How to measure the Chiral magnetic effect and phase transitions of topological semimetals under strong field

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Z.D. Song, et al, Phys. Rve. B, 94, 214306, 2016
Z.D. Song, et al, arXiv:1705.05119

Outline

- Introduce to the topological semimetal
- Chiral magnetic effect as the key property of TSM
- Detect the CME by the dynamics of Pseudo scalar phonon modes
- Nematic and charge density wave (CDW) instabilities for Dirac semimetal under magnetic field

Definition of Topological Semi-Metal(TSM)

- Topological Semi-metal: metal with vanishing FS, insulator with vanishing energy gap, band crossings at Fermi level
- Semi-metals defined above can all described by Topological invariance: Weyl, Dirac, Nodal lines
- TSM has very unique and fruitful transport properties (mostly under magnetic field)
- New Fermions: three-fold and six-fold points： arXiv:1603.03093

Proposed materials

Type	Compound	proposing reference
DSM, high symmetry line	Na_3Bi	39
DSM, high symmetry line	Cd_3As_2	41
DSM, high symmetry line	$BaAuBi$	42
DSM, high symmetry line	$LiGaGe$	42
DSM, high symmetry point	BiO_2	40
DSM, high symmetry point	HfI_3	42
WSM, Magnetic, type I	$Rn_2Ir_2O_7$	10
WSM, Magnetic,type I	$HgCr_2Se_4$	24
WSM, Magnetic,type II	$YbMnBi_2$	58
WSM, non-Magnetic,type I	$TaAs$ family	35,36
WSM, non-Magnetic,type I	Te and Se under pressure	34
WSM, non-Magnetic,type I	Ta_3S_2	59
WSM, non-Magnetic,type I	$CuTlSe_2$ family	60
WSM, non-Magnetic,type II	WTe_2 and $MoTe_2$	14
NLSM w/o SOC	Carbon Mackay-Terrones structure	51
NLSM w/o SOC	Cu_3PdN	56,57
NLSM w/o SOC	LaN	52
NLSM w/o SOC	Black Phosphorus under pressure	54
NLSM w/o SOC	Ca_3P_2	53
NLSM w/o SOC	$CaAgX$	55
NLSM with SOC	$TlTaSe_2$	50
NLSM with SOC	$SrIrO3$	49

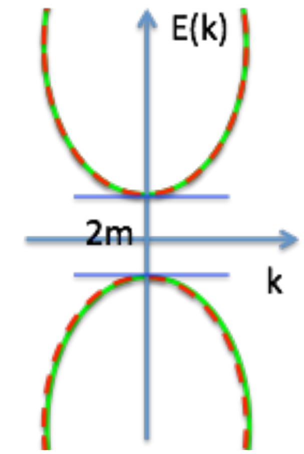
Dirac *vs.* Weyl

Quantum mechanics + Relativistic

Dirac Equation (1928) 4x4

$$\begin{pmatrix} \hat{E} - c\boldsymbol{\sigma}\cdot\hat{\mathbf{p}} & 0 \\ 0 & \hat{E} + c\boldsymbol{\sigma}\cdot\hat{\mathbf{p}} \end{pmatrix}\psi = mc^2\begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}\psi$$

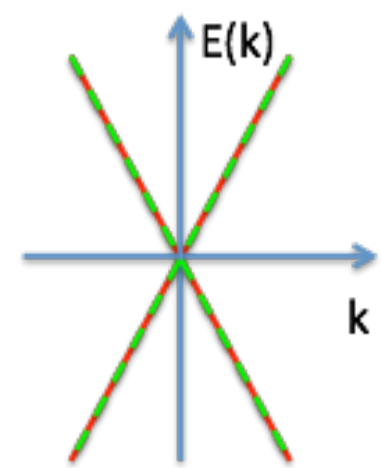
$$E(k) = \pm\sqrt{k^2 + m^2}$$



Massive Fermion

Weyl Equation (1929) 2x2

$$H(\vec{k}) = \vec{k}\cdot\vec{\sigma} = \begin{bmatrix} k_z & k_x - ik_y \\ k_x + ik_y & -k_z \end{bmatrix}$$



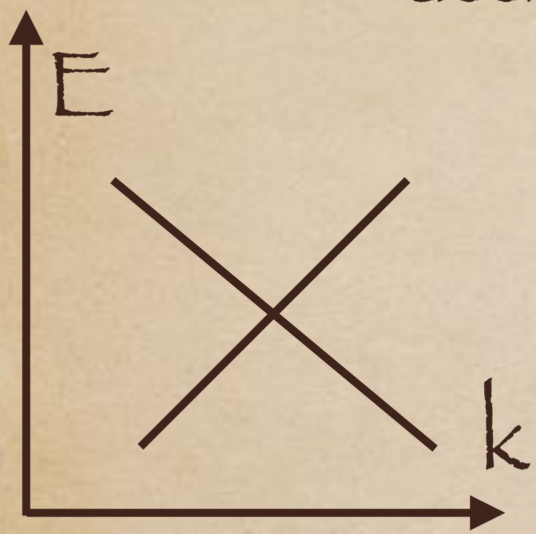
Massless Fermion

Two Weyl Equations with opposite Chirality

H. Weyl, "Electron and gravitation," Z. Phys. 56, 330 (1929)

Weyl Fermion in solid

"accidental" band crossing in the band structure



$$H = \vec{v}_x \cdot \vec{\sigma} k_x + \vec{v}_y \cdot \vec{\sigma} k_y + \vec{v}_z \cdot \vec{\sigma} k_z$$

$$\chi = sgn[(\vec{v_x} \times \vec{v_y}) \cdot \vec{v_z}]$$

Principle axises:

singular value decomposition

$$H = \sum_{\alpha\beta = x,y,z} v_{\alpha\beta} \sigma_\alpha k_\beta = \sum_i \lambda_i \bar{k}_i \bar{\sigma}_i \qquad \hat{v} = \hat{L} \hat{\lambda} \hat{R}$$

$$\bar{\sigma}_i = \sum_\alpha \sigma_\alpha L_{\alpha i} \quad \bar{k}_i = \sum_\beta R_{\beta i} k_\beta \quad \chi = sgn[det(R) \cdot det(L)]$$

$$\epsilon_k = \sqrt{\lambda_1^2 k_1^2 + \lambda_2^2 k_2^2 + \lambda_3^2 k_3^2}$$

Moving the Weyls around by smoothly changing the Hamiltonian

$$H = \sum_{\alpha\beta=x,y,z} v_{\alpha\beta}\sigma_\alpha k_\beta = \sum_i \lambda_i \bar{k}_i \bar{\sigma}_i$$

$$H' = \sum_i c_i \bar{\sigma}_i$$

$$\Downarrow$$

$$\lambda_i \bar{k}_i + c_i = 0$$

Weyl points and singularity of Berry's Curvature

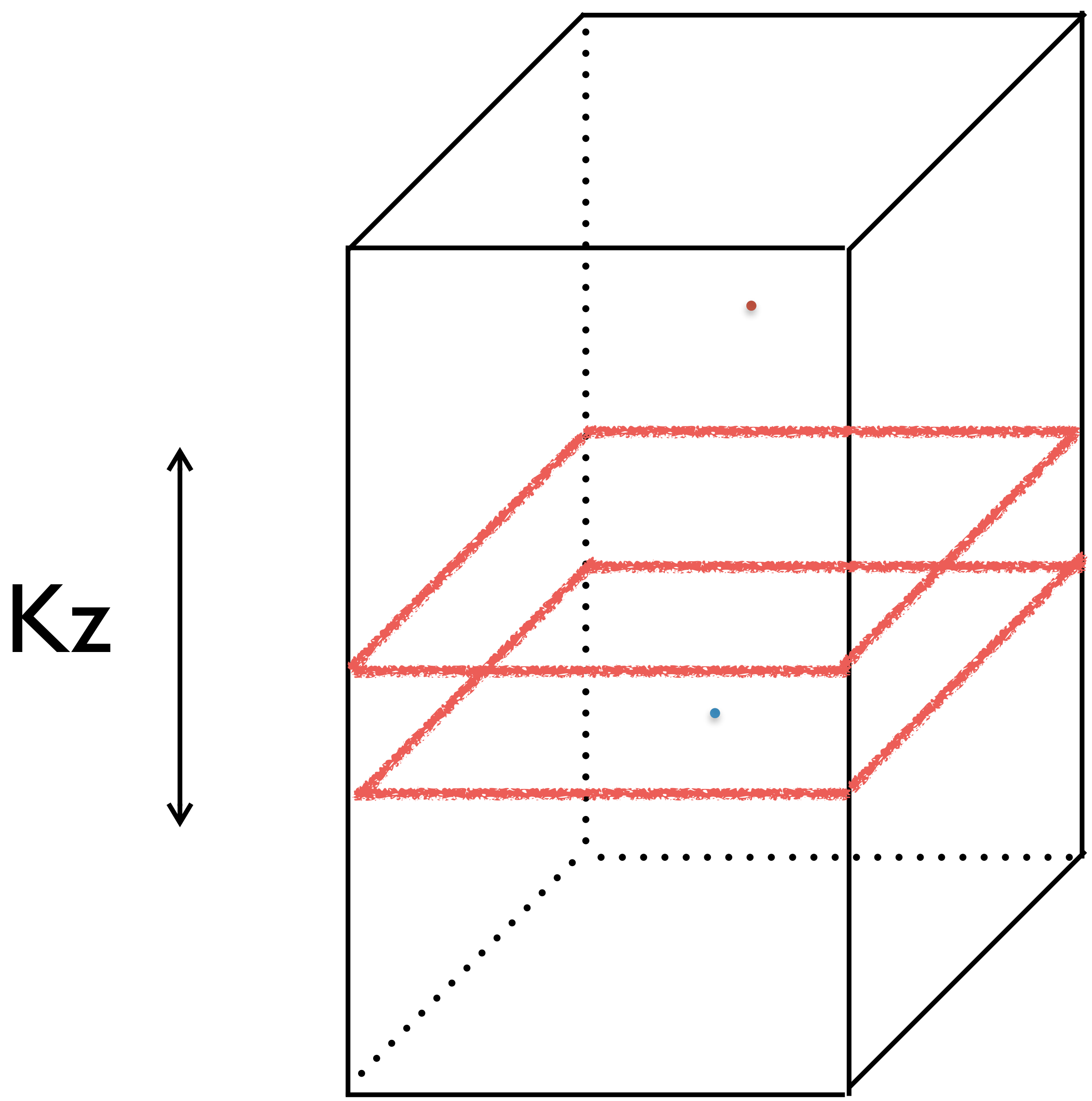
- Weyl points are always come in pairs with opposite chirality for any lattice model.
- Weyl points are the singular point of the Berry's Curvature

