vec{B}$$

$$\left. \begin{array}{l} \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{array} \right\} \text{PAULI MATRICES}$$

$$\vec{\sigma} \cdot \vec{B} = \begin{pmatrix} B_z & B_x - iB_y \\ B_x + iB_y & -B_z \end{pmatrix} = \begin{pmatrix} B_z & B_- \\ B_+ & -B_z \end{pmatrix}$$

$$\sigma_z |\pm\rangle = \pm |\pm\rangle$$

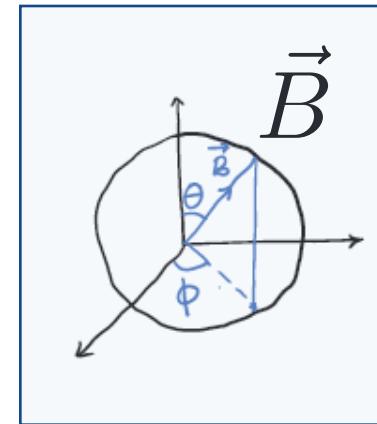
$$\sigma_x |\pm\rangle = |\mp\rangle$$

$$\sigma_y |\pm\rangle = \pm i |\mp\rangle$$

Eigen spectrum:

$$\lambda_1 = +B \quad \chi_+ = \begin{pmatrix} \cos \theta/2 \\ \sin \theta/2 e^{i\phi} \end{pmatrix}$$

$$\lambda_2 = -B \quad \chi_- = \begin{pmatrix} \sin \theta/2 e^{-i\phi} \\ -\cos \theta/2 \end{pmatrix}$$

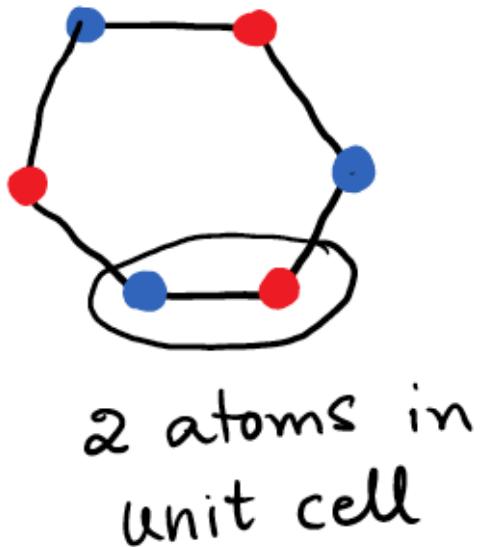


$$\theta = 0 \quad \chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \chi_- = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$$

$$\theta = \pi/2, \phi = 0 \quad \chi_+ = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \chi_- = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

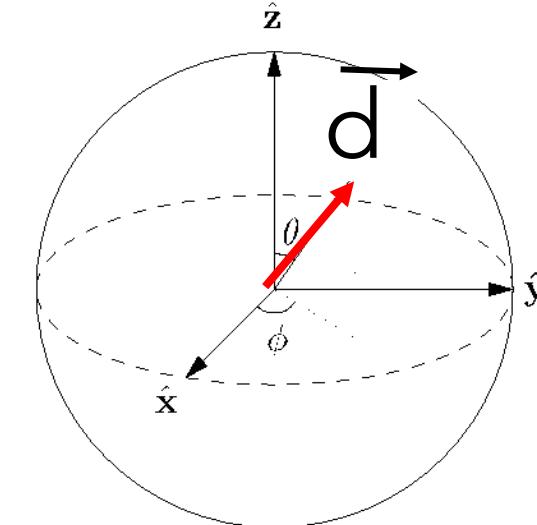
Apply to graphene:

Hamiltonian at momentum  $\mathbf{k}$  can be written in terms of Pauli matrices in sublattice space



$$A = \uparrow$$

$$B = \downarrow$$



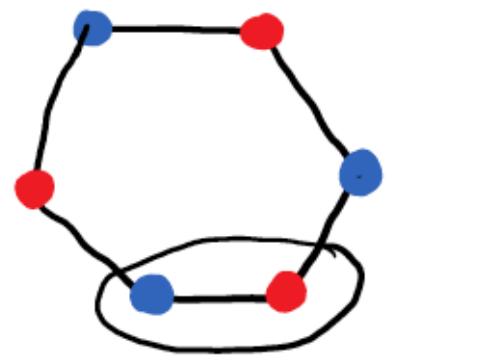
$$H_{\mathbf{k}} = \begin{pmatrix} 0 & h_{\mathbf{k}} \\ h_{\mathbf{k}}^* & 0 \end{pmatrix} = \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\tau}$$

↗

$\tau_i$  for  $i=1,2,3$   
: Pauli matrices  
in sublattice  
basis

Formally,  $\mathbf{d}(\mathbf{k})$  in sublattice basis is analogous to “magnetic field” acting on spin

$$H_{\mathbf{k}} = \begin{pmatrix} 0 & h_{\mathbf{k}} \\ h_{\mathbf{k}}^* & 0 \end{pmatrix} = \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\tau}$$



