KITP Program “New Phases and Emergent Phenomena in
Correlated Materials with Strong Spin-Orbit Coupling”
@KITP, UCSB, Sep 3,2015

topological semimetals in inversion asymmetric systems

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CREST, JST

Inversion asymmetric systems
i.e. chiral systems: Te (tellurium)

- Weyl semimetals
- Chiral transport in crystals with chiral lattice structure

Hirayama, Okugawa, Ishibashi, SM, Miyake, PRL 114, 206401 (2015)
Yoda, Yokoyama, SM, Sci. Rep. 5, 12024 (2015)

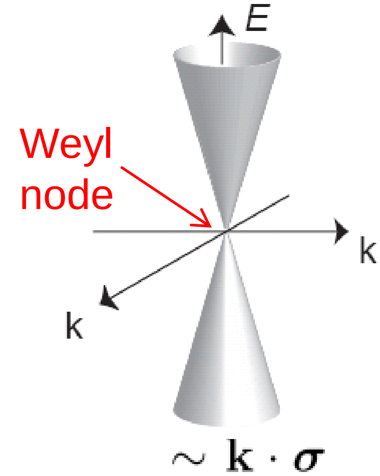
Collaborators:

- Tokyo Tech.
  M. Hirayama, T. Yoda, T. Yokoyama, R. Okugawa

- AIST, Tsukuba, Japan
  T. Miyake, S. Ishibashi

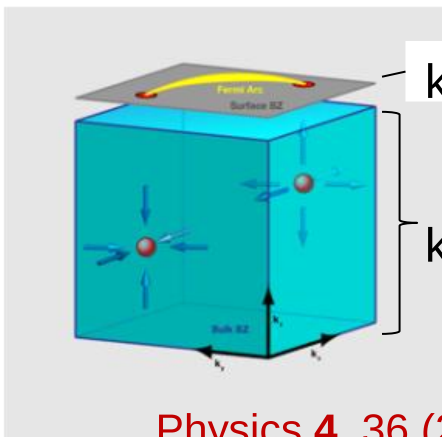
Weyl semimetal

Weyl semimetal =
Bulk 3D Dirac cones without degeneracy
either time-reversal or inversion symmetry must be broken

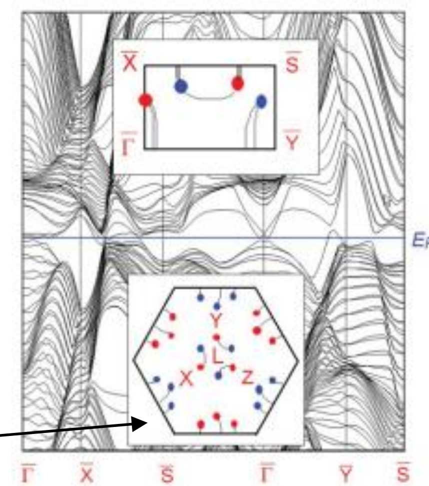


Dirac semimetal =
Bulk 3D Dirac cones with degeneracy

- Surface Fermi arc – connecting between Weyl nodes



Physics **4**, 36 (2011)



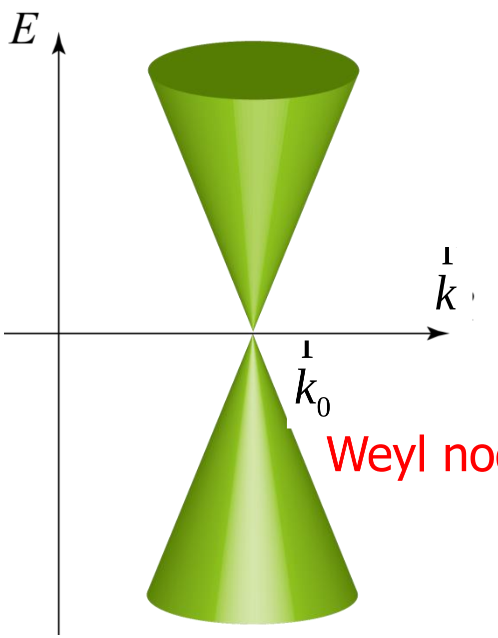
24 Weyl points predicted in $Y_2Ir_2O_7$

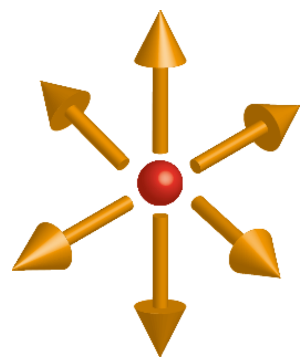
- pyrochlore iridates
  (Wan et al., PRB (2011), Yang et al., PRB(2011))
- TI multilayer (Burkov, Balents)
- TaAs ….

Wan et al., PRB (2011)

3D Weyl nodes

$$\begin{cases} \vec{B}_n(\vec{k}) = i\left\langle \dfrac{\partial u_{nk}}{\partial \vec{k}} \right| \times \left| \dfrac{\partial u_{nk}}{\partial \vec{k}} \right\rangle & \text{: Berry curvature} \\ \rho_n(\vec{k}) = \dfrac{1}{2\pi} \nabla_{\vec{k}} \cdot \vec{B}_n(\vec{k}) & \text{: monopole density} \end{cases}$$

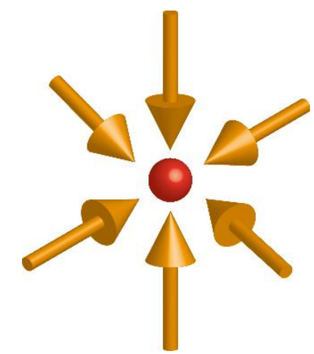




Monopole at $\vec{k} = \vec{k}_0$

$\rho_l(\vec{k}) = \delta(\vec{k} - \vec{k}_0)$

or



Antimonopole at $\vec{k} = \vec{k}_0$

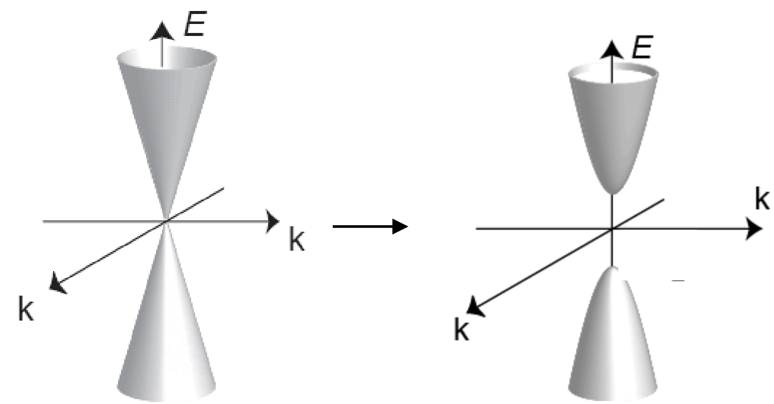
$\rho_l(\vec{k}) = -\delta(\vec{k} - \vec{k}_0)$

- Weyl nodes are either monopole or antimonopole
- Quantized monopole charge

C. Herring, Phys. Rev. 52, 365 (1937).
G. E. Volovik, The Universe in a Helium Droplet (2007).
S. Murakami, New J. Phys. 9, 356 (2007).

Weyl nodes in 2D and 3D

$m = 0$ $\qquad$ $m \neq 0$



2D Weyl node :

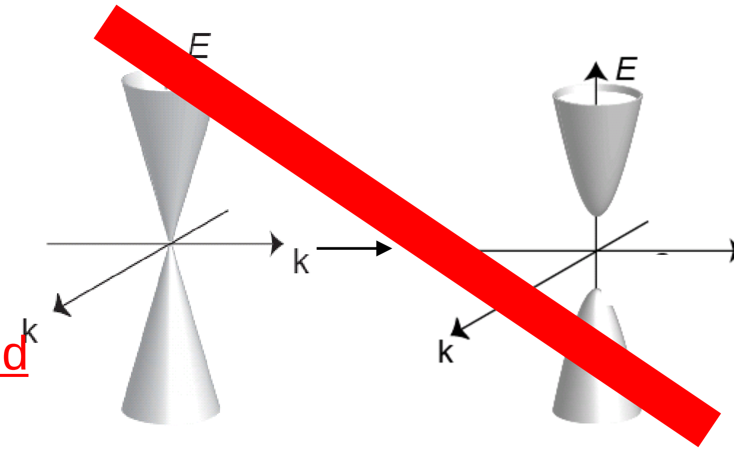
$$H(\vec{k},m) = k_x\sigma_x + k_y\sigma_y$$

parameter m opens a gap.

3D Weyl node :

$$H(\vec{k},m) = k_x\sigma_x + k_y\sigma_y + k_z\sigma_z$$

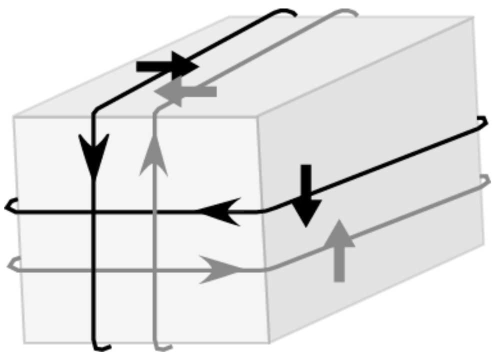
Weyl point moves but gap does not open.
(0,0,0)→(0,0,-m)



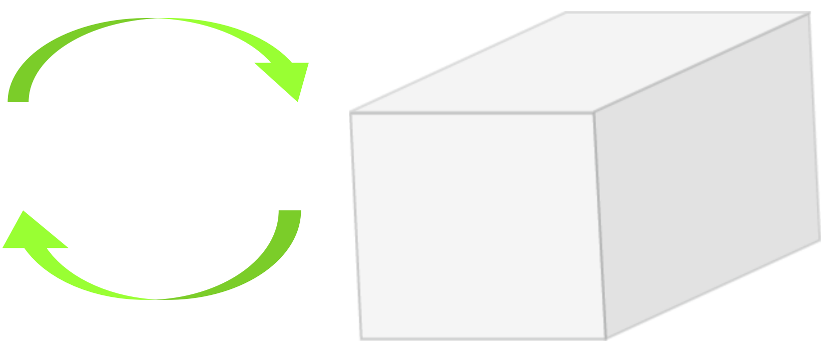
←Monopole charge (in 3D k-space) is conserved

3D Weyl node is topological.