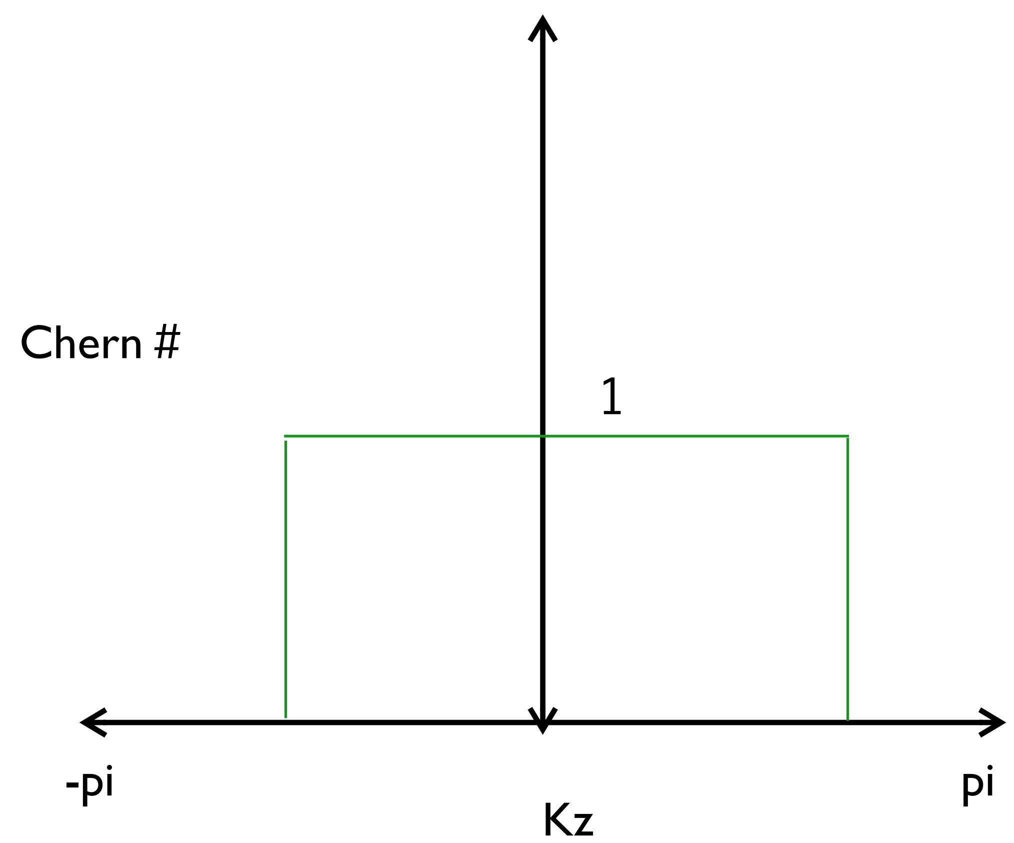
$$\vec{A}(\vec{k}) = \sum_n < n\vec{k}|\vec{\nabla}_k|n\vec{k} > \quad \vec{B}(\vec{k}) = \vec{\nabla}_k \times \vec{A}(\vec{k})$$

$$\vec{\nabla}_k \cdot \vec{B}(\vec{k}) = \pm\delta(\vec{k} - \vec{k}_0)$$

- integral of Berry curvature over a 2D closed manifold gives Chern number: Chern number for a 2D BZ: quantum Hall effect
  Chern number for a FS in 3D: Chiral anomaly!

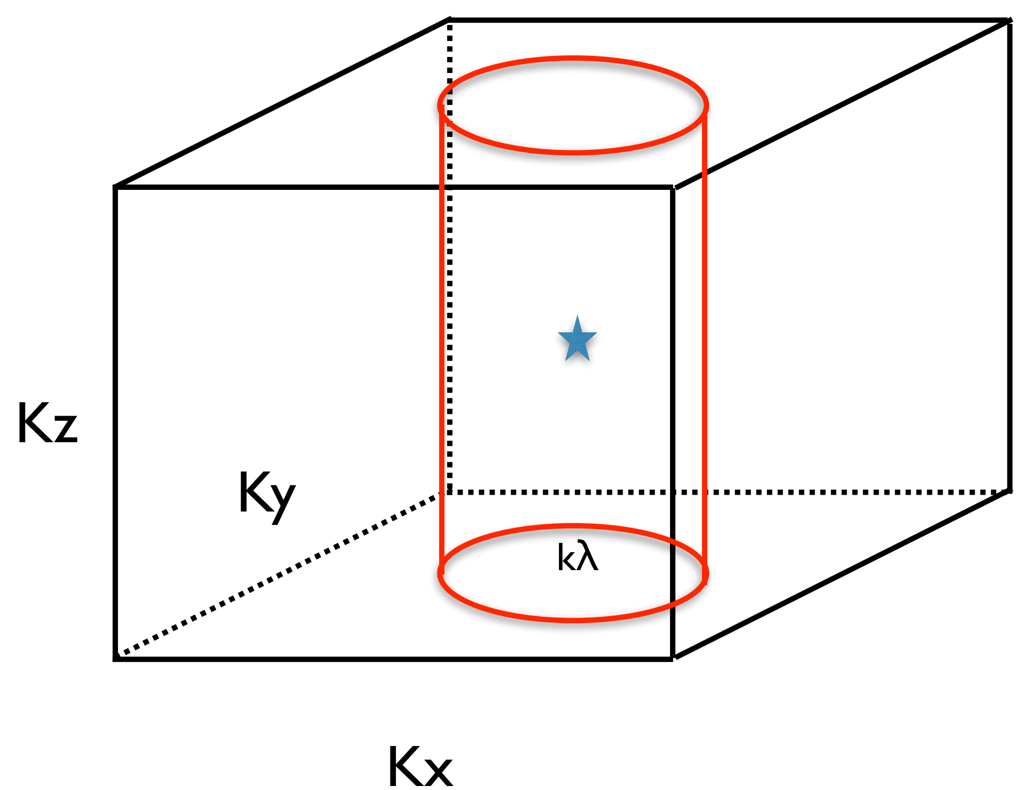
Why Weyl points must appear in pairs?

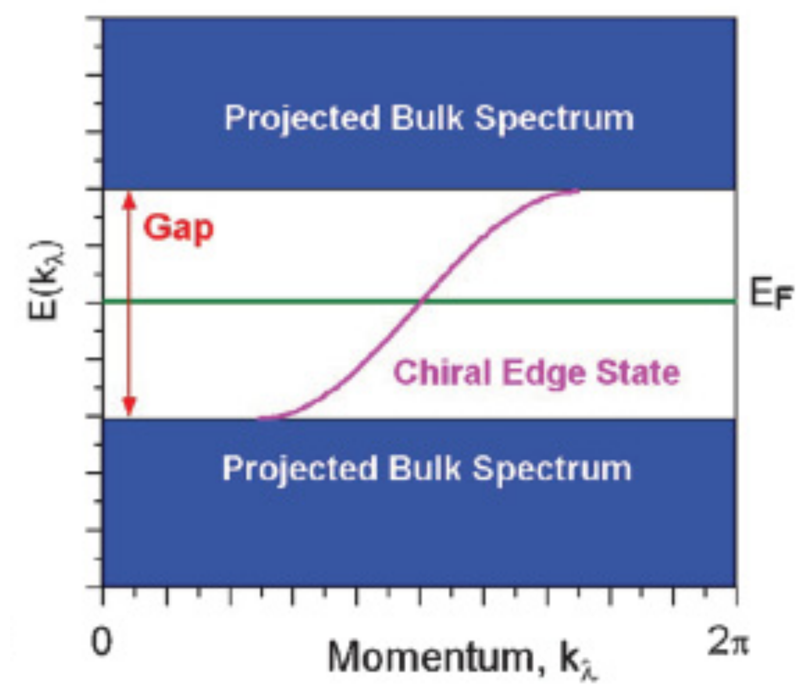


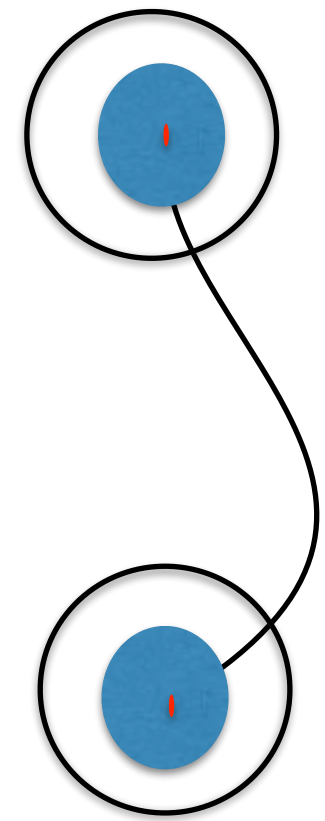


Properties of WSM:
Fermi arcs on the surface, what protects it?

fully gapped between nth and (n+1)th bands!
Weyl points are located between nth and (n+1)th bands!







