cem
Center for Emergent Materials
an NSF MRSEC

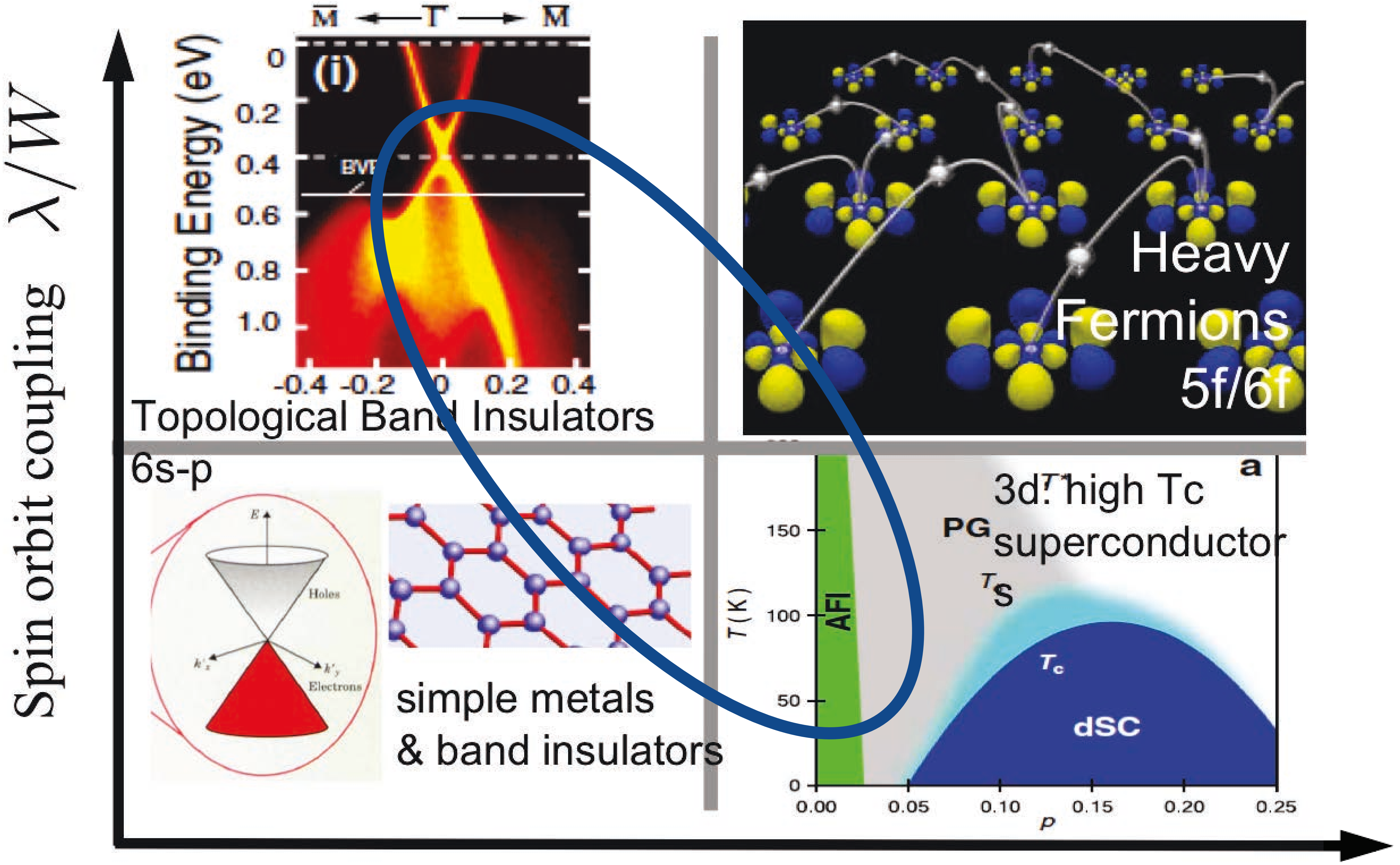
POEM: Physics of Emergent Materials

Nandini Trivedi

L1: Spin Orbit Coupling
L2: Topology and Topological Insulators

Reference: Bernevig Topological Insulators and Topological Superconductors

Tutorials: May 24, 25 (2017)



Spin orbit coupling λ/W
Topological Band Insulators
Heavy Fermions 5f/6f
6s-p
simple metals & band insulators
3d: high Tc superconductor
Binding Energy (eV)
AFI
PG
dSC
T (K)
p

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 #

Scope of Lectures and Anchor Points:

DAY1

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DAY2

3. The many Hall effects
   - integer qhe and chern #

My philisophy….
choose simplicity and insight over completeness

<u>Toy Problems:</u>

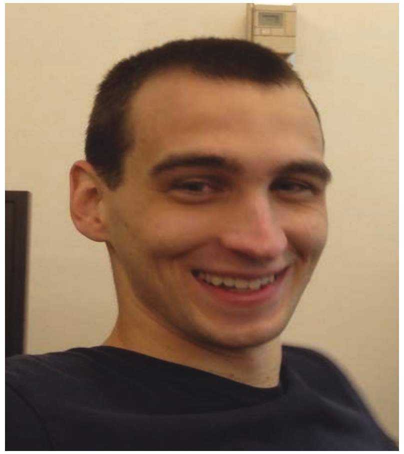
<u>Day 1:</u>

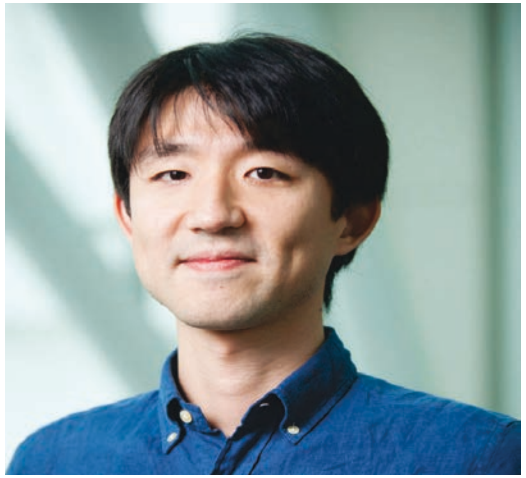
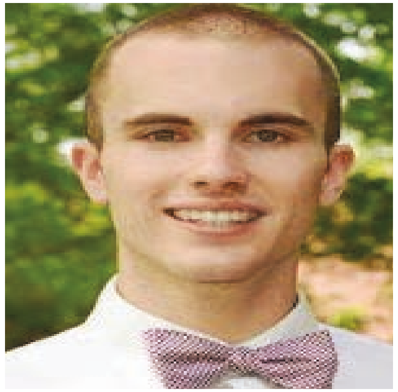
1) 1d SOC: spin-momentum locking
2) Two level system (Spin ½ in a magnetic field) and Berry Phase
3) Graphene: dirac points protected by inversion and TR

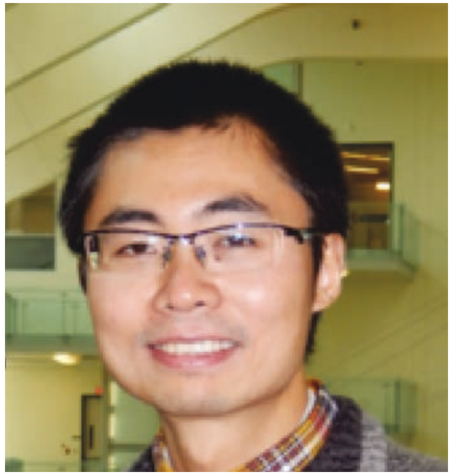
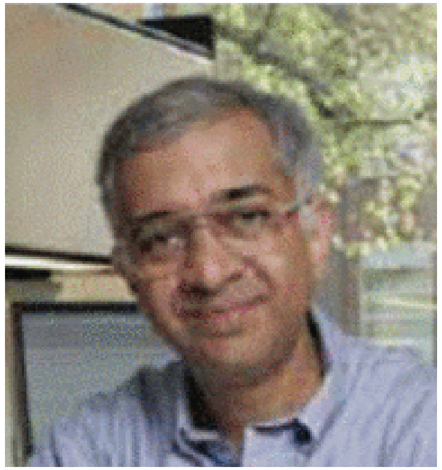
<u>Day 2:</u>

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

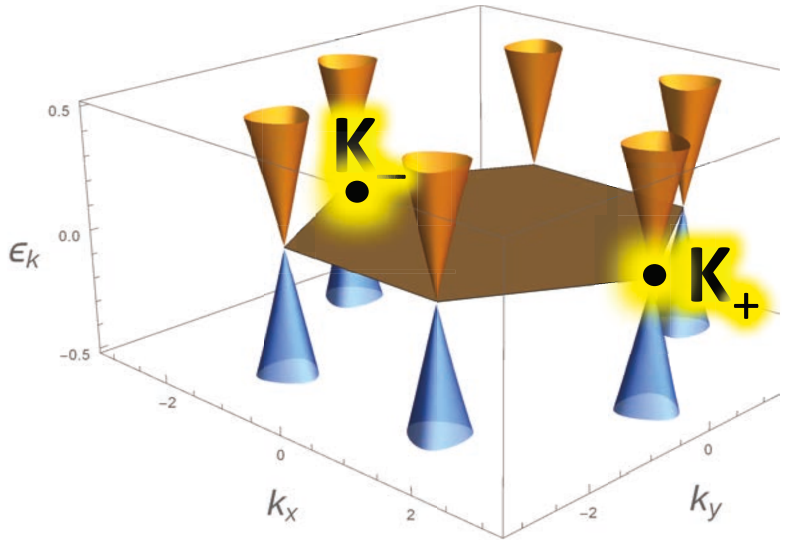
Pauli spin matrices

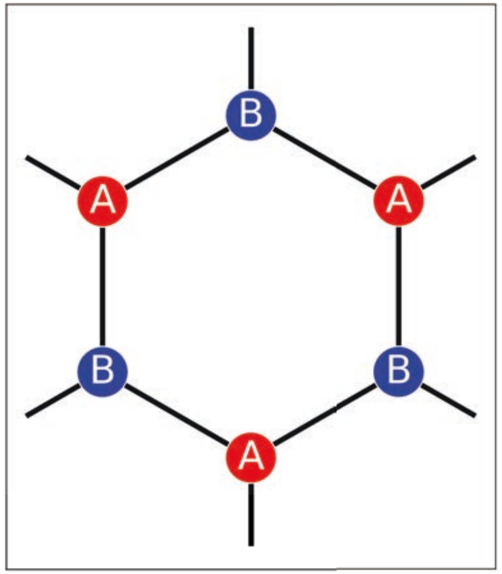
$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

σ Spin

τ Sublattice

χ Valley





Symmetries:

- Time Reversal
- Inversion
- Mirror

Time Reversal (without spin)

Definition:

$$T : t \to -t \qquad\qquad TR \Rightarrow [H, T] = 0$$

Transformation of various operators under T

$$\boxed{\begin{array}{l} T\hat{x}T^{-1} = \hat{x} \qquad T\hat{p}T^{-1} = -\hat{p} \qquad TiT^{-1} = -i \\ T[\hat{x}, \hat{p}]T^{-1} = Ti\hbar T^{-1} = -[\hat{x}, \hat{p}] = -i\hbar \end{array}} \qquad T\hat{L}T^{-1} = -\hat{L}$$

$$Tc_jT^{-1} = c_j \qquad\qquad Tc_kT^{-1} = c_{-k} \qquad Th(k)T^{-1} = h(-k)$$

$$\boxed{T = K \qquad\qquad T^2 = 1}$$

K:Complex conjugate

Definition: Time Reversal (with half integer spin)

$$T : t \to -t \qquad TR \Rightarrow [H,T] = 0 \quad \Rightarrow T|\Psi\rangle \quad and \quad |\Psi\rangle$$

are both eigenvectors with eigenvalue E

$$\boxed{T = e^{-i\pi S_y} K \qquad T^2 = -1 \\ T^2 = -i\sigma_y i\sigma_y KK = -\sigma_y^2 = -1}$$

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

$$\vec{S} = (\hbar/2)\vec{\sigma} \qquad e^{-i\pi\sigma_y/2} = -i\sigma_y = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

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

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

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

Same for dagger operators

Polar vs Axial vectors

Saturday, May 20, 2017 7:43 PM

Polar ≡ "usual" vector

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

under a transformation A

$\vec{v}_p \longrightarrow A\,\vec{v}_p$

polar

Axial ≡ pseudo vector

e.g. $\vec{L} = \vec{r} \times \vec{p}$, $\vec{S}$, $\vec{B}$

$\vec{v}_a \longrightarrow (\det A)\, A\, \vec{v}_a$

Inversion

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

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

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

$\vec{S} \rightarrow \vec{S}$

$B \rightarrow \vec{B}$

$\det I = \underline{\underline{-1}}$

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

- polar x polar = axial

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

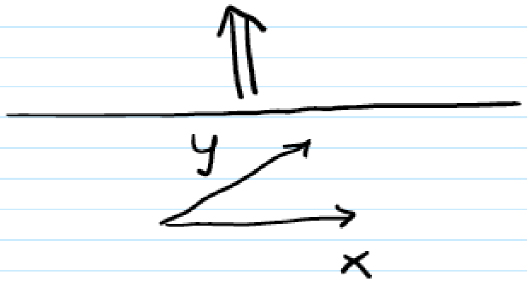
- polar x axial = polar

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

- axial x axial = axial

Mirror:

z - Mirror $\sigma_h(xy)$



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

$L_x = y p_z - z p_y$

$L_y = z p_x - x p_z$

$L_z = x p_y - y p_x$

$x \to x$

$y \to y$

$z \to -z$

$L_x \to -L_x$

$L_y \to -L_y$

$L_z \to L_z$

$\sigma_v(xz)$

Y-mirror

$$\boxed{\begin{array}{l} x \to x \\ y \to -y \\ z \to z \end{array}}$$

$$\boxed{\begin{array}{l} L_x \to -L_x \\ L_y \to L_y \\ L_z \to -L_z \end{array}}$$

$\sigma_v(yz)$

X-mirror

$$\boxed{\begin{array}{l} x \to -x \\ y \to y \\ z \to z \end{array}}$$

$$\boxed{\begin{array}{l} L_x \to L_x \\ L_y \to -L_y \\ L_z \to -L_z \end{array}}$$

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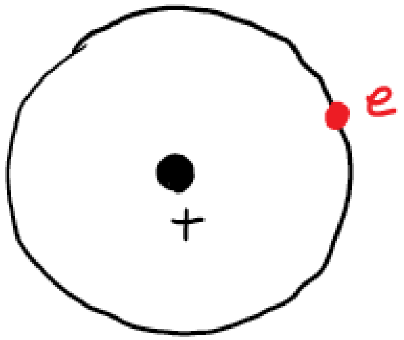
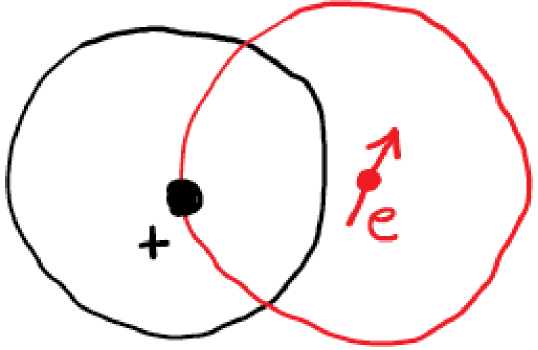
Atom SOC