NI-TI phase transitions and Weyl semimetals



TI: topological insulator



NI: normal insulator

SM, New J. Phys. (‘07).
SM. Kuga, PRB (’08)
SM, Physica E43, 748 (‘11)

Z_2 topological number ν

ν=0: normal insulator (NI)
ν=1: topological insulator (TI)

(A) systems without inversion symmetry

$$(-1)^{\nu} = \prod_i \frac{\sqrt{\det\left[w(\Gamma_i)\right]}}{\mathrm{Pf}\left[w(\Gamma_i)\right]}$$

$$w_{mn}(\vec{k}) = \langle u_{-k,m} | \Theta | u_{k,n} \rangle \qquad \Gamma_i : \text{TRIM}$$

Fu,Kane, PRB(2006)

(B) systems with inversion symmetry

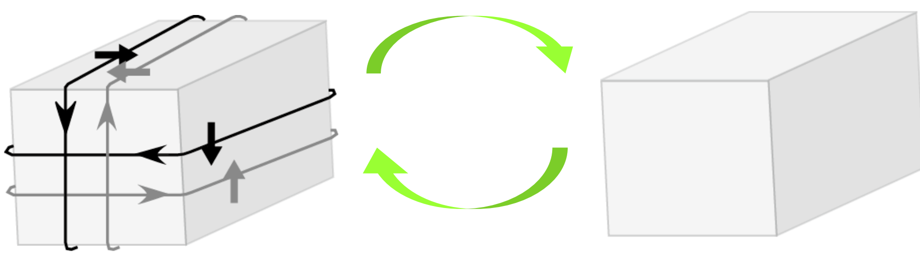
$$(-1)^{\nu} = \prod_i \prod_{m=1}^{N} \xi_{2m}(\Gamma_i)$$

Parity eigenvalue
+1 or -1

Fu,Kane, PRB(2007)

different formulae between (A) & (B)

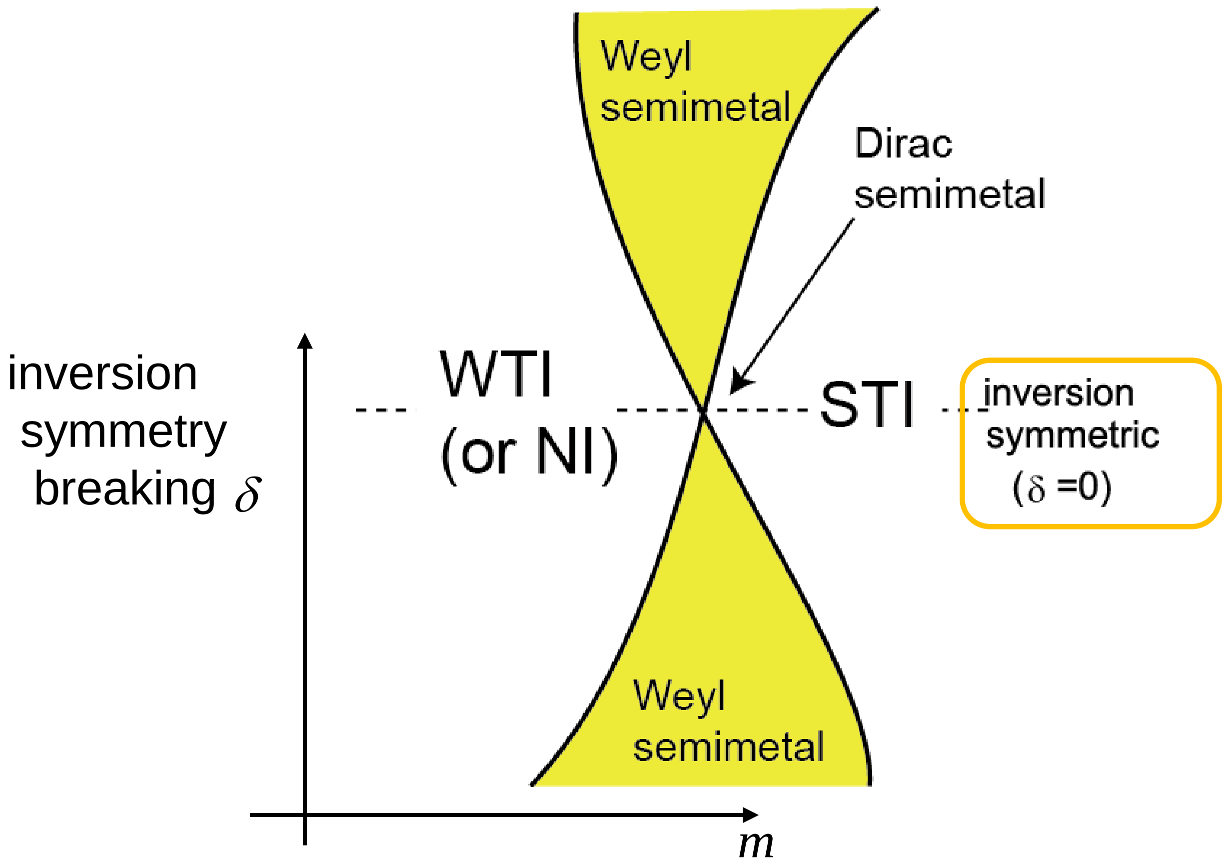
→ TI-NI phase transition in (A) & (B)



TI: topological insulator NI: normal insulator

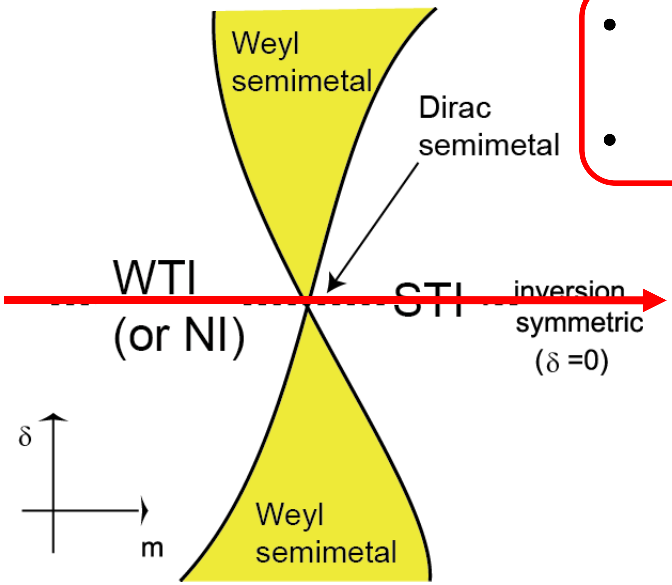
Universal phase diagram in 3D

SM, New J. Phys. (‘07).
SM. Kuga, PRB (’08)
SM, Physica E43, 748 (‘11)

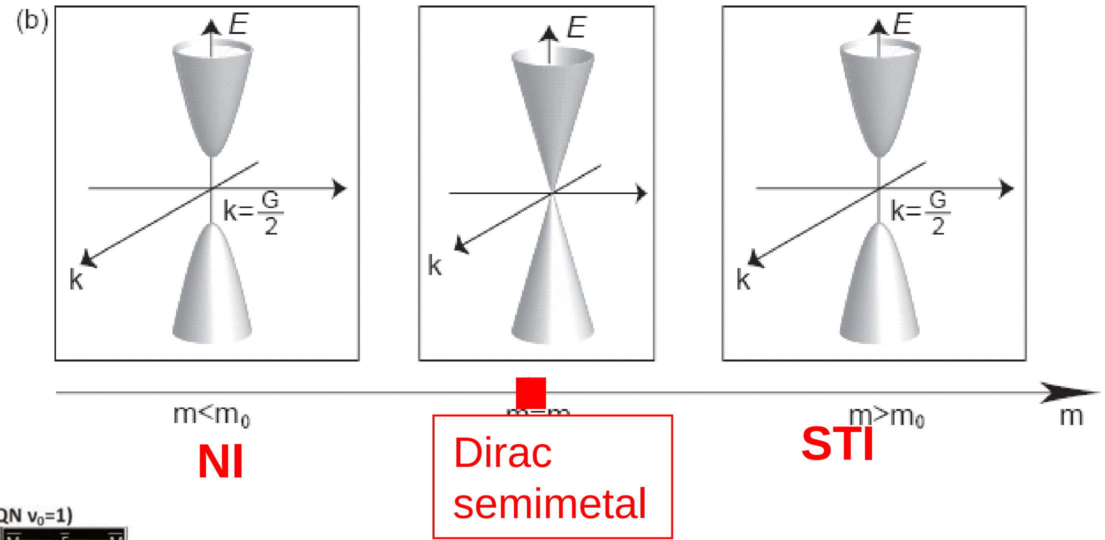


external parameter
(e.g.: pressure, atomic composition, SOC etc.)

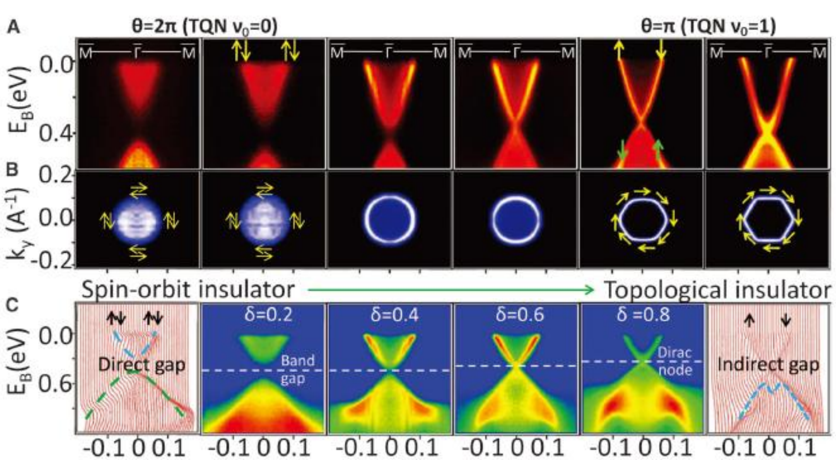
Systems with inversion symmetry



- Gap closes at TRIM
  inversion of bands with opposite parities.
- Insulator-to-insulator transition

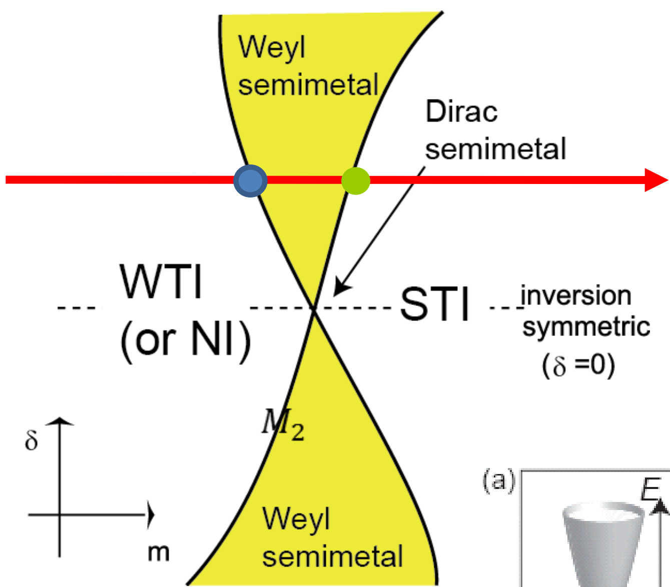


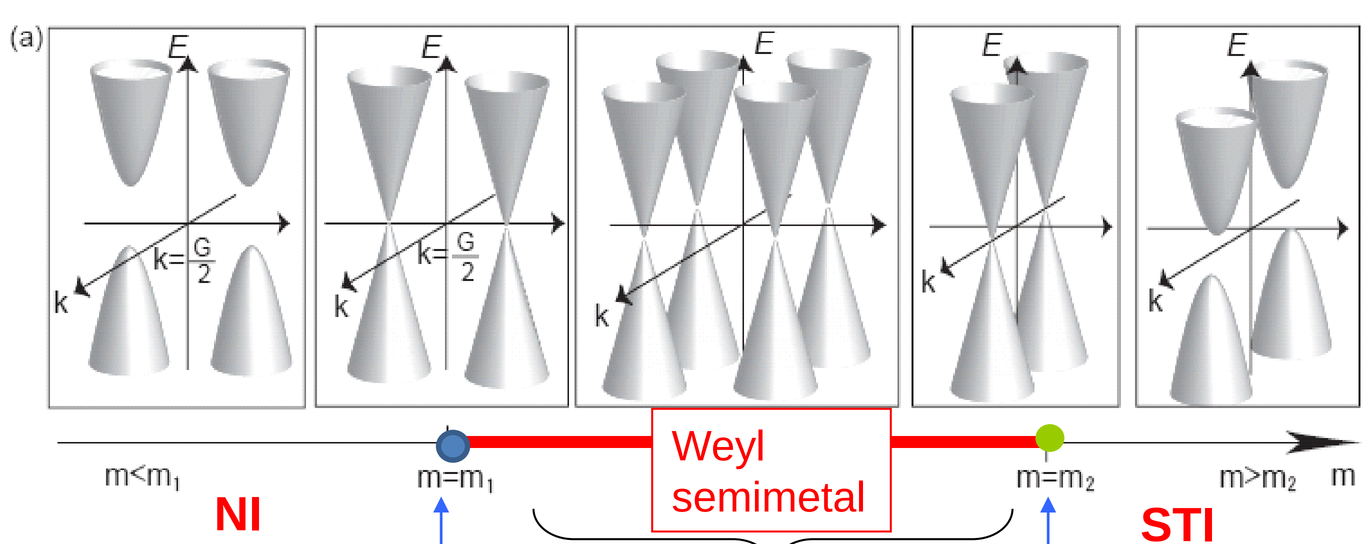
e.g. $TlBi(S_{1-x}Se_x)2$



Xu et al., Science.332, 560 ('11)