Topview

Wan et al, Phys.Rev.B 83,205101

The most important Physics in TSM:

1. Chiral anomaly: non-conservation of electron number with fixed chirality under parallel electric and magnetic fields

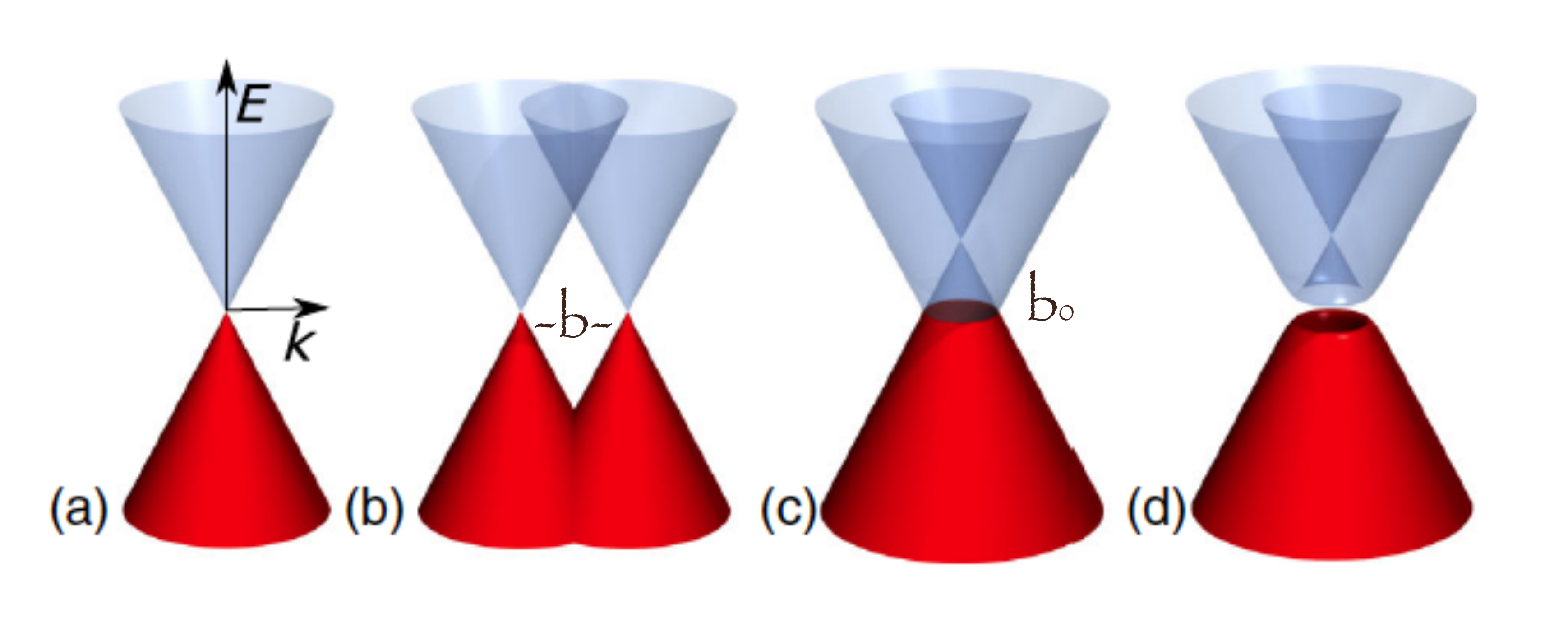
2. Chiral magnetic effect: Weyl fermions can carry current under external magnetic field with unbalanced chemical potential

Anomalous Hall effect (AHE) and CME for a single WP pair

$$\rho = \frac{e^2}{2\pi^2}\boldsymbol{b}\cdot\boldsymbol{B},$$

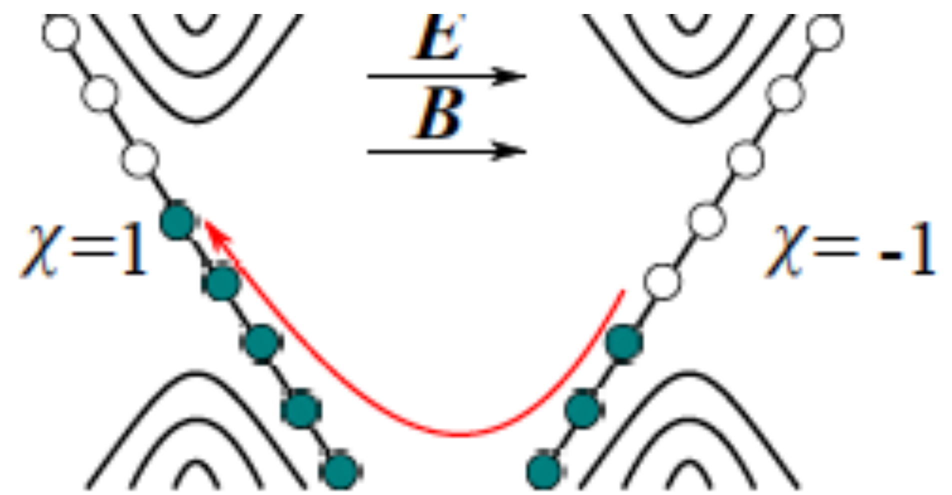
$$\boldsymbol{j} = \frac{e^2}{2\pi^2}(\boldsymbol{b}\times\boldsymbol{E} - b_0\boldsymbol{B}).$$

AHE CME



Chiral anomaly under U(1) gauge field: E and B
Full quantum mechanical(strong field) point of view

The Chiral density(N_L-N_R) won't be conserved under parallel magnetic and electric fields:
adiabatic pumping of particles from One Weyl point to another one with opposite chirality



$$\epsilon_n = v_F \mathrm{sign}(n)\sqrt{2\hbar|n|eB + (\hbar \boldsymbol{k}\cdot\hat{B})^2},\ n = \pm1, \pm2, \ldots$$
$$\epsilon_0 = -\chi\hbar v_F \boldsymbol{k}\cdot\hat{B}$$

The equation of motion for the zeroth Landau level

$$\hbar\frac{dk}{dt} = -eE$$

Will generate negative Magneto-resistance in WSM materials

Derive the CME using quantum mechanics

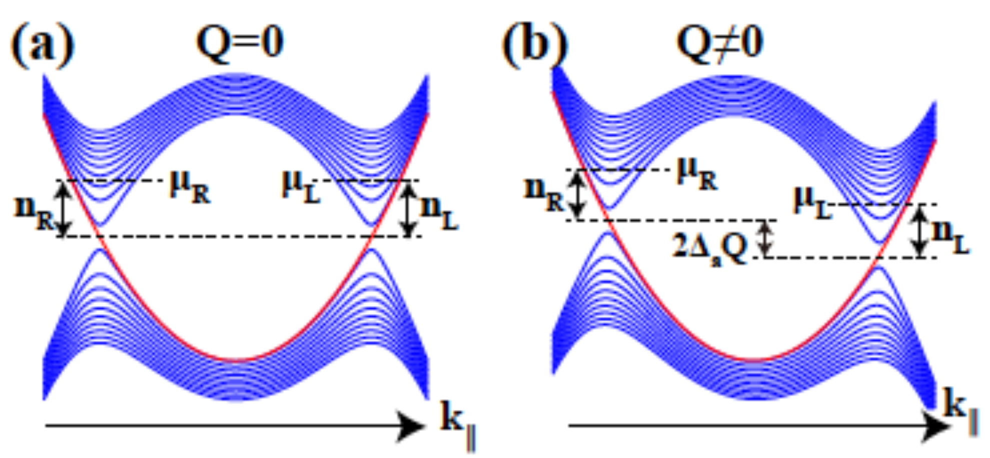


FIG. 1: Landau bands and deformation potential in a two WPs model. The red and blue lines represent the zeroth (chiral) Landau band and other Landau bands respectively. Chiral charge density is defined as $n_a = n_R - n_L$. (a) is the case of $Q = 0$ and (b) is the case of $Q \neq 0$.

$$\mathbf{j}_{\mathrm{CME}} = -\frac{e^2\mathbf{B}}{4\pi^2\hbar}\int_{occ} dk_\parallel \frac{\partial\epsilon_0\left(k_\parallel\right)}{\hbar\partial k_\parallel} = \frac{e^2\mathbf{B}}{4\pi^2\hbar^2}\left(\mu_R - \mu_L\right)$$