2 atoms in  
unit cell

$$d_x(\mathbf{k}) = -t \sum_{j=1}^3 \cos(\mathbf{k} \cdot \delta_j)$$

$$d_y(\mathbf{k}) = -t \sum_{j=1}^3 \sin(\mathbf{k} \cdot \delta_j)$$

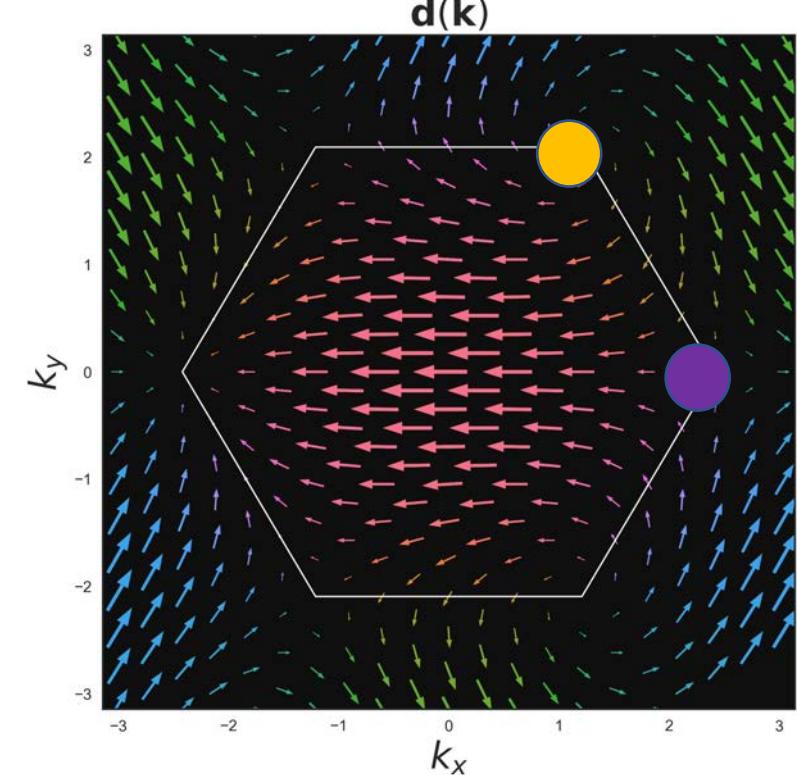
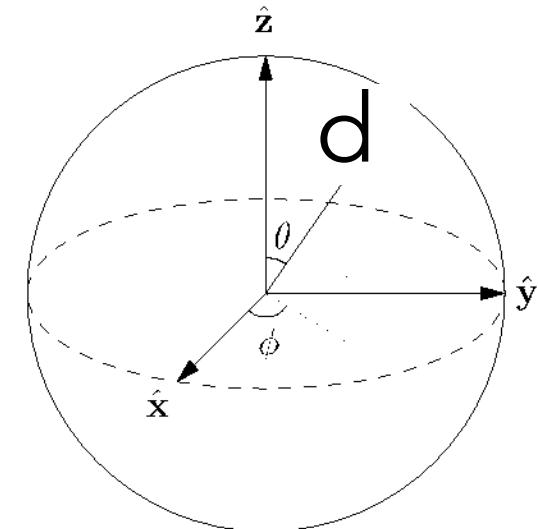
$$d_z(\mathbf{k}) = 0$$

$$\lambda_1 = +|\vec{d}|$$

$$\lambda_2 = -|\vec{d}|$$

$$\chi_+ = \begin{pmatrix} \cos \theta/2 & e^{i\phi} \\ \sin \theta/2 & \end{pmatrix}$$

$$\chi_- = \begin{pmatrix} \sin \theta/2 & e^{-i\phi} \\ -\cos \theta/2 & \end{pmatrix}$$



*My philosophy....*  
choose simplicity and insight over completeness

### Toy Problems:

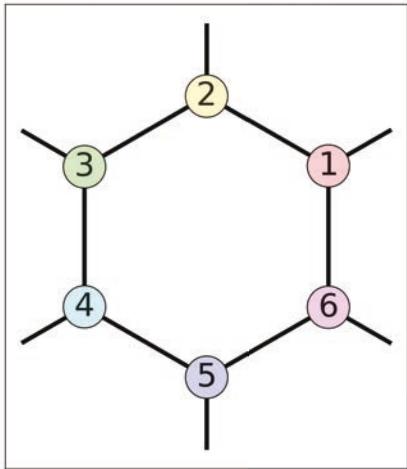
#### Day 1:

- 1) 1d SOC: spin-momentum locking
- 2) Two level system (Spin  $\frac{1}{2}$  in a magnetic field) and Berry Phase
- 3) Graphene: dirac points protected by inversion and TR

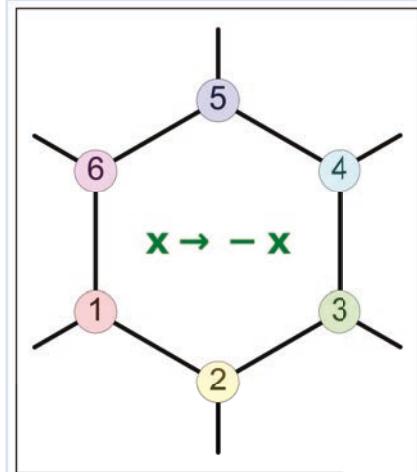
#### Day 2:

- 4) 1d SSH [polyacetylene] model and topological invariant
- 5) Graphene continued:
  - Break inversion: sublattice potential
  - Break TR: Haldane mass

# Dirac points protected by TR and inversion symmetry



## Inversion Symmetry



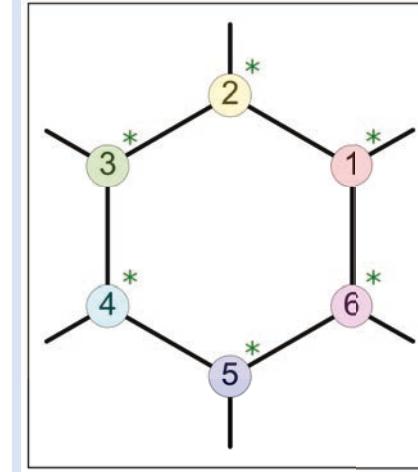
Wavefunction transforms as  
 $\Psi(\mathbf{x}) \rightarrow \Psi(-\mathbf{x})$

- Changes sublattice ( $A \leftrightarrow B$ )

$$H_{\mathbf{k}} = \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\tau}$$

$$d_z(\mathbf{k}) \rightarrow -d_z(-\mathbf{k})$$

## Time Reversal Symmetry



Wavefunction transforms as  
 $\Psi(\mathbf{x}) \rightarrow \Psi(\mathbf{x})^*$

- Complex conjugation
- Does not change sublattice

$$d_z(\mathbf{k}) \rightarrow d_z(-\mathbf{k})$$

- With *both* inversion and time-reversal symmetry,  $d_z(\mathbf{k}) = 0$   
 → Zeros of  $\mathbf{d}(\mathbf{k})$  exist (Dirac points)