Systems without inversion symmetry





Monopole-antimonopole pair creation

2 monopoles and 2 antimonopoles

Monopole-antimonopole pair annihilation

SM, New J. Phys. ('07).
SM. Kuga, PRB ('08)
SM, Physica E('11)
Okugawa, SM, PRB('14)

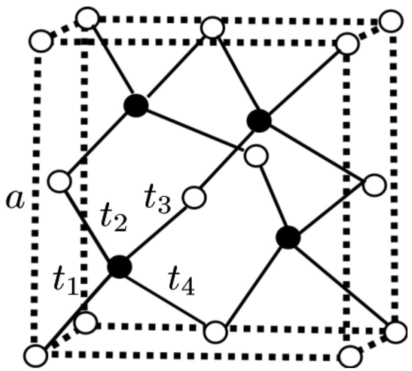
Lattice model: Fu-Kane-Mele model + staggered on-site energy

$$H = \sum_{\langle i,j \rangle} t_{ij} c_i^\dagger c_j + i\frac{8\lambda_{so}}{a^2} \sum_{\langle\langle i,j \rangle\rangle} c_i^\dagger \boldsymbol{s} \cdot (\boldsymbol{d}_{ij}^1 \times \boldsymbol{d}_{ij}^2) c_j + \lambda_v \sum_i \xi_i c_i^\dagger c_i$$

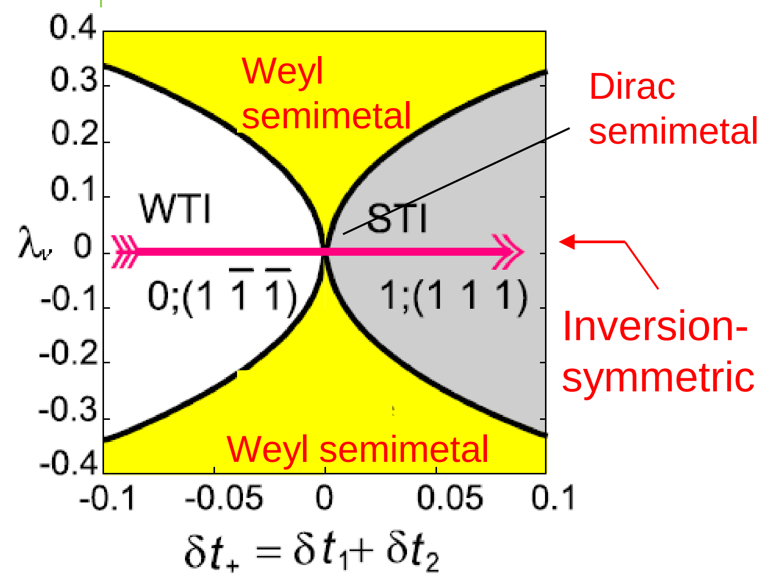
Fu-Kane-Mele model
(PRL98, 106803 (2007))

On-site staggered potenial
→ breaks inversion

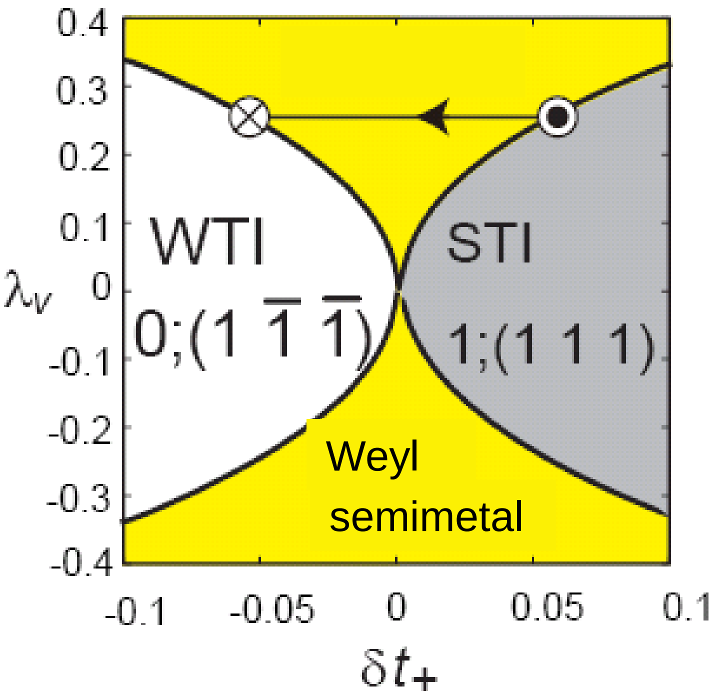
- Diamond lattice
- nearest neighbor: spin-indep. hopping
- next nearest neighbor: spin-orbit coupling



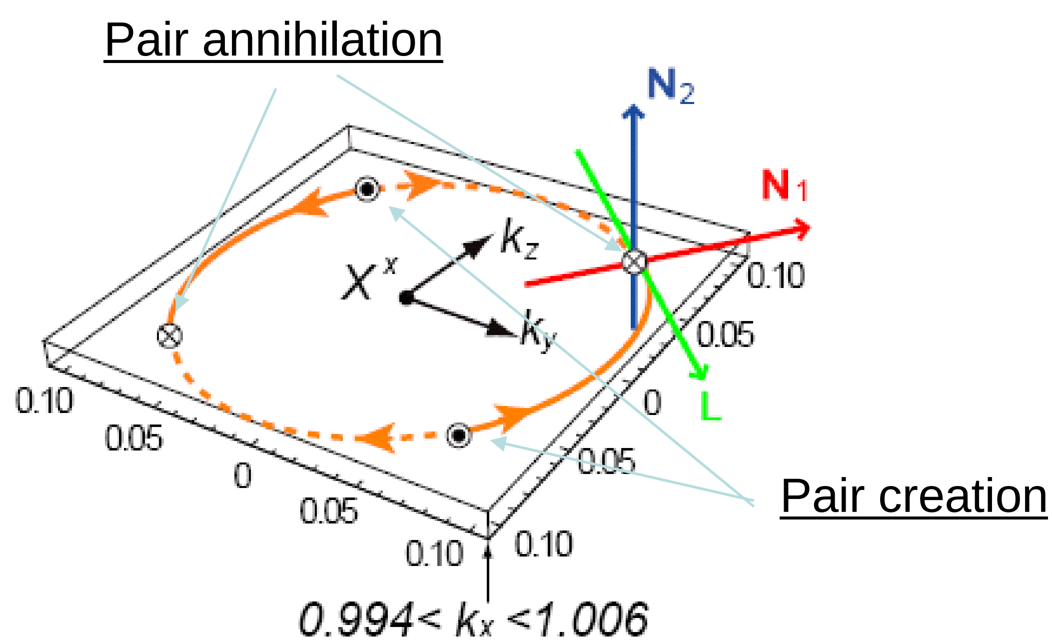
Weyl semimetal appears!
(SM, Kuga,
PRB78, 165313(2008))



Fu-Kane-Mele model
+ inversion-symmetry breaking



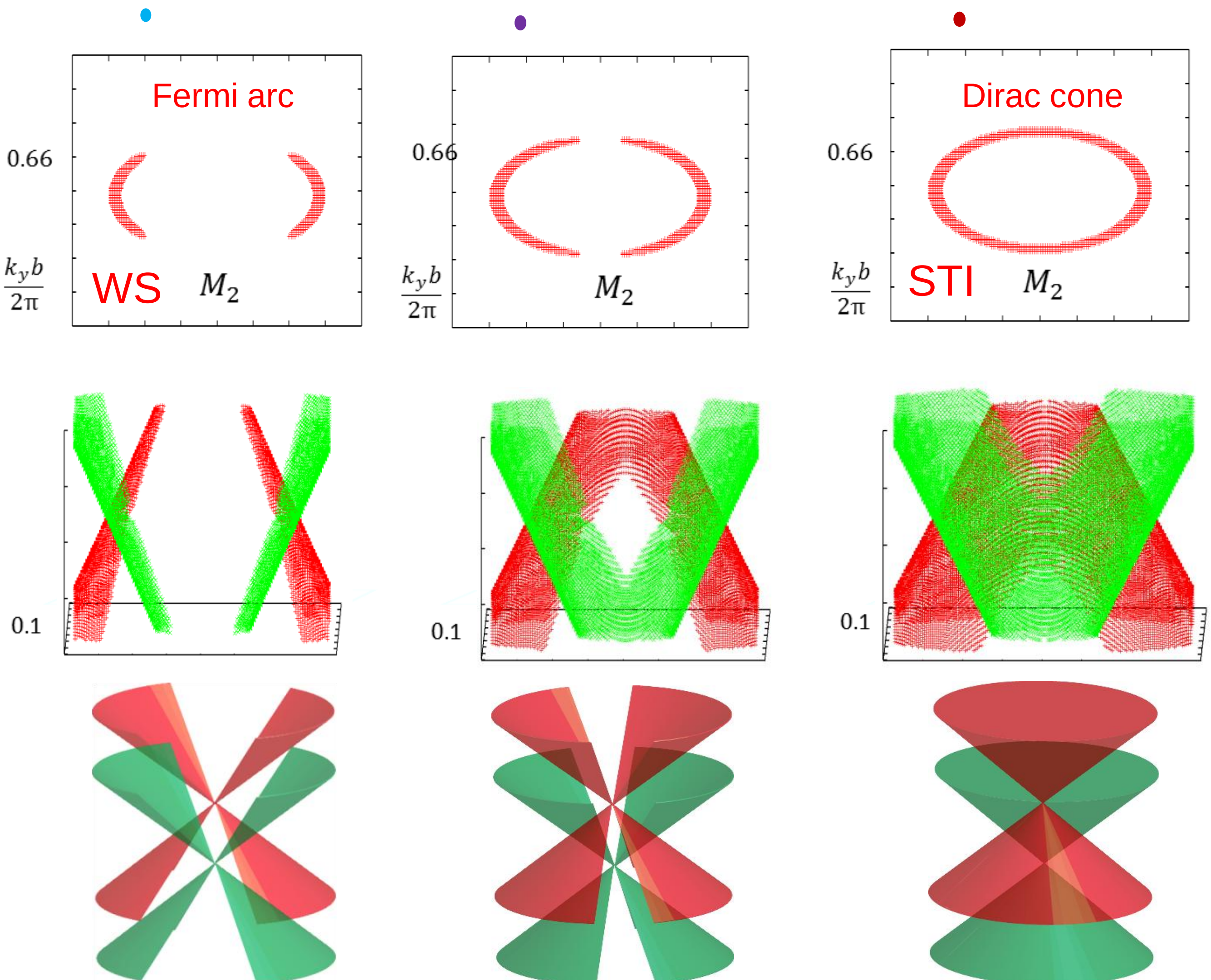
k-space trajectory of the monopoles

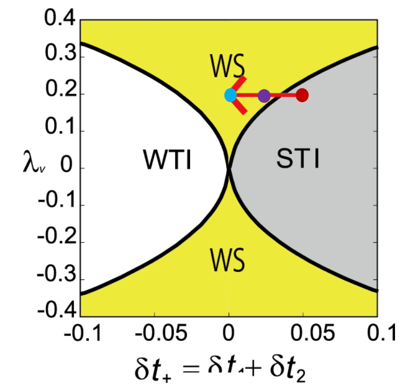


Evolution of surface states

Fermi arcs in the Weyl semimetal → (merge) → Dirac cones in the TI phase

Okugawa, Murakami, PRB (2014)