1. No current at the thermal equilibrium state!!!

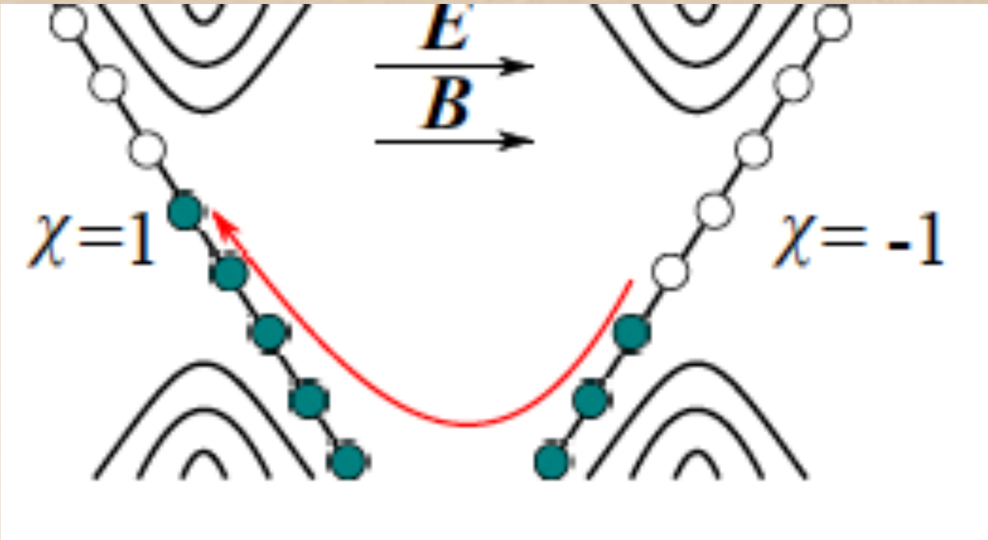
M. Franz et al, Phys. Rev. Lett. 111, 027201 (2013)

2. Need clean limit to detect the effect

Where to find WSM?

- Remove the spin degeneracy of the band
- Spin-orbital coupling is essential?
- SOC+Either break of time reversal or spacial inversion symmetries
- First proposed real material by X. Wan, S. Savrasov et al: Y2Ir2O7 with all in all out spin structure Phys.Rev.B 83,205101
- Ferromagnetic metal proposed by us: HgCr2Se4 PRL 107,186806
- Tellurium and Selenium under pressure by S. Murakami, and T. Miyake's groups: cond-mat:1409.7517
- critical point between normal and topological insulators by Vanderbilt's group: PRB90,155316
- Nonmagnetic material without inversion center: TaAs, TaP, NbAs, NbP
  HM Weng, et al, Phys. Rev. X 5, 011029 (2015)

Negative MR in DC transport:
Generate CME by steady state



$$\begin{aligned}\epsilon_n &= v_F \mathrm{sign}(n)\sqrt{2\hbar|n|eB + (\hbar \boldsymbol{k}\cdot\hat{B})^2},\ n = \pm 1, \pm 2, \ldots \\ \epsilon_0 &= -\chi\hbar v_F \boldsymbol{k}\cdot\hat{B}\end{aligned}$$

$$j_e = v_F \frac{e^3}{4\pi^2\hbar}\tau_{int}(\mathbf{E}\cdot\mathbf{B})\hat{\mathbf{B}},$$

(I) :Generating CME by time dependent state:
much bigger territory to explore!!

Our proposal: detect CME by lattice dynamics (more are on the way!)

- There are certain phonon modes called pseudo scalar phonons which can couple to CME
- Some phonon modes can be non-polarized, which is decouple from EM wave without CME
- With CME, these pseudo scalar phonons can be optically active

What kind of Zone centre phonon mode can couple to CME?

$$\hat{H}_{ep} = \frac{1}{V}\sum_{\mathbf{K}_i\mathbf{p}} \hat{\psi}^{\dagger}_{\mathbf{K}_i+\mathbf{p}} \Delta_{\mathbf{K}_i,Q} \hat{\psi}_{\mathbf{K}_i+\mathbf{p}} Q$$

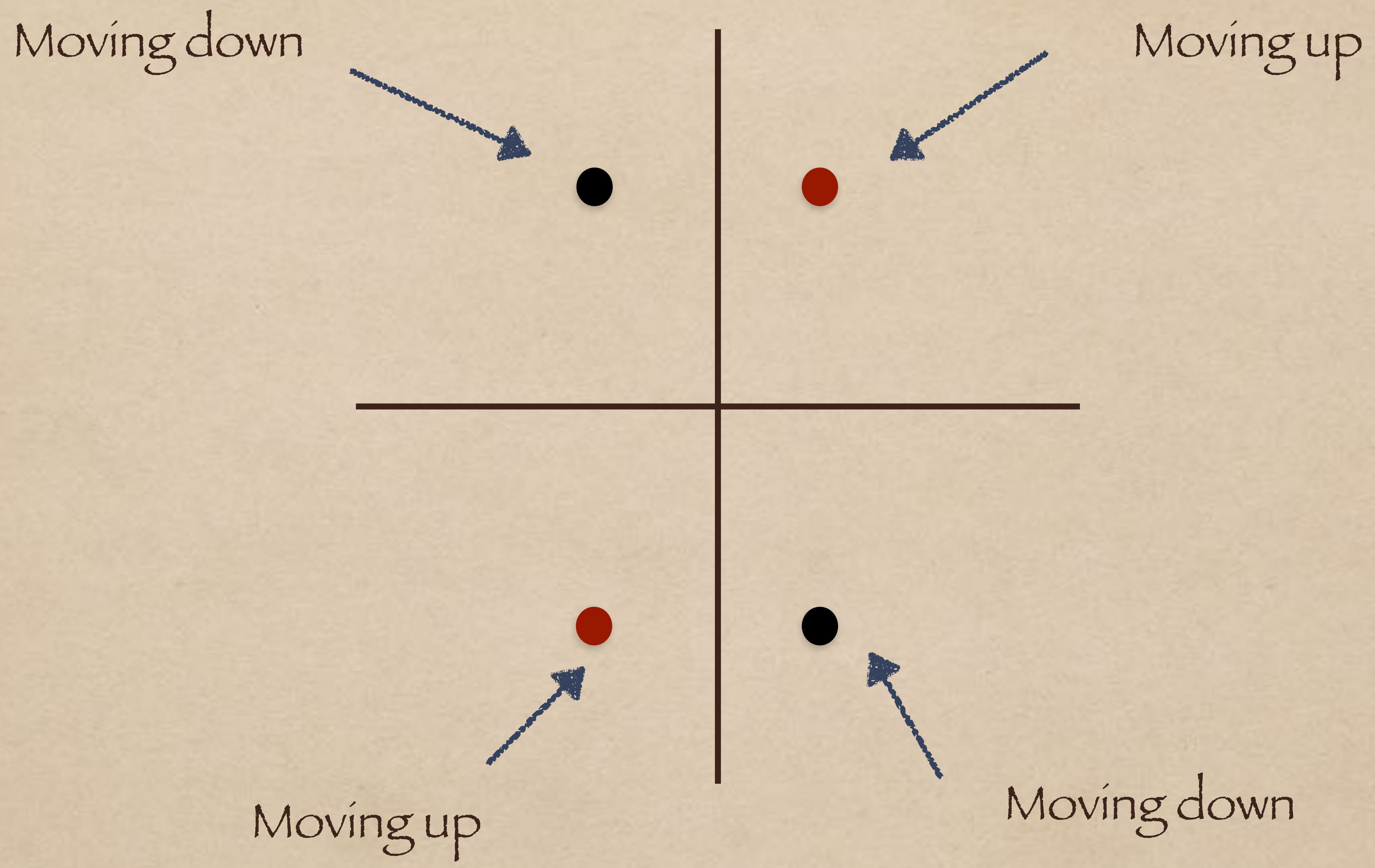
electron-phonon coupling term

$$\mathbf{j}_{\mathrm{CME},Q} = \frac{N_W e^2 \mathbf{B}}{4\pi^2\hbar^2}\Delta_{a,Q} Q$$

where $\Delta_{a,Q} = \frac{1}{N_W}\sum_i^{N_W} \chi_i \Delta_{\mathbf{K}_i,Q}$

In order to have nonzero coupling, the phonon mode Q must transform in the same way with chirality, which is a pseudo scalar