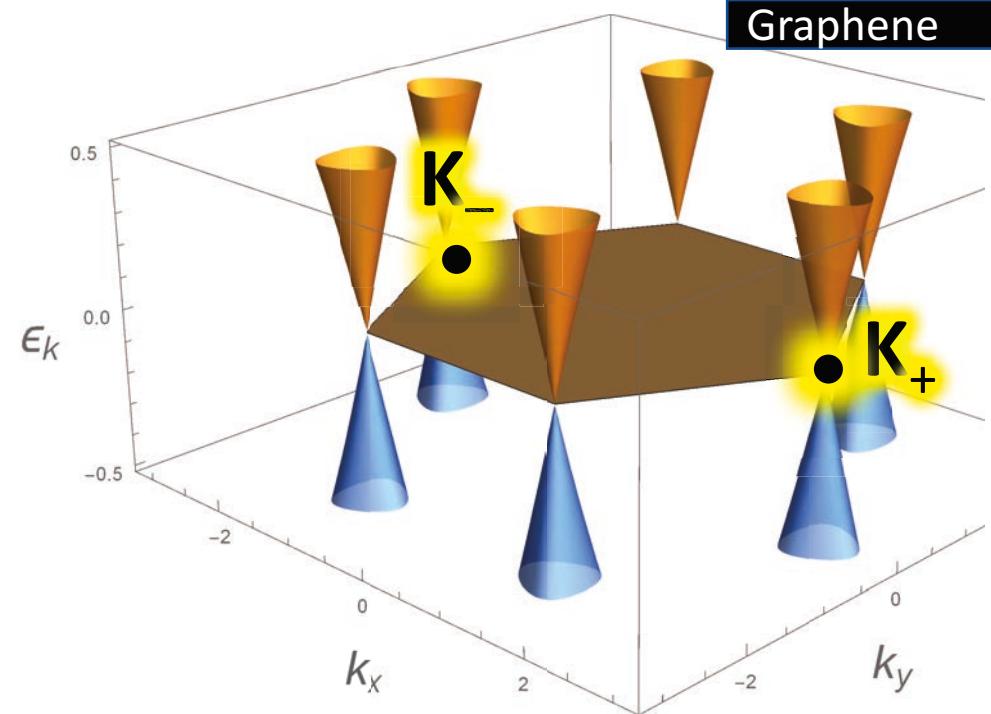
Proof: TR and I protect Dirac points

The “Full” tight binding Hamiltonian can be expanded around each “valley”

- Dirac nodes at  $\mathbf{K}_{\pm} = \left( \pm \frac{4\pi}{3\sqrt{3}a}, 0 \right)$
- Keep only low energy states
- Expand  $H_{\mathbf{k}}$  near  $\mathbf{K}_+$  and  $\mathbf{K}_-$

$$h_{\mathbf{k}} = -t \sum_j e^{i\mathbf{k}\cdot\delta_j}$$

$$\mathcal{H} \approx \sum_{\mathbf{q}} \begin{pmatrix} c_{\mathbf{K}_+ + \mathbf{q}, A}^\dagger, & c_{\mathbf{K}_+ + \mathbf{q}, B}^\dagger, & c_{\mathbf{K}_- + \mathbf{q}, A}^\dagger, & c_{\mathbf{K}_- + \mathbf{q}, B}^\dagger \end{pmatrix} \begin{pmatrix} 0 & h_{\mathbf{K}_+ + \mathbf{q}} & 0 & 0 \\ h_{\mathbf{K}_+ + \mathbf{q}}^* & 0 & 0 & 0 \\ 0 & 0 & 0 & h_{\mathbf{K}_- + \mathbf{q}} \\ 0 & 0 & h_{\mathbf{K}_- + \mathbf{q}}^* & 0 \end{pmatrix} \begin{pmatrix} c_{\mathbf{K}_+ + \mathbf{q}, A} \\ c_{\mathbf{K}_+ + \mathbf{q}, B} \\ c_{\mathbf{K}_- + \mathbf{q}, A} \\ c_{\mathbf{K}_- + \mathbf{q}, B} \end{pmatrix}$$



Two independent “valleys” with Dirac cones

$$\mathcal{H} \approx \frac{3}{2}ta \sum_{\mathbf{q}} \left( c_{\mathbf{K}_+ + \mathbf{q}, A}^\dagger, c_{\mathbf{K}_+ + \mathbf{q}, B}^\dagger \right) \begin{pmatrix} 0 & q_x - iq_y \\ q_x + iq_y & 0 \end{pmatrix} \begin{pmatrix} c_{\mathbf{K}_+ + \mathbf{q}, A} \\ c_{\mathbf{K}_+ + \mathbf{q}, B} \end{pmatrix}$$

$$+ \left( c_{\mathbf{K}_- + \mathbf{q}, A}^\dagger, c_{\mathbf{K}_- + \mathbf{q}, B}^\dagger \right) \begin{pmatrix} 0 & -q_x - iq_y \\ -q_x + iq_y & 0 \end{pmatrix} \begin{pmatrix} c_{\mathbf{K}_- + \mathbf{q}, A} \\ c_{\mathbf{K}_- + \mathbf{q}, B} \end{pmatrix}$$

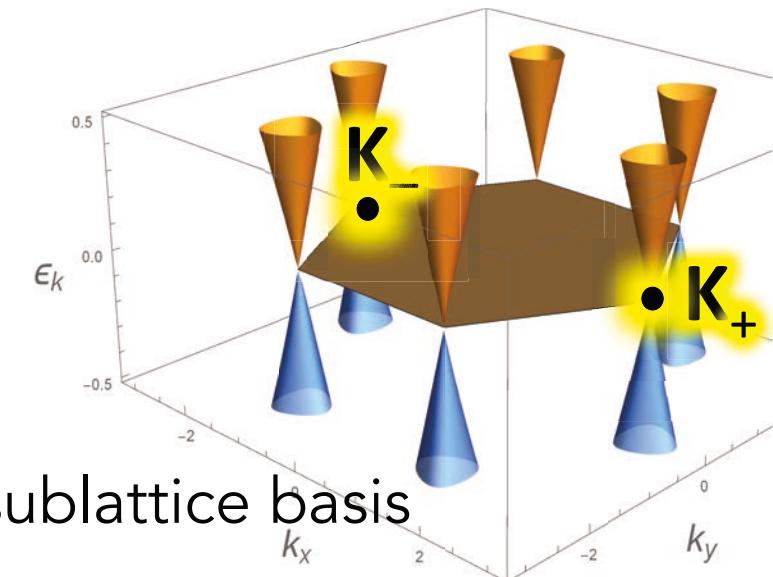
Each block can be written in terms of Pauli matrices in sublattice basis

$$h_{K_+ + q} = \frac{3}{2}ta(q_x \tau_x + q_y \tau_y) = \vec{d}_+(\vec{q}) \cdot \vec{\tau}$$

$$h_{K_- + q} = \frac{3}{2}ta(-q_x \tau_x + q_y \tau_y) = \vec{d}_-(\vec{q}) \cdot \vec{\tau}$$

Include valley index

$$H_q = \hbar v_F (q_x \chi_z \tau_x - q_y \tau_y)$$



$\tau_i$  for  $i=1,2,3$

: Pauli matrices in sublattice basis

$\chi_i$  for  $i=1,2,3$

: Pauli matrices in valley basis

By expanding the honeycomb band structure around the points  $\vec{K}_+$  and  $\vec{K}_-$  we get the following two Dirac Ham.

$$\frac{\text{Around } \vec{K}_+}{h(\vec{k}_+ + \vec{q})} = q_x \tau_x + q_y \tau_y \quad - (1) \quad = \begin{pmatrix} 0 & q_x - iq_y \\ q_x + iq_y & 0 \end{pmatrix}$$

$$\frac{\text{Around } \vec{K}_-}{h(\vec{k}_- + \vec{q})} = h(-\vec{k}_+ + \vec{q}) = -q_x \tau_x + q_y \tau_y \quad - (2) \quad = \begin{pmatrix} 0 & -q_x - iq_y \\ -q_x + iq_y & 0 \end{pmatrix}$$