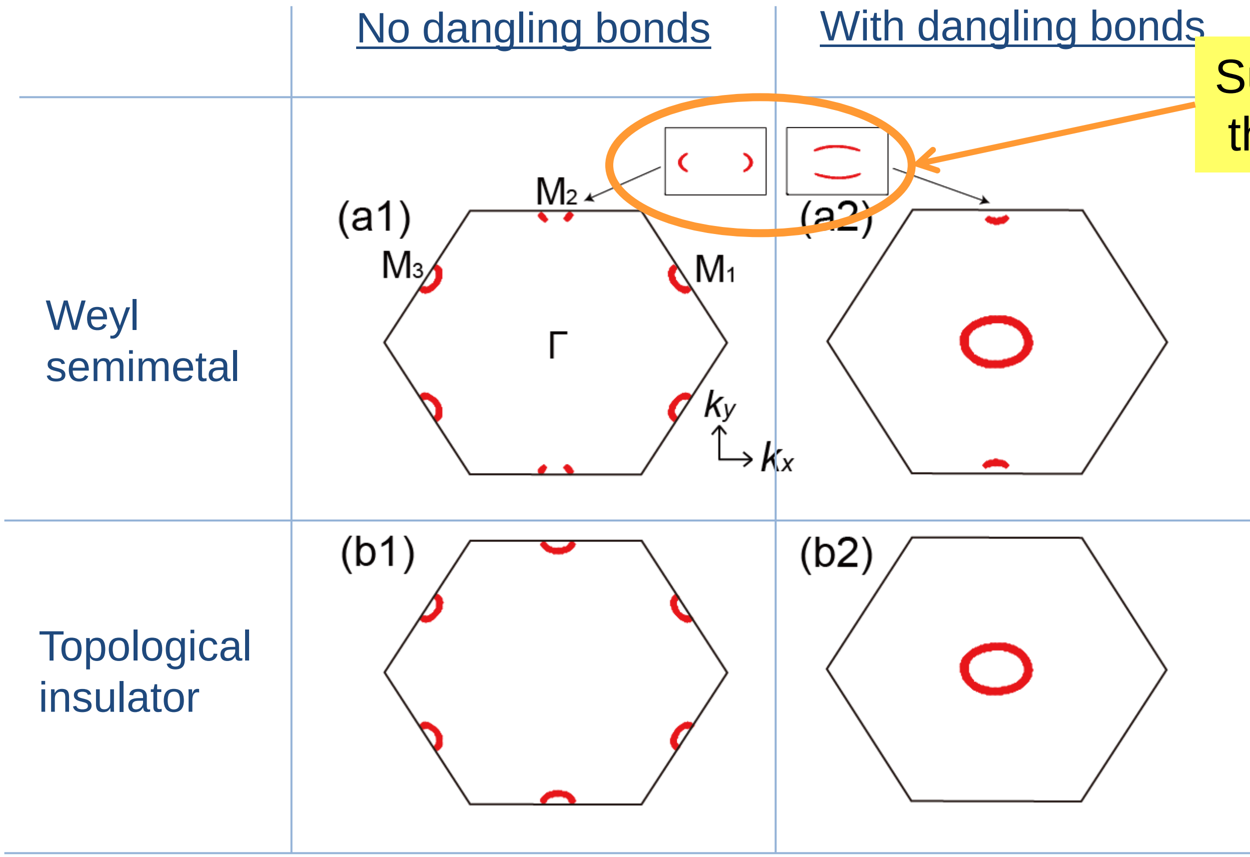
$\delta t_+ = 0$ → $\delta t_+ = 0.05t$

$\lambda_v = 0.2 \qquad t = 1.0$

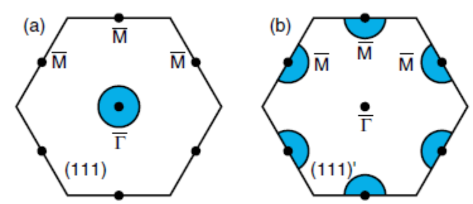
Red: top surface

Green: bottom surface

Change of surface terminations



Surface termination change the pairing of Weyl nodes

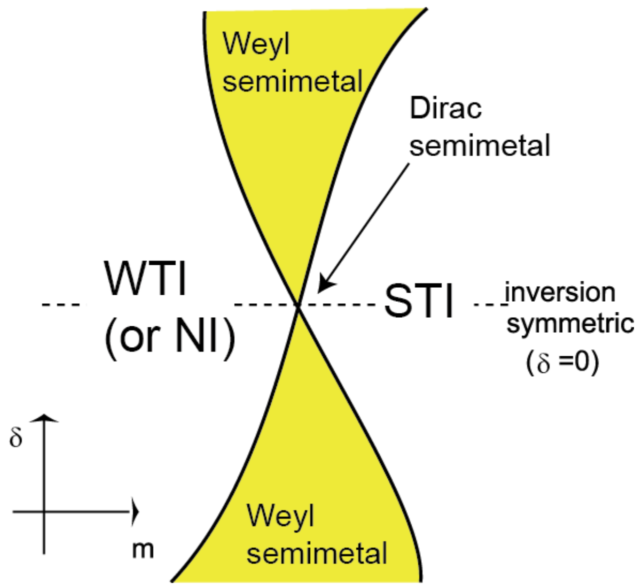


Surface Fermion parity →
surface termination changes the inside and outside of surface FS.
(for inversion symmetric systems)
Teo, Fu, Kane, PRB78, 045426 (2008)

Okugawa, Murakami, PRB (2014)

Universal phase diagram in 3D

SM, New J. Phys. ('07).
SM. Kuga, PRB ('08)
SM, Physica E43, 748 ('11)

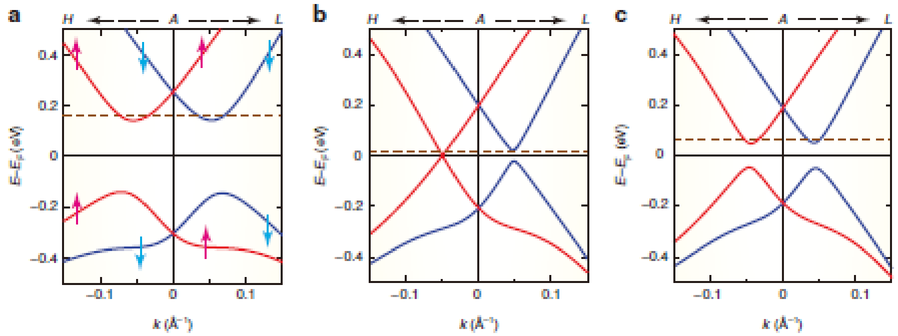


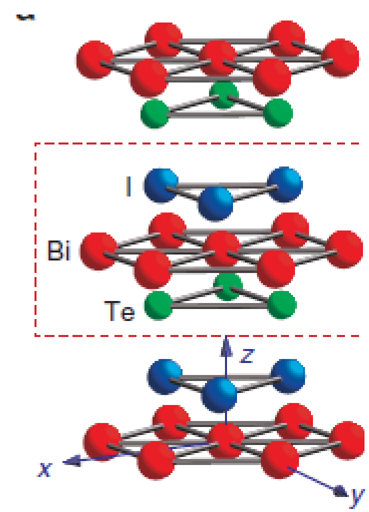
Only the inversion and time-reversal symmetries are considered.

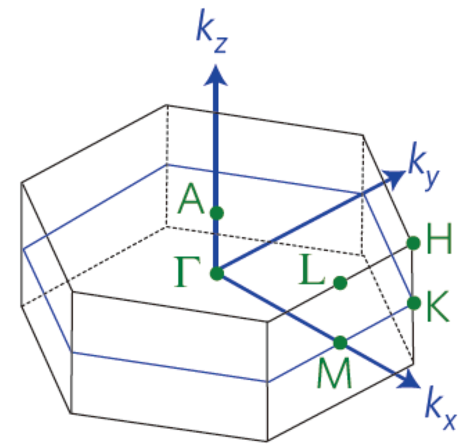
Question:
Is it valid for crystals with crystallographic symmetries?

BiTeI at high pressure: ab initio calc.

Bahramy, Nat. Commun. 3, 679 (2012)
Yang et al. PRL 110, 086402 (2013)







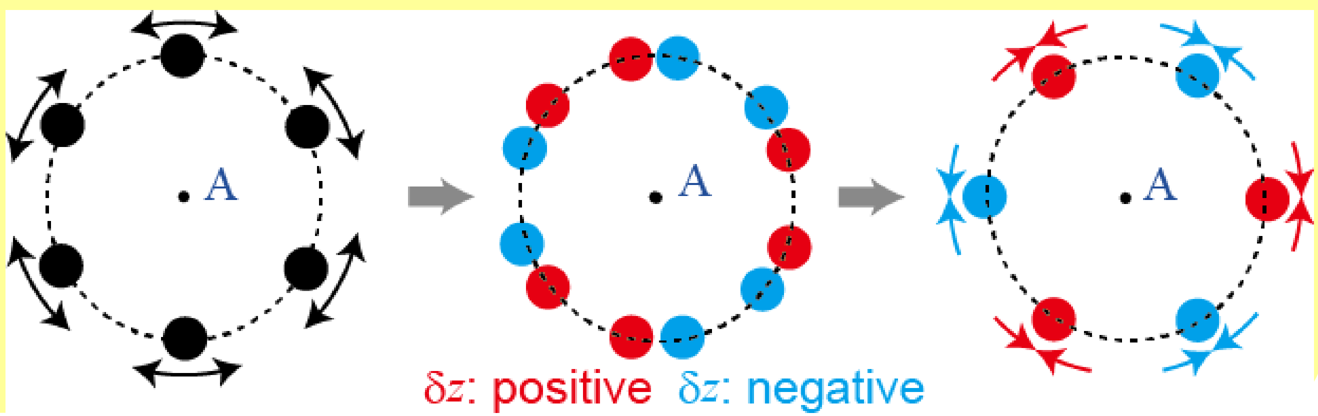
NI

TI

Phase transition at $p=p_c$

No Inversion symmetry

Weyl nodes move with increasing pressure



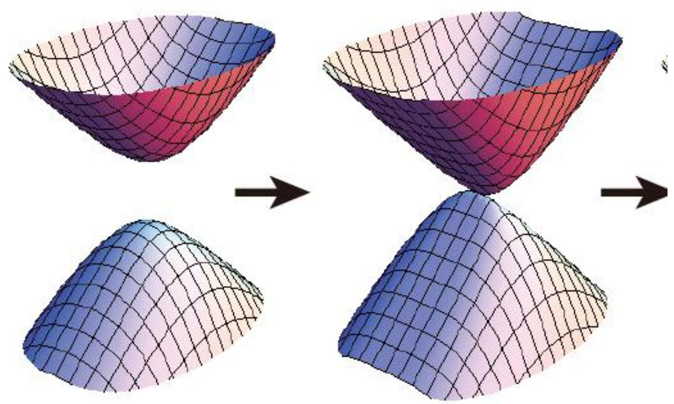
ween A and H
at $p=p_c$
etal phase

Search for Weyl semimetals without inversion symmetry

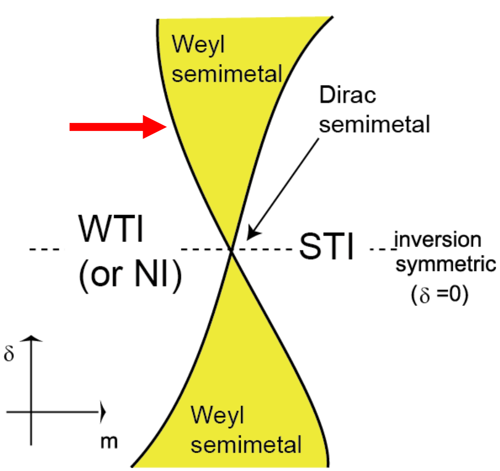
Start from any band insulator

→ suppose a gap closes by changing a parameter *m*

→ *m*



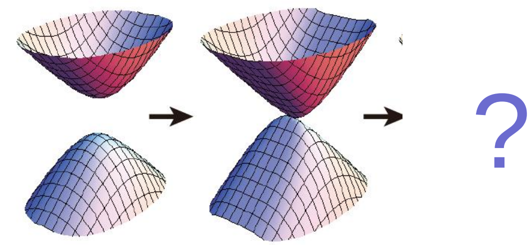
?



Classification by space groups & *k*-points.

230 space groups

138 space groups without inversion sym.



1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40
41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60
61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80
81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100
101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120
121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	139	140
141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	160
161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180
181	182	183	184	185	186	187	188	189	190	191	192	193	194	195	196	197	198	199	200
201	202	203	204	205	206	207	208	209	210	211	212	213	214	215	216	217	218	219	220
221	222	223	224	225	226	227	228	229	230										

No inversion sym.

156 $P3m1$ C_{3v}^1

($F1$; $K6$; $K7$; $M5$; $Z1$.)

