Topological phase transition in 3D noncentrosymmetic systems

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- Hiroki Isobe (U. Tokyo)
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Reference

- M. S. Bahramy, **B. -J. Yang**, R. Arita, and N. Nagaosa, Nature Communications, 3, 679 (2011).
- **B. -J. Yang**, M. S. Bahramy, R. Arita, H. Isobe, E.-G. Moon and N. Nagaosa, Phys. Rev. Letts. 110, 086402 (2013).
- **B. -J. Yang** ,E.-G. Moon, H. Isobe, and N. Nagaosa, in preparation

Outline

1. Accidental band crossing and topological phase transition

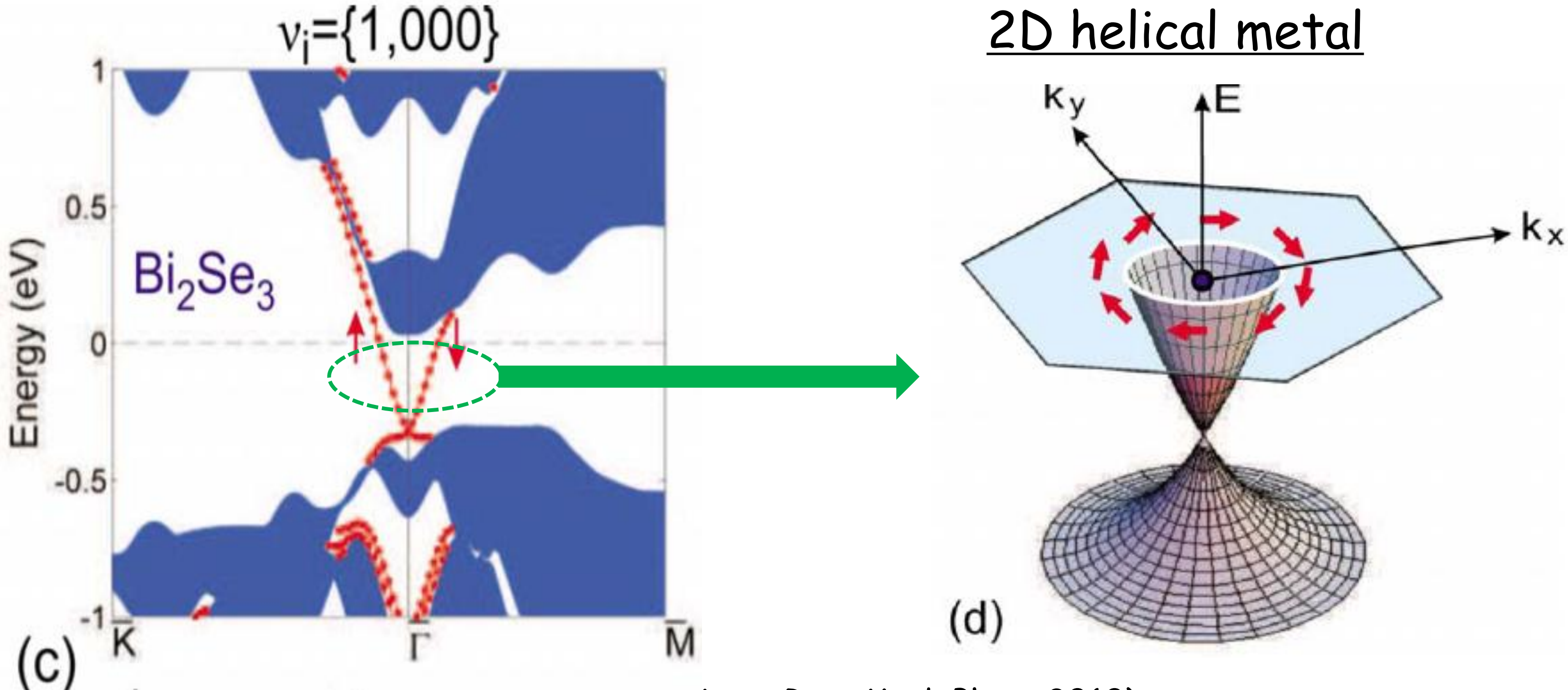
- Introduction to 3D topological insulators.
- Topological phase transition via accidental band touching
- Direct topological transition between two insulators

2. (Direct) topological phase transition in BiTeI

- Topological phase transition of pressured BiTeI (First-principle cal.)
- Unusual band dispersion near the quantum critical point
- Physical properties at the quantum critical point

3D topological insulator

3D narrow gap semi-conductors with 2D helical Dirac metal on the surface



(Hasan and Kane, Rev. Mod. Phys. 2010)

Topologcal stability of the surface states :

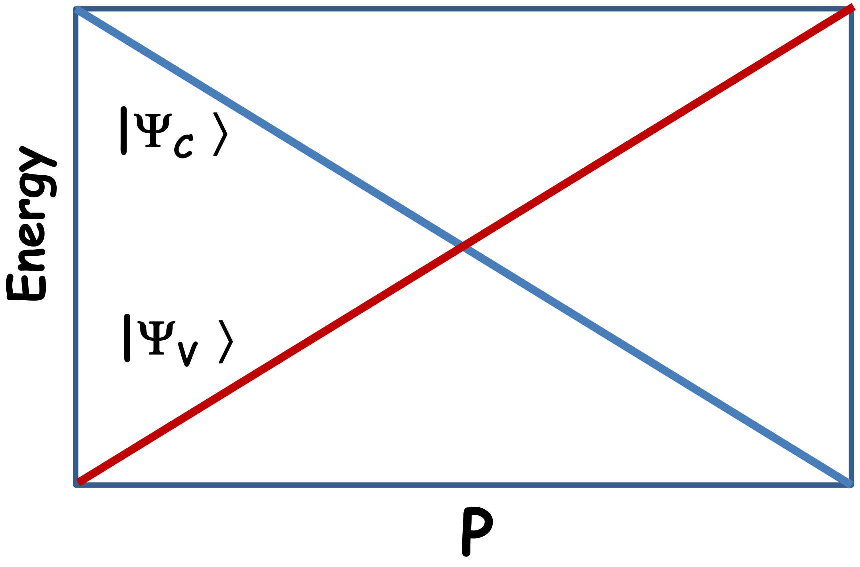
bulk gap and time-reversal symmetry

Topological phase transition

Accidental band crossing

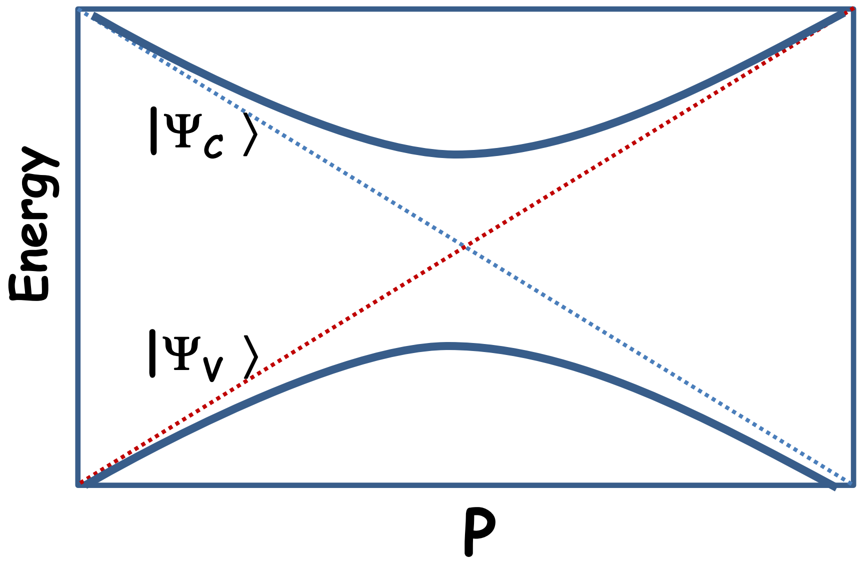
A single tuning parameter : P

Level crossing



v.s.

Level repulsion (anti-crossing)



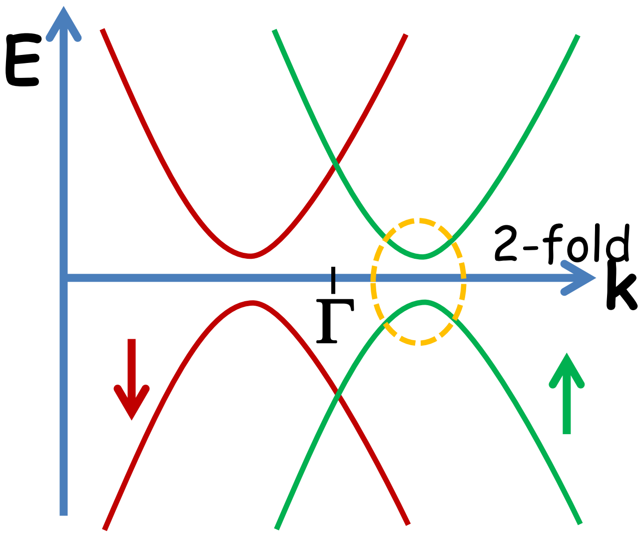
Accidental band crossing is not easy to achieve !