Time reversal:

(see notes)

$$\underbrace{T h(\vec{k}) T^{-1}}_{\parallel} = h(-\vec{k})$$

$[h(\vec{k})]^*$

for general  $\vec{k}$

$$\Rightarrow [h(\vec{k})]^* = h(-\vec{k})$$

Check

Consider the point  $K_+$ 

$$\underbrace{[h(\vec{K}_+ + \vec{q})]}_{\parallel}^* = h(-\vec{K}_+ - \vec{q})$$

From(2)

From (1)

$$q_x \tau_x - q_y \tau_y \quad \text{Smiley Face} \quad q_x \tau_x - q_y \tau_y \quad \text{--- (3)}$$

$\Rightarrow$  Once we know the form of  $h(\vec{k})$  near  $\vec{K}_+$   
 TR fixes the form of  $h(\vec{k})$  at  $\vec{K}_-$

From (3)

$$h(\vec{K}_- + \vec{q}) = h(-\vec{K}_+ + \vec{q}) = -q_x \tau_x + q_y \tau_y$$

(4)

What kind of term can we add to  $h(\vec{R})$   
so that it opens a gap in the spectrum  
but preserves TR symmetry.

Consider:

$$h(\vec{K}_+ + \vec{q}) = q_x \tau_x + q_y \tau_y + m \sigma_z$$

$$[h(\vec{K}_+ + \vec{q})]^* = q_x \tau_x - q_y \tau_y + m \sigma_z \quad \checkmark$$

||

$$\xrightarrow{\text{TR}} h(-\vec{K}_+ - \vec{q}) = q_x \tau_x - q_y \tau_y + m \sigma_z$$

from (4)

↓ Preserves TR  
Breaks I

Inversion symmetry

$$I : (x, y) \rightarrow (-x, -y)$$

$$\left\{ I C_{i,A} I^{-1} = C_{-i,B} \right.$$

$$\left[ I C_{i,B} I^{-1} = C_{-i,A} \right]$$

$$\Rightarrow I C_{i,\alpha} I^{-1} = \tilde{\sigma}_{\alpha, \beta}^x C_{-i\beta}$$

$$I H I^{-1} = H$$

$$\Rightarrow h(\vec{r}) = \sigma_x h(-\vec{r}) \sigma_x$$

Dirac points are protected when both TR and Inv are present

Under TR

$$h(\vec{k}) = [h(-\vec{k})]^* \quad (1)$$

Under I

$$h(\vec{k}) = \tau_x h(-\vec{k}) \tau_x \quad (2)$$

When both I and T are present

$$\begin{aligned} [h(-\vec{k})]^* &= \tau_x h(-\vec{k}) \tau_x \\ \Rightarrow h(\vec{k}) &= \tau_x h^*(\vec{k}) \tau_x \end{aligned}$$

Now consider a generic 2-level Hamiltonian

$$H = \vec{d}(\vec{k}) \cdot \vec{\tau} + \epsilon(\vec{k}) \tau_0$$

T & I  $\Rightarrow$

$$\begin{aligned} d_i \tau_i + \epsilon &= \tau_x (d_i \tau_i + \epsilon)^* \tau_x \\ &= [d_x \tau_x \tau_x \tau_x + d_y \tau_x \tau_y \tau_x \\ &\quad + d_z \tau_x \tau_z \tau_x + \epsilon \tau_x \tau_x]^* \\ \text{Pauli matrices} \quad \sigma_x^2 &= \sigma_y^2 = \sigma_z^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ \{\sigma_\mu, \sigma_\nu\} &= 0 \\ \text{anti commute} &= (d_x \tau_x - d_y \tau_y - d_z \tau_z + \epsilon) \\ &= (d_x \tau_x + d_y \tau_y - d_z \tau_z + \epsilon) \\ \tau_y^* &= -\tau_y \end{aligned}$$

Thus the combined action of TR and I gives:

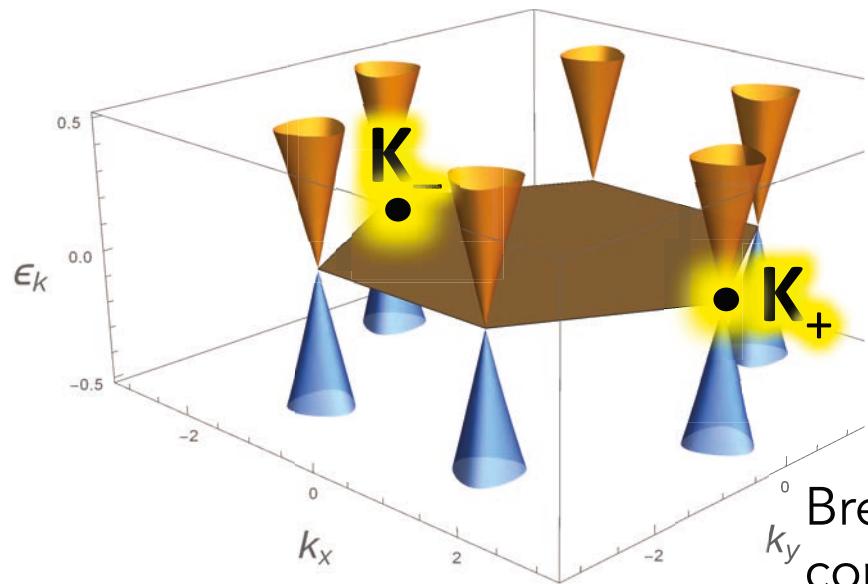
$$d_z(\vec{k}) = -d_z(\vec{k}) = 0$$

around Dirac points.

$$H = \sum_q \begin{pmatrix} c_{\mathbf{K}_+ + \mathbf{q}, A}^+ & c_{\mathbf{K}_+ + \mathbf{q}, B}^+ & c_{\mathbf{K}_- + \mathbf{q}, A}^+ & c_{\mathbf{K}_- + \mathbf{q}, B}^+ \end{pmatrix} \begin{pmatrix} 0 & h_q & 0 & 0 \\ h_q^* & 0 & 0 & 0 \\ 0 & 0 & 0 & h_q^* \\ 0 & 0 & h_q & 0 \end{pmatrix} \begin{pmatrix} c_{\mathbf{K}_+ + \mathbf{q}, A} \\ c_{\mathbf{K}_+ + \mathbf{q}, B} \\ c_{\mathbf{K}_- + \mathbf{q}, A} \\ c_{\mathbf{K}_- + \mathbf{q}, B} \end{pmatrix}$$