Γ $\mathbf{G}_{12}^4$: $\{C_3^+ \mid 000\}$, $\{\sigma_{v1} \mid 000\}$: 3, 3; 4, 3; 6, 2: a.
M $\mathbf{G}_4^1 \otimes \mathbf{T}_2$: $\{\sigma_{v1} \mid 000\}$; $\mathbf{t}_2$: 2, 3; 4, 3: b.
A $\mathbf{G}_{12}^4 \otimes \mathbf{T}_2$: $\{C_3^+ \mid 000\}$, $\{\sigma_{v1} \mid 000\}$; $\mathbf{t}_3$: 3, 3; 4, 3; 6, 2: a.
L $\mathbf{G}_4^1 \otimes \mathbf{T}_2$: $\{\sigma_{v1} \mid 000\}$; $\mathbf{t}_2$ or $\mathbf{t}_3$: 2, 3; 4, 3: b.

high-symmetry points (TRIM)

K $\mathbf{G}_6^1 \otimes \mathbf{T}_3$: $\{C_3^+ \mid 000\}$; $\mathbf{t}_1$ or $\mathbf{t}_2$: 2, 2; 4, 2; 6, 2: a.
H $\mathbf{G}_6^1 \otimes \mathbf{T}_3 \otimes \mathbf{T}_2$: $\{C_3^+ \mid 000\}$; $\mathbf{t}_1$ or $\mathbf{t}_2$; $\mathbf{t}_3$: 2, 2; 4, 2; 6, 2: a.

high-symmetry points (non TRIM)

Δ^x $\mathbf{G}_{12}^4$: $(C_3^+, 0)$, $(\sigma_{v1}, 0)$: 3, x; 4, x; 6, x: a.
U^x $\mathbf{G}_4^1$: $(\sigma_{v1}, 0)$: 2, x; 4, x: b.
P^x $\mathbf{G}_6^1$: $(C_3^+, 0)$: 2, x; 4, x; 6, x: a.
T^x $\mathbf{G}_2^1$: $(\bar{E}, 0)$: 2, 2: a.
S^x $\mathbf{G}_2^1$: $(\bar{E}, 0)$: 2, 2: a.
T'^x $\mathbf{G}_2^1$: $(\bar{E}, 0)$: 2, 2: a.
S'^x $\mathbf{G}_2^1$: $(\bar{E}, 0)$: 2, 2: a.
Σ^x $\mathbf{G}_4^1$: $(\sigma_{v1}, 0)$: 2, x; 4, x: b.
R^x $\mathbf{G}_4^1$: $(\sigma_{v1}, 0)$: 2, x; 4, x: b.

high-symmetry lines

"The Mathematical Theory of Symmetry in Solids", Bradley, Cracknell

Each k point → little group→ irreps.

Gap closing in systems without inversion symmetry.

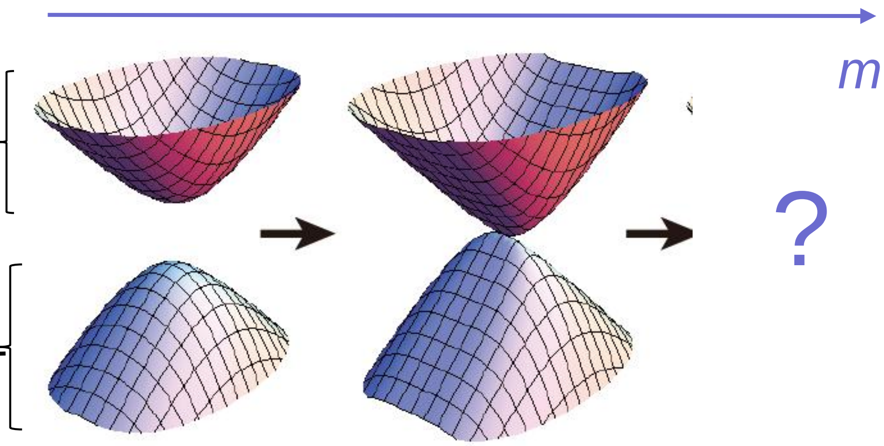
Start from an insulator → the gap closes by changing a parameter *m*

effective model

$$H(\vec{k},m)=\begin{pmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{pmatrix}$$

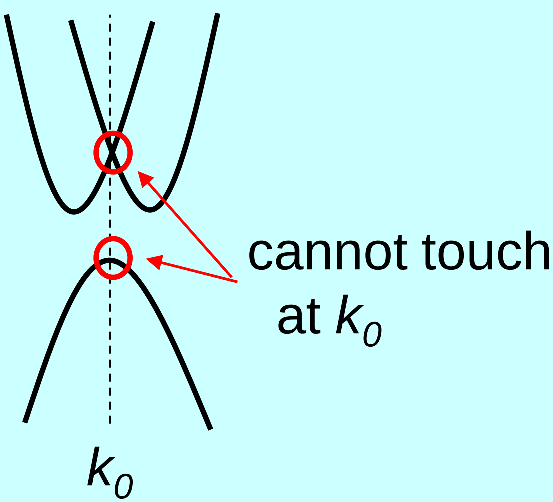
irrep. R_c

irrep. R_v

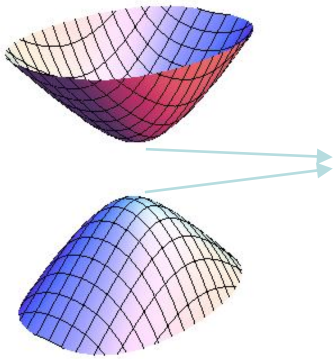


R_c and R_v should be one-dimensional
(Otherwise the gap does not close at k_0)

$$H(\vec{k},m)=\begin{pmatrix} * & * \\ * & * \end{pmatrix}=\sum_i a_i(\vec{k},m)\sigma_i$$



(Example #1): mirror symmetry (i.e. *k* : invariant under *M*)



M eigenvalue = +i or -i

k

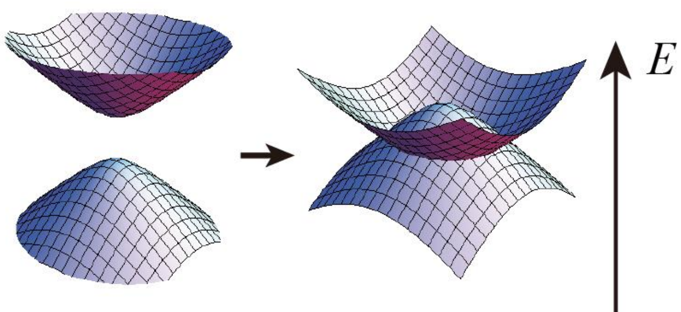
(i) <u>Same signs of *M*</u>

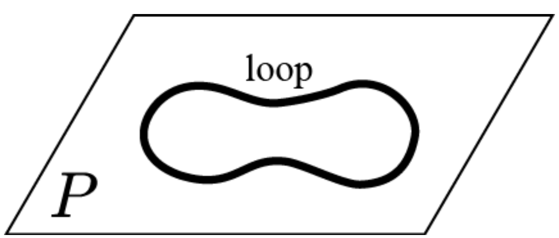
gap cannot close at *k* – level repulsion

(ii) <u>Different signs of *M*</u>

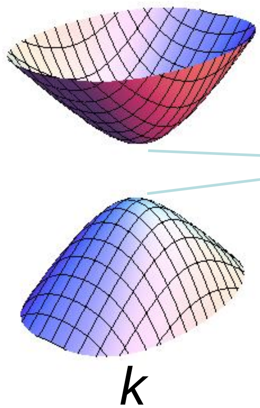
nodal-line semimetal

(gap closing along a loop on a mirror plane)





(Example #2): C_2 symmetry (i.e. *k* : invariant under C_2)