Conditions for accidental band crossing

Depends on the symmetry and dimensionality of the system

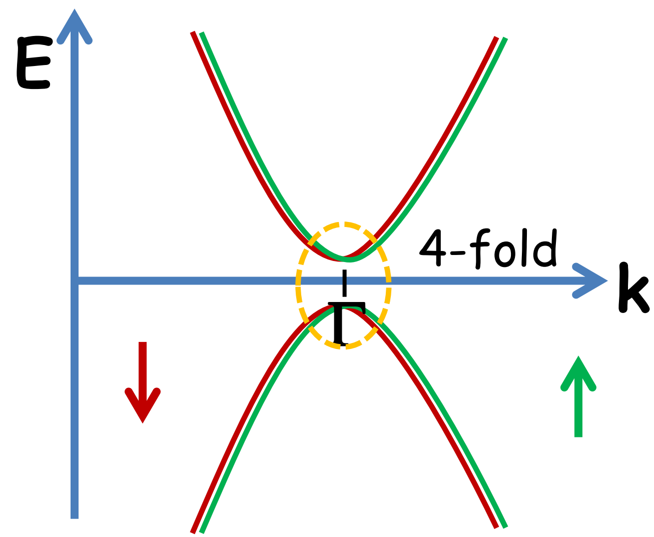
(1) Symmetry : number of equations to be satisfied (D_C: codimension)

TRS(O), inversion (X)



D_C=3

TRS(O), inversion (O)



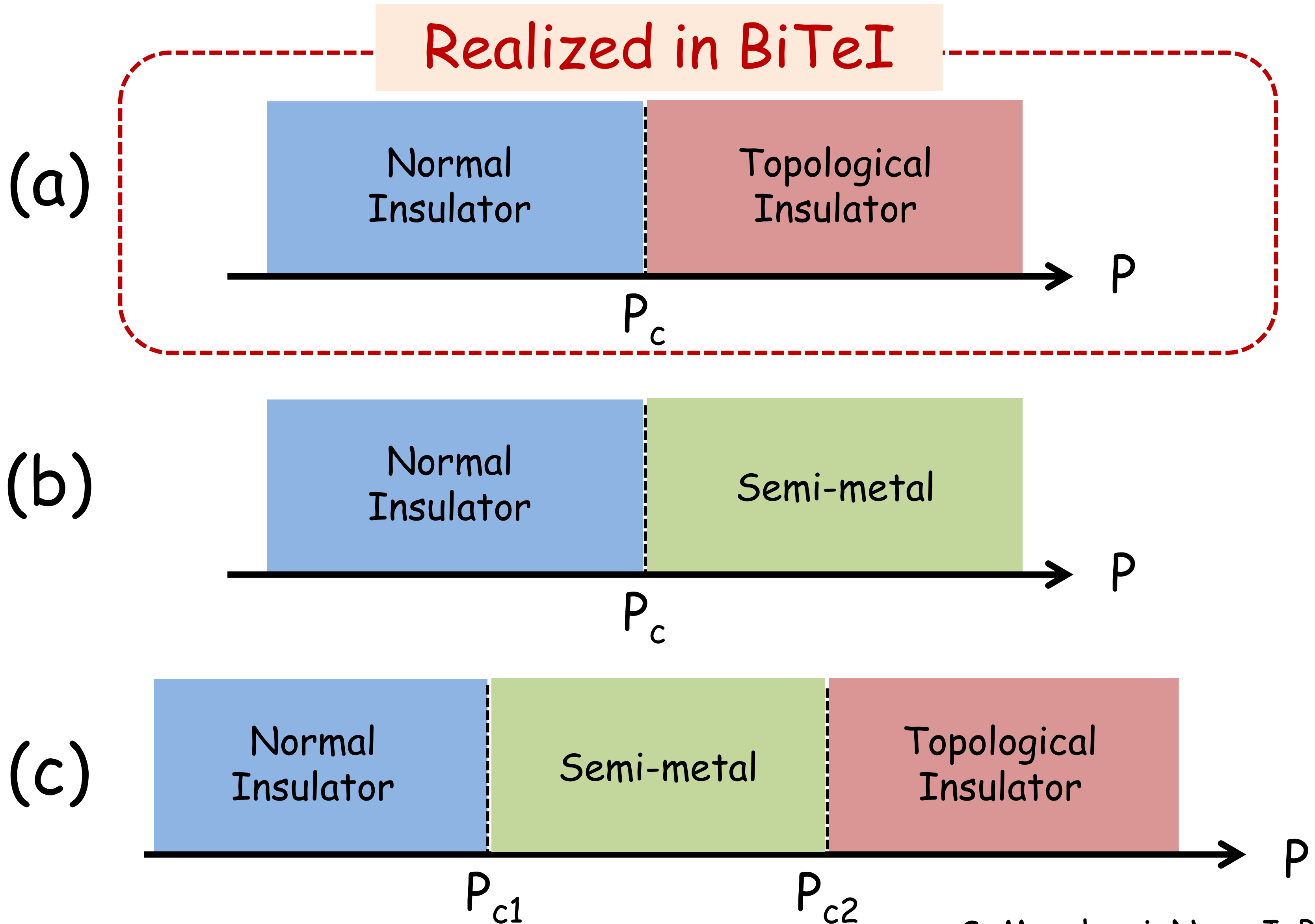
D_C=5

(2) Dimensionality : total number of parameters (N_P) of $\Psi(\mathbf{k},P)$

(i) N_P = 3 in 2D (kx,ky,P), (ii) N_P = 4 in 3D (kx,ky,kz,P)