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

$$\propto \vec{L}$$

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

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

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

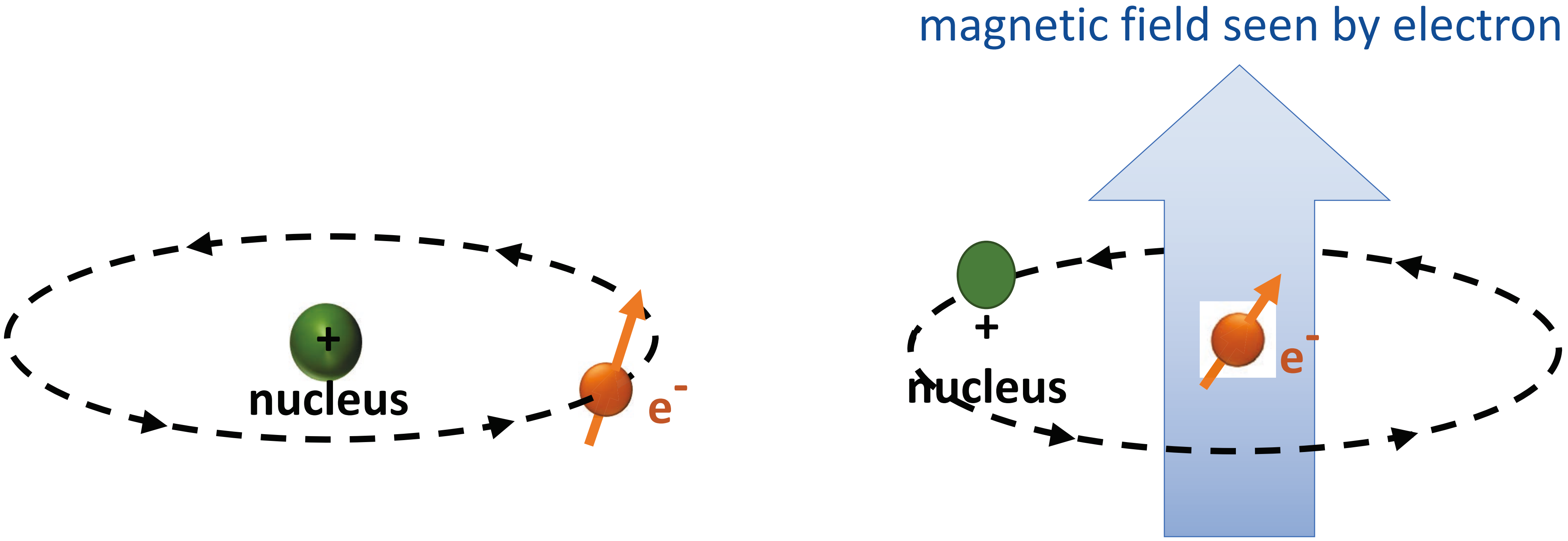
$$\mathcal{H} = \vec{\sigma} \cdot \vec{B} = \lambda\, \vec{\sigma} \cdot \vec{L}$$

Zeeman Effect

spin orbit

coupling

Spin-Orbit Coupling

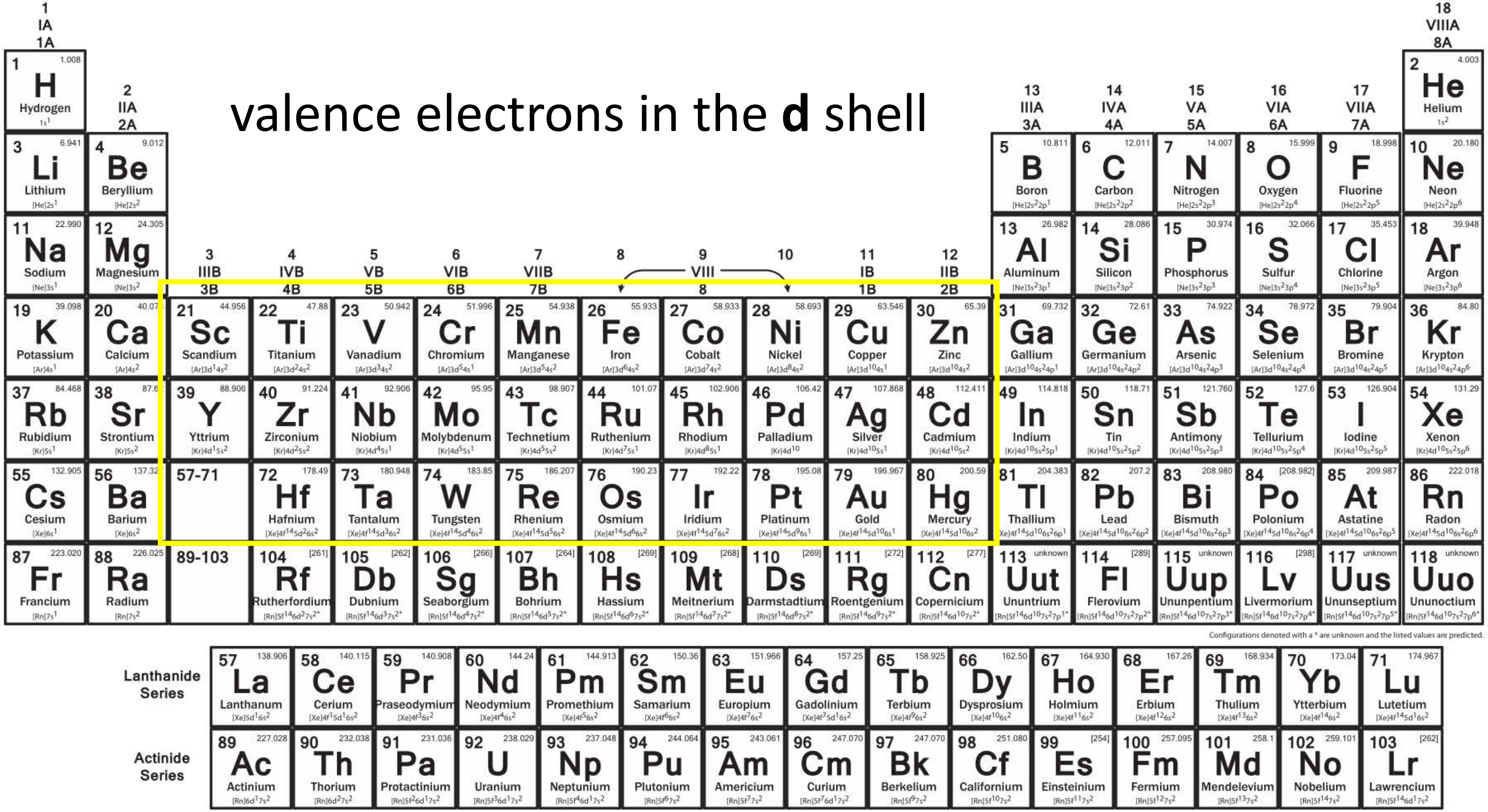


$$H_{\mathrm{SO}} = \frac{1}{m_e^2 c^2} \frac{1}{r} \frac{dV}{dr} \vec{S} \cdot \vec{L} \quad \rightarrow \quad \lambda \vec{L} \cdot \vec{S}$$

When is Spin Orbit coupling large?
What materials?

Transition Metals

valence electrons in the **d** shell



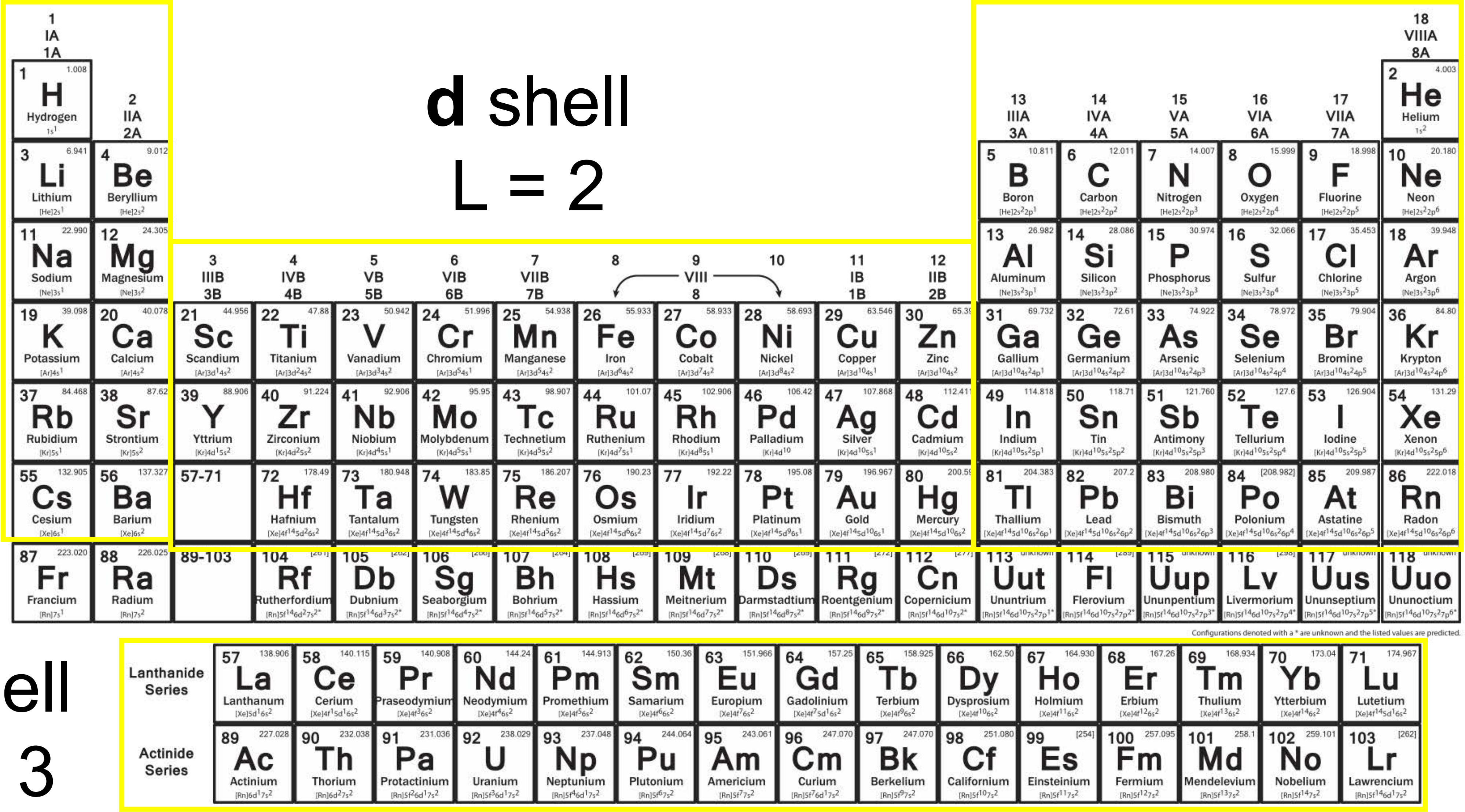
Transition Metals

s shell
L = 0

p shell
L = 1

d shell
L = 2

f shell
L = 3



Spherical Symmetry

- Wavefunction for atomic orbitals

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

radial part

angular part (spherical Harmonics)

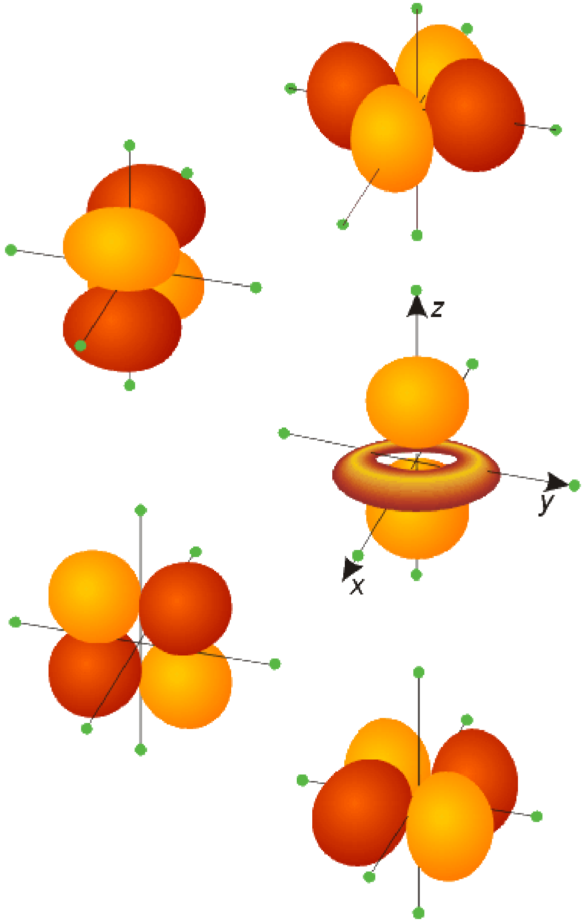
- For the **d** shell:

$$\Omega(\theta, \phi) = Y_l^m(\theta, \phi)$$ with $l = 2$

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

d Orbitals

- Atomic orbitals are linear combinations of spherical harmonics



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

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

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

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

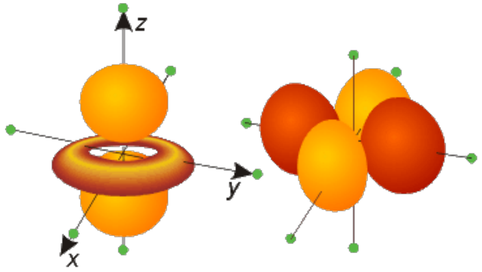
$$d_{xy} = \frac{i}{\sqrt{2}}\left(Y_2^{-2} - Y_2^{+2}\right)$$

Crystal Field Splitting

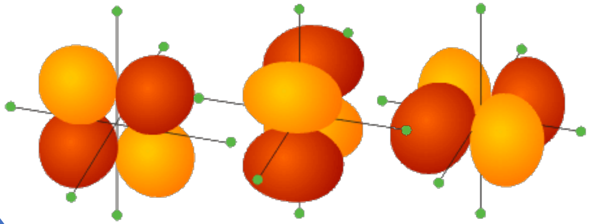
***Spherical** Symmetry* *… reduced to …* ***Octahedral** Symmetry*

Energy

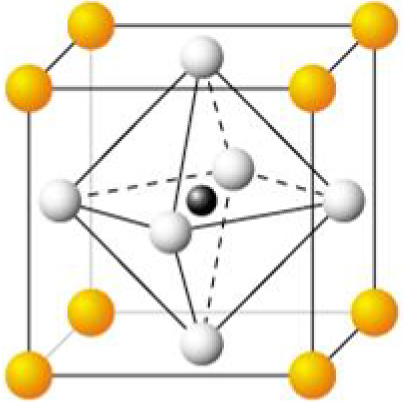
degenerate **d** orbitals



degenerate
e_g orbitals



degenerate
t_{2g} orbitals



** Omiting the ħ factor from ***L***.

L = 2 Angular Momentum

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

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

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

Eigenbasis of $\mathbf{L_z}$

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

$\longleftarrow \; |L = 2, m = +2\rangle$

$\longleftarrow \; |L = 2, m = +1\rangle$

$\longleftarrow \; |L = 2, m = 0\rangle$

$\longleftarrow \; |L = 2, m = -1\rangle$

$\longleftarrow \; |L = 2, m = -2\rangle$

** Omiting the ħ factor from ***L***.

L = 2 Angular Momentum

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

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

Orbital basis

$$L_z = \begin{array}{cl} \left(\begin{array}{ccc|cc} 0 & +i & 0 & 0 & 0 \\ -i & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & +2i \\ \hline 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -2i & 0 & 0 \end{array}\right) & \begin{array}{l} \longleftarrow \quad |d_{yz}\rangle \\ \longleftarrow \quad |d_{zx}\rangle \\ \longleftarrow \quad |d_{xy}\rangle \\ \longleftarrow \quad |d_{z^2}\rangle \\ \longleftarrow \quad |d_{x^2-y^2}\rangle \end{array} \end{array}$$