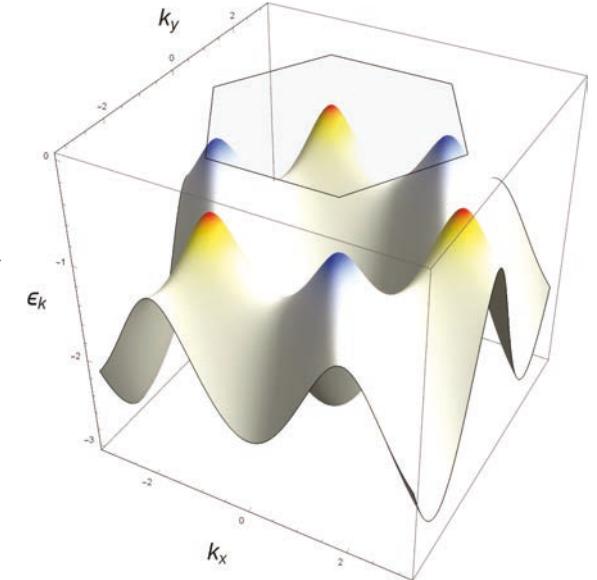
Graphene

where  $h_{\mathbf{q}} = \frac{3ta}{2}(-q_x + i q_y)$

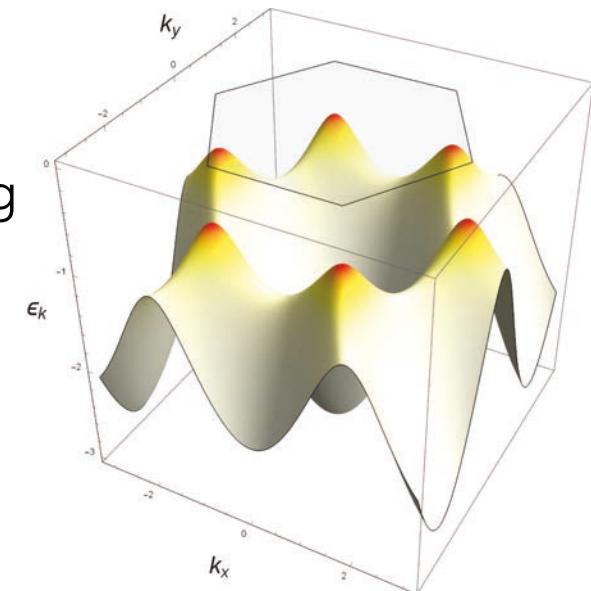


Dirac points  
protected by  
inversion and time  
reversal symmetry

Break inversion  
Sublattice potential



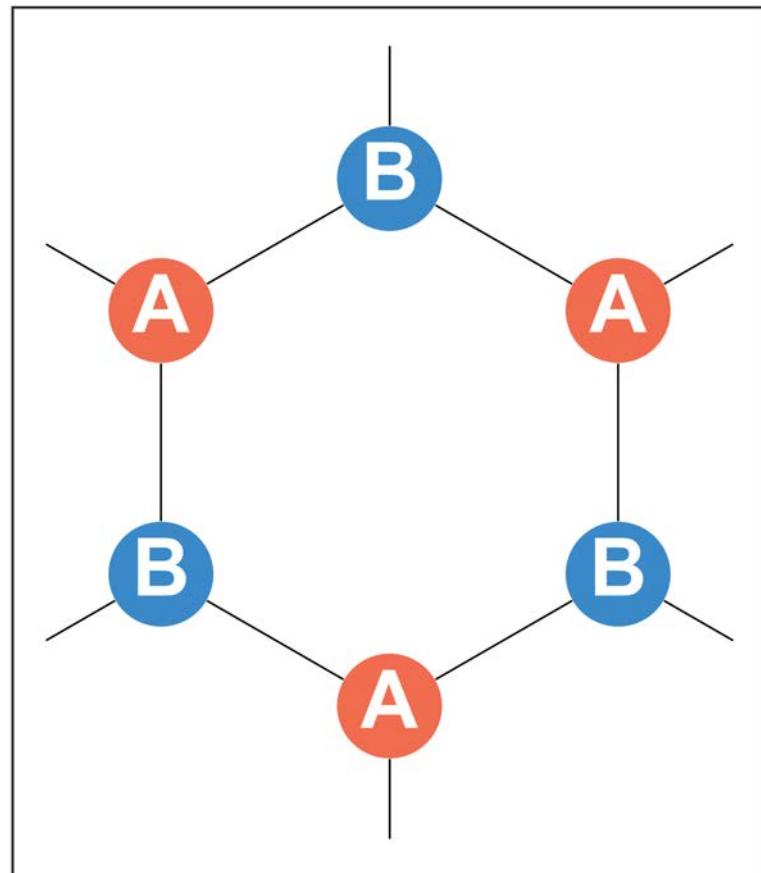
Break TR  
complex nn hopping



(Color: Berry curvature = Berry flux density)

# Introduce Dirac mass by breaking symmetry

To introduce “mass” to the Dirac cones,  
need to break either inversion or time-reversal symmetry



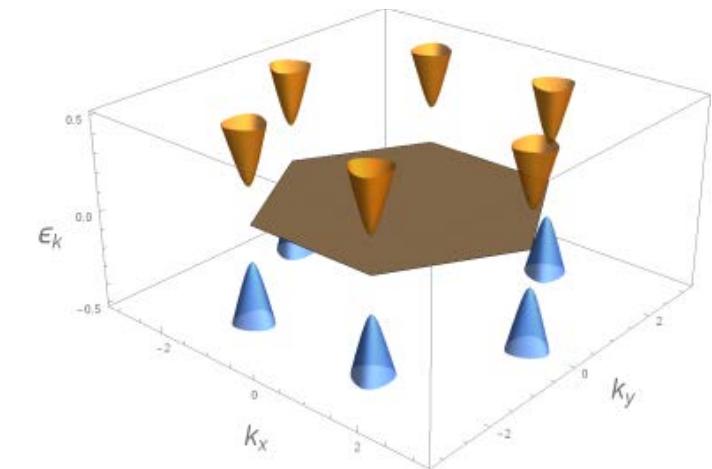
Potential energy difference  
between sublattices

$$\mathcal{H}_{AB} = m_{AB} \left( \sum_{i_A} c_{i_A}^\dagger c_{i_A} - \sum_{i_B} c_{i_B}^\dagger c_{i_B} \right)$$

breaks inversion (and  $C_6$   
rotation, etc.).