Accidental band crossing is possible for $\mathbf{N_P \geq D_C}$

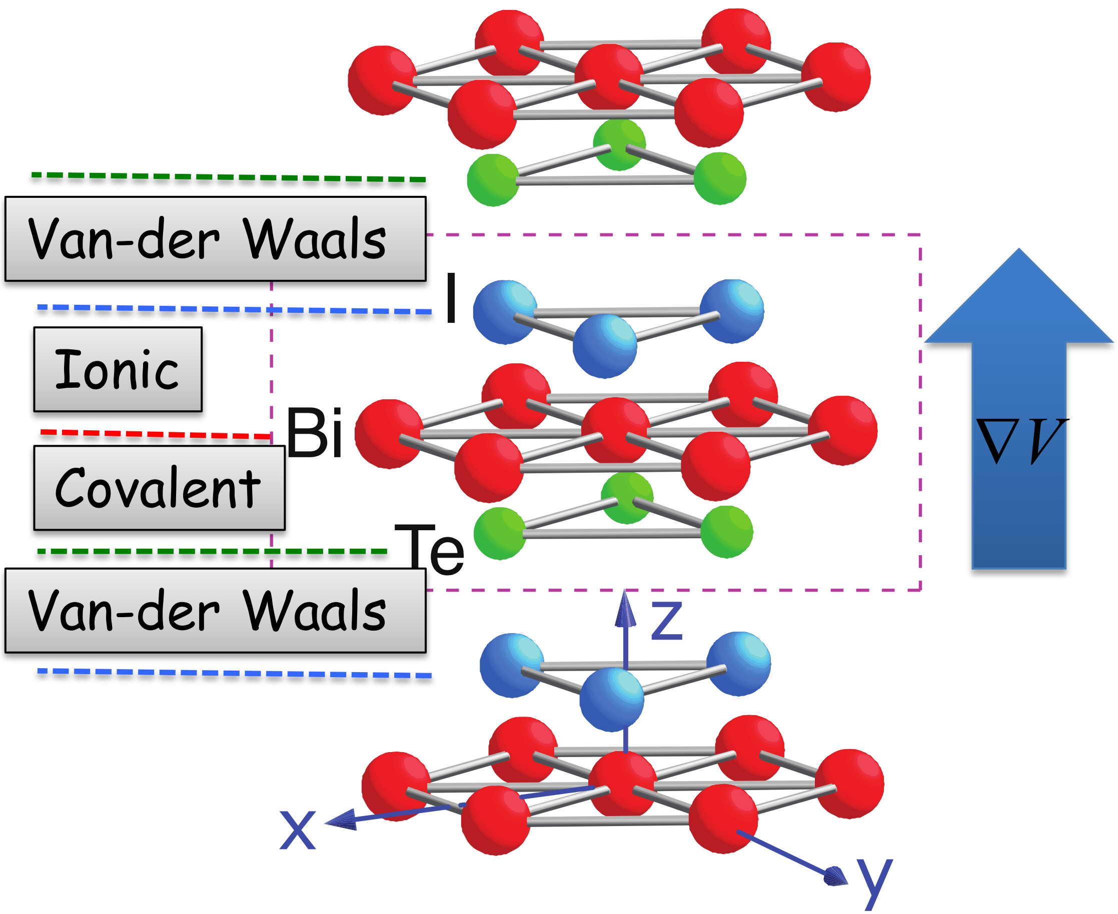
Phase diagram in 3D noncentrosymmetric

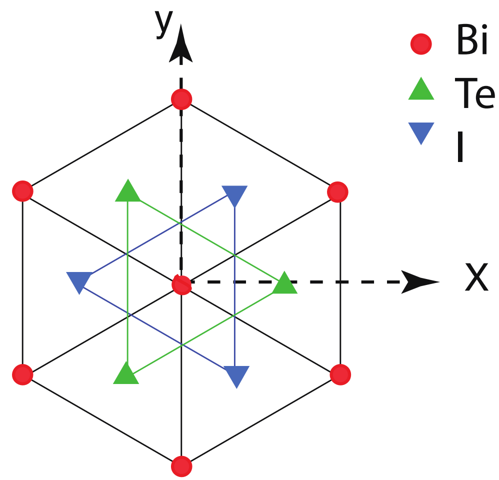


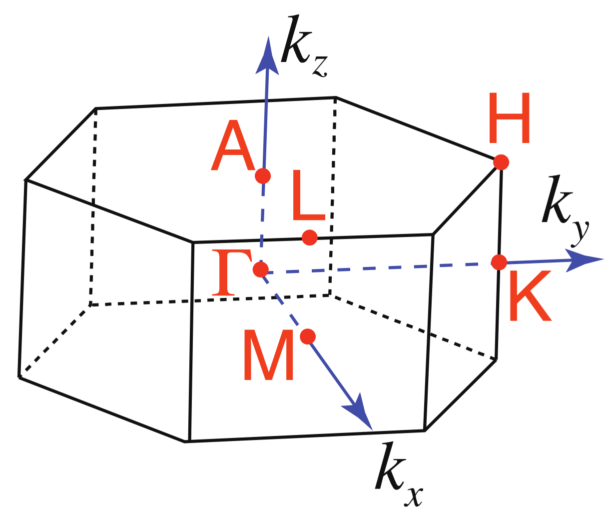
S. Murakami, New. J. Phys.

Lattice structure of BiTeI

- BiTeI : polar layered semiconductor





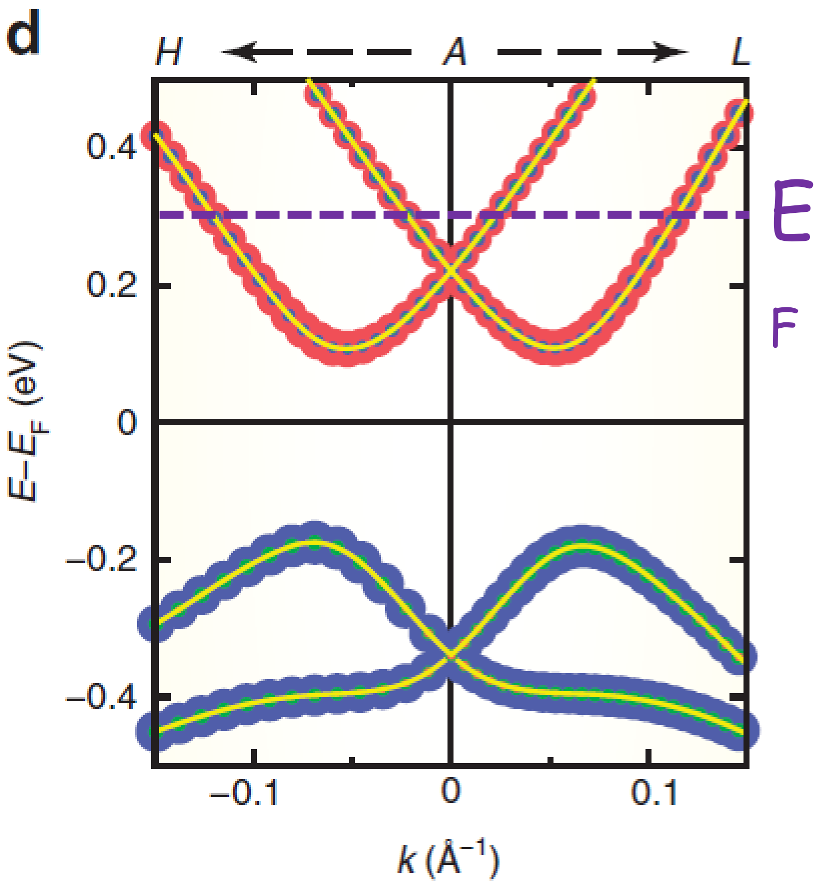


Broken I-symmetry + Strong atomic SOI of Bi

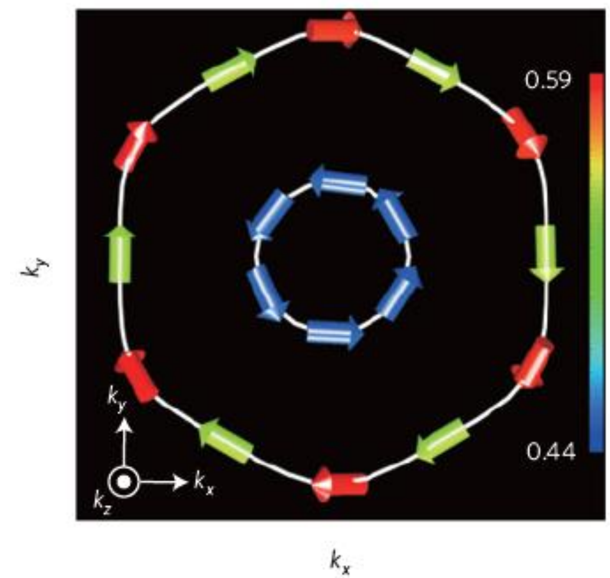
Bulk band structure : Rashba spin-splitting

Broken inversion symmetry → Spin splitting due to spin-orbit coupling (SOC)

$$H_{SO} = \frac{\hbar}{4m^2c^2}(\vec{\nabla}V \times \vec{p}) \cdot \vec{\sigma}$$