** Omiting the ħ 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.

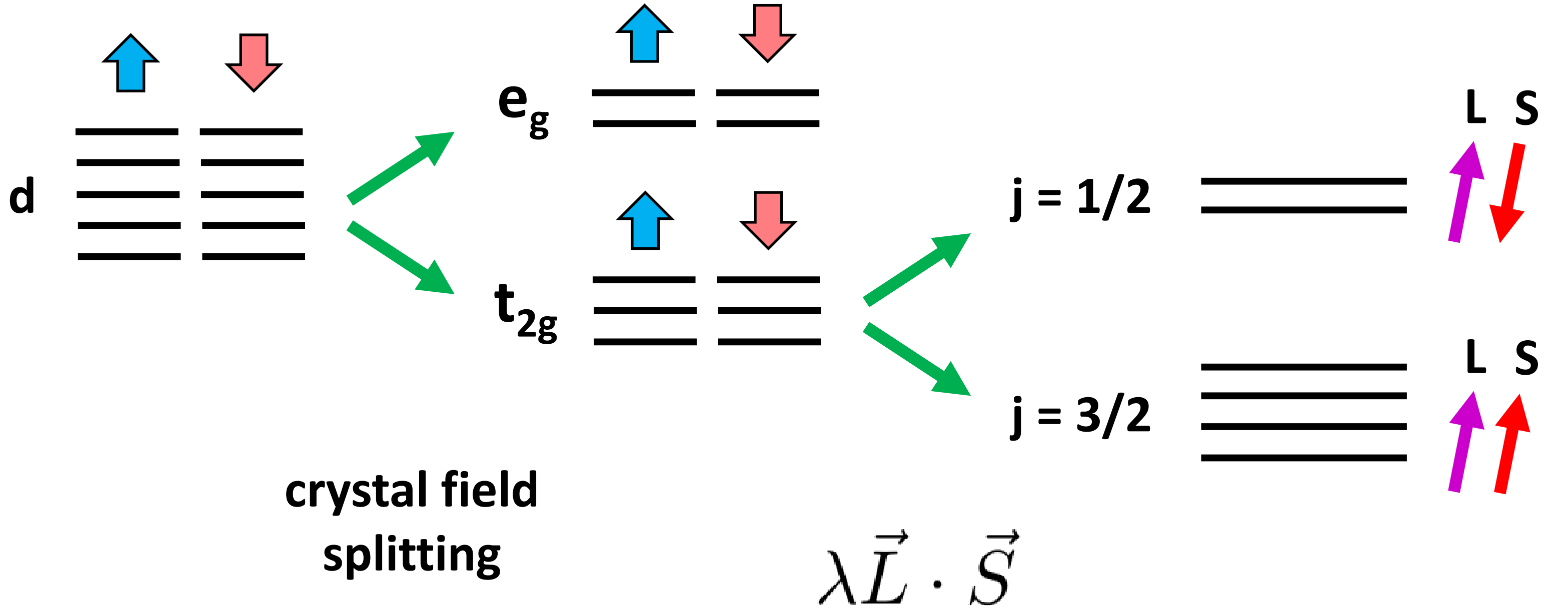
$$L_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & +i \\ 0 & -i & 0 \end{pmatrix} \quad L_y = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ +i & 0 & 0 \end{pmatrix} \quad L_z = \begin{pmatrix} 0 & +i & 0 \\ -i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

- 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

Sr_2XO_4 tetragonal BCC crystal structure

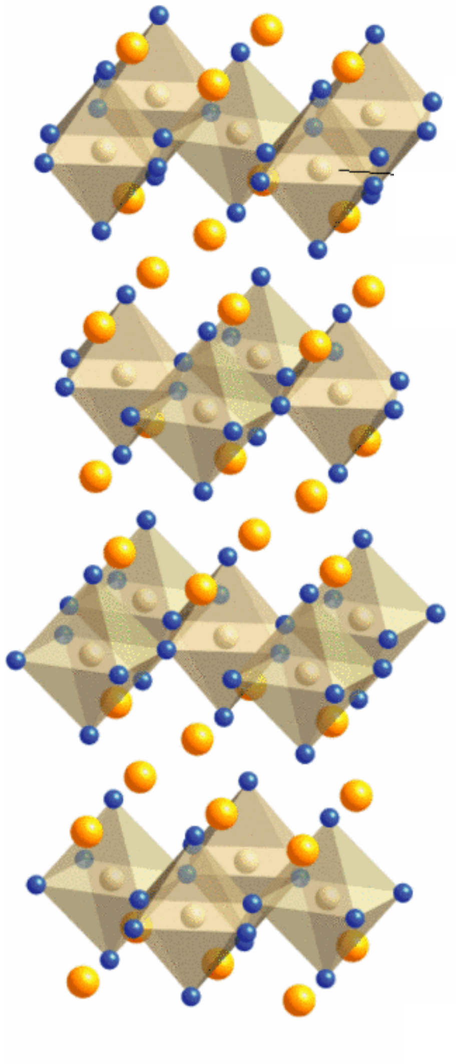
U

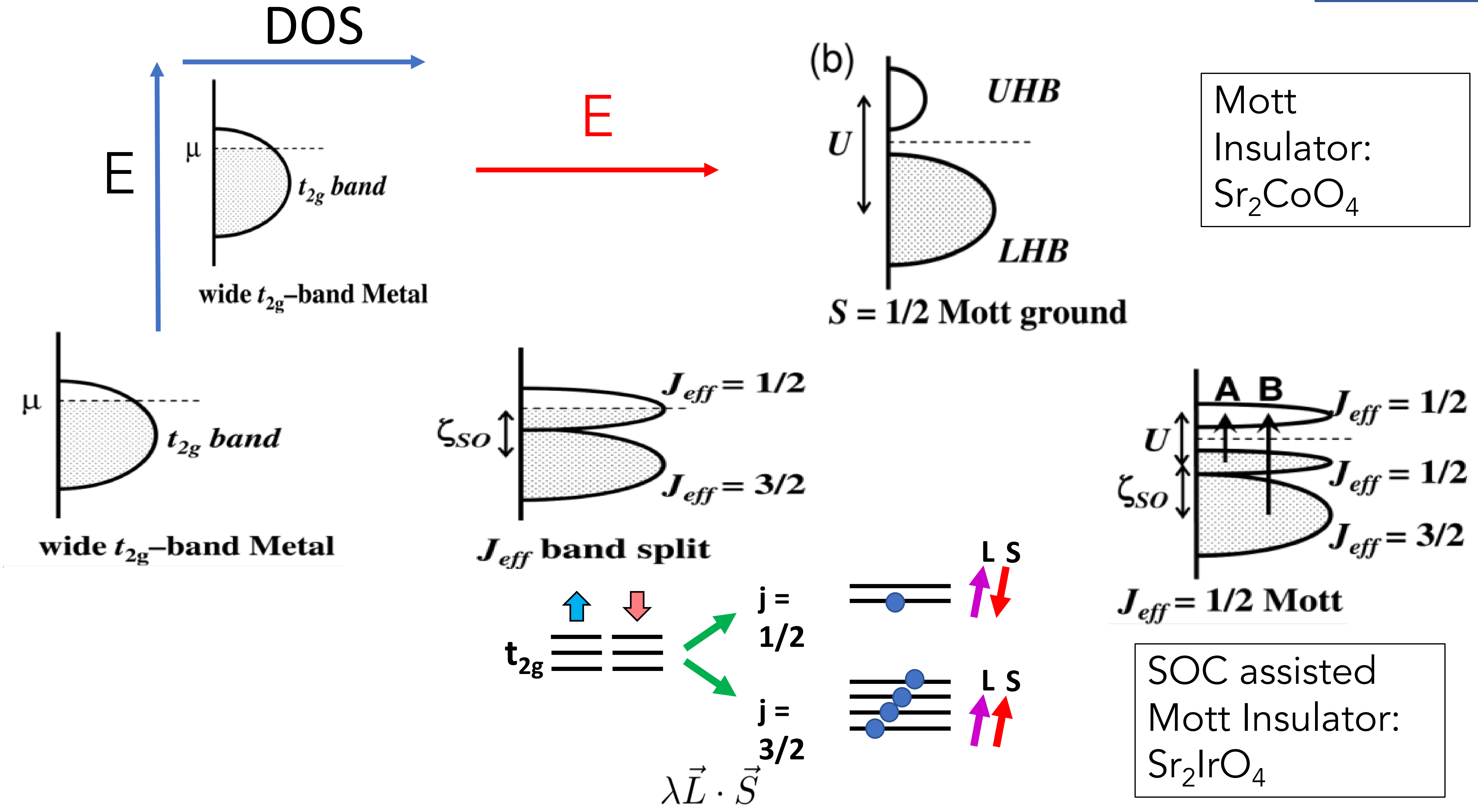
λ

26 Fe Iron 55.933 $[Ar]3d^6 4s^2$	27 Co Cobalt 58.933 $[Ar]3d^7 4s^2$	28 Ni Nickel 58.693 $[Ar]3d^8 4s^2$
44 Ru Ruthenium 101.07 $[Kr]4d^7 5s^1$	45 Rh Rhodium 102.906 $[Kr]4d^8 5s^1$	46 Pd Palladium 106.42 $[Kr]4d^{10}$
76 Os Osmium 190.23 $[Xe]4f^{14} 5d^6 6s^2$	77 Ir Iridium 192.22 $[Xe]4f^{14} 5d^7 6s^2$	78 Pt Platinum 195.08 $[Xe]4f^{14} 5d^9 6s^1$

Yet….

Sr_2CoO_4 (Mott Insulator)
Sr_2RhO_4 (metal)
Sr_2IrO_4 (insulator)




DOS
E
μ
t_{2g} band
wide t_{2g}–band Metal
E
(b)
UHB
U
LHB
S = 1/2 Mott ground
Mott Insulator: Sr_2CoO_4
μ
t_{2g} band
wide t_{2g}–band Metal
ζ_{SO}
$J_{eff} = 1/2$
$J_{eff} = 3/2$
J_{eff} band split
A B
U
ζ_{SO}
$J_{eff} = 1/2$
$J_{eff} = 1/2$
$J_{eff} = 3/2$
$J_{eff} = 1/2$ Mott
t_{2g}
j = 1/2
j = 3/2
L S
L S
$\lambda\vec{L}\cdot\vec{S}$
SOC assisted Mott Insulator: Sr_2IrO_4

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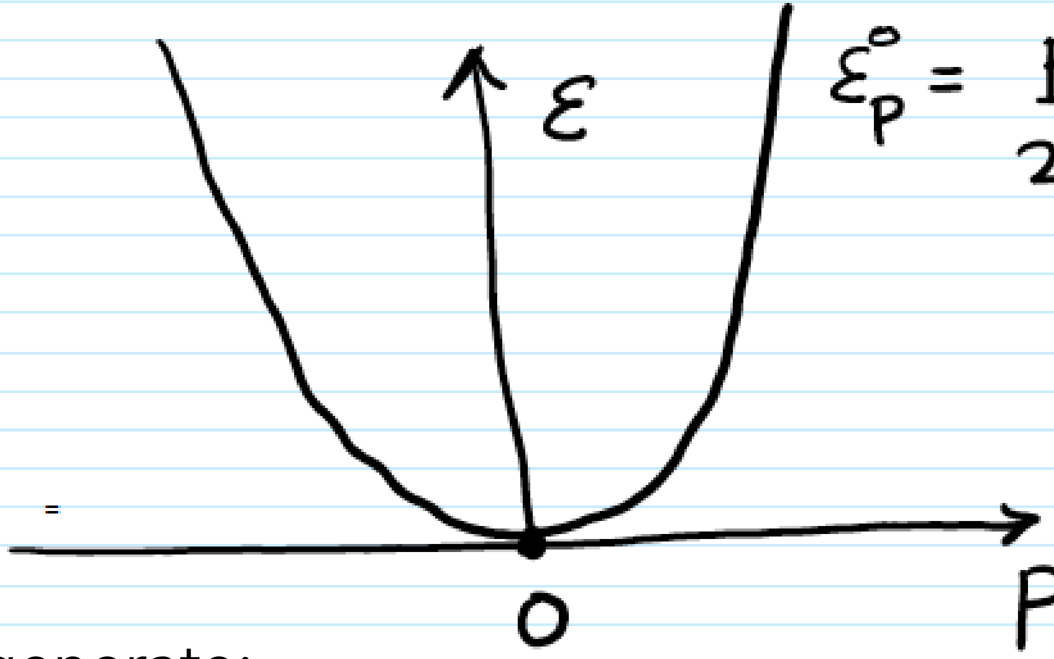
Spin-orbit coupling in bands
Example in 1d: spin-momentum locking