Example of Pseudo Scalar Phonon mode



Materials			Space Group	Little Group at Γ	Relevant Wyckoff Sites	SSGs	Pseudo Scalar Phonon [a]	Polarised
Weyl	non magnetic	$A\mathrm{Bi}_{1-x}\mathrm{Se}_x\mathrm{Te}_3$ [1]	160	C_{3v}	-	-	-	-
		BiTeI under pressure [1]	156	C_{3v}	-	-	-	-
		Se/Te under pressure [2]	152/153	D_3	$3a$	C_2	A_1	No
		TaAs [3, 4]	109	C_{4v}	-	-	-	-
	magnetic	$A_2\mathrm{Ir}_2\mathrm{O}_7$ [5]	227.131 [b]	$\mathcal{O}_h$ [c]	-	-	-	-
		$\mathrm{HgCr_2Se_4}$ [6]	141.557 [b]	$\mathcal{D}_{4h}$ [c]	$8c$, $16h$	C_{2h}, C_s	$2 \times A_{1u}$	No
Dirac	Class I [d]	$\mathrm{Cu_3PdN}$ [7]	221	O_h	-	-	-	-
		$A_3\mathrm{Bi}$ [8]	194	D_{6h}	-	-	-	-
		BaAuBi-family [9]	194	D_{6h}	-	-	-	-
		LiGaGe-family [9]	186	C_{6v}	-	-	-	-
		$\mathrm{SrSn_2As_2}$[9]	160	C_{3v}	-	-	-	-
		$\mathrm{Cd_3As_2}$ [10]	137	D_{4h}	$3 \times 8g$, $8f$	C_s, C_2	$4 \times A_{1u}$	No
		$\mathrm{Cd_3As_2}$ [10]	110	C_{4v}	$9 \times 16b$, $2 \times 8a$	C_1, C_2	$29 \times A_2$	No
	Class II	β-cristobalite $\mathrm{BiO_2}$ [11]	227	O_h	-	-	-	-
		$\mathrm{HfI_3}$ [9]	193	D_{6h}	-	-	-	-
		$A\mathrm{Mo}_3X_3$-family [9]	176	C_{6h}	$2 \times 6h$, $2c$	C_s, C_{3h}	$3 \times A_u$	Yes
		Distorted Spinel [12]	74	D_{2h}	$4a$, $4d$, $8h$, $8i$	C_{2h}, C_{2h}, C_s, C_s	$4 \times A_u$	No

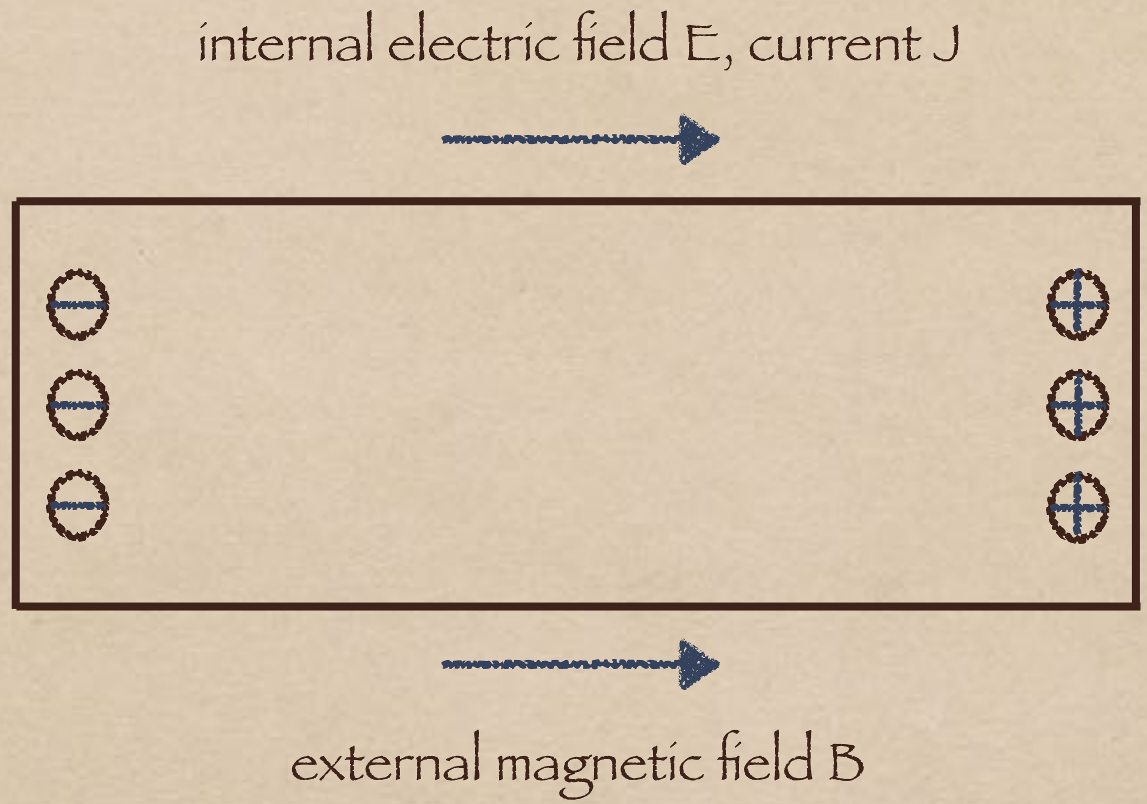
[a] The pseudo scalar representation may have different symbols in different groups. In the first class point groups (consisting of proper rotations), it is just the identity representation A_1. While in the second (centrosymmetric) and third (non-centrosymmetric but with improper rotations) class point groups, it is usually referred as A_{1u} and A_2, respectively. The prefactor is the number of pseudo scalar phonon modes. "-" means there is no pseudo scalar phonon.

[b] The magnetic space group is referred to Ref. [13].

[c] The magnetic little group is defined as $\mathcal{O}_h = T_h + \mathcal{T} \cdot (O_h - T_h)$ and $\mathcal{D}_{4h} = C_{4h} + \mathcal{T} \cdot (D_{4h} - C_{4h})$, respectively, where $\mathcal{T}$ is the time reversal operator.

[d] The classification follows Ref. [14].

Coupled Dynamics for anomalous current, current, electric field and pseudo scalar phonons



Coupled equations of motion:

$$\ddot{Q} + \omega_{ph}^2 Q + \frac{\Delta_a \Omega}{M_{ph}} n_a = 0$$

phonon mode

$$\dot{n}_a = \frac{e^2 N_W}{4\pi^2 \hbar^2} \mathbf{E} \cdot \mathbf{B}$$

Chiral charge

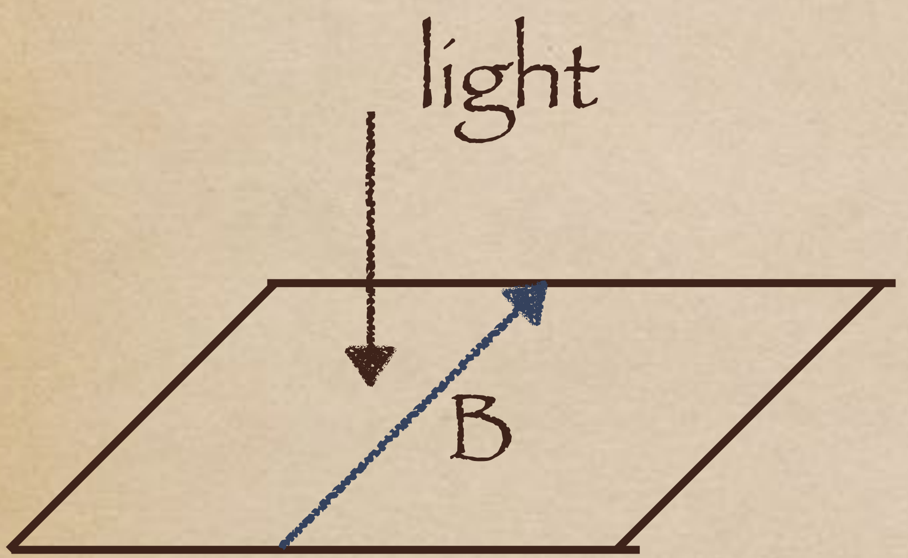
$$\ddot{\mathbf{D}} + \dot{\mathbf{J}} + \frac{1}{\mu} \nabla (\nabla \cdot \mathbf{E}) - \frac{1}{\mu} \nabla^2 \mathbf{E} = 0$$

internal electric field

$$\mathbf{J}_{\mathrm{CME}} = \frac{e^2 \mathbf{B}}{4\pi^2 \hbar^2} \left(N_W \Delta_a Q + \frac{n_a}{\nu_D} \right)$$

Chiral current induced by CME

Case I: Transverse optical response —reflectivity



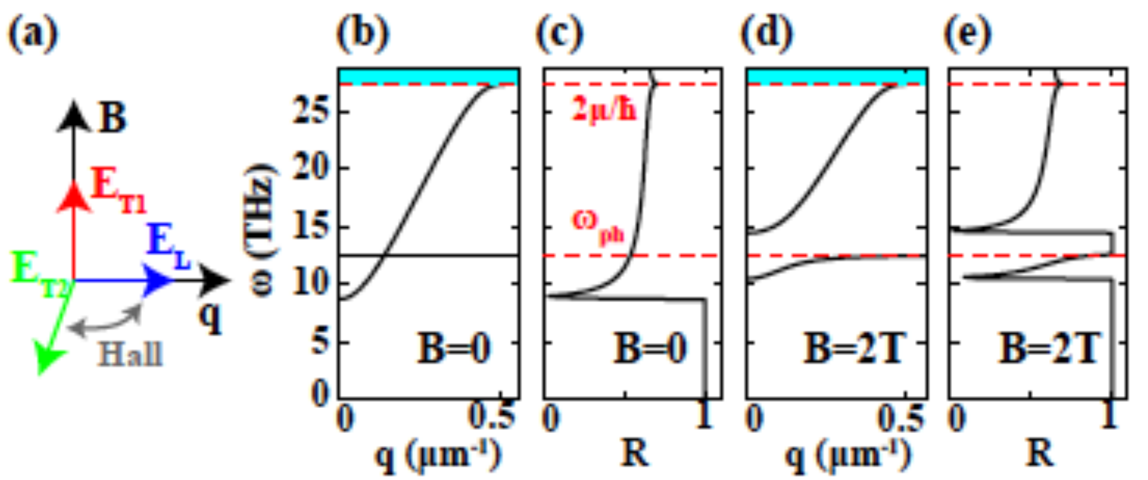


FIG. 2: EM wave coupled with unpolarised pseudo scalar phonon. (a) illustrates the fields configuration, which ensures that the mode coupled with CME current (E_{T1}) and is free from Hall effects. (b) and (c) are the numerically calculated dispersion and reflectivity for E_{T1} at $|\mathbf{B}| = 0$. (d) and (e) are the dispersion and reflectivity at $|\mathbf{B}| = 2\mathrm{T}$. The cyan areas are the inter-band single particle excitation zones [37].