Fermi surface

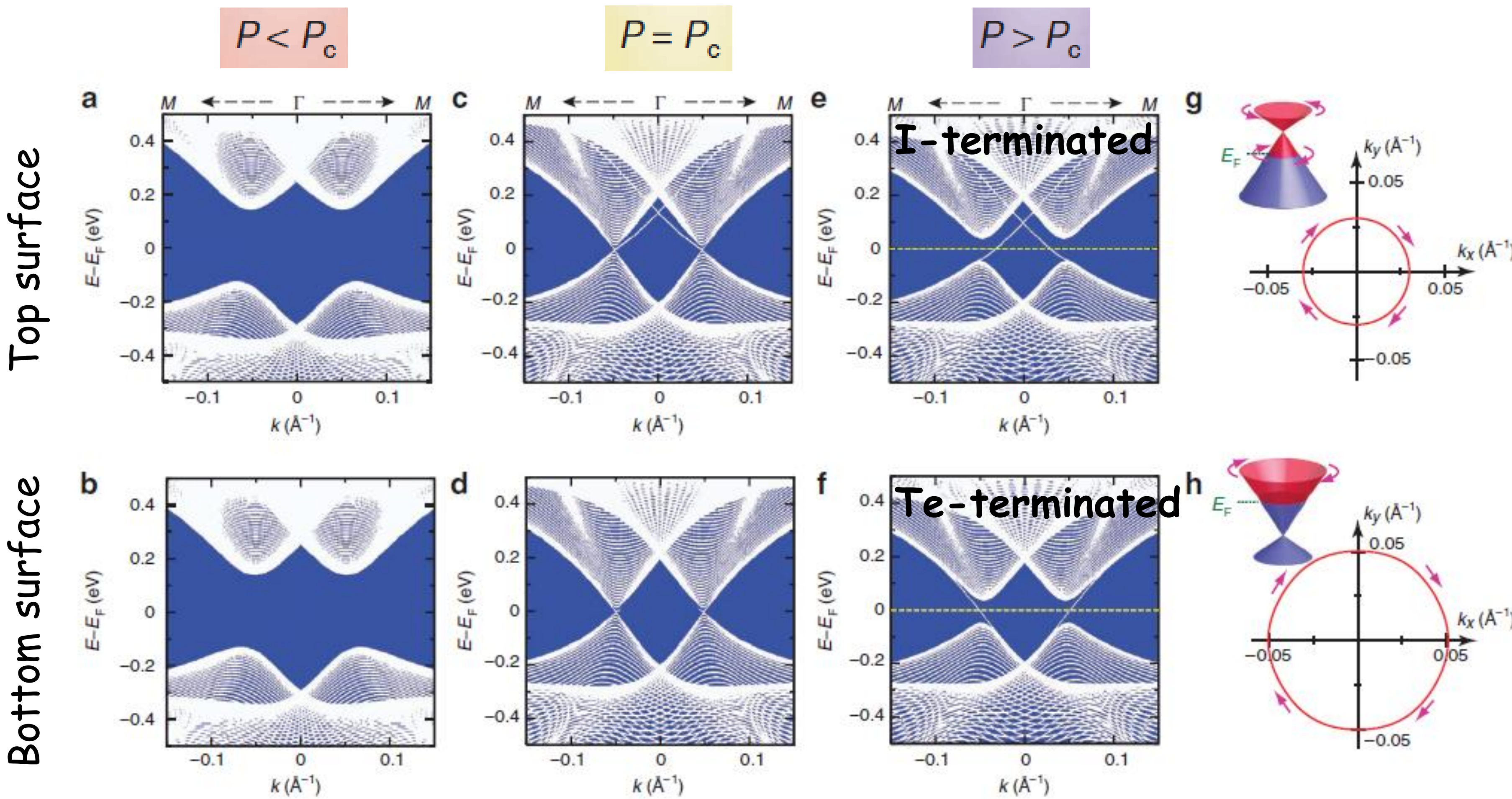


Ishizaka et al. (2011)

Rashba spin splitting in bulk bands !

Topological phase transition under pressure

- Energy spectrum $E(k_x,k_y;z)$ of a system with finite length along the z-direction

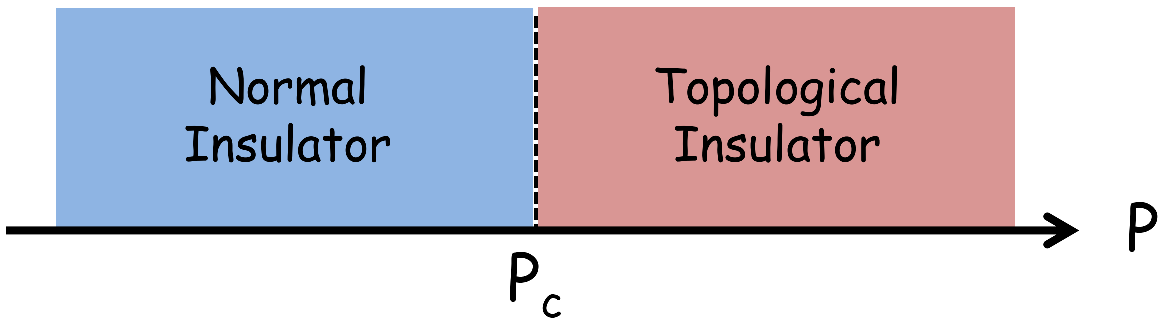


- Spin helicity of the top and bottom surface states are the same !

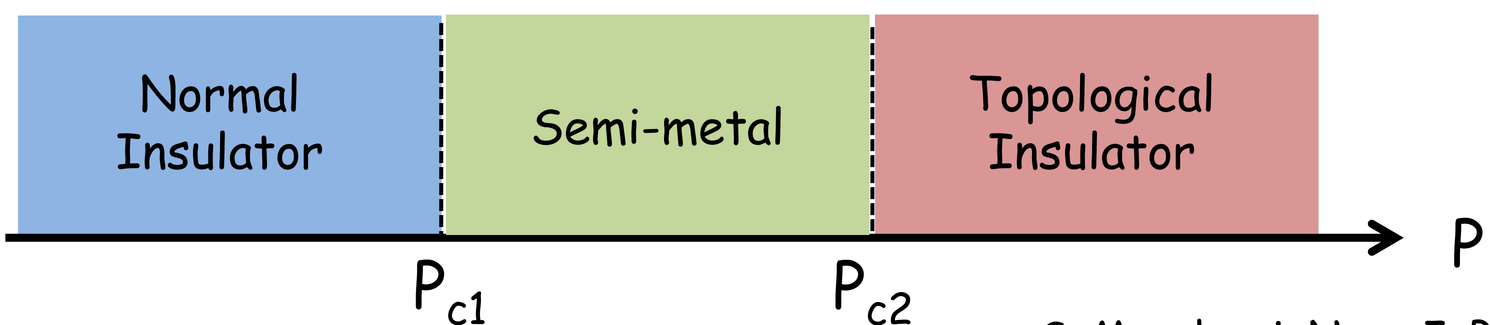
cf) Inversion symmetric TI : opposite spin helicity

Direct insulator-insulator transition

Highly unusual phase diagram !



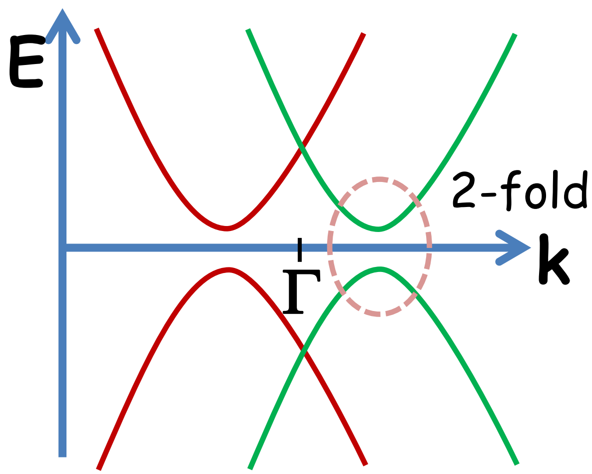
cf) Generic phase diagram in 3D noncentrosymmetric systems



S. Murakami, New. J. Phys.

Band crossing in 3D non-centrosymmetric systems

TRS(O), inversion (X)



$$H = f_0 + f_1\sigma_1 + f_2\sigma_2 + f_3\sigma_3$$

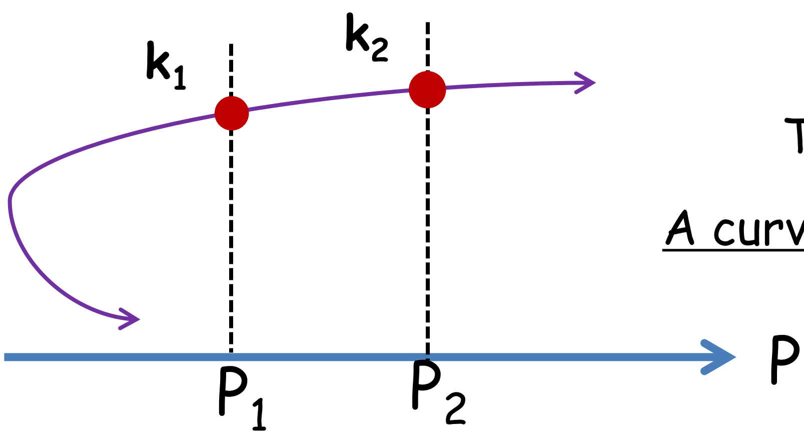
$$E_{conduction} = f_0 + (f_1^2 + f_2^2 + f_3^2)^{1/2},$$

$$E_{valence} = f_0 - (f_1^2 + f_2^2 + f_3^2)^{1/2}$$

Crossing of two bands

$$\begin{cases} f_1(k_x, k_y, k_z, P) = 0 \\ f_2(k_x, k_y, k_z, P) = 0 \\ f_3(k_x, k_y, k_z, P) = 0 \end{cases}$$