C_2 eigenvalue = +i or -i

(i) <u>Same signs of C_2</u>

gap cannot close at *k* – level repulsion

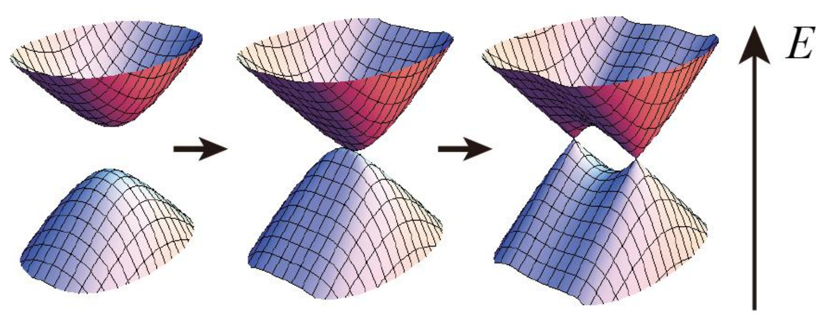
(ii) <u>Different signs of C_2</u>

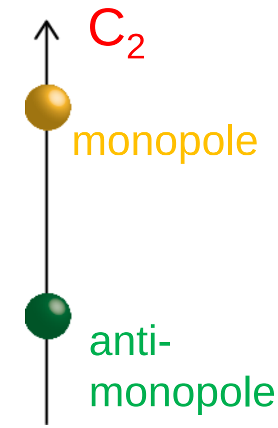
gap closing

→ Weyl semimetal

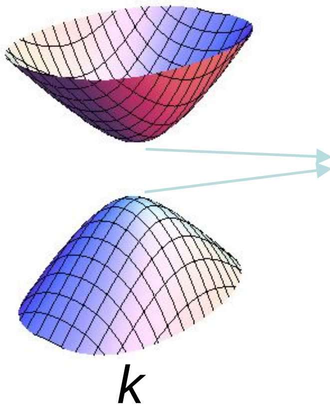
pair creation of Weyl nodes

→ move along C_2 line

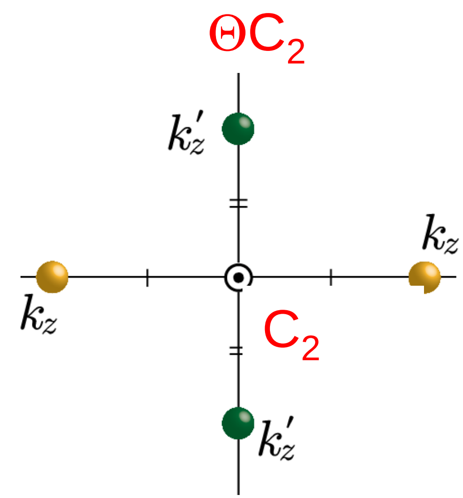




(Example #3): C_2 and ΘC_2 symmetries



C_2 eigenvalue = +i or -i

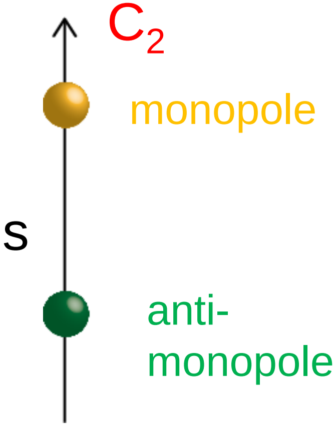


(i) Same signs of C_2

no level repulstion

Weyl semimetal

two pairs of Weyl nodes →

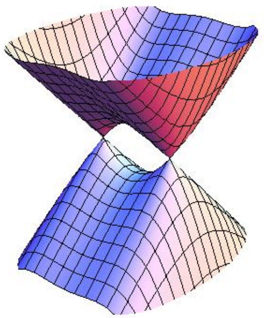


(ii) Different signs of C_2

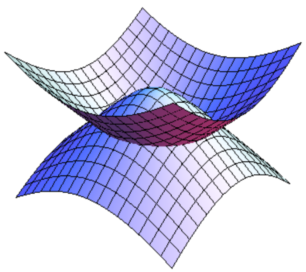
Weyl semimetal

one pair of Weyl nodes along C_2 axis

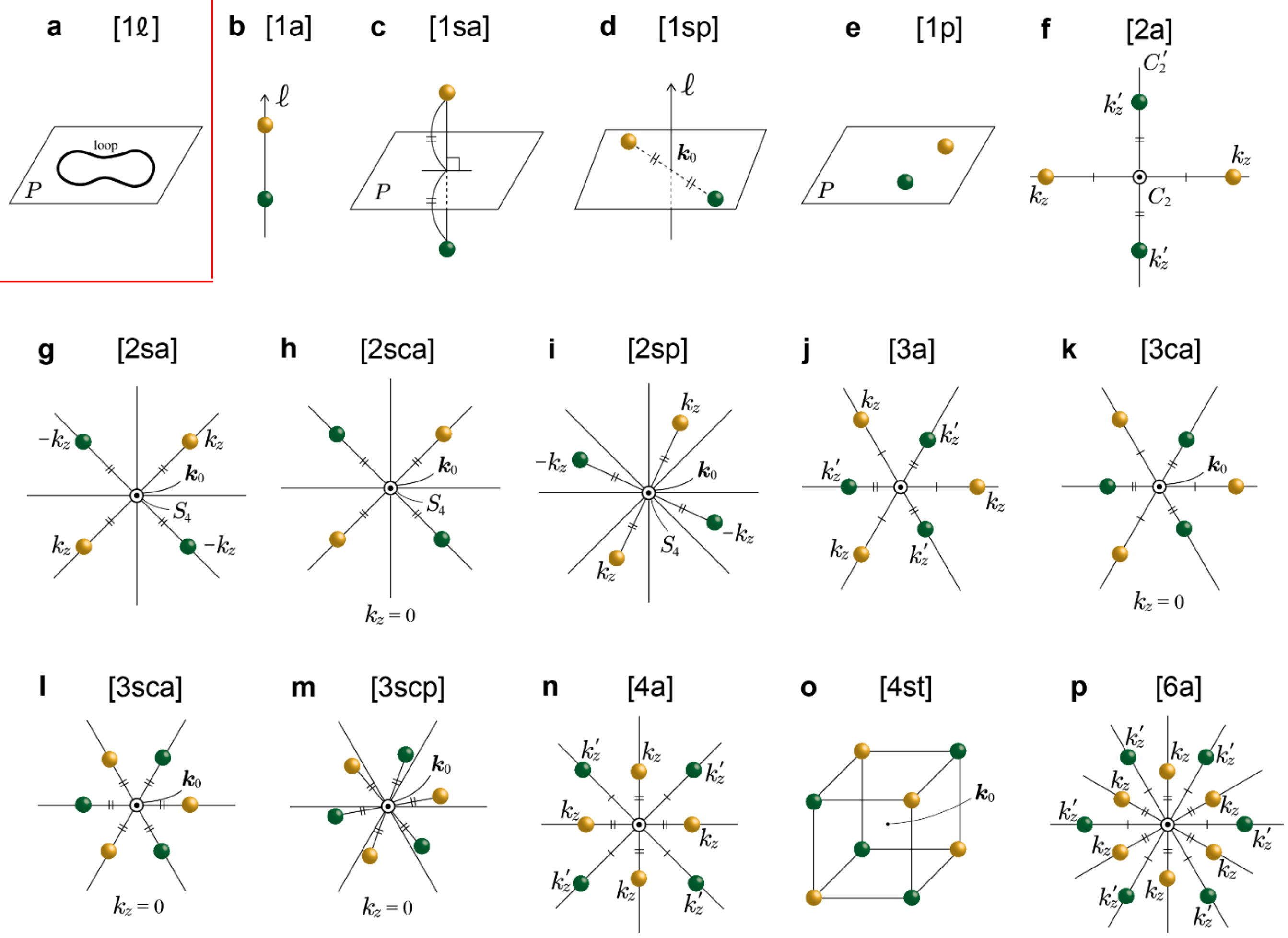
Systems without inversion symmetry
→ Classification of parametric gap-closing



Nodal line semimetal



Weyl semimetal



tetragonal

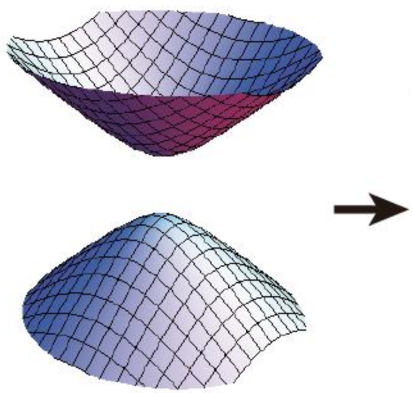
		point	line
75	$P4$		ΔUΣSYT:1p ΛVW:ij;1a
76	$P4_1$		ΔΣY:1p ΛVW:ij;1a
77	$P4_2$		ΔUΣSYT:1p ΛVW:ij;1a
78	$P4_3$		ΔΣY:1p ΛVW:ij;1a
79	$I4$		ΛVW:ij;1a ΣFΔUY:1p
80	$I4_1$		ΛVW:ij;1a ΣFΔUY:1p
81	$P\bar{4}$		ΔUΣSYT:1p W:ij;1a
82	$I\bar{4}$	P:[2]	W:ij;1a ΣFΔUY:1p
89	$P422$		ΔUΣSYTW:ii;2a,ij;1a ΛV:ii;4a,ij;1a
90	$P42_12$		ΔUΣS:ii;2a,ij;1a Λ:ii;4a,ij;1a
91	$P4_122$		ΔΣYW:ii;2a,ij;1a ΛV:ii;4a,ij;1a
92	$P4_12_12$		ΔΣ:ii;2a,ij;1a Λ:ii;4a,ij;1a
93	$P4_222$		ΔUΣSYTW:ii;2a,ij;1a ΛV:ii;4a,ij;1a
94	$P4_22_12$		ΔUΣS:ii;2a,ij;1a Λ:ii;4a,ij;1a
95	$P4_322$		ΔΣYW:ii;2a,ij;1a ΛV:ii;4a,ij;1a
96	$P4_32_12$		ΔΣ:ii;2a,ij;1a Λ:ii;4a,ij;1a
97	$I422$		ΛV:ii;4a,ij;1a WΣFΔUY:ii;2a,ij;1a Q:ij;1a
98	$I4_122$	P:(2,3);4a	ΛV:ii;4a,ij;1a WΣFΔUY:ii;2a,ij;1a Q:ij;1a
99	$P4mm$		ΔUΣSYT:ii;1sa,ij;1l
100	$P4bm$		ΔUΣS:ii;1sa,ij;1l W:[3]
101	$P4_2cm$		ΔΣSY:ii;1sa,ij;1l
102	$P4_2nm$		ΔΣST:ii;1sa,ij;1l W:[3]
103	$P4cc$		ΔΣY:ii;1sa,ij;1l
104	$P4nc$		ΔΣT:ii;1sa,ij;1l W:[3]
105	$P4_2mc$		ΔUΣYT:ii;1sa,ij;1l
106	$P4_2bc$		ΔUΣ:ii;1sa,ij;1l W:[3]
107	$I4mm$		ΣFΔUY:ii;1sa,ij;1l Q:1sp
108	$I4cm$		ΣFΔUY:ii;1sa,ij;1l
109	$I4_1md$	P:(13,14);2l	W:[3] ΣFΔ:ii;1sa,ij;1l Q:1sp
110	$I4_1cd$		W:[3] ΣFΔ:ii;1sa,ij;1l
111	$P\bar{4}2m$		ΔUYTW:ii;2a,ij;1a ΣS:ii;1sa,ij;1l
112	$P\bar{4}2c$		ΔUYTW:ii;2a,ij;1a Σ:ii;1sa,ij;1l
113	$P\bar{4}2_1m$		ΔU:ii;2a,ij;1a ΣS:ii;1sa,ij;1l
114	$P\bar{4}2_1c$		ΔU:ii;2a,ij;1a Σ:ii;1sa,ij;1l
115	$P\bar{4}m2$		ΔUYT:ii;1sa,ij;1l ΣS:ii;2a,ij;1a
116	$P\bar{4}c2$		ΔY:ii;1sa,ij;1l ΣS:ii;2a,ij;1a
117	$P\bar{4}b2$		ΔU:ii;1sa,ij;1l ΣS:ii;2a,ij;1a W:[3]
118	$P\bar{4}n2$		ΔT:ii;1sa,ij;1l ΣS:ii;2a,ij;1a W:[3]
119	$I\bar{4}m2$	P:[4]	WΔUY:ii;2a,ij;1a ΣF:ii;1sa,ij;1l Q:1sp
120	$I\bar{4}c2$		WΔUY:ii;2a,ij;1a ΣF:ii;1sa,ij;1l
121	$I\bar{4}2m$		ΣF:ii;2a,ij;1a Q:ij;1a ΔUY:ii;1sa,ij;1l
122	$I\bar{4}2d$	P:[5]	W:[3] ΣF:ii;2a,ij;1a Δ:ii;1sa,ij;1l Q:ij;1a

trigonal & hexagonal

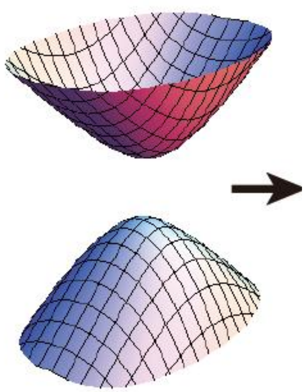
		point	line
143	$P3$		ΔP:ij;1a
144	$P3_1$		ΔP:ij;1a
145	$P3_2$		ΔP:ij;1a
146	$R3$		ΛP:ij;1a
149	$P312$		ΔP:ii;3a,ij;1a UTST'S':1p ΣR:ij;1a
150	$P321$	KH:(3,4);3ca	Δ:ii;3a,ij;1a UΣR:1p PTST'S':ij;1a
151	$P3_112$		ΔP:ii;3a,ij;1a UTST'S':1p ΣR:ij;1a
152	$P3_121$	KH:(3,4);3ca	Δ:ii;3a,ij;1a UΣR:1p PTST'S':ij;1a
153	$P3_212$		ΔP:ii;3a,ij;1a UTST'S':1p ΣR:ij;1a
154	$P3_221$	KH:(3,4);3ca	Δ:ii;3a,ij;1a UΣR:1p PTST'S':ij;1a
155	$R32$		ΛP:ij;3a,ij;1a BΣQY:ij;1a
156	$P3m1$	KH:ij;1a	Δ:(3,4);3l UΣR:ij;1l P:ij;1a TST'S':1sp
157	$P31m$		ΔP:(3,4);3l UTST'S':ij;1l ΣR:1sp
158	$P3c1$	K:ij;1a	Δ:(3,4);3l P:ij;1a UΣR:ij;1l TT':1sp
159	$P31c$		ΔP:(3,4);3l UTST'S':ij;1l Σ:1sp
160	$R3m$		ΛP:(3,4);3l BΣQY:1sp
161	$R3c$		ΛP:(3,4);3l ΣQ:1sp
168	$P6$		ΔUP:ij;1a TST'S'ΣR:1p
169	$P6_1$		ΔUP:ij;1a TT'Σ:1p
170	$P6_5$		ΔUP:ij;1a TT'Σ:1p
171	$P6_2$		ΔUP:ij;1a TST'S'ΣR:1p
172	$P6_4$		ΔUP:ij;1a TST'S'ΣR:1p
173	$P6_3$		ΔUP:ij;1a TT'Σ:1p
174	$P\bar{6}$	KH:[6]	Δ:(4,4):3scp U:1sp P:ij;1a TST'S'ΣR:ij;1l
177	$P622$	KH:(3,4);3ca	Δ:ii;6a,ij;1a UTST'S'ΣR:ii;2a,ij;1a P:ii;3a,ij;1a
178	$P6_122$	K:(3,4);3ca	Δ:ii;6a,ij;1a UTT'Σ:ii;2a,ij;1a P:ii;3a,ij;1a
179	$P6_522$	K:(3,4);3ca	Δ:ii;6a,ij;1a UTT'Σ:ii;2a,ij;1a P:ii;3a,ij;1a
180	$P6_222$	KH:(3,4);3ca	Δ:ii;6a,ij;1a UTST'S'ΣR:ii;2a,ij;1a P:ii;3a,ij;1a
181	$P6_422$	KH:(3,4);3ca	Δ:ii;6a,ij;1a UTST'S'ΣR:ii;2a,ij;1a P:ii;3a,ij;1a
182	$P6_322$	K:(3,4);3ca	Δ:ii;6a,ij;1a UTT'Σ:ii;2a,ij;1a P:ii;3a,ij;1a
183	$P6mm$	KH:(3,4);3l	P:(3,4);3l TST'S'ΣR:ii;1sa,ij;1l
184	$P6cc$	K:(3,4);3l	P:(3,4);3l TT'Σ:ii;1sa,ij;1l
185	$P6_3cm$	K:(3,4);3l	P:(3,4);3l TT'Σ:ii;1sa,ij;1l
186	$P6_3mc$	K:(3,4);3l	P:(3,4);3l TT'Σ:ii;1sa,ij;1l
187	$P\bar{6}m2$	KH:[6]	Δ:(3,4);3l (3,3)(4,4);3sca UTST'S':ii;1sa,ij;1l P:ii;3a,ij;1a
188	$P\bar{6}c2$	K:[6]	Δ:(3,4);3l (3,3)(4,4);3sca UTT':ii;1sa,ij;1l P:ii;3a,ij;1a R:[1]
189	$P\bar{6}2m$		Δ:(3,4);3l (3,3)(4,4);3sca UΣR:ii;1sa,ij;1l P:(3,4);3l
190	$P\bar{6}2c$	H:[8]	Δ:(3,4);3l (3,3)(4,4);3sca UΣ:ii;1sa,ij;1l P:(3,4);3l SS':[1]