Spin – momentum coupling

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

$\lambda = 0$



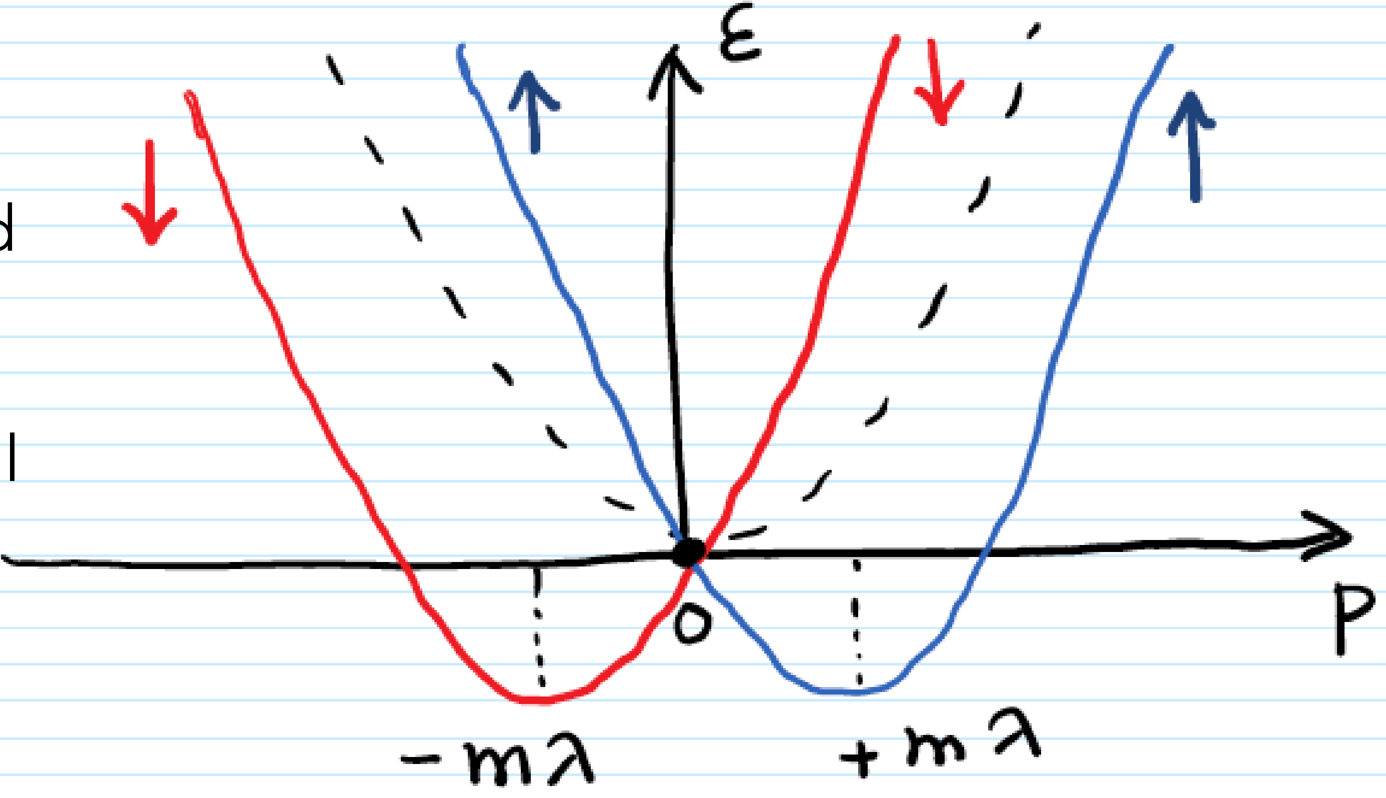
$$\varepsilon_p^0 = \frac{p^2}{2m}$$

Each eigenstate is doubly degenerate:
Kramer's degeneracy

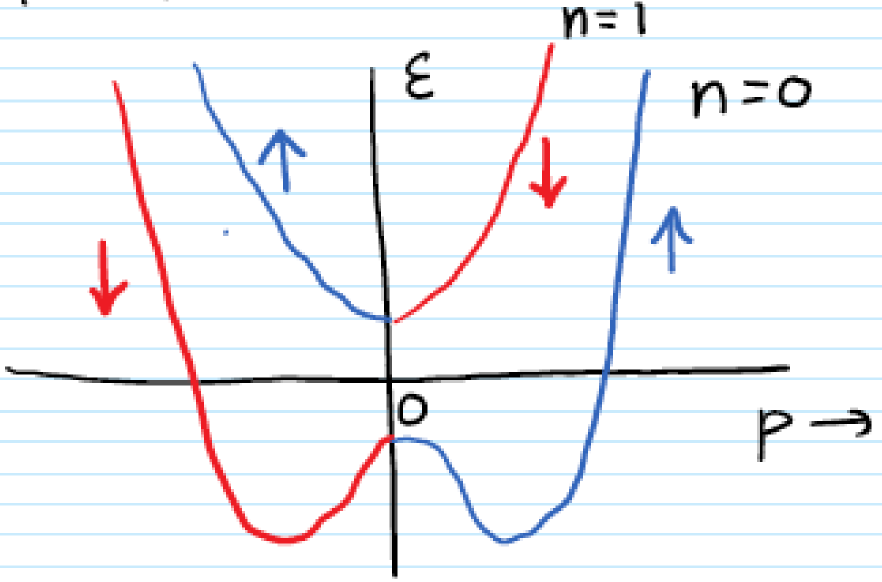
$\lambda \neq 0$

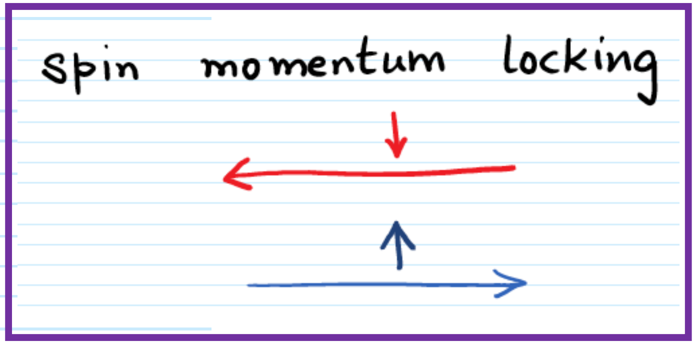
$$\mathcal{H} = \begin{array}{c} \\ \uparrow \\ \downarrow \end{array} \begin{array}{c} \begin{array}{cc} \uparrow & \downarrow \end{array} \\ \begin{pmatrix} \varepsilon_p^0 - \lambda p & 0 \\ 0 & \varepsilon_p^0 + \lambda p \end{pmatrix} \end{array}$$

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 x





Gap opens up at the degenerate point.

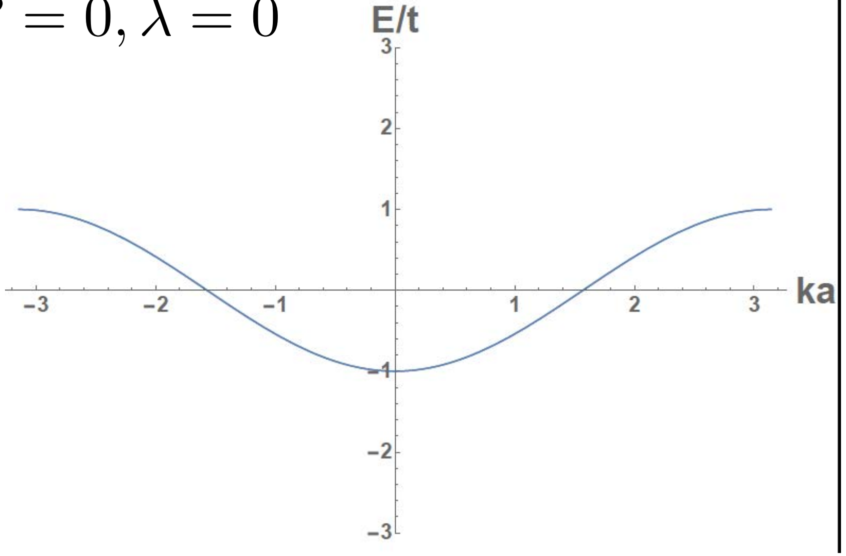
Traverse the BZ always remaining in the lowest band. (adiabatic evolution).

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

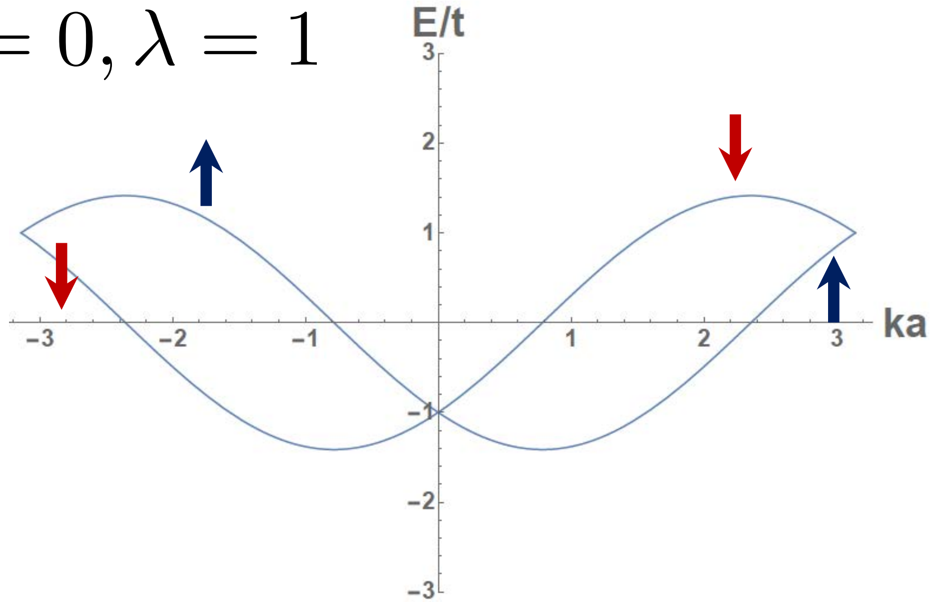
$$h(k) = -\cos(k)\sigma_0 - \lambda\sin(k)\sigma_z - B\sigma_x = -\cos(k)\sigma_0 + \vec{d}(k).\vec{\sigma}$$

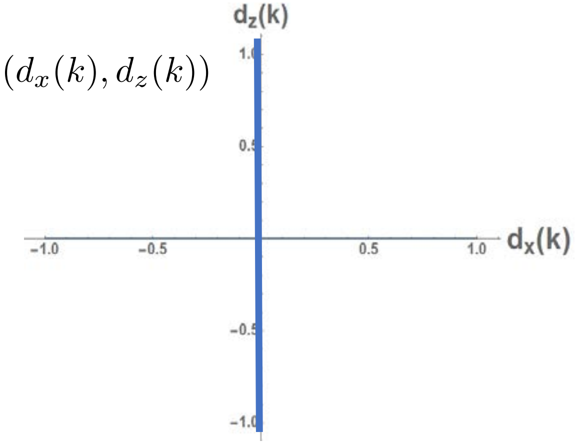
$$d_x(k) = -B \quad d_z(k) = -\lambda\sin(k)$$

$B = 0, \lambda = 0$



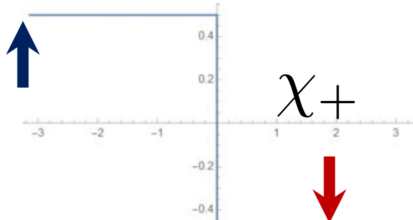
$B = 0, \lambda = 1$





$\chi-$

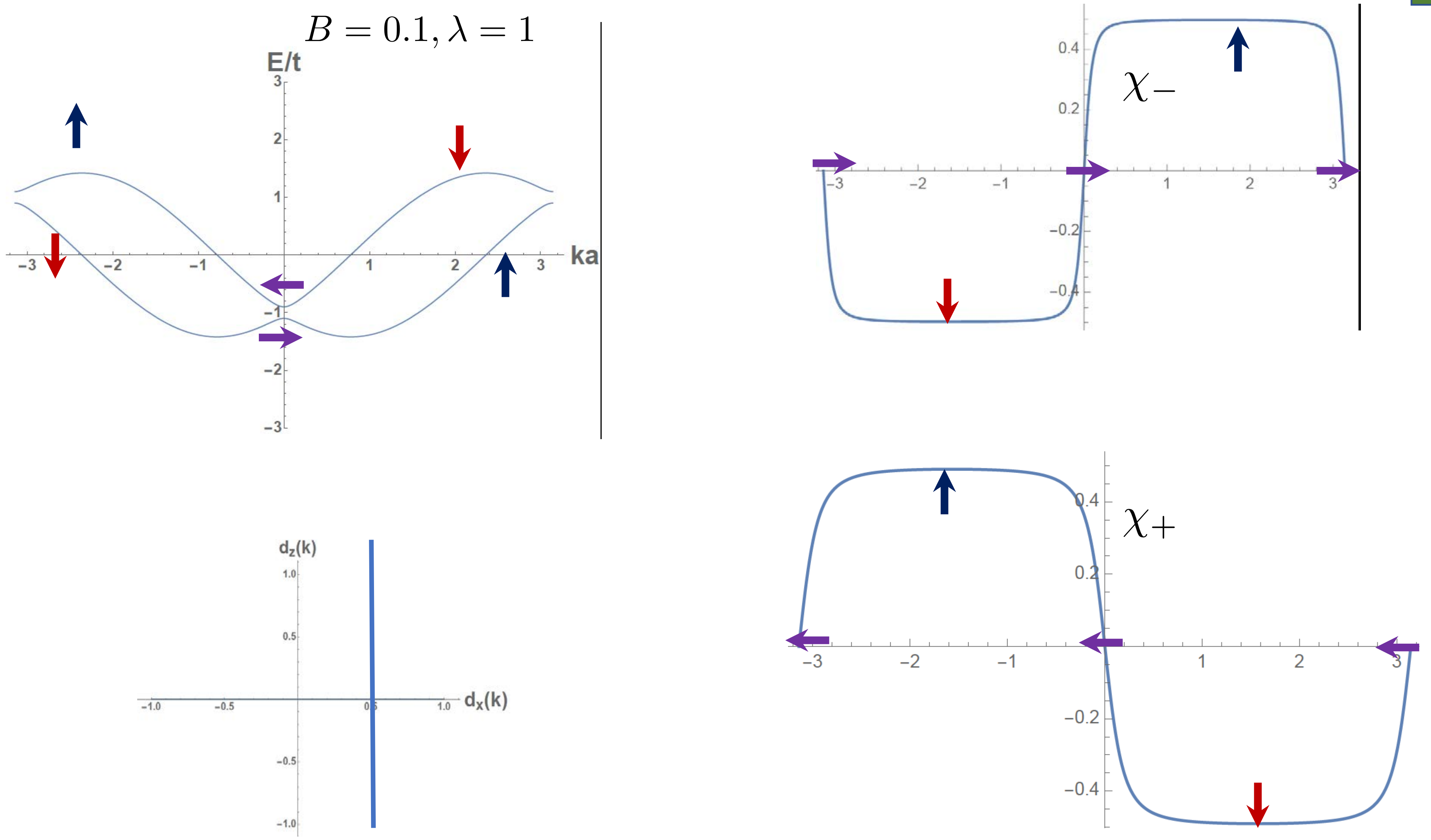
Eigenvector corresponding to lower energy



$\chi+$

Eigenvector corresponding to upper energy

Bands SOC



No Winding: hence topologically trivial

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Graphene

- topological quantum matter
- quantum criticality at Dirac point

Electronic structure

Carbon : $Z = 6$

$\underbrace{1s^2}_{\text{He-core (ignore)}} \quad \underbrace{2s^2\ 2p^2}_{\text{valence electrons}}$

4 orbitals : $(n=2)$

$[\underbrace{s, p_x, p_y}_{sp^2 \text{ bonding}}, p_z]$ → π bond

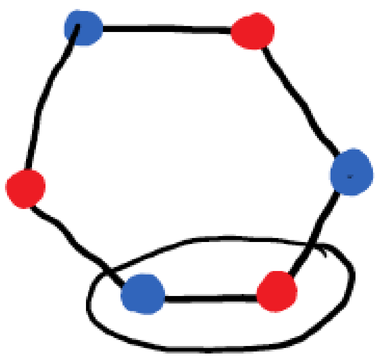
planar structure

Honeycomb lattice

⇓

not a Bravais lattice

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



2 atoms in unit cell

Aside :