Case II: longitudinal mode —Plasmon

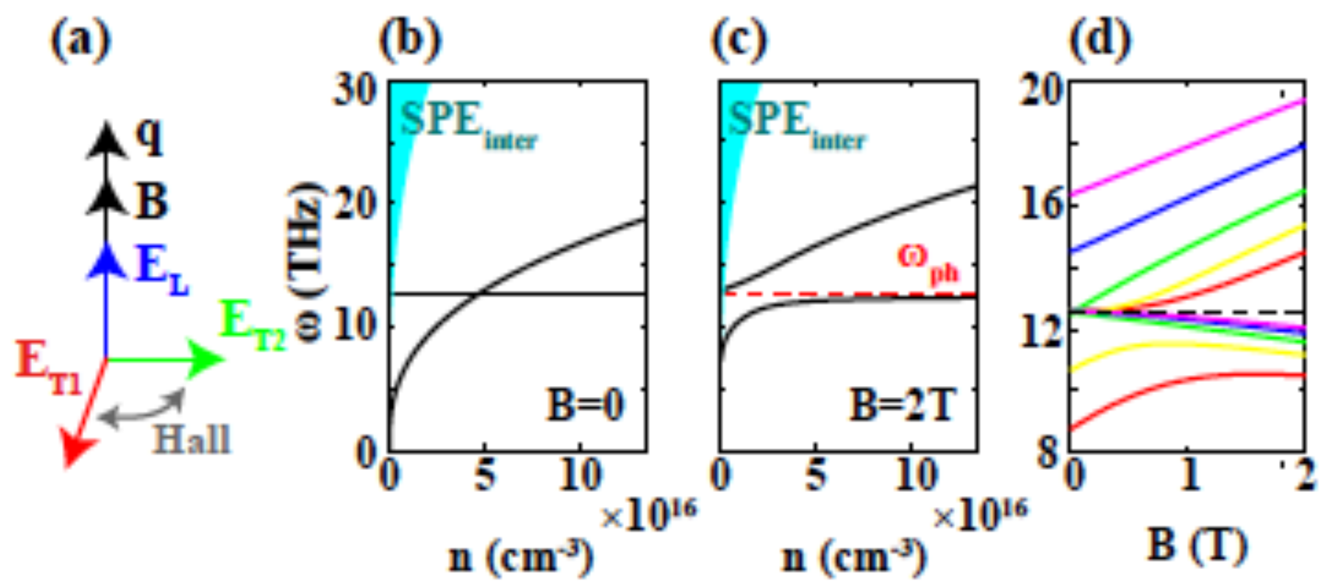


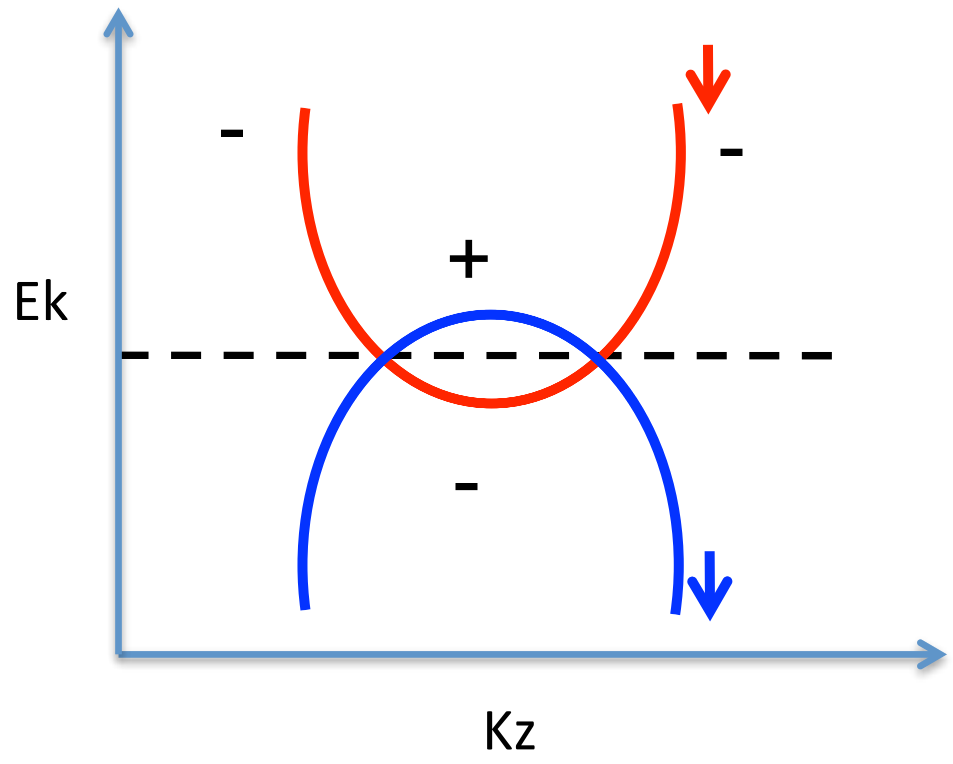
FIG. 3: Plasmon coupled with unpolarised pseudo scalar phonon. (a) illustrates the fields configuration, which ensures that the mode coupled with CME current (E_L) is free from Hall effect. (b) and (c) are the eigen frequencies of the coupled modes as functions of carrier density at $|\mathbf{B}| = 0$ and $|\mathbf{B}| = 2\mathrm{T}$, respectively, where the cyan areas are the inter-band single particle excitation zones [38]. In (d) we plot the eigen frequencies of the coupled modes as functions of the magnetic field. Different colored lines represent different intrinsic plasmon frequencies (carriers densities).

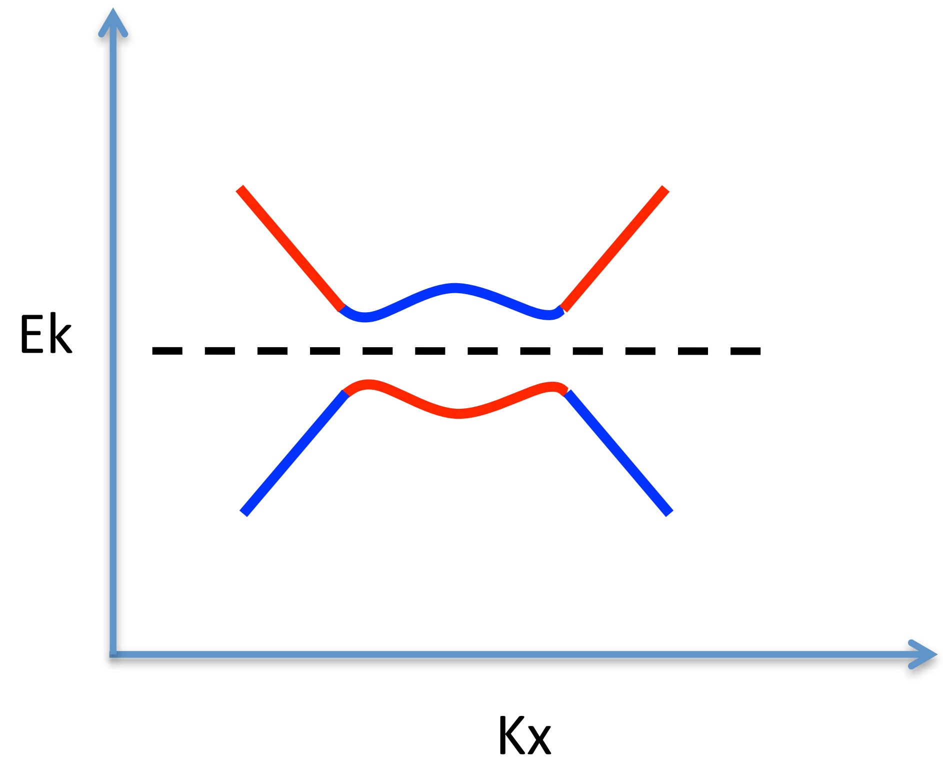
(II) Instability of Dirac semimetal under strong magnetic field

Topological semi-metal with TRS:

3D Dirac semi-metal

3D Dirac semi-metal generated by band inversion

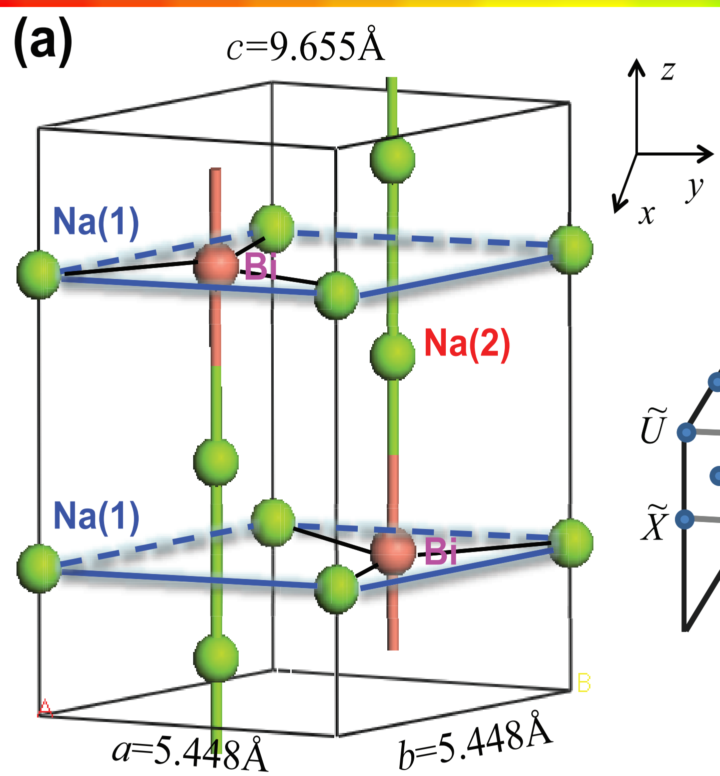


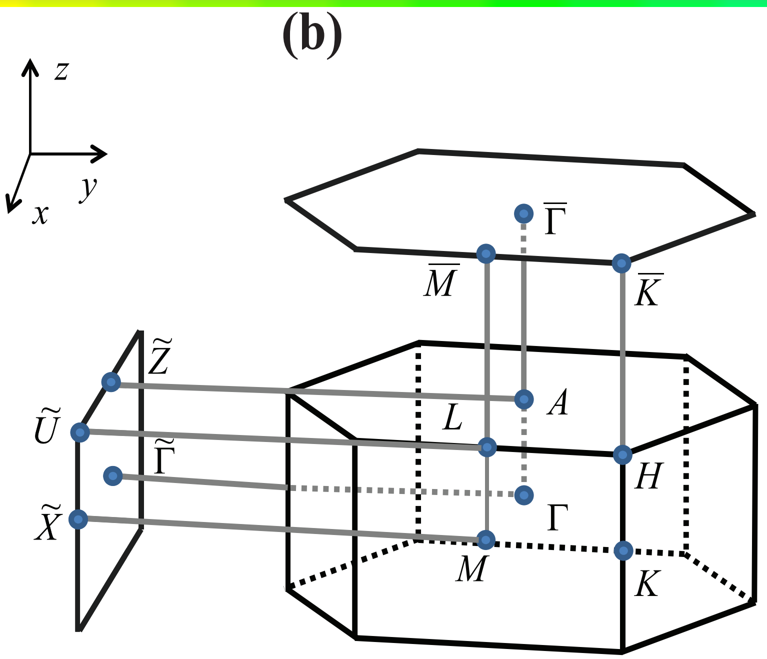


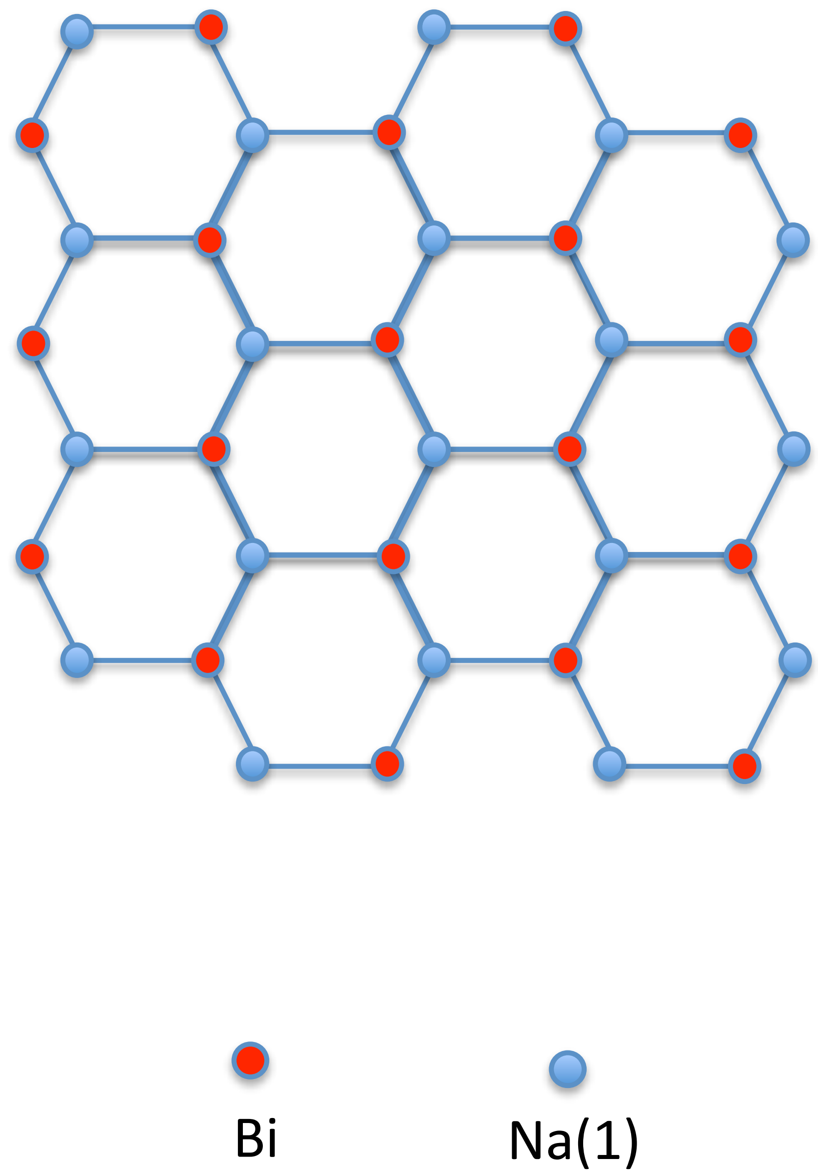
Along Z-axis with extra crystal symmetry
Which protects the band crossing

Along any other direction where
the crossing is no longer protected

3D Dirac semi-metal: A_3Bi (A=Na, K, Rb)







Layered hexagonal structure
Space group: $P6_3/mmc$
Stacking of NaBi Honeycomb layers along the C-axis

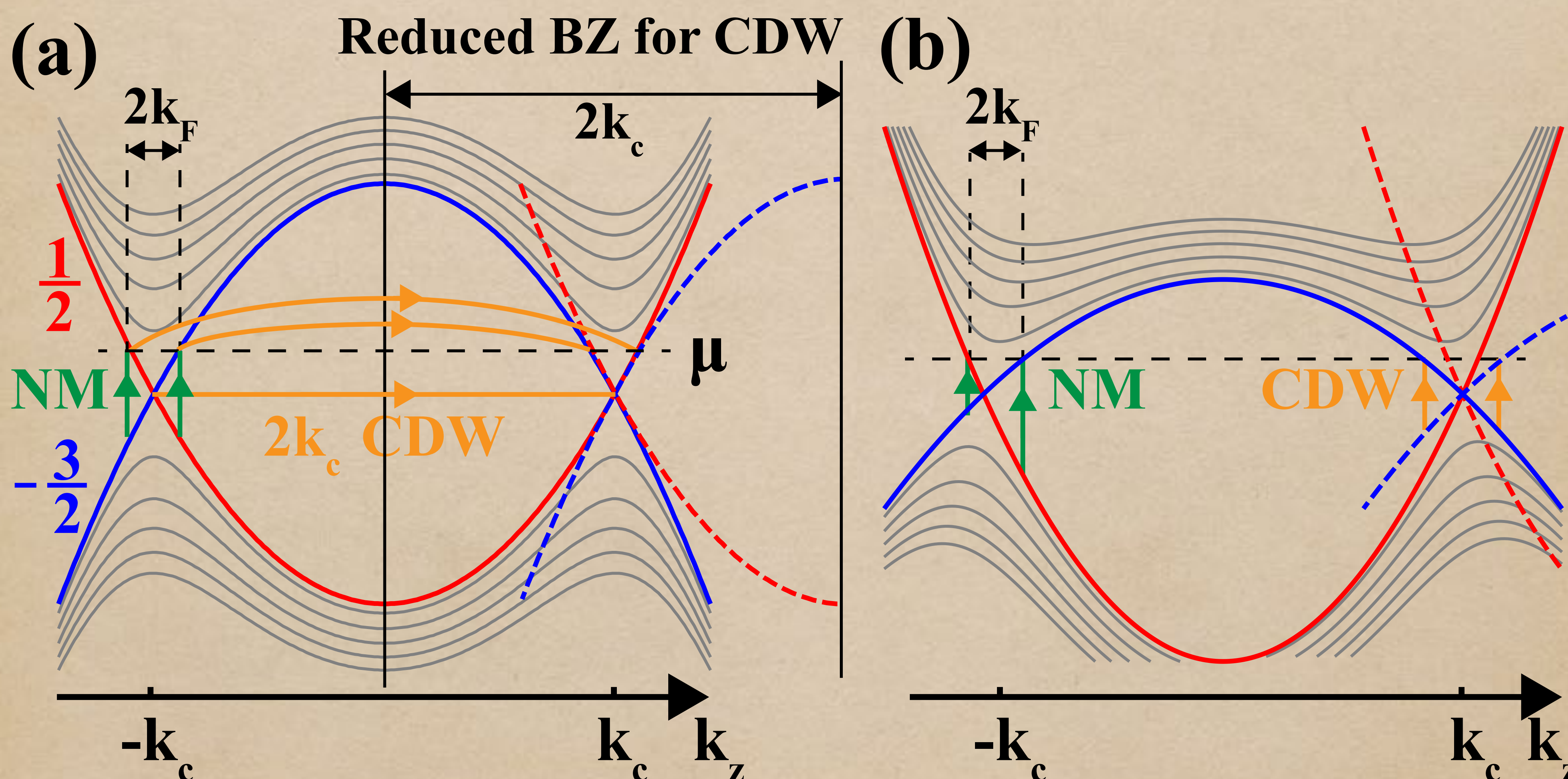
kp model for Na3Bi

$$H^0 = C(k_z) + \begin{pmatrix} M(k_z) & -v\hbar k_- & \gamma(\mathbf{k}) & 0 \\ -v\hbar k_+ & -M(k_z) & 0 & \gamma(\mathbf{k}) \\ \gamma^*(\mathbf{k}) & 0 & -M(k_z) & v\hbar k_- \\ 0 & \gamma^*(\mathbf{k}) & v\hbar k_+ & M(k_z) \end{pmatrix} \quad (1)$$