This introduces uniform  $d_z(\mathbf{k})$ .

$$d_z(\mathbf{k}) = m_{AB}$$



## Graphene

$$H = \sum_q$$

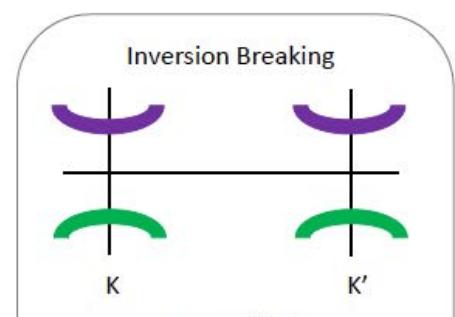
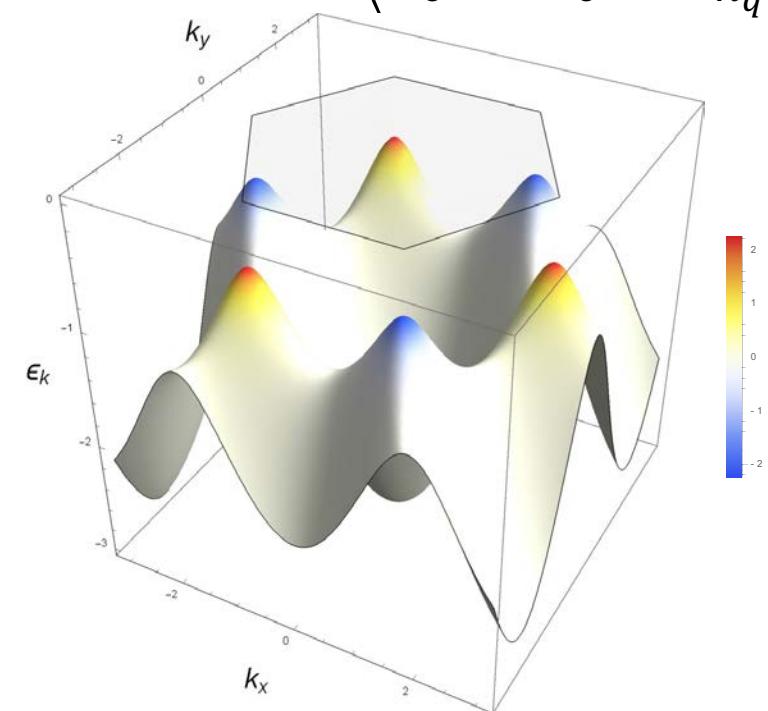
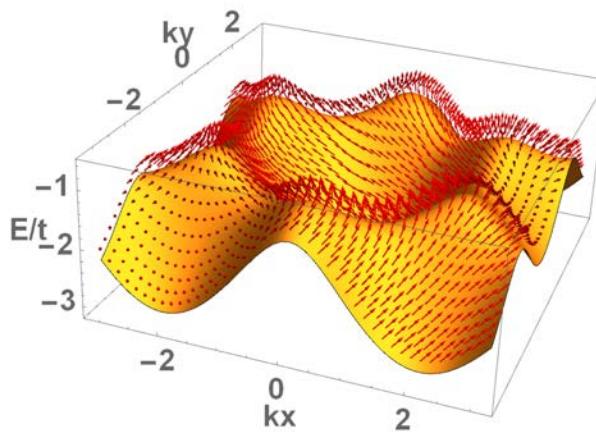
$$\begin{pmatrix} c_{\mathbf{K}_+ + \mathbf{q}, A}^+ & c_{\mathbf{K}_+ + \mathbf{q}, B}^+ & c_{\mathbf{K}_- + \mathbf{q}, A}^+ & c_{\mathbf{K}_- + \mathbf{q}, B}^+ \end{pmatrix} \begin{pmatrix} 0 & h_q & 0 & 0 \\ h_q^* & 0 & 0 & 0 \\ 0 & 0 & 0 & h_q^* \\ 0 & 0 & h_q & 0 \end{pmatrix} \begin{pmatrix} c_{\mathbf{K}_+ + \mathbf{q}, A} \\ c_{\mathbf{K}_+ + \mathbf{q}, B} \\ c_{\mathbf{K}_- + \mathbf{q}, A} \\ c_{\mathbf{K}_- + \mathbf{q}, B} \end{pmatrix}$$

where  $h_{\mathbf{q}} = \frac{3ta}{2}(-q_x + i q_y)$

With sublattice potential

$$H = \sum_q$$

$$\begin{pmatrix} c_{\mathbf{K}_+ + \mathbf{q}, A}^+ & c_{\mathbf{K}_+ + \mathbf{q}, B}^+ & c_{\mathbf{K}_- + \mathbf{q}, A}^+ & c_{\mathbf{K}_- + \mathbf{q}, B}^+ \end{pmatrix} \begin{pmatrix} m_{AB} & h_q & 0 & 0 \\ h_q^* & -m_{AB} & 0 & 0 \\ 0 & 0 & m_{AB} & h_q^* \\ 0 & 0 & h_q & -m_{AB} \end{pmatrix} \begin{pmatrix} c_{\mathbf{K}_+ + \mathbf{q}, A} \\ c_{\mathbf{K}_+ + \mathbf{q}, B} \\ c_{\mathbf{K}_- + \mathbf{q}, A} \\ c_{\mathbf{K}_- + \mathbf{q}, B} \end{pmatrix}$$

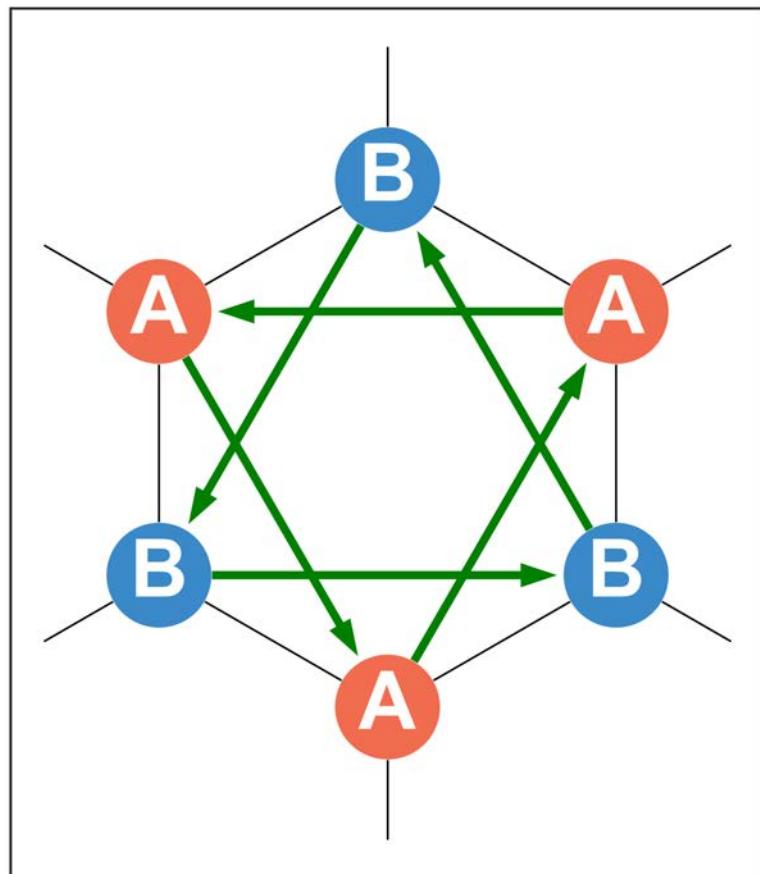


# Introduce Dirac mass by breaking symmetry

To introduce “mass” to the Dirac cones,  
need to break either inversion or time-reversal symmetry

