Superconductivity in Cu:Bi_2Se_3

model order parameters and surface states

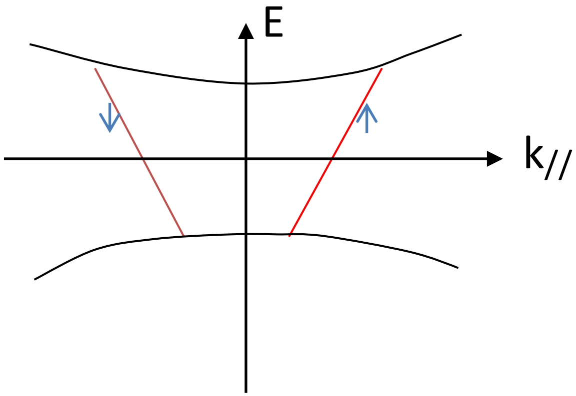
Sungkit Yip
Institute of Physics
Academia Sinica, Taipei, Taiwan

Topological states (bulk)

Surface /edge states

Quantum Hall

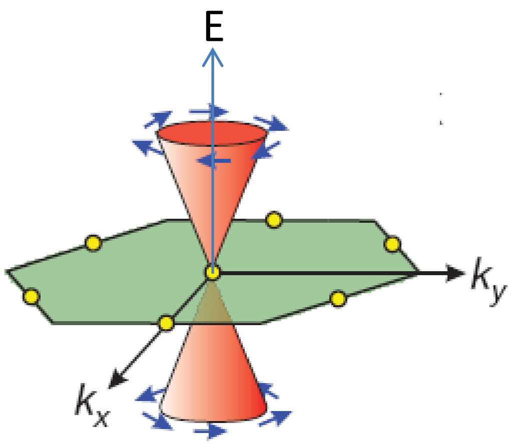
chiral



Quantum Spin Hall

Topological Insulators

3D Dirac cone



Bi_2Se_3, Bi_2Te_3, ….

Spin-ARPES

(Hsieh et al (Princeton))

Superconductor:

can be topological non-trivial due to superconducting order parameter even though normal state band structure trivial

Examples:

$$-(k_x - ik_y)\,|\uparrow\uparrow> + (k_x + ik_y)\,|\downarrow\downarrow>$$

$$\begin{pmatrix} -k_x + ik_y & 0 \\ 0 & k_x + ik_y \end{pmatrix}$$

~(2D TI) planar state

$$\begin{pmatrix} -k_x + ik_y & k_z \\ k_z & k_x + ik_y \end{pmatrix}$$

~(3D TI) ^{3}He-B

Balian-Werthamer

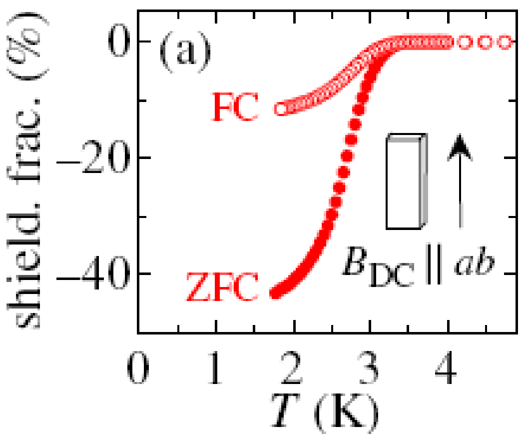
(c.f. s-wave, topologically trivial; no surface states)

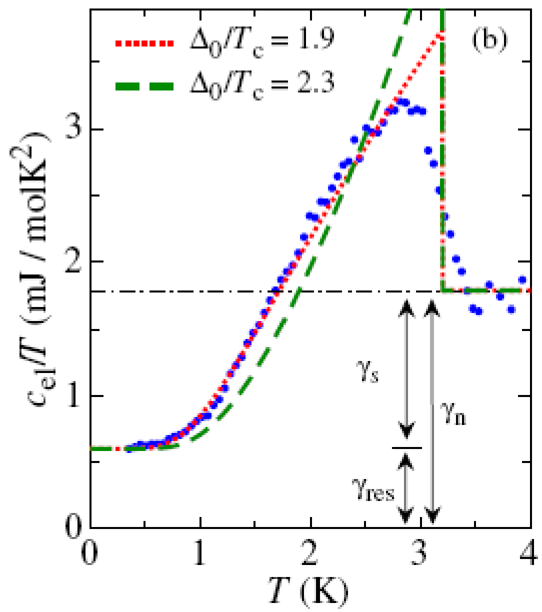
$Cu:Bi_2Se_3$

superconducting (Princeton)