Systems without inversion symmetry
→ Classification of parametric gap-closing

(a) Nodal-line semimetal (← mirror plane)

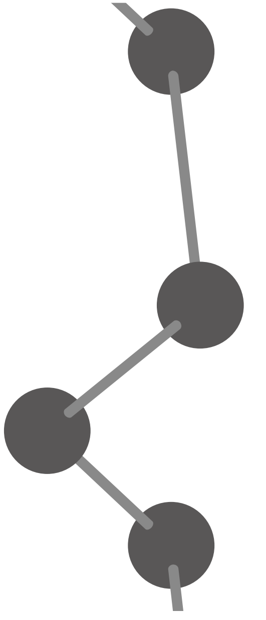


(b) Weyl semimetal



Only two possibilities. No insulator-to-insulator transition happens.

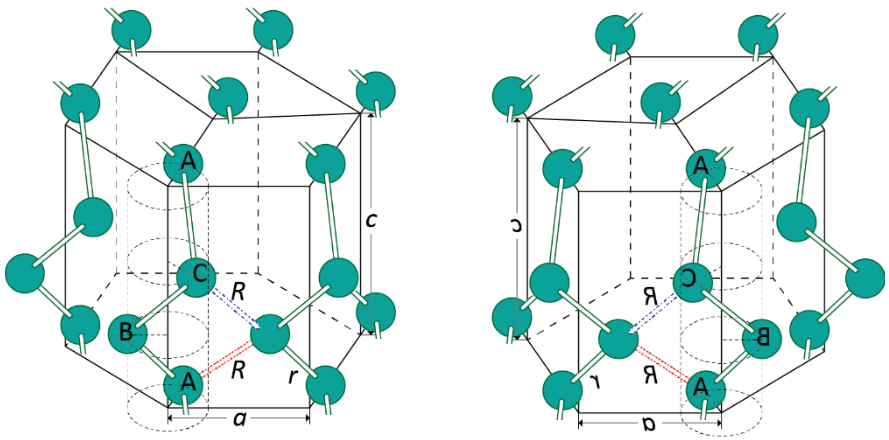
Topological Effects in Tellurium and Selenium



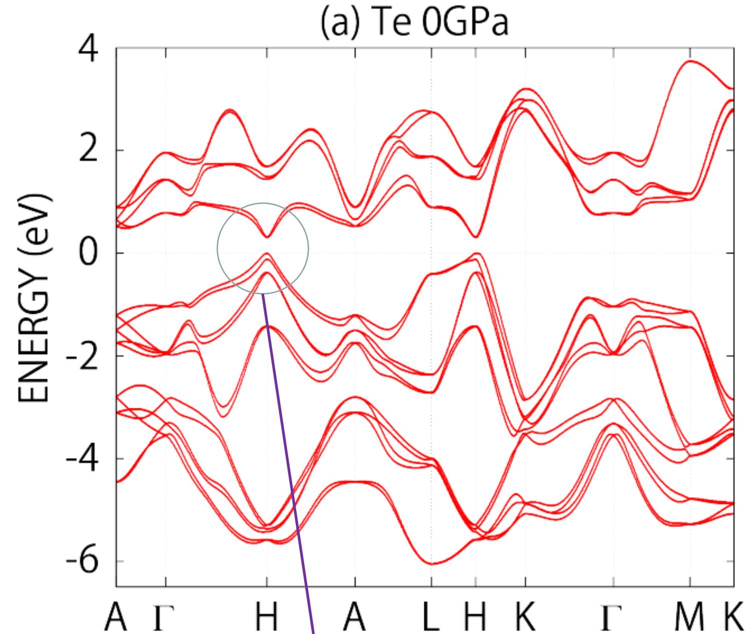
Hirayama, Okugawa, Ishibashi, Murakami, Miyake,
PRL 114, 206401 (2015)

Te : lattice with helical chains

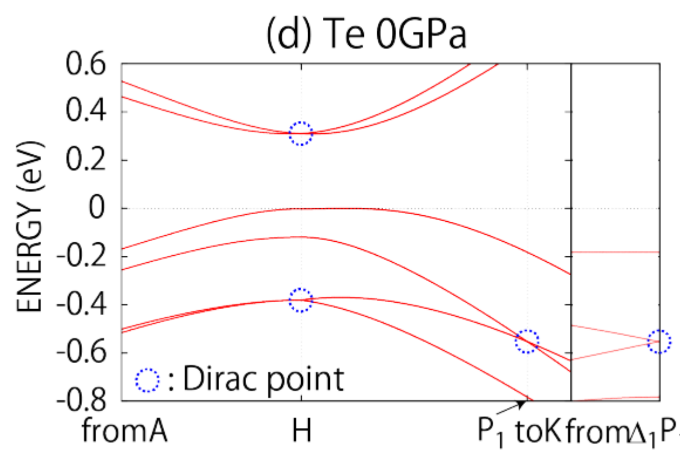
M. Hirayama, R. Okugawa, S. Ishibashi,
S. Murakami, T. Miyake,
PRL (2015)

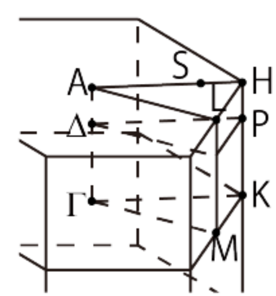


$P3_121$ $P3_221$



Band gap: 0.3eV



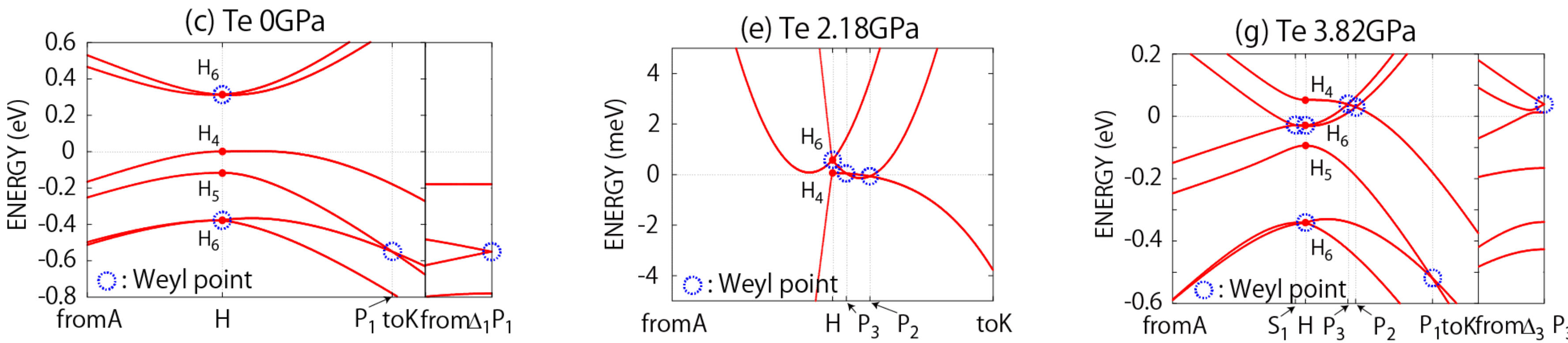


- Lattice with helical chains
- No inversion symmetry
- No mirror symmetry

→ Allow Weyl nodes

Te becomes Weyl semimetal at high pressure

pressure

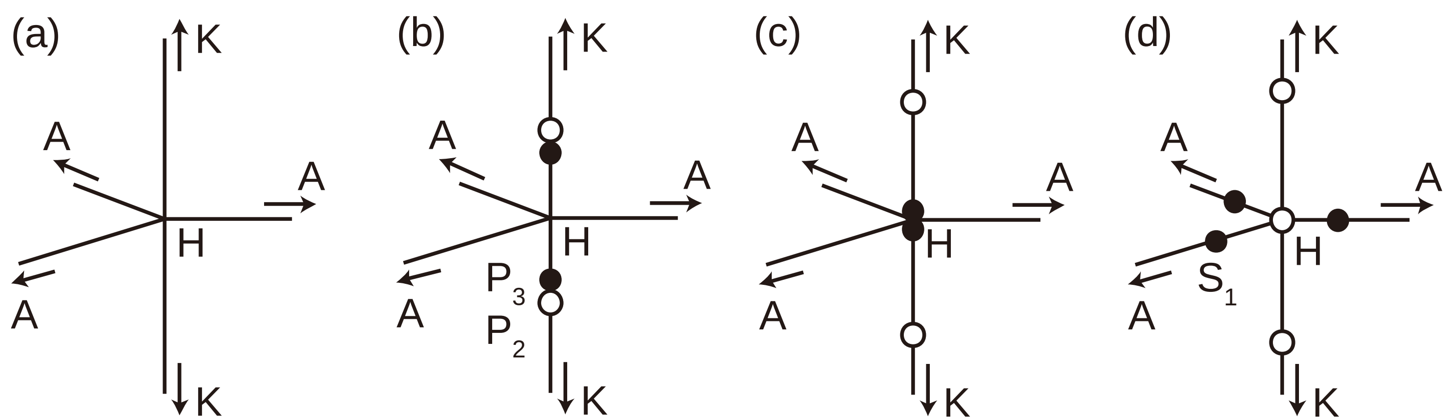


insulator

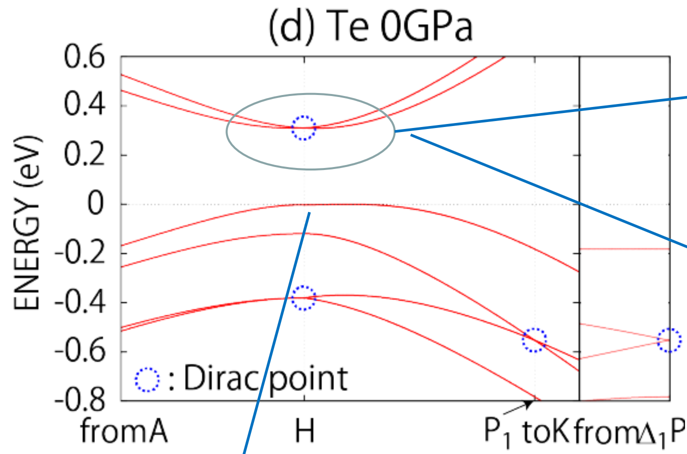
Weyl semimetal

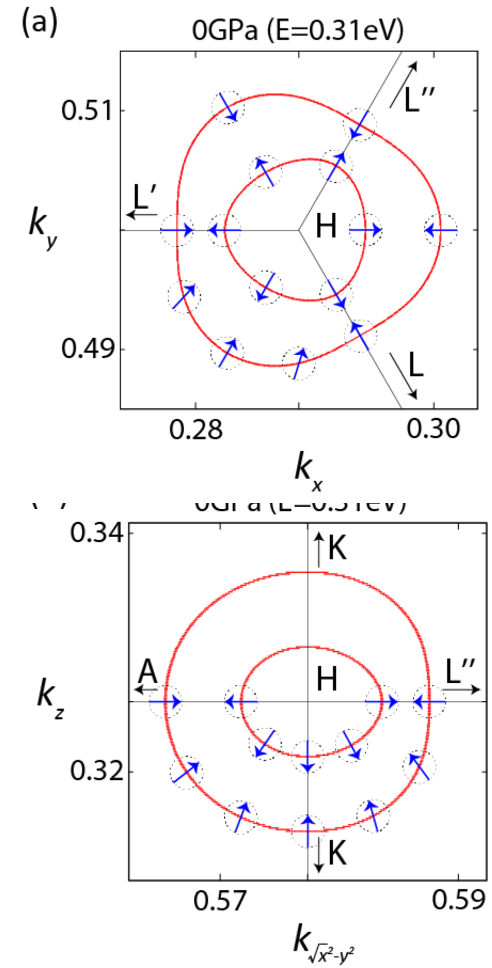
metal

Motion of Weyl Nodes

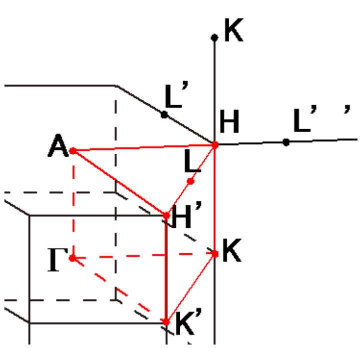


Te: spin structure at ambient pressure





Valence band
spin // z axis
: opposite spins for H and H' points
valley degree of freedom
similar to MoS_2