Next nearest neighbor hopping with  
imaginary amplitude

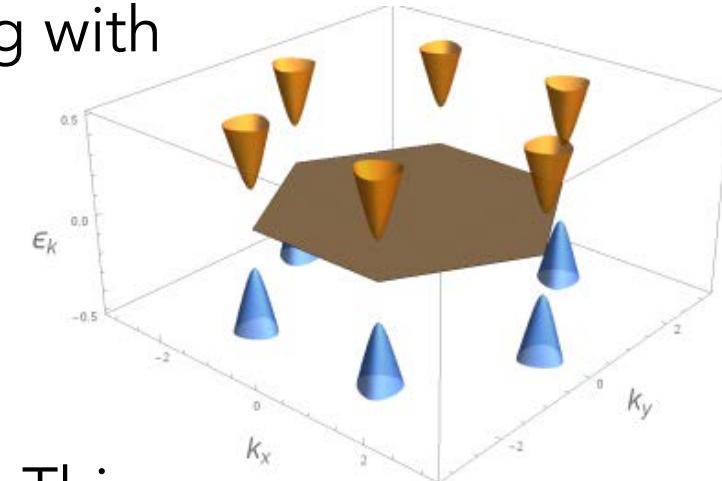
$$\mathcal{H}_H = i\lambda_H \sum_{\langle\langle i,j \rangle\rangle} c_i^\dagger c_j + \text{H.c.}$$



breaks time-reversal symmetry. This  
introduces valley dependent  $d_z(\mathbf{k})$ .

$$d_z(\mathbf{k}) = m_H \varepsilon_z \tau_z$$

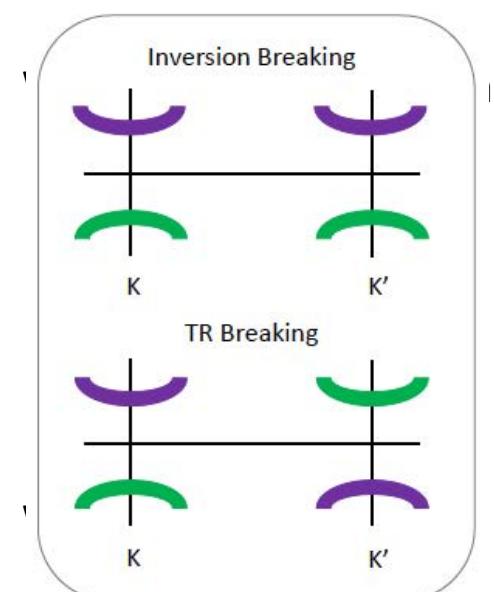
$$m_H = 3\sqrt{3}\lambda_H$$



$$H = \sum_q (c_{\mathbf{K}_+ + \mathbf{q}, A}^+ c_{\mathbf{K}_+ + \mathbf{q}, B}^+ c_{\mathbf{K}_- + \mathbf{q}, A}^+ c_{\mathbf{K}_- + \mathbf{q}, B}^+) \begin{pmatrix} 0 & h_q & 0 & 0 \\ h_q^* & 0 & 0 & 0 \\ 0 & 0 & 0 & h_q^* \\ 0 & 0 & h_q & 0 \end{pmatrix} \begin{pmatrix} c_{\mathbf{K}_+ + \mathbf{q}, A} \\ c_{\mathbf{K}_+ + \mathbf{q}, B} \\ c_{\mathbf{K}_- + \mathbf{q}, A} \\ c_{\mathbf{K}_- + \mathbf{q}, B} \end{pmatrix}$$

Graphene  
where  $h_{\mathbf{q}} = \frac{3ta}{2}(-q_x + i q_y)$

$$H = \sum_q (c_{\mathbf{K}_+ + \mathbf{q}, A}^+ c_{\mathbf{K}_+ + \mathbf{q}, B}^+ c_{\mathbf{K}_- + \mathbf{q}, A}^+ c_{\mathbf{K}_- + \mathbf{q}, B}^+) \begin{pmatrix} m_{AB} & h_q & 0 & 0 \\ h_q^* & -m_{AB} & 0 & 0 \\ 0 & 0 & m_{AB} & h_q^* \\ 0 & 0 & h_q & -m_{AB} \end{pmatrix} \begin{pmatrix} c_{\mathbf{K}_+ + \mathbf{q}, A} \\ c_{\mathbf{K}_+ + \mathbf{q}, B} \\ c_{\mathbf{K}_- + \mathbf{q}, A} \\ c_{\mathbf{K}_- + \mathbf{q}, B} \end{pmatrix}$$



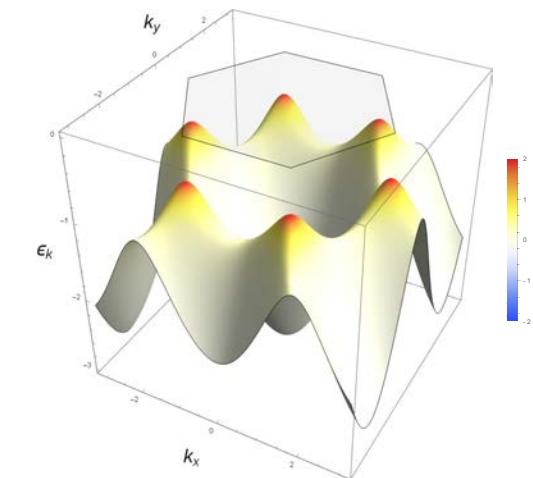
$$H = \sum_q (c_{\mathbf{K}_+ + \mathbf{q}, A}^+ c_{\mathbf{K}_+ + \mathbf{q}, B}^+ c_{\mathbf{K}_- + \mathbf{q}, A}^+ c_{\mathbf{K}_- + \mathbf{q}, B}^+) \begin{pmatrix} m_H & h_q & 0 & 0 \\ h_q^* & -m_H & 0 & 0 \\ 0 & 0 & -m_H & h_q^* \\ 0 & 0 & h_q & m_H \end{pmatrix} \begin{pmatrix} c_{\mathbf{K}_+ + \mathbf{q}, A} \\ c_{\mathbf{K}_+ + \mathbf{q}, B} \\ c_{\mathbf{K}_- + \mathbf{q}, A} \\ c_{\mathbf{K}_- + \mathbf{q}, B} \end{pmatrix}$$