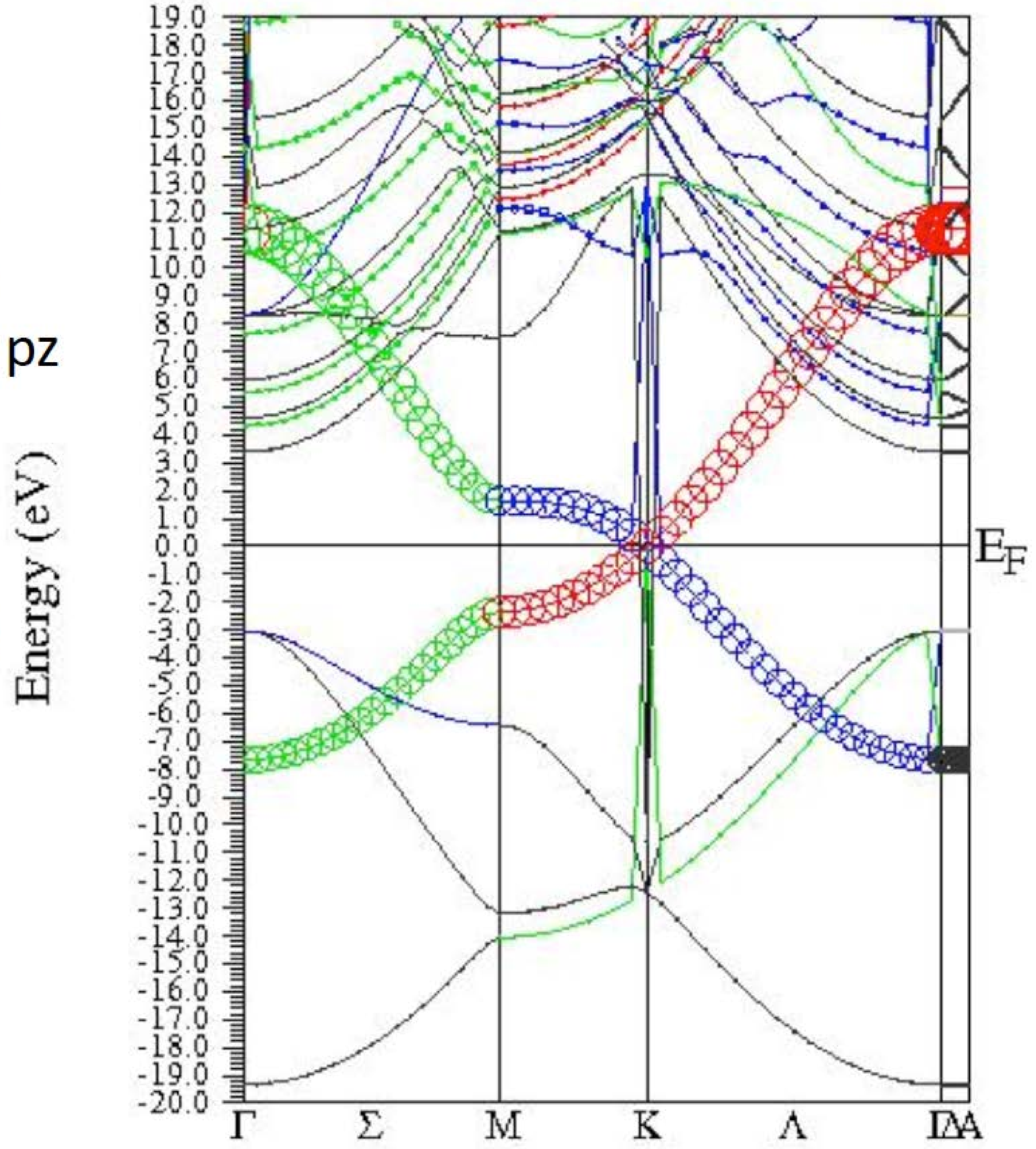
$2s^2\ 2p^2$ → total spin $S=1$

total orbital $L=1$

total g.s. $J=0$

Graphene

Bands at the chemical potential are derived from p_z orbitals



Within unit cell:

atoms = 2

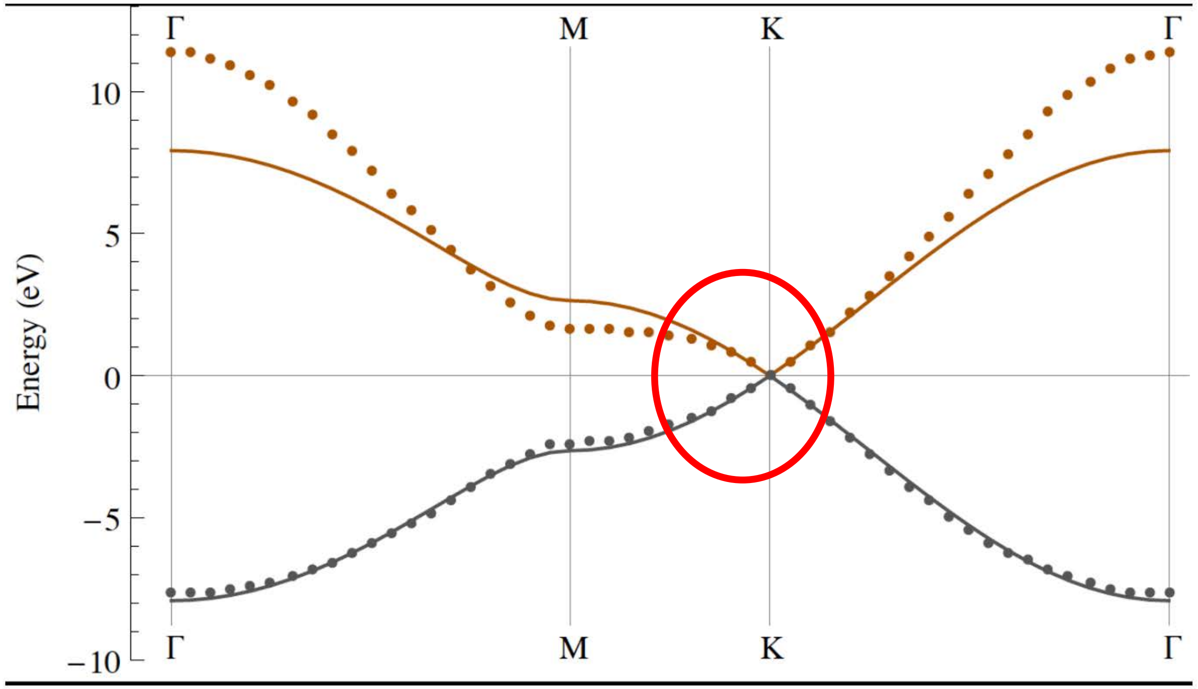
orbitals (4×2) = 8

electrons (4×2) = 8

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

∵ each orbital can hold 2 elections (spin up & down)

When the atoms come together they form bands.



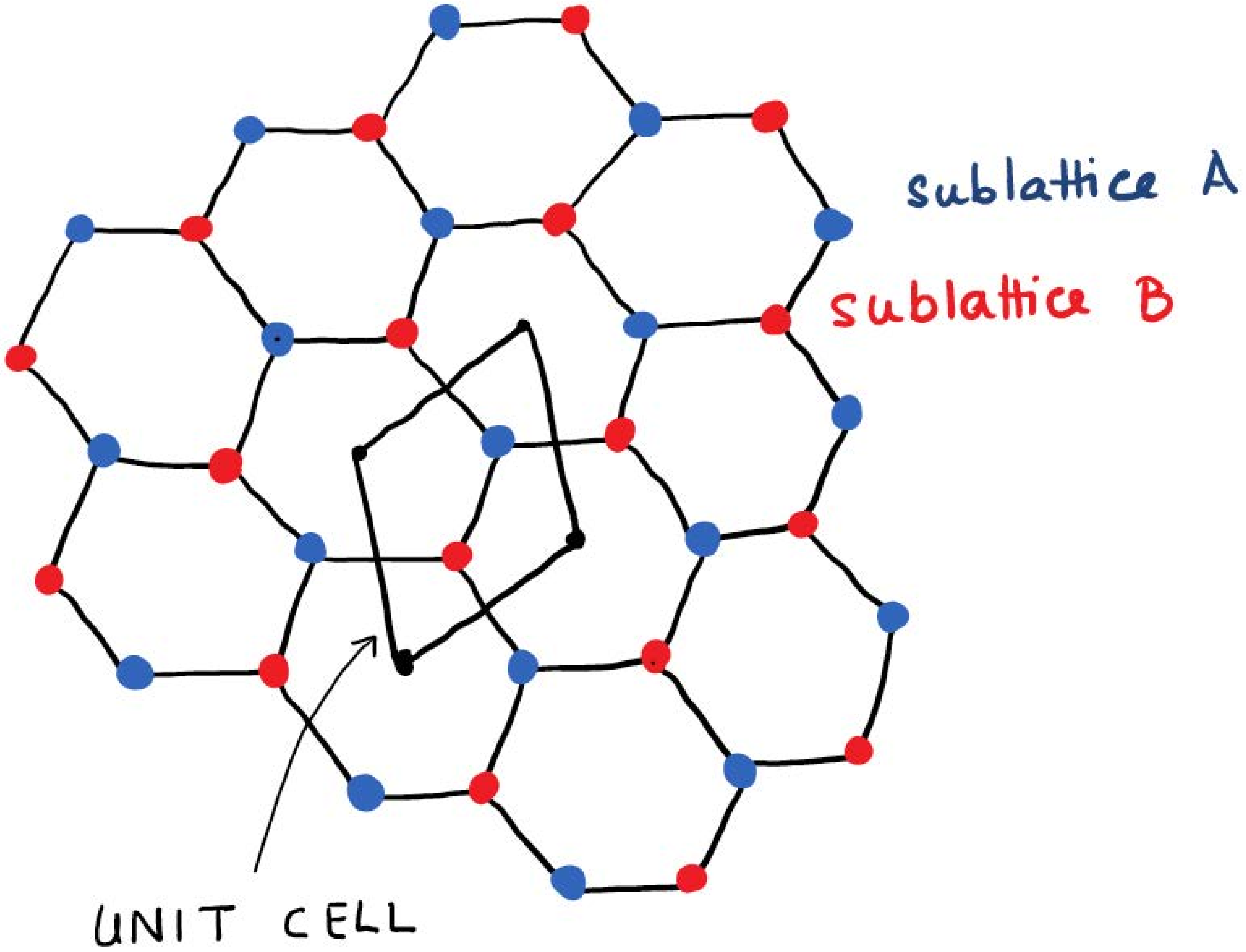
Tightbinding Fits: t=2.64 eV

$$v_F \approx c/350$$

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

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

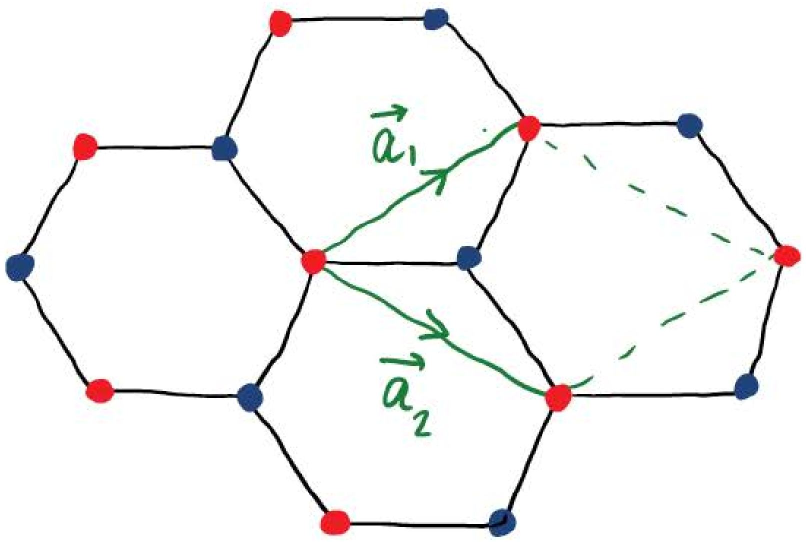
Graphene Material → Honeycomb



When the atoms come together they form bands.

Real Space Structure

Sunday, April 30, 2017 8:45 PM



$a_0 \equiv a_{c-c} = 1.42\,A^\circ$
nearest neighbor carbon-carbon

2 atoms in unit cell.

$$\vec{a}_1 = \left(\frac{3}{2}\hat{x} + \frac{\sqrt{3}}{2}\hat{y}\right)a_0 = a\hat{x} + b\hat{y}$$

$$\vec{a}_2 = \left(\frac{3}{2}\hat{x} - \frac{\sqrt{3}}{2}\hat{y}\right)a_0 = a\hat{x} - b\hat{y}$$

basis vectors

$a \equiv \frac{3}{2}a_0 \qquad b \equiv \frac{\sqrt{3}}{2}a_0$

Lattice spanned by

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

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

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

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

The magnitude of a_3 cancels in the evaluation of the b_i

Definitions:

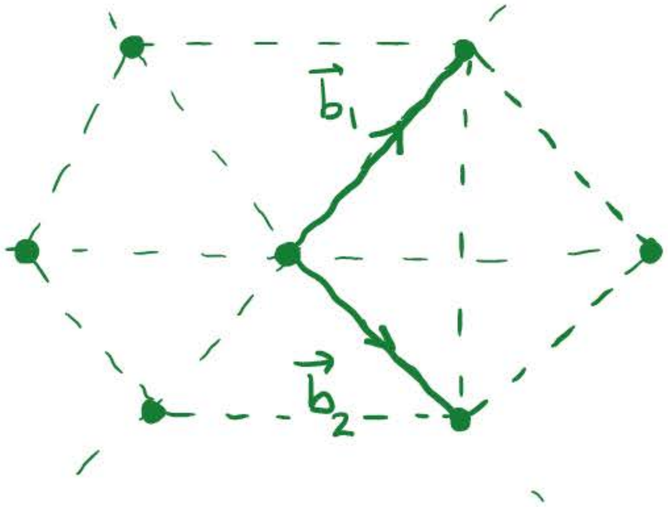
$a = \frac{3}{2} a_0$

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

Reciprocal lattice in momentum space

$\vec{G} = n\vec{b}_1 + m\vec{b}_2$

$(n, m \in \mathbb{Z})$

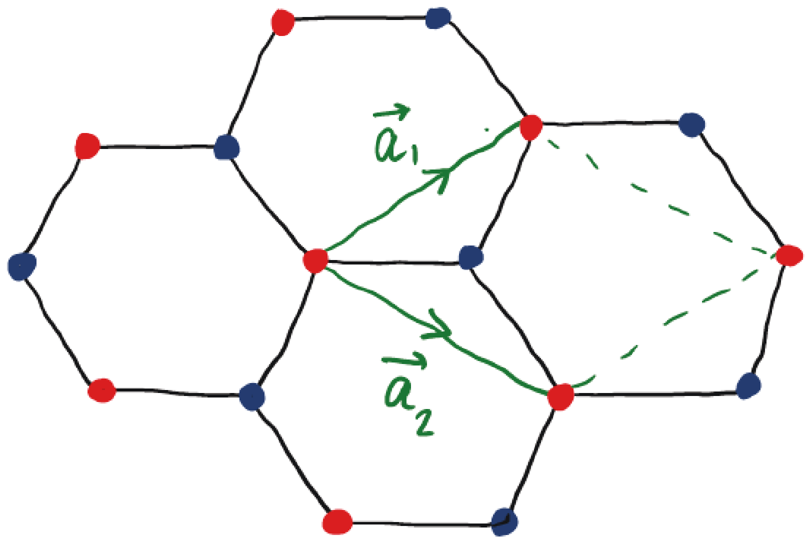


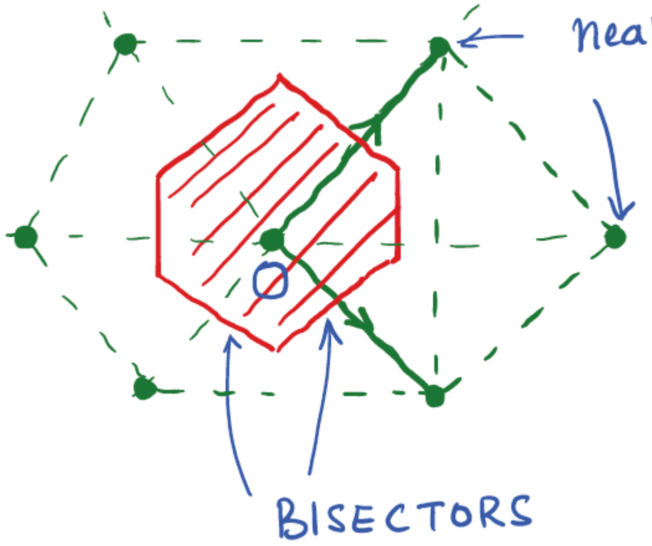
BRILLOUIN ZONE: UNIT CELL IN MOMENTUM SPACE

Find region enclosed by bisectors of vectors to nearest neighbor points in reciprocal space