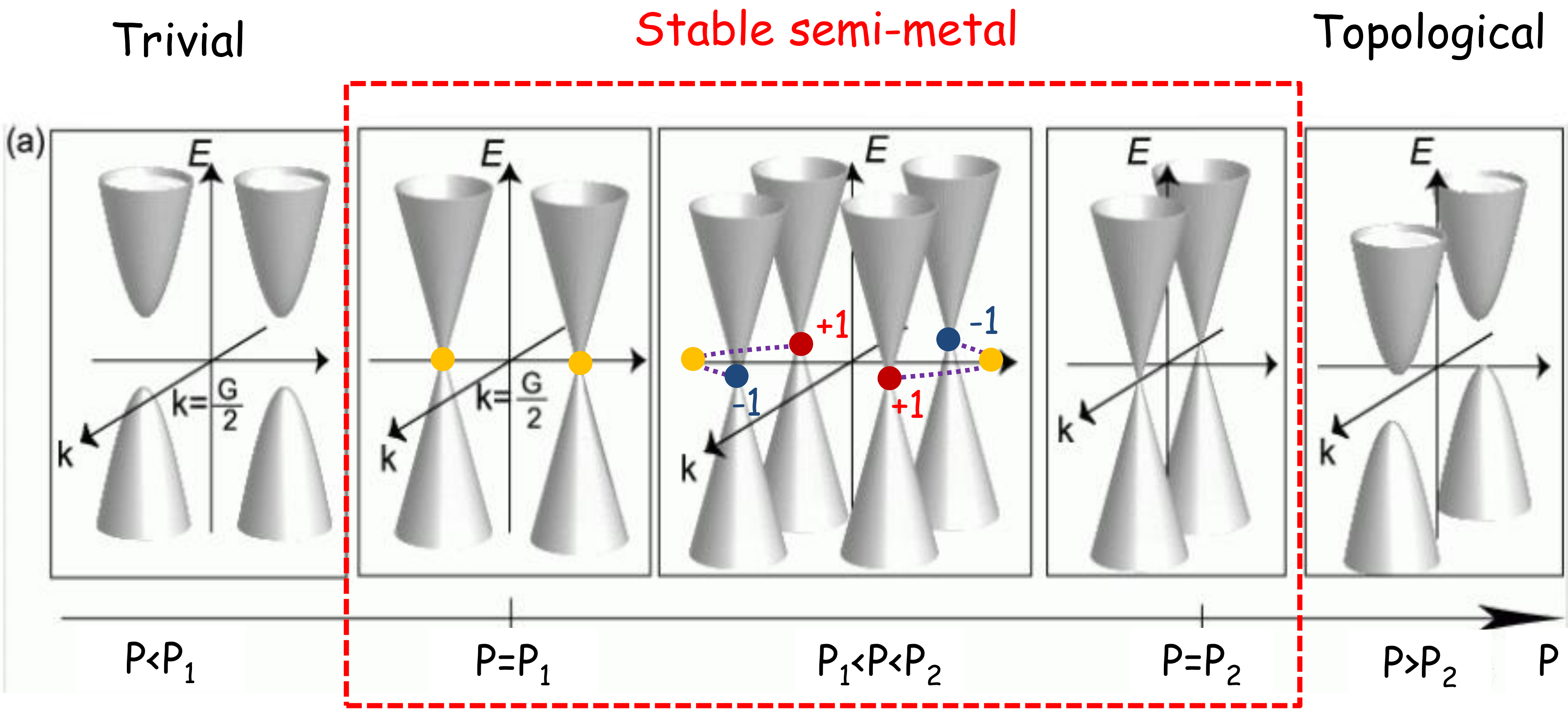
One free parameter !



Trajectory of gap-closing point : $\mathbf{k}_c = \mathbf{k}_c(P)$

A curve in 3D momentum space with a parameter P !

Intermediating semi-metallic states



S. Murakami, New. J. Phys.

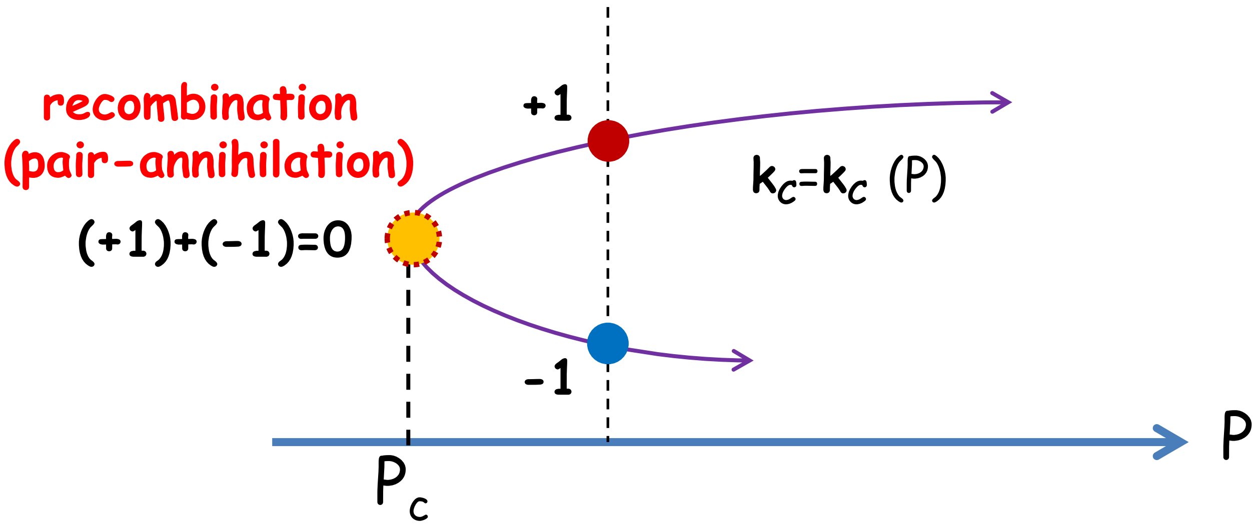
"Weyl fermions !"

$$H = (\mathbf{v}_1 \cdot \mathbf{k})\sigma_1 + (\mathbf{v}_2 \cdot \mathbf{k})\sigma_2 + (\mathbf{v}_3 \cdot \mathbf{k})\sigma_3$$

$$\text{Chiral charge} = \frac{\mathbf{v}_1 \cdot (\mathbf{v}_2 \times \mathbf{v}_3)}{|\mathbf{v}_1 \cdot (\mathbf{v}_2 \times \mathbf{v}_3)|}$$

How to achieve a direct transition ?

1. Zero chiral charge at the critical point



2. Small number of constraints : $N_{Parameter}=4 > N_{Constraint}=3$

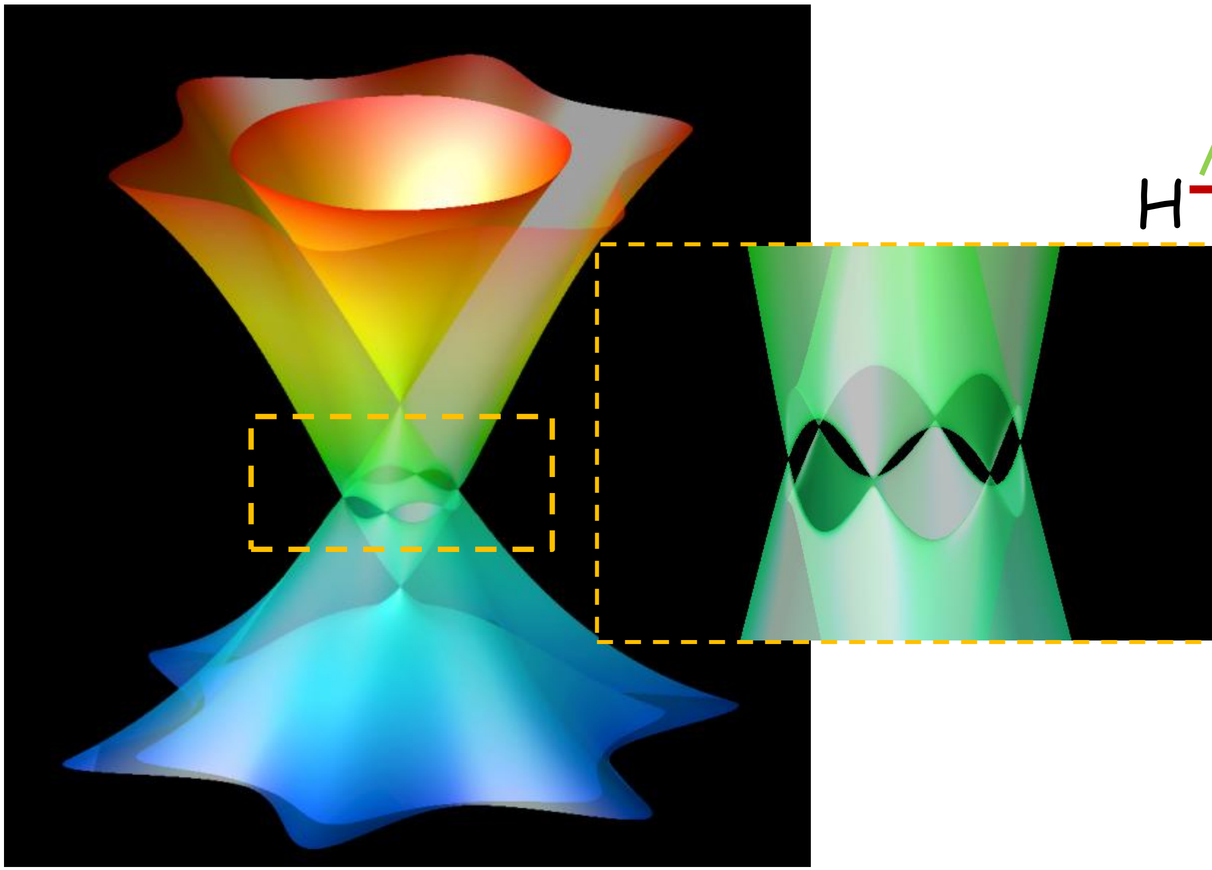
$$H= f_0 + f_1\sigma_1 + f_2\sigma_2 + f_3\sigma_3$$