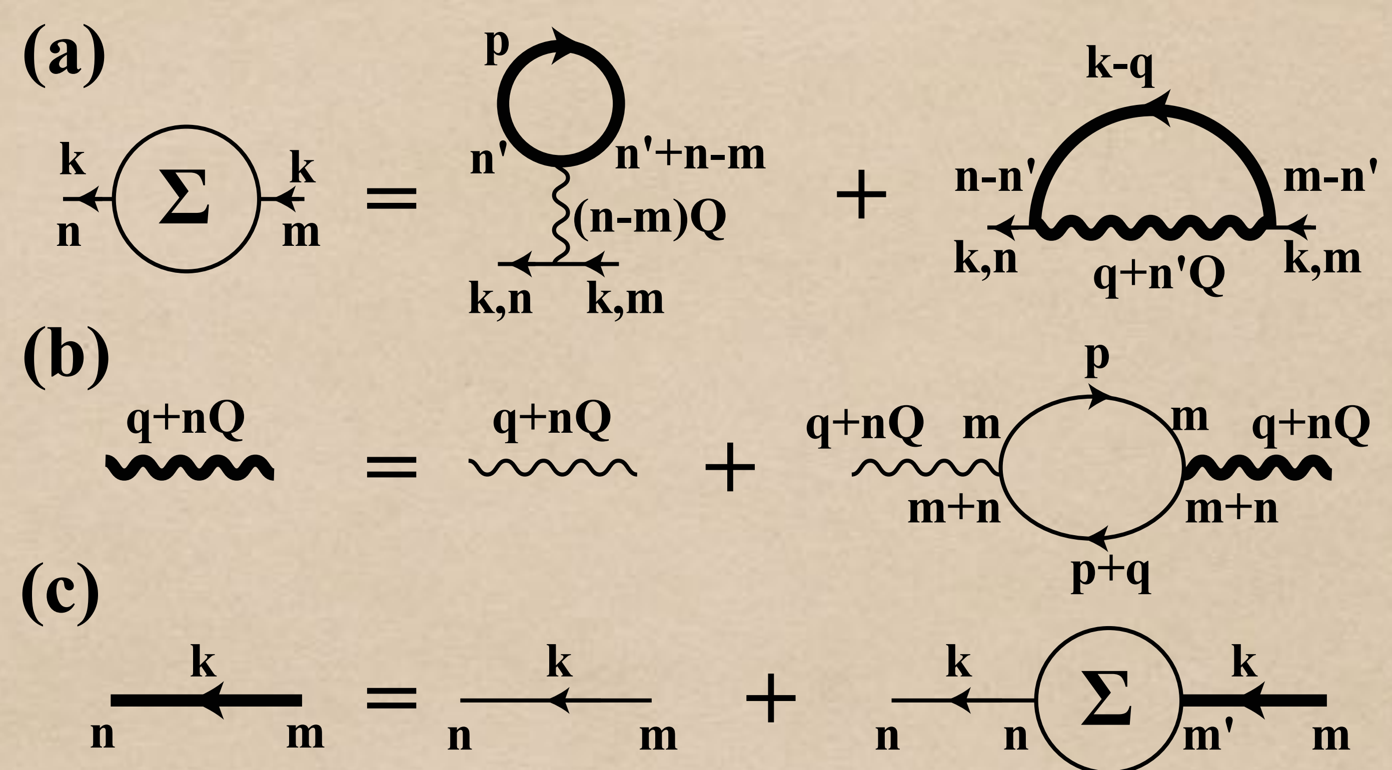
Here $C(k_z) = C_0(\cos a_0 k_z - \cos a_0 k_c)$, $M(k_z) = M_0(\cos a_0 k_z - \cos a_0 k_c)$, $k_\pm = k_x \pm i k_y$, v is the veloc-

the C_0 term tilt the Dirac cone

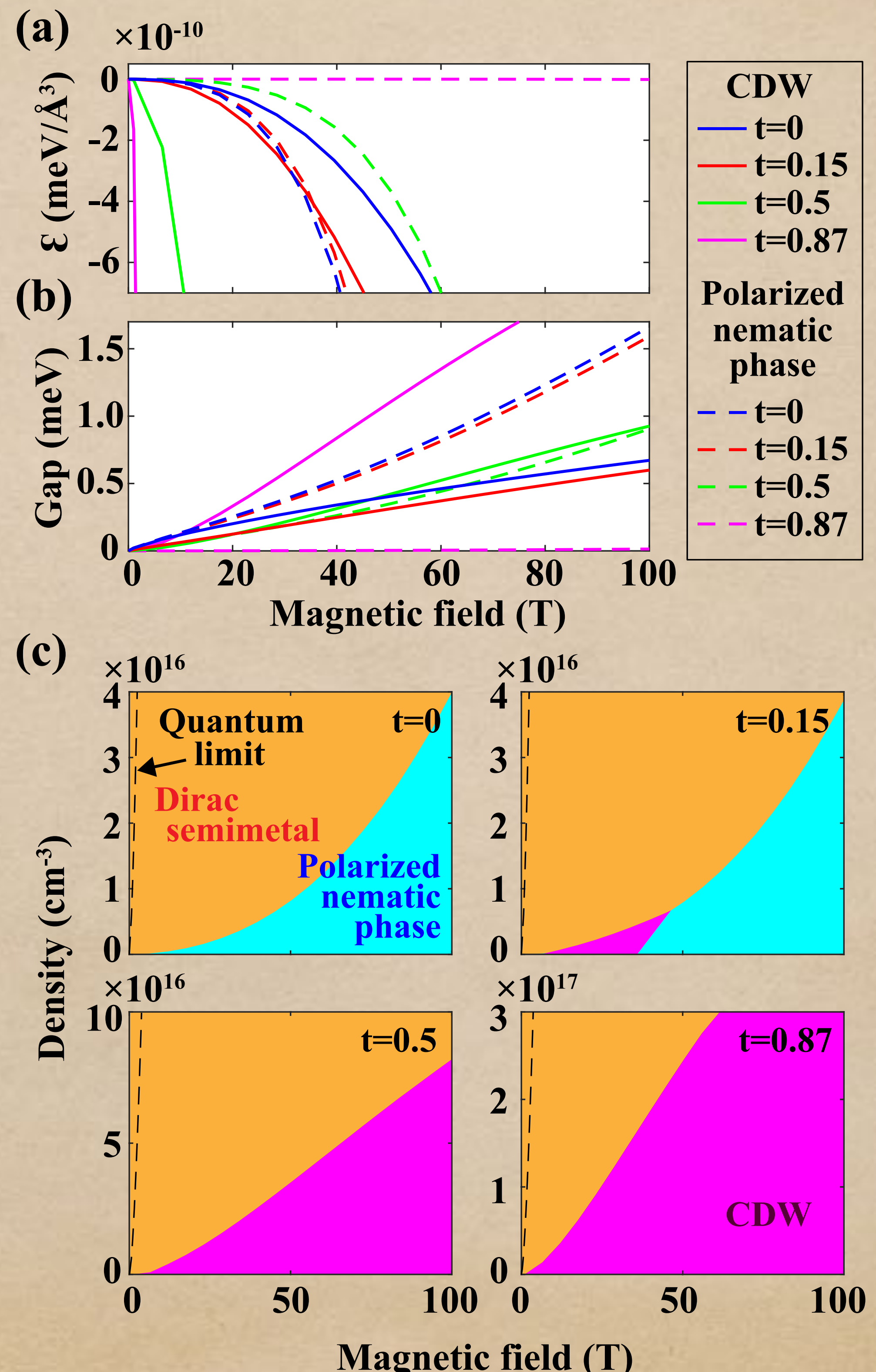
Two kinds of instability caused by "nesting FS" under strong magnetic field



GW type approach



Mean field phase diagram



Conclusions

- Dynamics of Pseudo scalar phonons can couple to CME
- non-polarized pseudo scalar phonon modes can be used as the detector of CME
- Two kinds of instability, CDW and nematic phases, can occur under magnetic field in topological Dirac semimetal

Thank you for your attention !