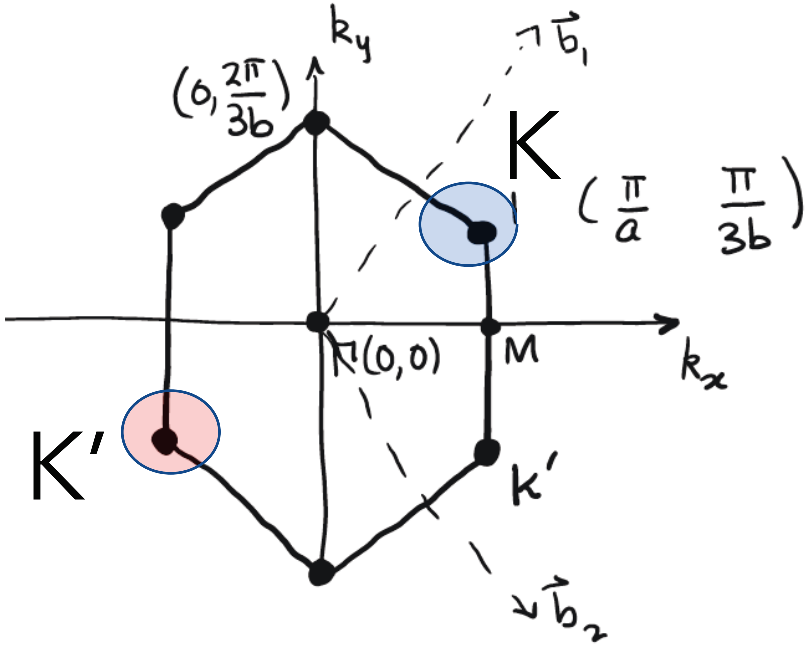
Real Space Structure

Sunday, April 30, 2017 8:45 PM





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



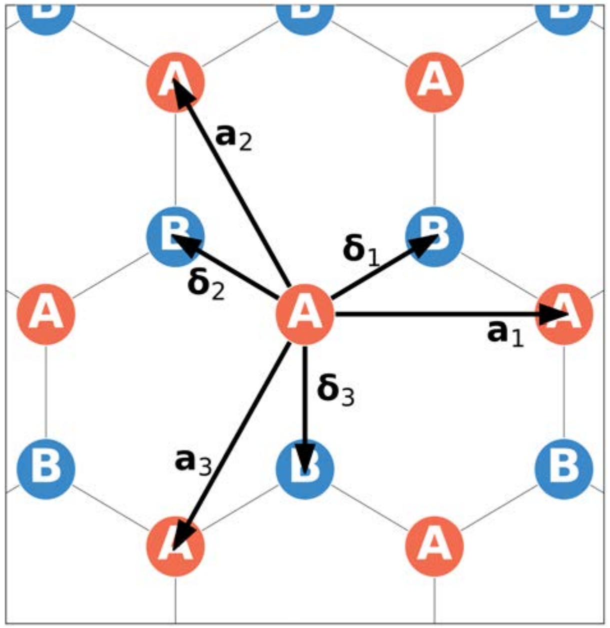
$\left(\frac{2\pi}{3a_0}, \frac{2\pi}{3\sqrt{3}a_0}\right)$

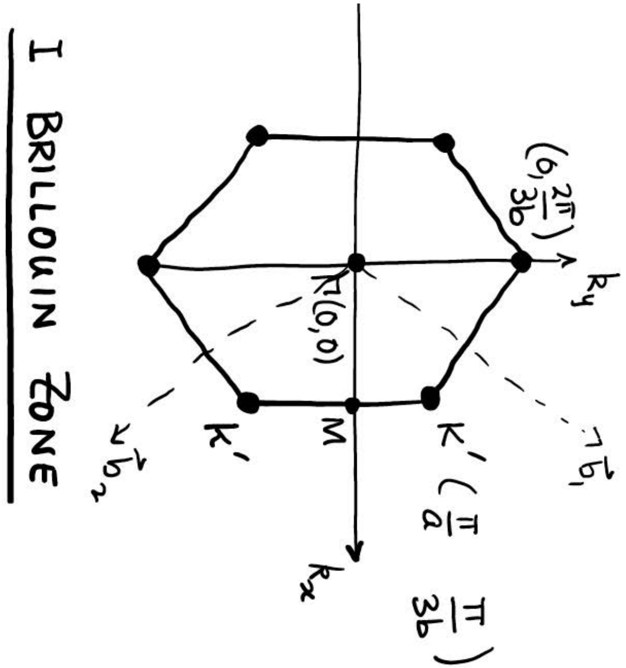
I BRILLOUIN ZONE

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

$$\boxed{\mathcal{H} = -t \sum_{\substack{\langle i_A, j_B \rangle \\ \sigma = \uparrow,\downarrow}} \left(c^{\dagger}_{i_A\sigma} c_{j_B\sigma} + \mathrm{H.c.} \right)}$$

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





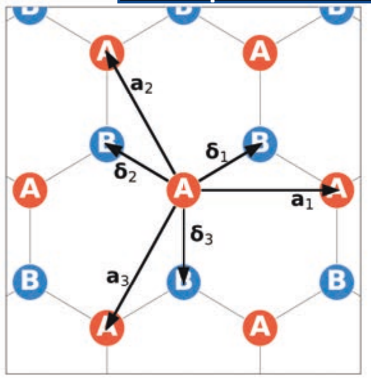
$$c_{i_\alpha} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_{i_\alpha}} c_{\mathbf{k}\alpha}$$

Here **α** is a sublattice index

Graphene

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

$$h_{\mathbf{k}} = -t\sum_{j} e^{i\mathbf{k}\cdot\boldsymbol{\delta}_j}$$

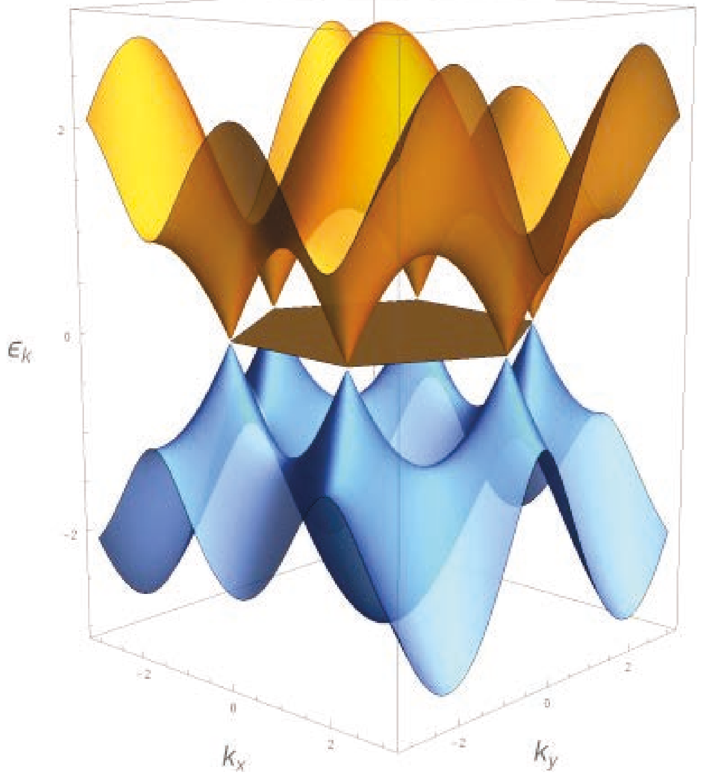


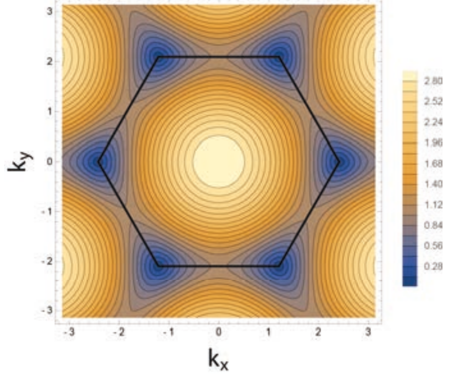
Eigenenergies at momentum **k**

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

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

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





My philisophy….
choose simplicity and insight over completeness

Toy Problems:

Day 1:

1) 1d SOC: spin-momentum locking
2) Two level system (Spin ½ 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

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

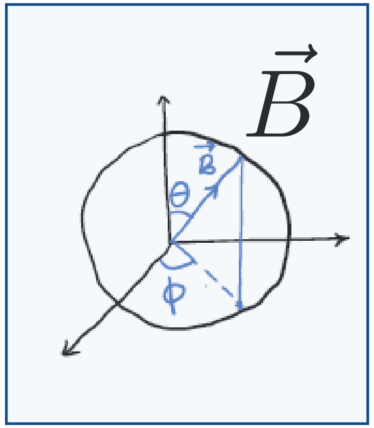
$$\left.\begin{aligned} \sigma_x &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ \sigma_y &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ \sigma_z &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{aligned}\right\} \text{PAULI MATRICES}$$

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

Eigenspectrum:

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

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

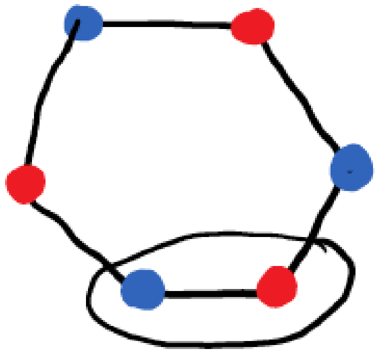


$$\sigma_z \mid \pm\rangle = \pm \mid \pm\rangle$$
$$\sigma_x \mid \pm\rangle = \mid \mp\rangle$$
$$\sigma_y \mid \pm\rangle = \pm i \mid \mp\rangle$$

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

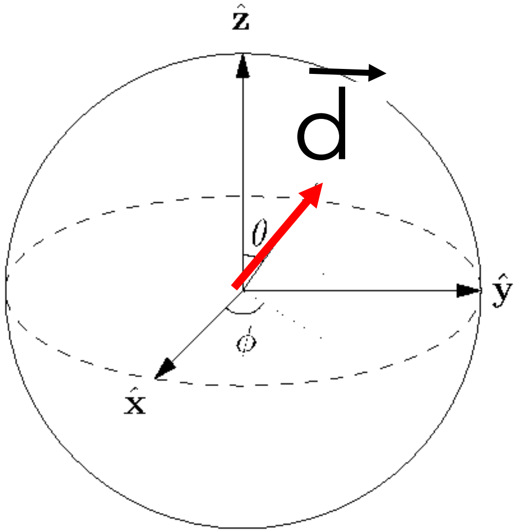
$$\theta = \pi/2, \phi = 0 \qquad \chi_+ = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \chi_- = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Apply to graphene:



2 atoms in unit cell

$$A = \uparrow$$
$$B = \downarrow$$



Hamiltonian at momentum k can be written in terms of Pauli matrices in sublattice space

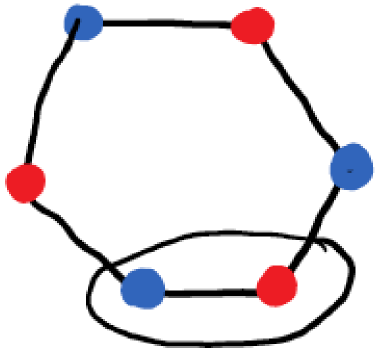
$$H_{\mathbf{k}} = \begin{pmatrix} 0 & h_{\mathbf{k}} \\ h_{\mathbf{k}}^* & 0 \end{pmatrix} = \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\tau}$$

τ_i for i=1,2,3 : Pauli matrices in sublattice basis

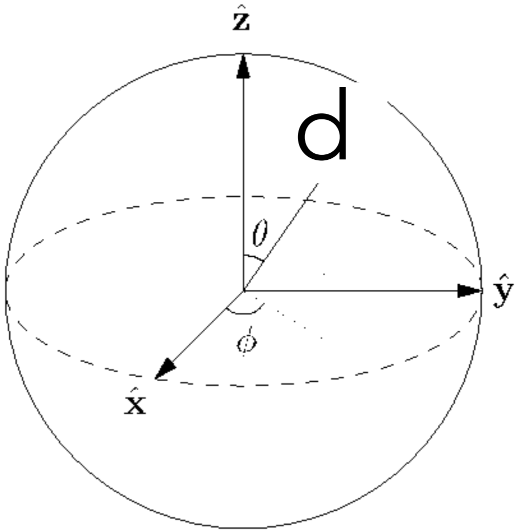
Formally, **d**(**k**) in sublattice basis is analogous to "magnetic field" acting on spin

Berry

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



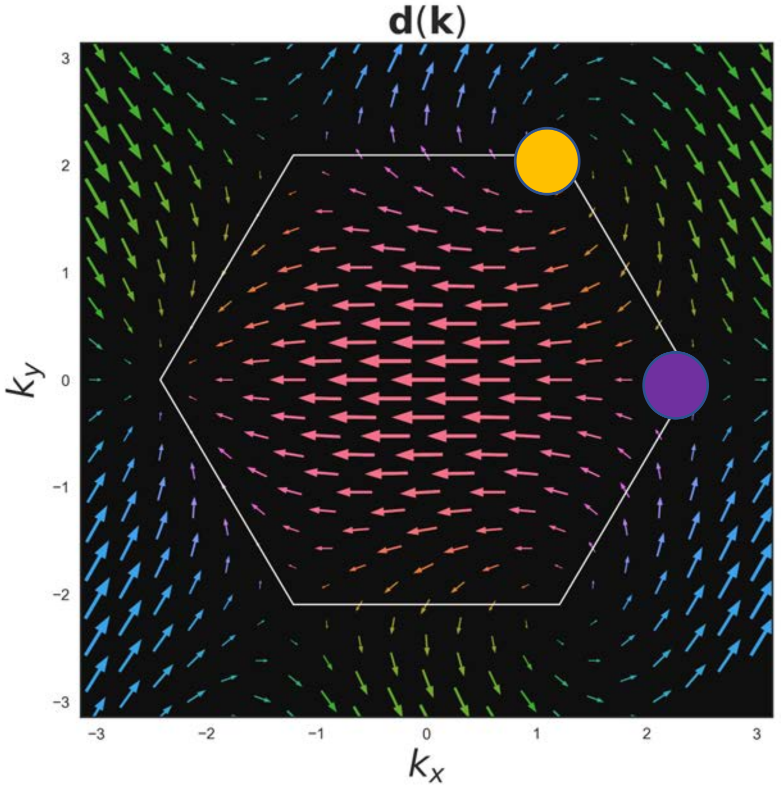
2 atoms in unit cell



$$d_x(\mathbf{k}) = -t \sum_{j=1}^{3} \cos\left(\mathbf{k}\cdot\boldsymbol{\delta}_j\right)$$

$$d_y(\mathbf{k}) = -t \sum_{j=1}^{3} \sin\left(\mathbf{k}\cdot\boldsymbol{\delta}_j\right)$$

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



$$\lambda_1 = +|\vec{d}| \qquad \chi_+ = \begin{pmatrix} \cos\theta/2 \\ \sin\theta/2 \; e^{i\phi} \end{pmatrix}$$

$$\lambda_2 = -|\vec{d}| \qquad \chi_- = \begin{pmatrix} \sin\theta/2 \; e^{-i\phi} \\ -\cos\theta/2 \end{pmatrix}$$

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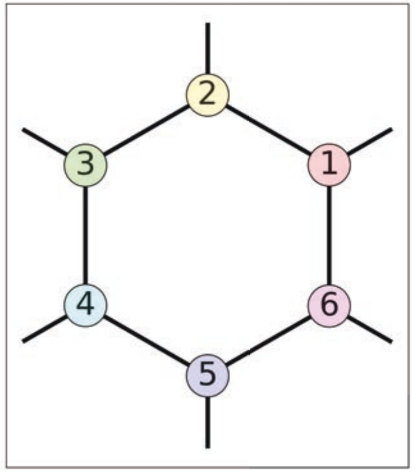
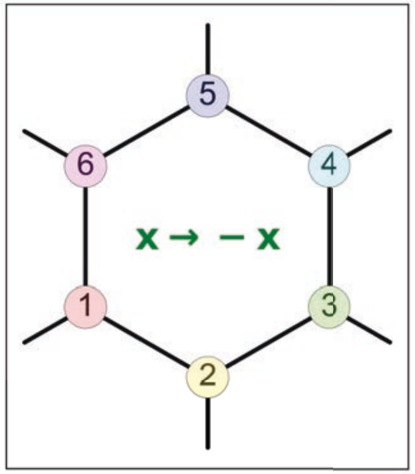
- Break inversion: sublattice potential
- Break TR: Haldane mass