where  $m_H = \frac{3\sqrt{3}}{2}\lambda_H$

With Haldane mass

$$H = \sum_q (c_{\mathbf{K}_+ + \mathbf{q}, A}^+ c_{\mathbf{K}_+ + \mathbf{q}, B}^+ c_{\mathbf{K}_- + \mathbf{q}, A}^+ c_{\mathbf{K}_- + \mathbf{q}, B}^+) \begin{pmatrix} m_H & h_q & 0 & 0 \\ h_q^* & -m_H & 0 & 0 \\ 0 & 0 & -m_H & h_q^* \\ 0 & 0 & h_q & m_H \end{pmatrix} (c_{\mathbf{K}_+ + \mathbf{q}, A} c_{\mathbf{K}_+ + \mathbf{q}, B} c_{\mathbf{K}_- + \mathbf{q}, A} c_{\mathbf{K}_- + \mathbf{q}, B})$$

$$\text{where } m_H = \frac{3\sqrt{3}}{2} \lambda_H$$



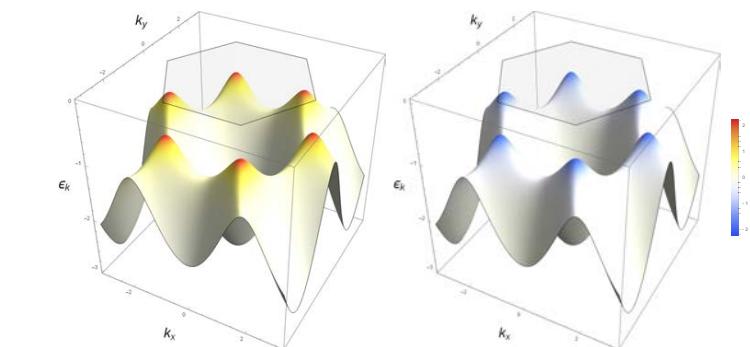
Kane-Mele:

With Haldane mass  $\times \sigma^z$

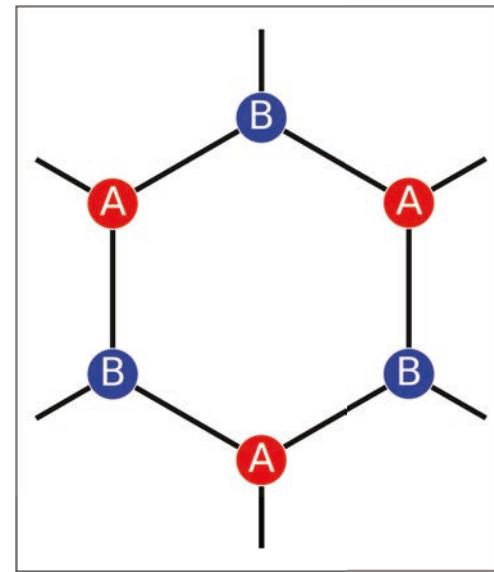
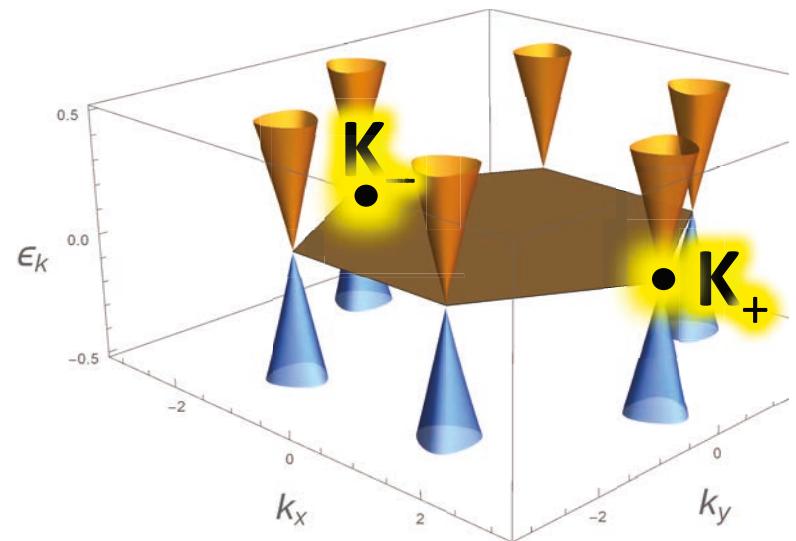
$$H = \sum_q (c_{\mathbf{K}_+ + \mathbf{q}, A\uparrow}^+ c_{\mathbf{K}_+ + \mathbf{q}, B\uparrow}^+ c_{\mathbf{K}_- + \mathbf{q}, A\uparrow}^+ c_{\mathbf{K}_- + \mathbf{q}, B\uparrow}^+ c_{\mathbf{K}_+ + \mathbf{q}, A\downarrow}^+ c_{\mathbf{K}_+ + \mathbf{q}, B\downarrow}^+ c_{\mathbf{K}_- + \mathbf{q}, A\downarrow}^+ c_{\mathbf{K}_- + \mathbf{q}, B\downarrow}^+)$$

$$\times \begin{pmatrix} m_H & h_q & 0 & 0 & 0 & 0 & 0 & 0 \\ h_q^* & -m_H & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -m_H & h_q^* & 0 & 0 & 0 & 0 \\ 0 & 0 & h_q & m_H & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -m_H & h_q & 0 & 0 \\ 0 & 0 & 0 & 0 & h_q^* & m_H & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & m_H & h_q^* \\ 0 & 0 & 0 & 0 & 0 & 0 & h_q & -m_H \end{pmatrix} (c_{\mathbf{K}_+ + \mathbf{q}, A\uparrow} c_{\mathbf{K}_+ + \mathbf{q}, B\uparrow} c_{\mathbf{K}_- + \mathbf{q}, A\uparrow} c_{\mathbf{K}_- + \mathbf{q}, B\uparrow} c_{\mathbf{K}_+ + \mathbf{q}, A\downarrow} c_{\mathbf{K}_+ + \mathbf{q}, B\downarrow} c_{\mathbf{K}_- + \mathbf{q}, A\downarrow} c_{\mathbf{K}_- + \mathbf{q}, B\downarrow})$$

spin  $\uparrow$       spin  $\downarrow$



$\sigma$  Spin  
 $\tau$  Sublattice  
 $\chi$  Valley



*....sheer poetry*