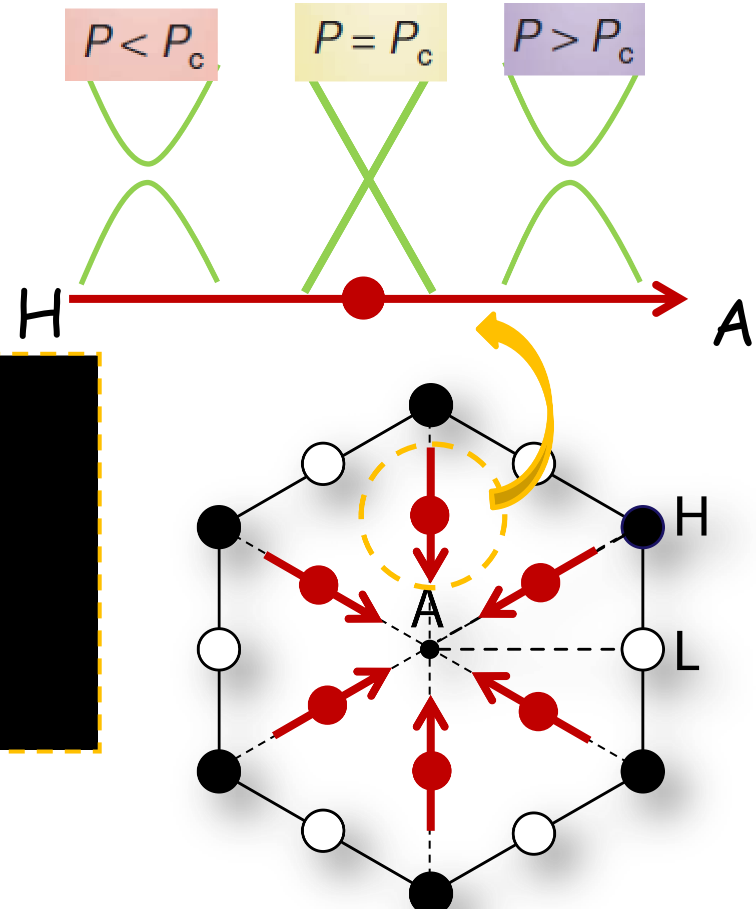
Impose additional constraint from crystalline symmetry ! ($N_c \rightarrow N_c +1$)

Add $f_4 (k_x , k_y , k_z , P) = 0$

Constraint from crystalline symmetry

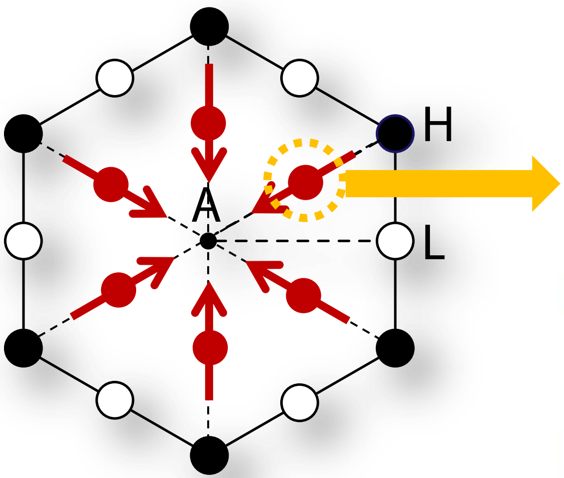
$P = P_c$



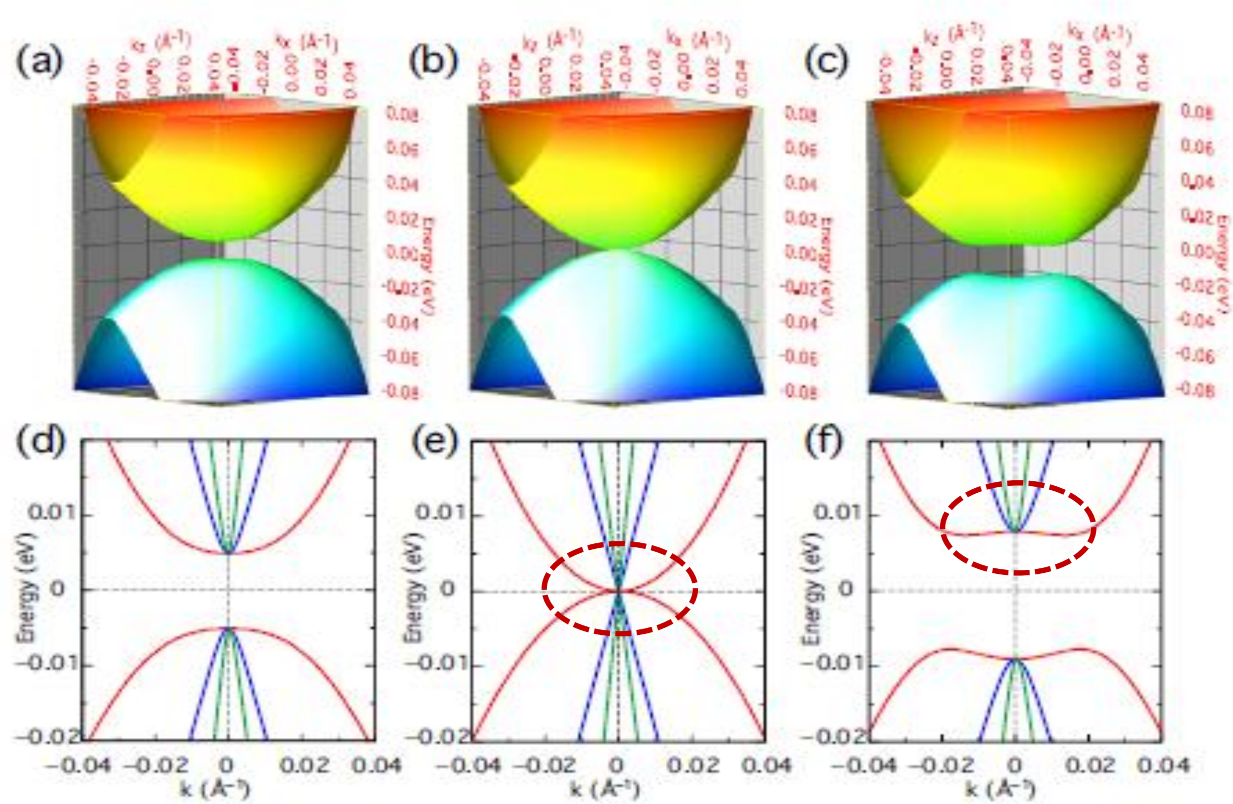


Conduction band: $H_c(k) = \frac{k_x^2 + k_y^2}{2m^*_{\perp,c}} + \frac{(k_z - \pi/c)^2}{2m^*_{\parallel,c}} + \underbrace{v_{k,c}(k_x\sigma_y - k_y\sigma_x)}_{\text{Rashba}} + \underbrace{\lambda_c\left(3k_x^2 - k_y^2\right)k_y\sigma_z}_{\text{Warping}},$

Evidence for direct insulator-insulator transition



$P < P_c$ $P = P_c$ $P > P_c$



$P = P_c$ → Anisotropic dispersion $H_{\mathrm{QCP}}(\mathbf{p}) = A p_1^2 \tau_1 + v p_2 \tau_2 + v p_3 \tau_3,$

$P > P_c$ → Saddle point

Unusual properties at the quantum critical point

$$H_{\mathrm{QCP}}(\mathbf{p}) = A p_1^2 \tau_1 + v p_2 \tau_2 + v p_3 \tau_3,$$

1. Unusual temperature dependence

specific heat ($C_V(T)$), compressibility ($\kappa(T)$), diamagnetic susceptibility ($\chi_D(T)$), DC conductivity ($\sigma_{DC}(T)$)

	$D(\varepsilon)$	$C_V(T)$	$\kappa(T)$	$\chi_D(T)$	$\sigma_{DC}(T)$
Weyl semi-metal	ε^2	T^3	T^2	$\ln T$	T
At the QCP	$\varepsilon^{3/2}$	$T^{5/2}$	$T^{3/2}$	$T^{-1/2}$	$T^{1/2}$