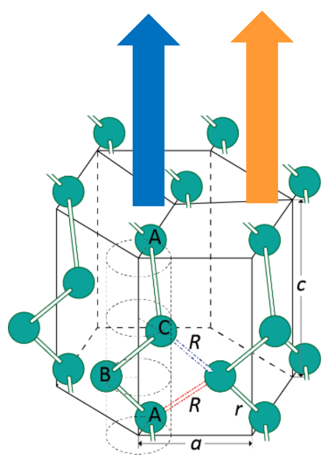
Conduction band
hedgehog spin structure
: unique to systems without mirror symmetry

Chiral transport
in crystals with helical structure

Yoda, Yokoyama, Murakami,Sci. Rep. 5, 12024 (2015)

Chiral crystal

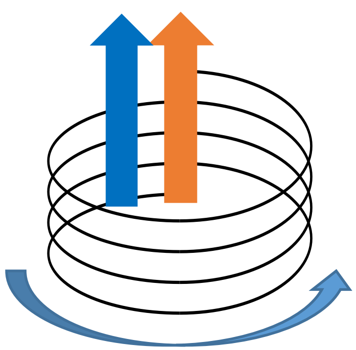
Current Magnetization



=

solenoid

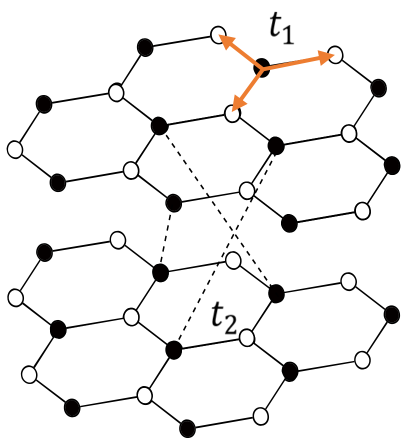
Current Magnetization



Current-induced orbital magnetization

Model

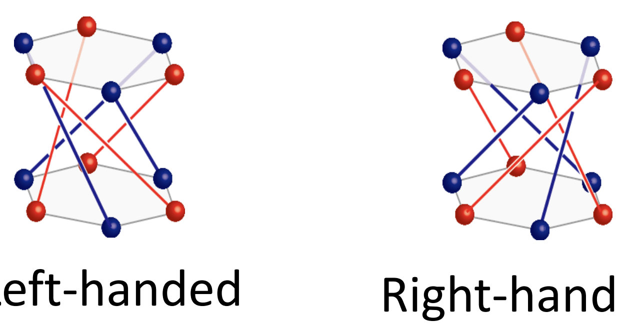
An infinite stack of honeycomb lattice layers with a helical structure



$$H = t_1 \sum_{\langle ij \rangle} c_i^\dagger c_j + t_2 \sum_i \xi_i c_i^\dagger c_j$$

t_1: nearest neighbor hopping

t_2:helical hopping within
the same sublattice in the neighboring layers



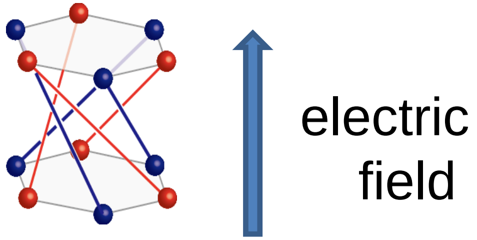
It reduces to Haldane model by replacement: kz→ϕ

Formalism for current induced orbital magnetization

Orbital magnetization (Ceresoli et al, Xiao et al. (2006))

$$\boldsymbol{M}_{\mathrm{orb}} = \frac{e}{2\hbar} \mathrm{Im} \sum_{n} \int_{\mathrm{BZ}} \frac{d^3\boldsymbol{k}}{(2\pi)^3} f_{n\boldsymbol{k}} \langle \partial_{\boldsymbol{k}} u_{n\boldsymbol{k}} | \times (H_{\boldsymbol{k}} + \varepsilon_{n\boldsymbol{k}} - 2\varepsilon_F) | \partial_{\boldsymbol{k}} u_{n\boldsymbol{k}} \rangle$$

Apply electric field (// helical axis)



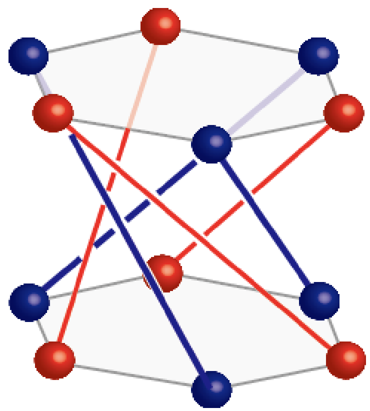
Boltzmann approximation

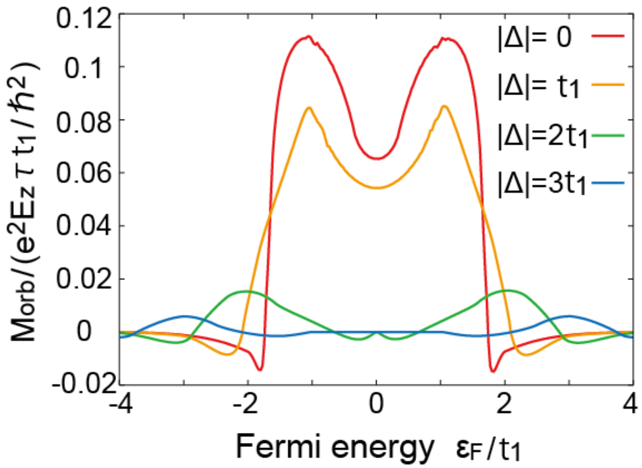
distribution function : $f_{n\boldsymbol{k}} = f^0_{n\boldsymbol{k}} + eE_z \tau v_{n,z} \left. \frac{df}{d\varepsilon} \right|_{\varepsilon=\varepsilon_{n\boldsymbol{k}}}$

For a metal, the orbital magnetization is induced by an electric current.

▪ Current-induced orbital magnetization (no SOC needed)

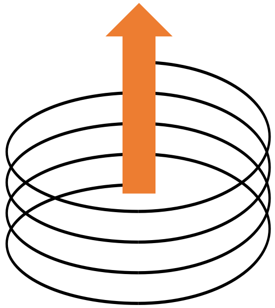
Left-handed crystal





opposite for the right-handed and left-handed helix.

Current
& magnetization



Current-induced orbital magnetization

- Inter-site (inter-unit-cell)
  - Tellurium: Present work (Yoda, Yokoyama, Murakami, Sci. Rep. (2015))

- Intra-site (intra-unit-cell)
  - Tellurium (Shalygin et al., Phys. Solid State 56, 2362 (2012))

    Current → different population for $j_z>0$ and $j_z<0$ states

  - zeolite-templated carbon

    Koretsune, Arita, Aoki,

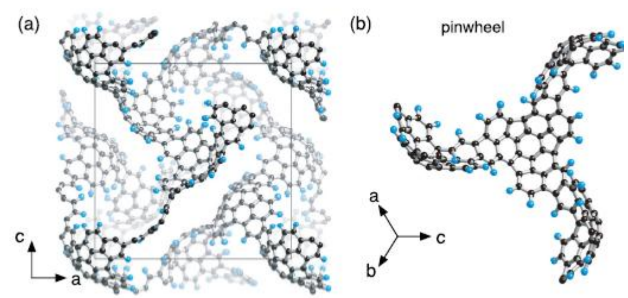
    PRB **86**, 125207 (2012)

    Network of $C_{36}H_9$

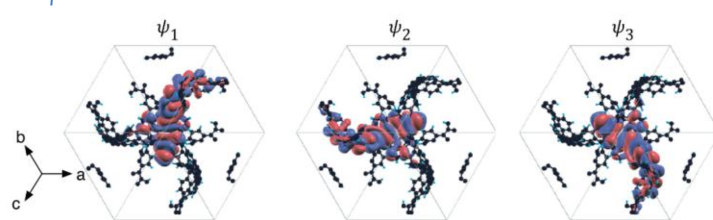
    At each $C_{36}H_9$

$$\psi_E^{\pm} = \frac{1}{\sqrt{3}}\left(p_x + e^{\pm 2\pi i/3} p_y + e^{\pm 4\pi i/3} p_z\right)$$

$$\longrightarrow \quad l_z = \pm 1$$

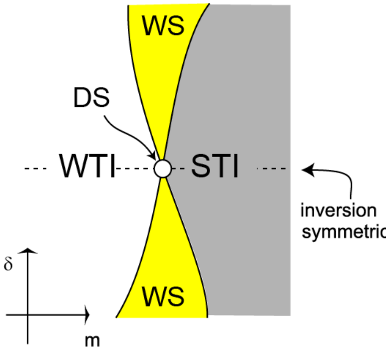


$C_{36}H_9$

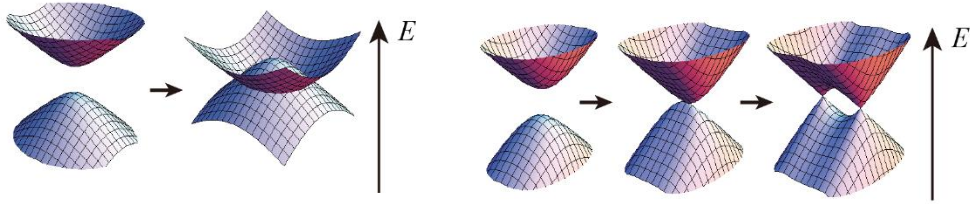


"p_x" "p_y" "p_z"

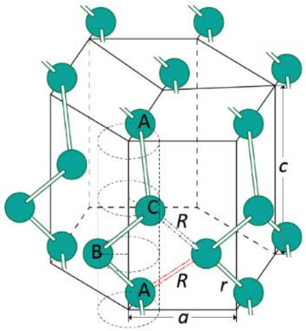
Conclusions



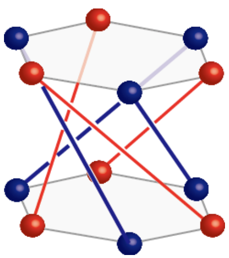
- Weyl semimetals (in inversion asymmetric systems)
  - In TI-NI phase transition, Weyl semimetals naturally appear.
  - Under space group symmetry
    e.g. Tellurium: Weyl semimetal at high pressure



Murakami, New J. Phys. 9, 356 (2007)
Murakami, Kuga, PRB78, 165313 (2008)
Okugawa, Murakami, Phys. Rev. B 89, 235315 (2014)
Hirayama et al., PRL 114, 206401 (2015)



- Chiral transport in crystals with helical lattice structure
  - analogy with solenoid
  - Current induced orbital & spin magnetization
  - Example:
    - 3D chiral crystals: Tellurium etc.



Yoda, Yokoyama, Murakami, Sci. Rep. 5, 12024 (2015)