Dirac points protected by TR and inversion symmetry



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

Inversion Symmetry



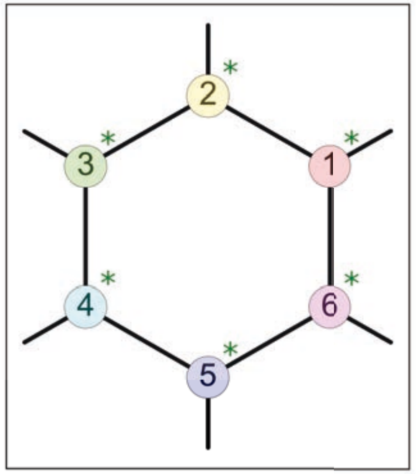
Wavefunction transforms as

$$\Psi(\mathbf{x}) \rightarrow \Psi(-\mathbf{x})$$

- Changes sublattice (A ⟷ B)

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

Time Reversal Symmetry



Wavefunction transforms as

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

- Complex conjugation
- Does not change sublattice

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

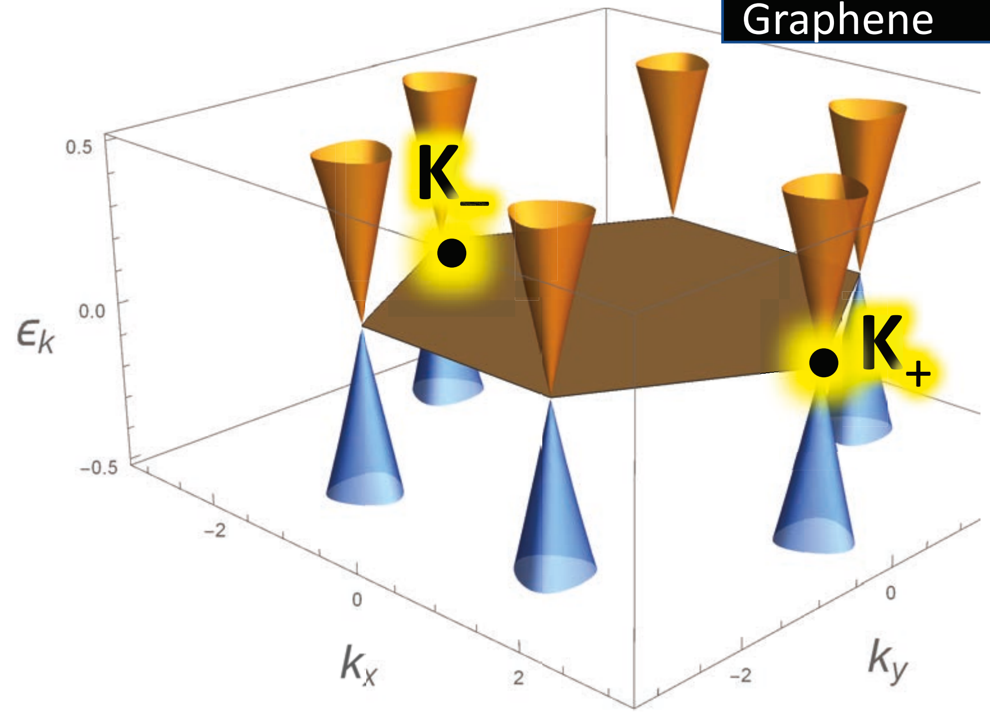
➔ With *both* inversion and time-reversal symmetry, $d_z(\mathbf{k}) = 0$

➔ Zeros of **d**(**k**) exist (Dirac points)

Proof: TR and I protect Dirac points

Graphene

The "Full" tight binding Hamiltonian can be expanded around each "valley"



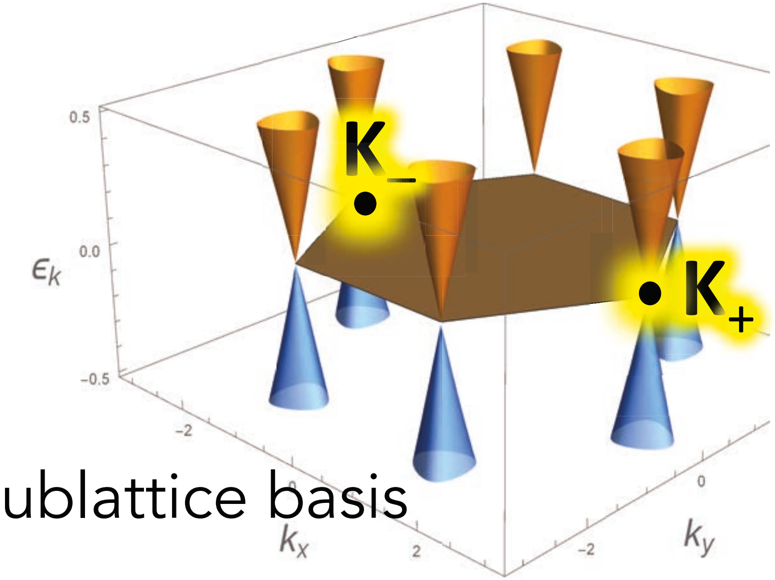
- Dirac nodes at $\mathbf{K}_\pm = \left(\pm\frac{4\pi}{3\sqrt{3}a}, 0\right)$
- Keep only low energy states
- Expand H_k near K_+ and K_-

$$h_\mathbf{k} = -t\sum_j e^{i\mathbf{k}\cdot\boldsymbol{\delta}_j}$$

$$\mathscr{H} \approx \sum_\mathbf{q} \left(c^\dagger_{\mathbf{K}_+ +\mathbf{q},A}, c^\dagger_{\mathbf{K}_+ +\mathbf{q},B}, c^\dagger_{\mathbf{K}_- +\mathbf{q},A}, c^\dagger_{\mathbf{K}_- +\mathbf{q},B}\right) \begin{pmatrix} 0 & h_{\mathbf{K}_+ +\mathbf{q}} & 0 & 0 \\ h^*_{\mathbf{K}_+ +\mathbf{q}} & 0 & 0 & 0 \\ 0 & 0 & 0 & h_{\mathbf{K}_- +\mathbf{q}} \\ 0 & 0 & h^*_{\mathbf{K}_- +\mathbf{q}} & 0 \end{pmatrix} \begin{pmatrix} c_{\mathbf{K}_+ +\mathbf{q},A} \\ c_{\mathbf{K}_+ +\mathbf{q},B} \\ c_{\mathbf{K}_- +\mathbf{q},A} \\ c_{\mathbf{K}_- +\mathbf{q},B} \end{pmatrix}$$

Two independent "valleys" with Dirac cones

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



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

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

τ_i for i=1,2,3
: Pauli matrices in sublattice basis

Include valley index

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

χ_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.

Around $\vec{K}_+$ $\qquad \vec{k} = \vec{K}_+ + \vec{q}$

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

Around $\vec{K}_-$ $\qquad \vec{k} = \vec{K}_- + \vec{q}$

$$\vec{K}_- = -\vec{K}_+$$

$$h(\vec{K}_- + \vec{q}\,) = h(-\vec{K}_+ + \vec{q}\,) = -q_x \tau_x + q_y \tau_y = \begin{pmatrix} 0 & -q_x - iq_y \\ -q_x + iq_y & 0 \end{pmatrix}$$

(2)

Time reversal:

(see notes)

$$\underbrace{T\, h(\vec{k})\, T^{-1}}_{\displaystyle \| \atop \displaystyle [h(\vec{k})]^*} = h(-\vec{k}) \quad \text{for general } \vec{k}$$

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

Check

Consider the point K_+

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

From (1) $\qquad\qquad\qquad\qquad$ From (2)

$q_x \tau_x - q_y \tau_y$  $q_x \tau_x - q_y \tau_y$ —(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)

$$h(\vec{K}_- + \vec{q}) = h(-\vec{K}_+ + \vec{q}) = -q_x \tau_x + q_y \tau_y \quad (4)$$

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

$$\boxed{\underline{\text{Consider:}} \quad h(\vec{K}_+ + \vec{q}) = q_x \tau_x + q_y \tau_y + m\sigma_z}$$

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

$$\text{TR} \longrightarrow \quad \| \quad \checkmark$$

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

from (4)

Preserves TR

Breaks I

Inversion symmetry

$$I: \quad (x, y) \mapsto (-x, -y)$$

$$\begin{cases} I \, c_{i,A} \, I^{-1} = c_{-i,B} \\ I \, c_{iB} \, I^{-1} = c_{-i,A} \end{cases}$$

$$I \, c_{i,\alpha} \, I^{-1} = \tau^{x}_{\alpha,\beta} \, c_{-i\beta}$$

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

$$\Rightarrow \quad h(\vec{k}) = \sigma_x \, h(-\vec{k}) \, \sigma_x$$

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

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

$$\Rightarrow \boxed{h(\vec{k}) = \tau_x h^*(\vec{k}) \tau_x}$$

Now consider a generic 2-level Hamiltonian

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

T & I $\Rightarrow$

$$d_i \tau_i + \epsilon = \tau_x (d_i \tau_i + \epsilon)^* \tau_x$$

$$= [d_x \tau_x \tau_x \tau_x + d_y \tau_x \tau_y \tau_x + d_z \tau_x \tau_z \tau_x + \epsilon \tau_x \tau_x]^*$$

$$= (d_x \tau_x - d_y \tau_y - d_z \tau_z + \epsilon)^*$$

$$= (d_x \tau_x + d_y \tau_y - d_z \tau_z + \epsilon)$$

$\tau_y^* = -\tau_y$

Pauli matrices

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\{\sigma_\mu, \sigma_\nu\} = 0$$

anti commute

Thus the combined action of TR and I gives:

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

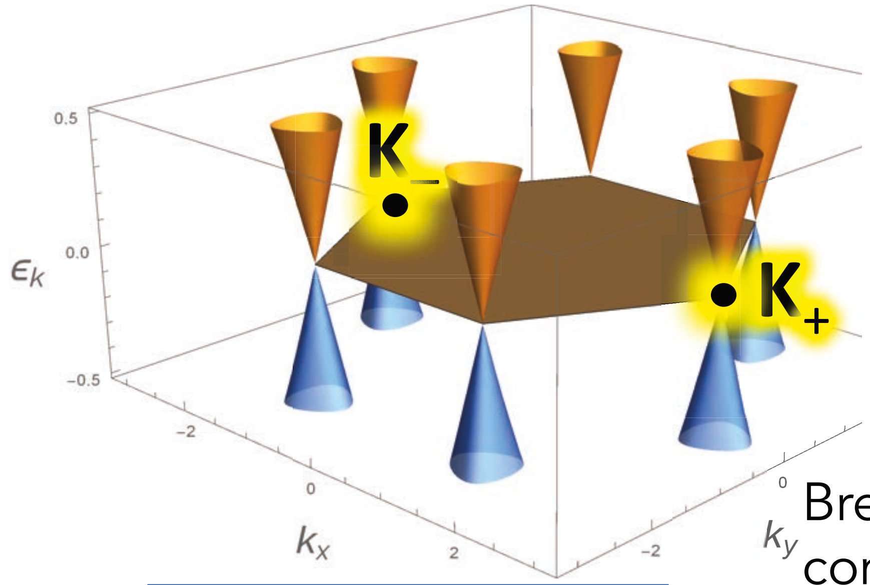
around Dirac points.

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

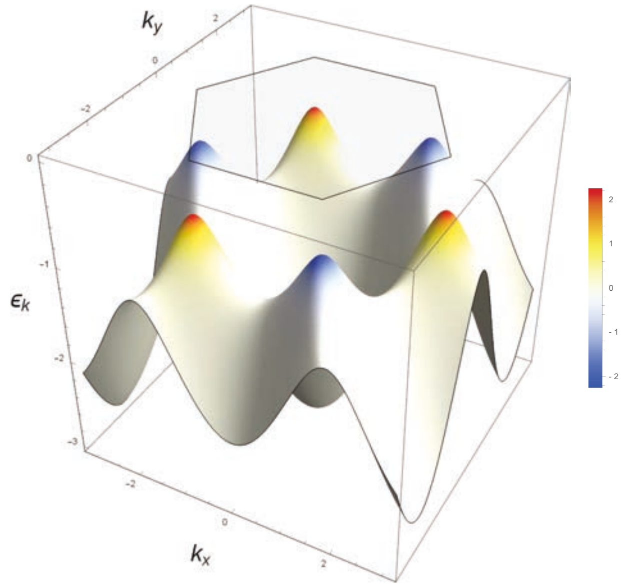
Graphene

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

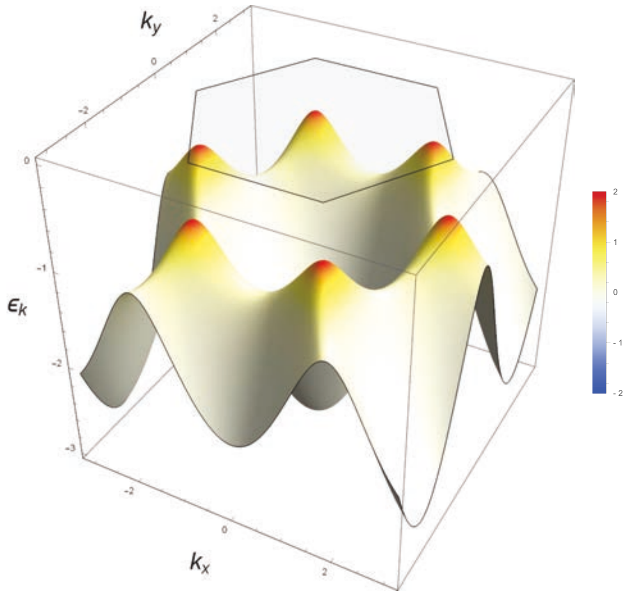
Graphene



Break inversion
Sublattice potential



Break TR
complex nn hopping

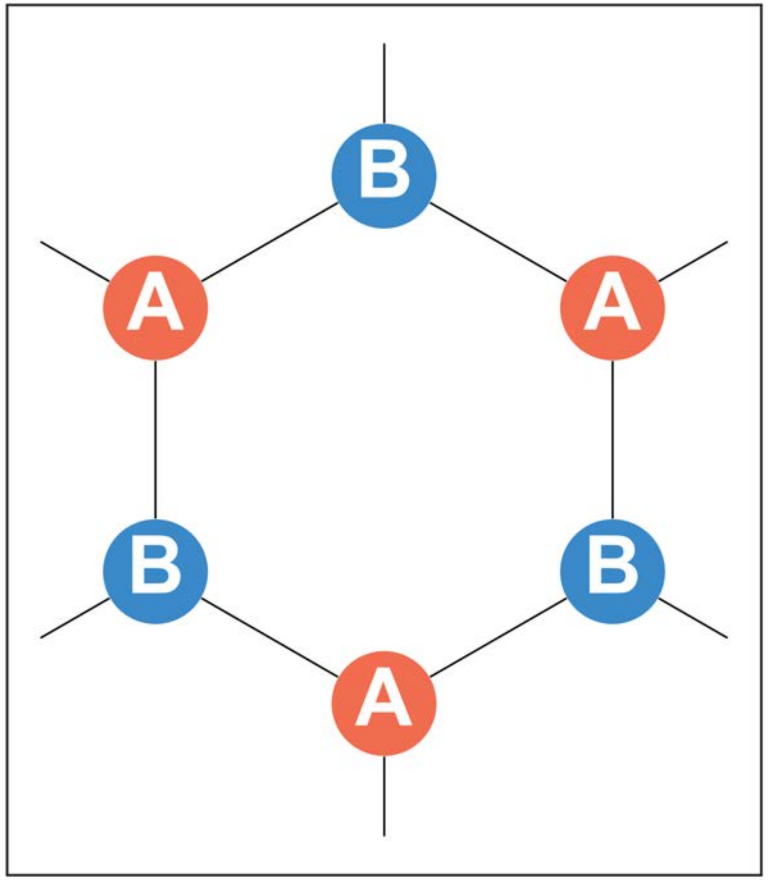


Dirac points protected by inversion and time reversal symmetry

(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

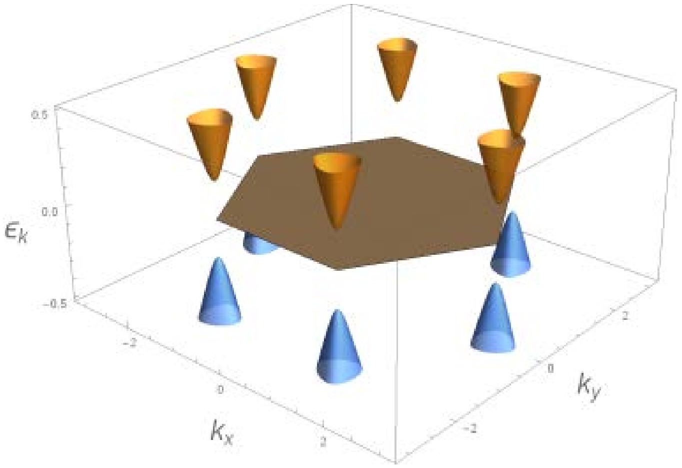


Potential energy difference between sublattices

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

breaks inversion (and C_6 rotation, etc.).
This introduces uniform $d_z(\mathbf{k})$.