2. Anisotropic DC conductivity : $\sigma_{11} / \sigma_{33} \propto T$

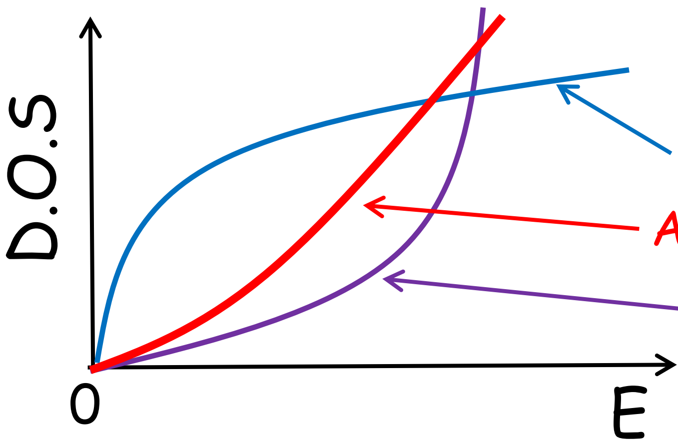
(1) Coulomb scattering (e-e interaction) : $\frac{1}{\tau} = \alpha^2 T$ with $\alpha = \frac{e^2}{4\pi\varepsilon v}$

$$\sigma_{11}(T) \propto T^{3/2} \quad \sigma_{22,33}(T) \propto T^{1/2}$$

(2) Disorder scattering (Born approx.): $\frac{1}{\tau(w)} \approx 2\pi\gamma_0 D(w)$ with $\gamma_0 = \frac{n_i V_0^2}{2}$

$$\sigma_{11} \propto T, \qquad \sigma_{22,33} = \text{const.}$$

Long-range Coulomb interaction at QCP



Quadratic dispersion (D~E $^{1/2}$) : relevant (E.G.Moon)

Anisotropic dispersion (D~E $^{3/2}$) : ???

Linear dispersion (D~E ^{2}) : marginally irrelevant

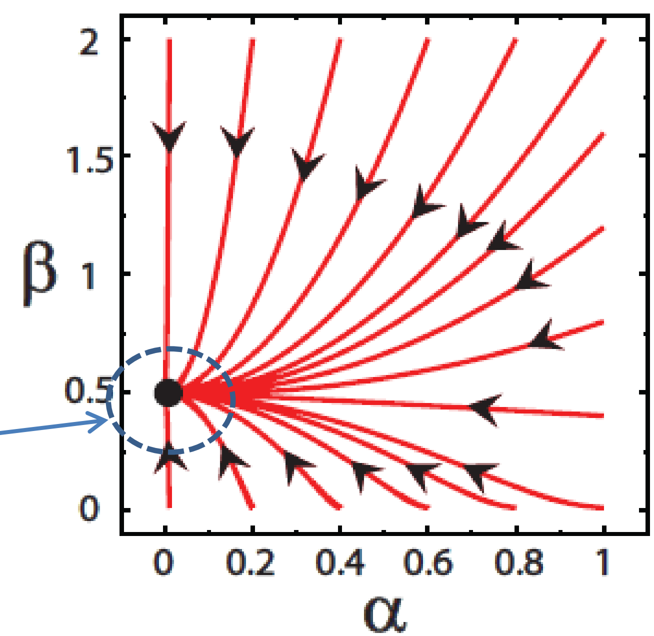
$$V_C(\mathbf{q}) = \frac{g^2}{\mathbf{q}^2}$$

- One loop RG analysis

$$H_{\rm QCP}(\mathbf{p}) = A p_1^2 \tau_1 + v p_2 \tau_2 + v p_3 \tau_3,$$

$$\alpha \sim \frac{g^2}{v} \qquad \beta \sim \frac{g^2}{A\Lambda}$$

Stable fixed point
(α=0,$\beta \neq$0)

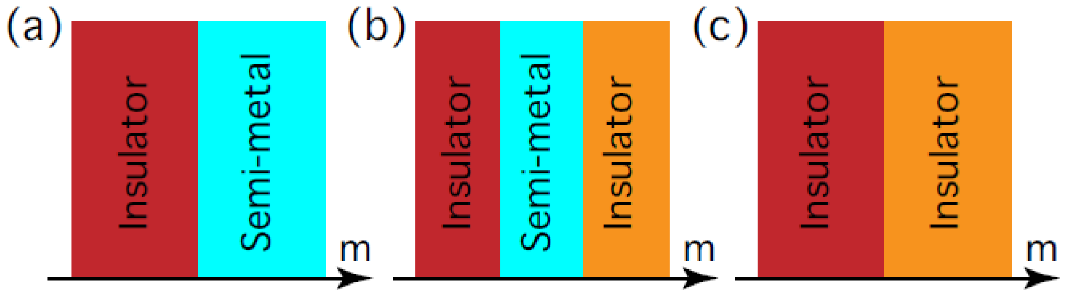


$$V_{\rm screened}(\mathbf{q}) \sim \frac{g^2}{q_1^2 + \eta q_\perp^{3/2}}$$

Anisotropic screened Coulomb interaction !

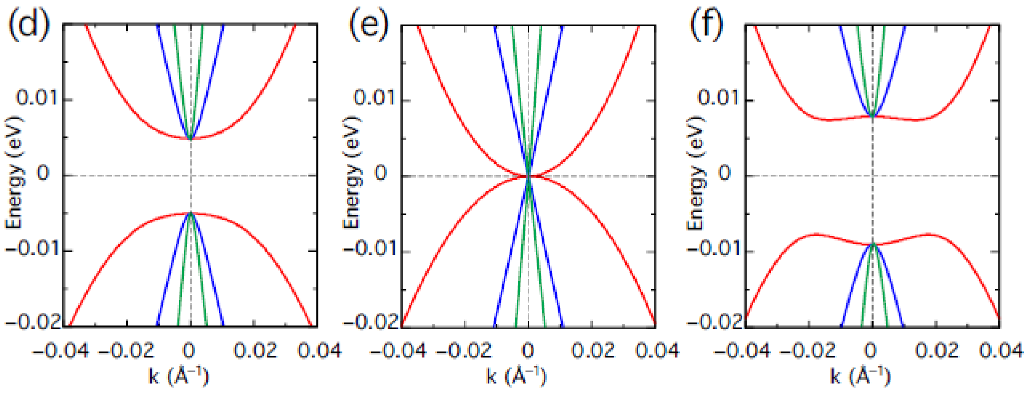
Summary

1. Generic phase diagram of 3D non-centrosymmetric system achievable via accidental band crossing



2. Direct insulator-insulator transition due to crystalline symmetry

3. Anisotropic dispersion at the critical point



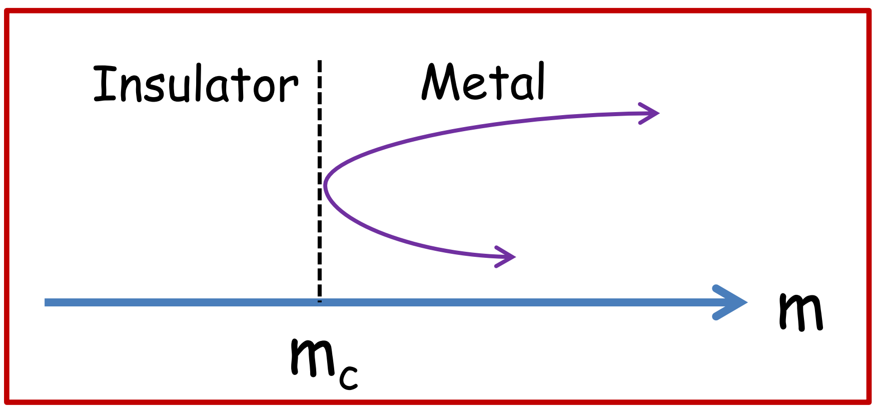
4. Unusual thermodynamic properties and anisotropic transport properties

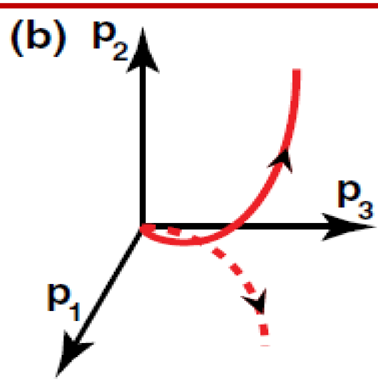
Fate of semi-metallic phase

- Semi-metal phase has topological stability !

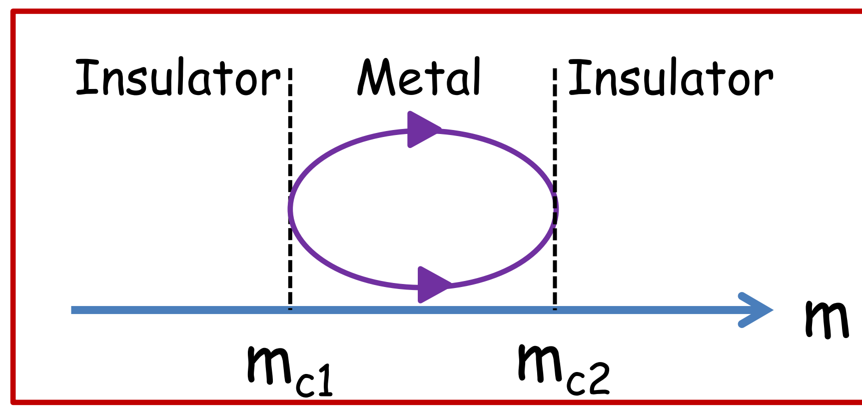
The shape of the trajectory of the gap-closing points determines the phase diagram!

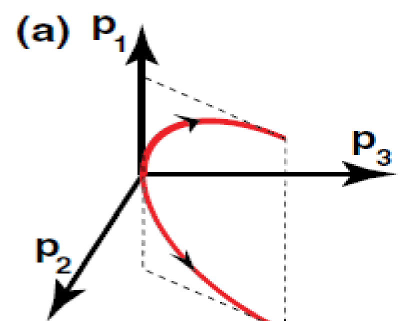
1. $k_c = k_c$ (m) open curve
: a curve with finite torsion





2. $k_c = k_c$ (m) closed curve
: a curve with zero torsion

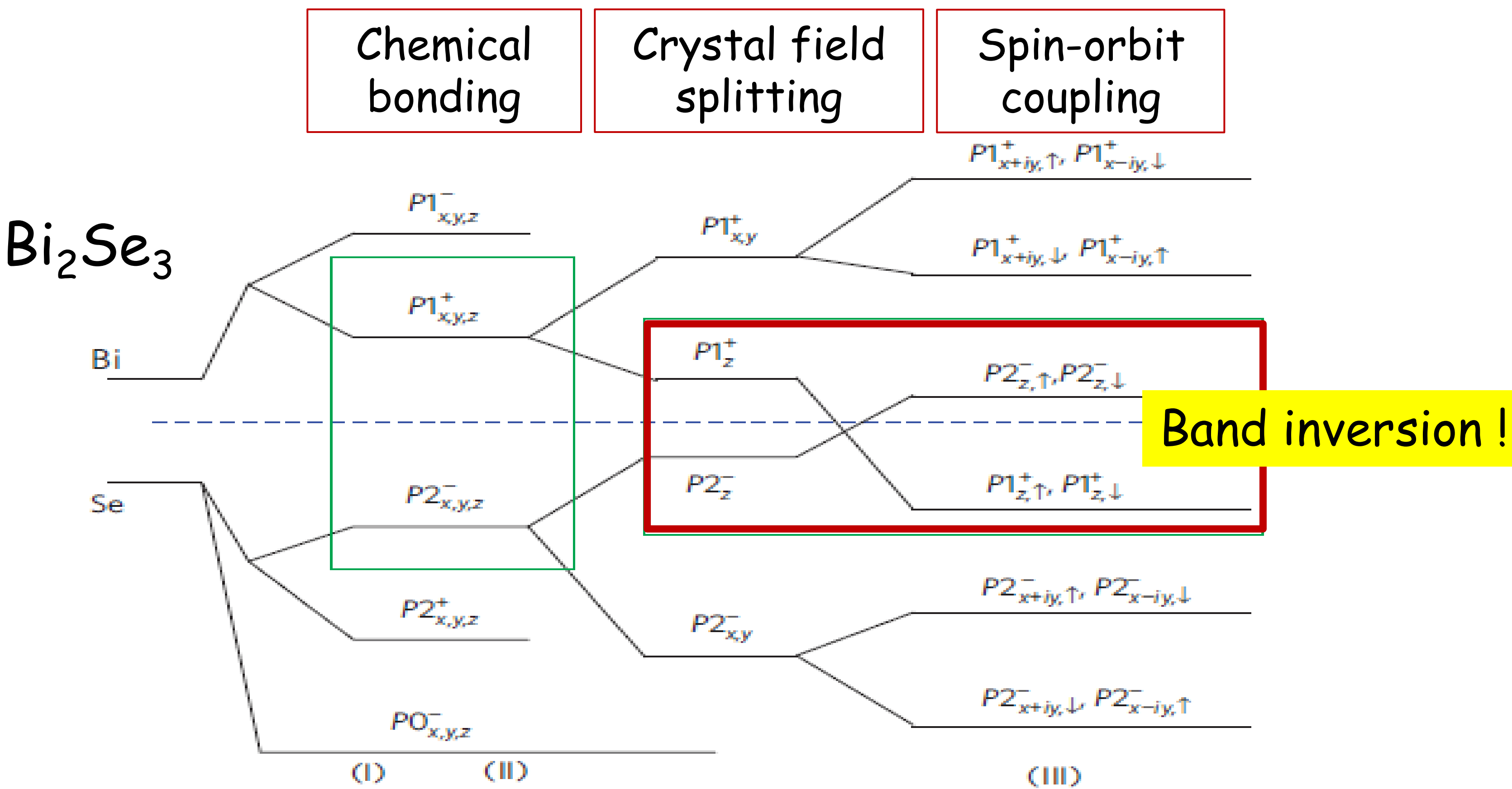




Spin-orbit coupling induced band inversion

Searching for new topological insulators

- Guiding principle: spin-orbit coupling induced band inversion (parity exchange through accidental band crossing)

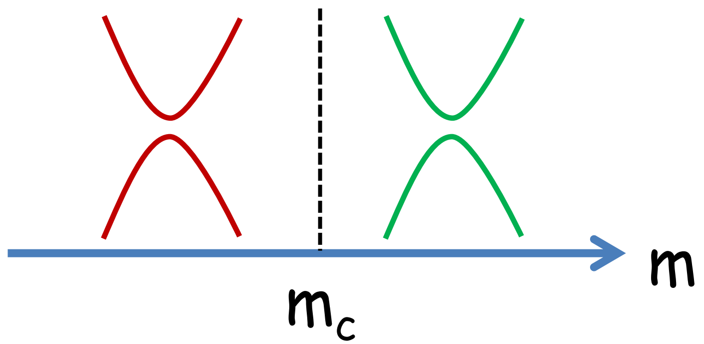


(H. Zhang et al., Nat. Phys. (2009))

Conditions for the direct insulator-insulator transition

- Away from the critical point ($m<m_c$ and $m>m_c$):

  Conduction and valence bands should have an extremum !



$H= f_1\sigma_1 + f_2\sigma_2 + f_3\sigma_3,$

$E^2 = f_1^2 + f_2^2 + f_3^2$

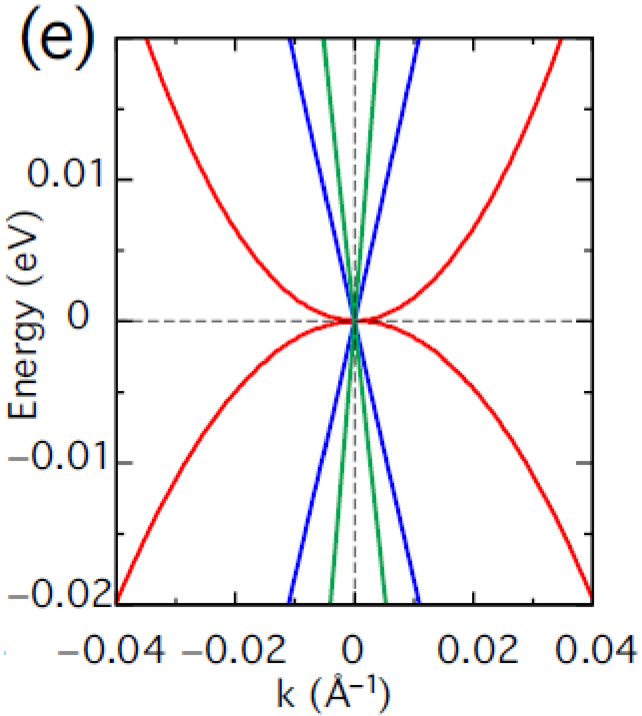
Examine the condition for extremum : $\partial E/\partial p_1 = \partial E/\partial p_2 = \partial E/\partial p_3 = 0$

- Condition for the direct transition

  :The location of the extremum should move along a straight line.

Anisotropic dispersion at the quantum critical point

- Anisotropic dispersion at QCP : direct consequence of zero chiral charge



$H_{Weyl} = (\mathbf{v}_1 \cdot \mathbf{k})\sigma_1 + (\mathbf{v}_2 \cdot \mathbf{k})\sigma_2 + (\mathbf{v}_3 \cdot \mathbf{k})\sigma_3$

↓ Unitary transform

$H_{Weyl} = c_1 Q_{chiral}\, p_1 \sigma_1 + c_2 p_2 \sigma_2 + c_3 p_3 \sigma_3$

↓ QCP with **zero chiral charge**

$$H_{\mathrm{QCP}}(\mathbf{p}) = A p_1^2 \tau_1 + v p_2 \tau_2 + v p_3 \tau_3$$

Density of states : $D(E) \propto E^{3/2}$

Cf) Weyl semi-metal $D(E) \propto E^2$,
Quadratic band dispersion $D(E) \propto E^{1/2}$