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



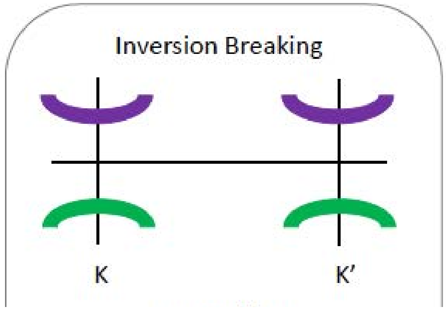
Graphene

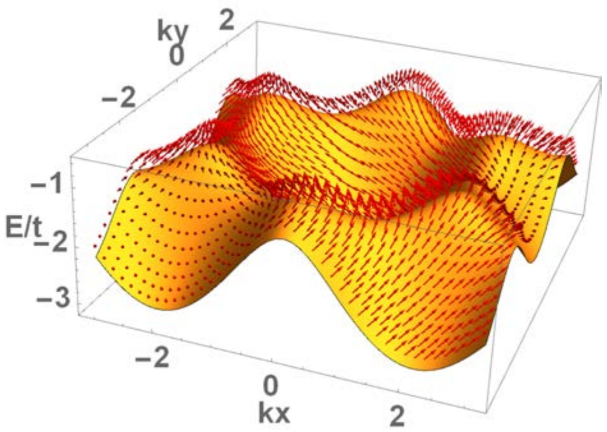
$$H=\sum_q\left(c^+_{\mathbf{K}_++\mathbf{q},A}\quad c^+_{\mathbf{K}_++\mathbf{q},B}\quad c^+_{\mathbf{K}_-+\mathbf{q},A}\quad c^+_{\mathbf{K}_-+\mathbf{q},B}\right)\begin{pmatrix}0 & h_q & 0 & 0\\ h_q^* & 0 & 0 & 0\\ 0 & 0 & 0 & h_q^*\\ 0 & 0 & h_q & 0\end{pmatrix}\begin{pmatrix}c_{\mathbf{K}_++\mathbf{q},A}\\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

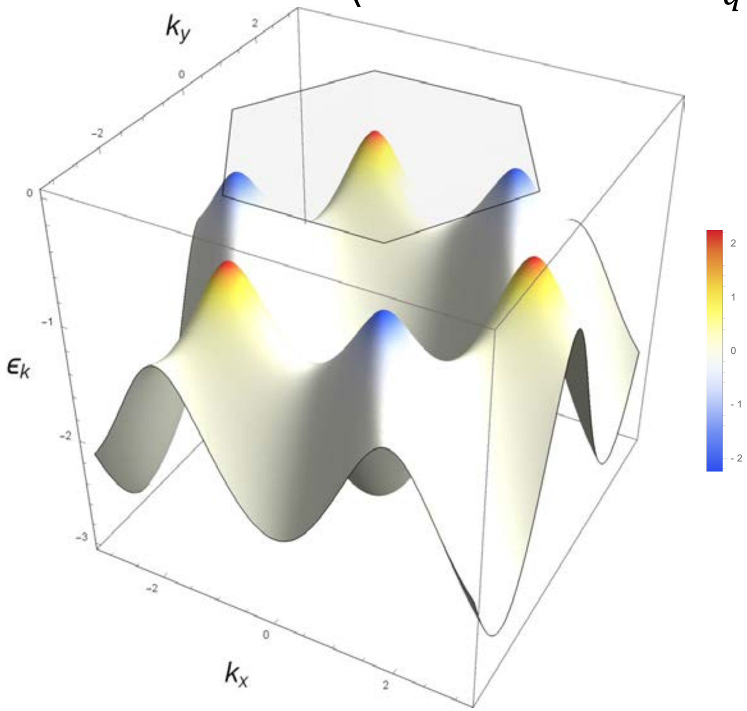
where $h_{\mathbf{q}}=\frac{3ta}{2}\left(-q_x+i\,q_y\right)$

With sublattice potential

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

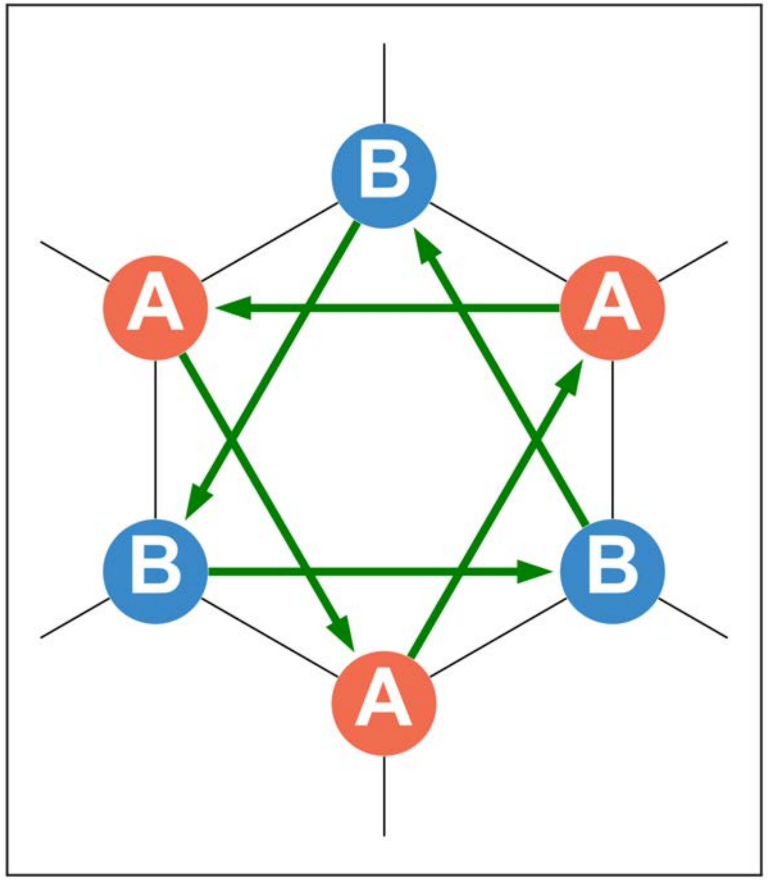






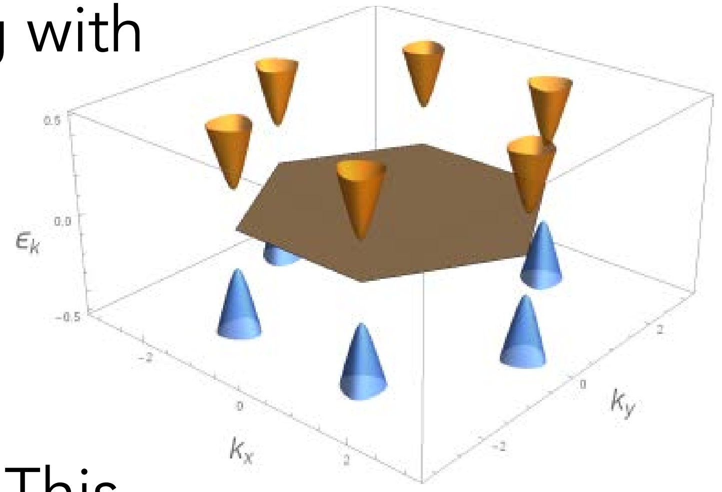
Introduce Dirac mass by breaking symmetry

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



Next nearest neighbor hopping with imaginary amplitude

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



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

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

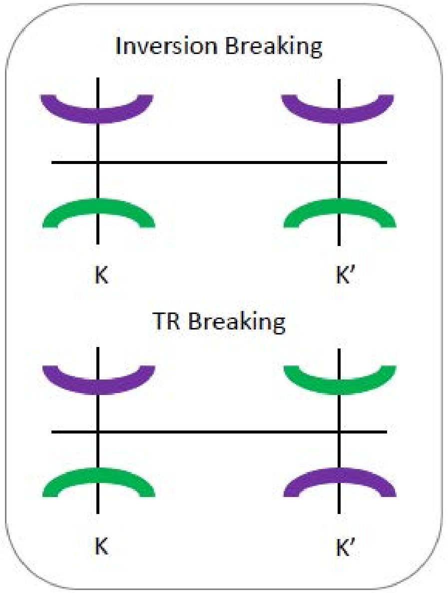
$$m_H = 3\sqrt{3}\lambda_H$$

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

Graphene

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

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

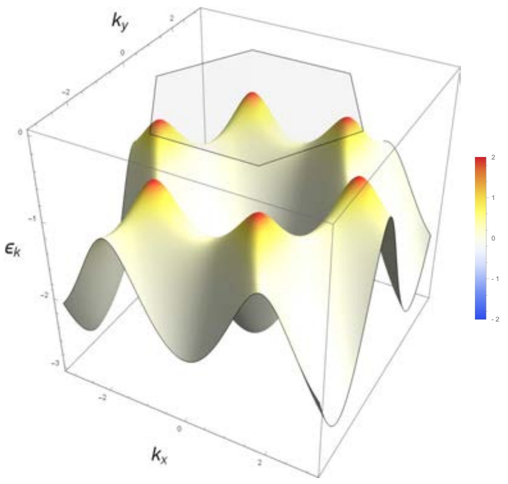


$$H=\sum_q \left(c^+_{\mathbf{K}_++\mathbf{q},A} \quad c^+_{\mathbf{K}_++\mathbf{q},B} \quad c^+_{\mathbf{K}_-+\mathbf{q},A} \quad c^+_{\mathbf{K}_-+\mathbf{q},B}\right)\begin{pmatrix} m_H & h_q & 0 & 0 \\ h_q^* & -m_H & 0 & 0 \\ 0 & 0 & -m_H & h_q^* \\ 0 & 0 & h_q & m_H \end{pmatrix}\begin{pmatrix}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

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

With Haldane mass

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



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

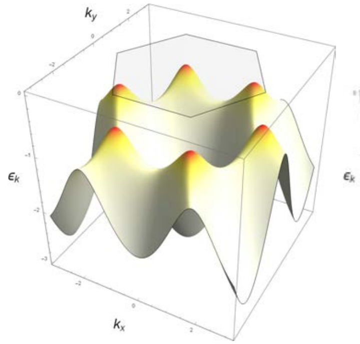
Kane-Mele:

With Haldane mass $\times\sigma^z$

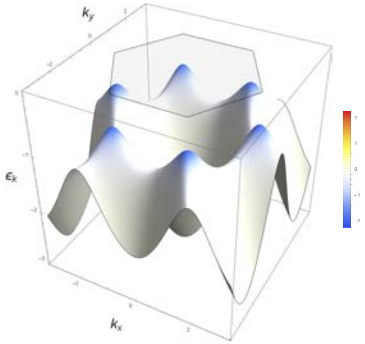
$$H=\sum_q \begin{pmatrix} c^+_{\mathbf{K}_+ +\mathbf{q},A\uparrow} & c^+_{\mathbf{K}_+ +\mathbf{q},B\uparrow} & c^+_{\mathbf{K}_- +\mathbf{q},A\uparrow} & c^+_{\mathbf{K}_- +\mathbf{q},B\uparrow} & c^+_{\mathbf{K}_+ +\mathbf{q},A\downarrow} & c^+_{\mathbf{K}_+ +\mathbf{q},B\downarrow} & c^+_{\mathbf{K}_- +\mathbf{q},A\downarrow} & c^+_{\mathbf{K}_- +\mathbf{q},B\downarrow} \end{pmatrix}$$

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

spin $\uparrow$



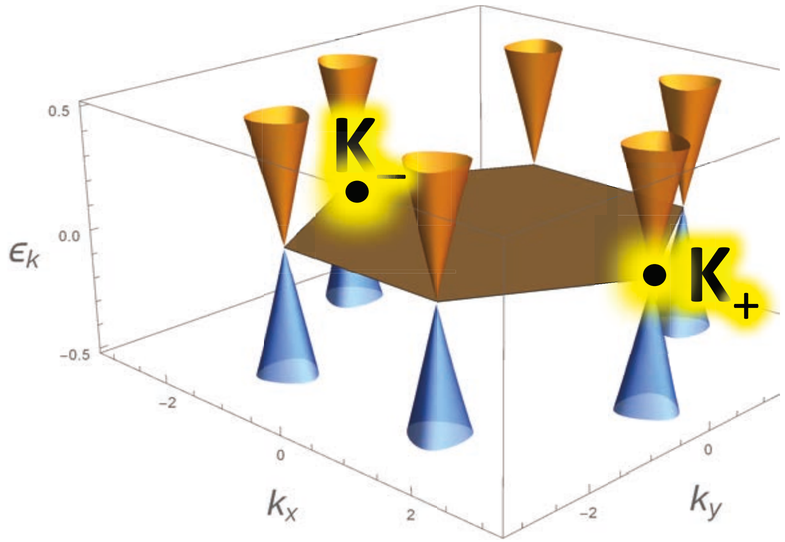
spin $\downarrow$

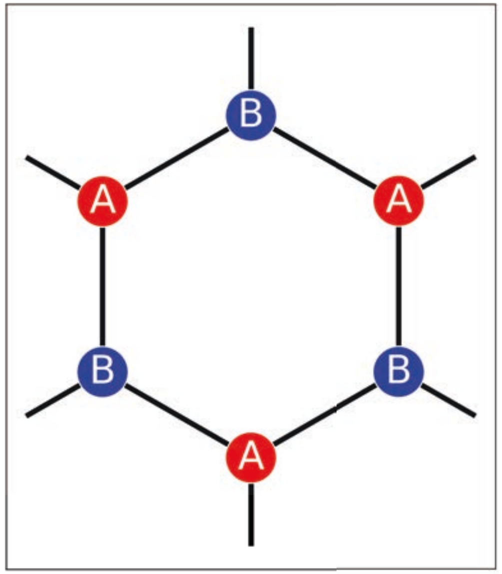


σ Spin

τ Sublattice

χ Valley





….sheer poetry

Material → Model