Tc varies with Cu concentration, up to ~ 4K

Ando:





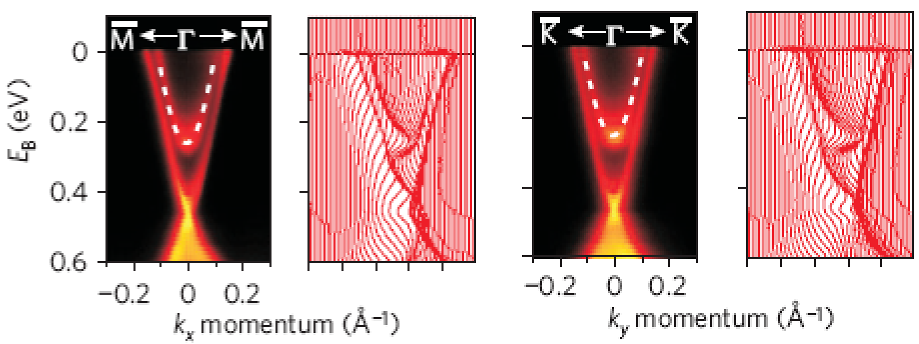
suggest fully gapped

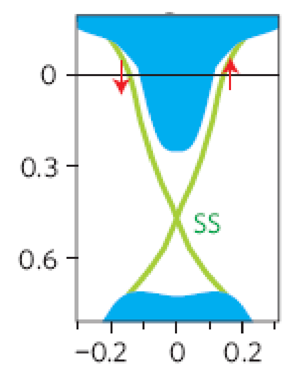
Cu intercalates

electron doped

chemical potential ~0.4 eV (>> Tc)

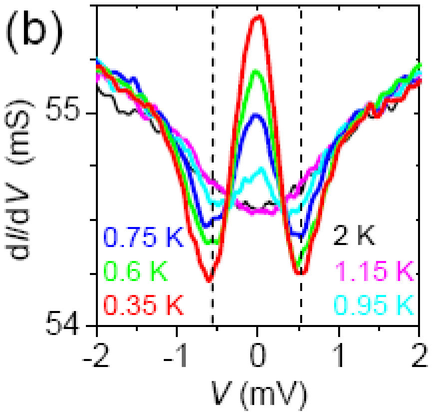
Wray et al, Nature, 10



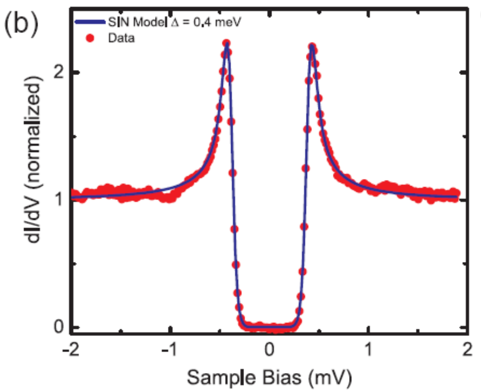


Tunneling experiments: -- controversial

Osaka 11:



NIST, MD



Q:

Superconducting order parameter ?

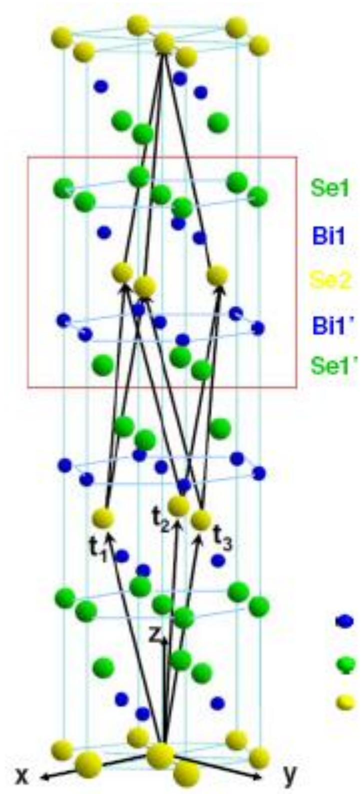
Topology of the superconducting state ?

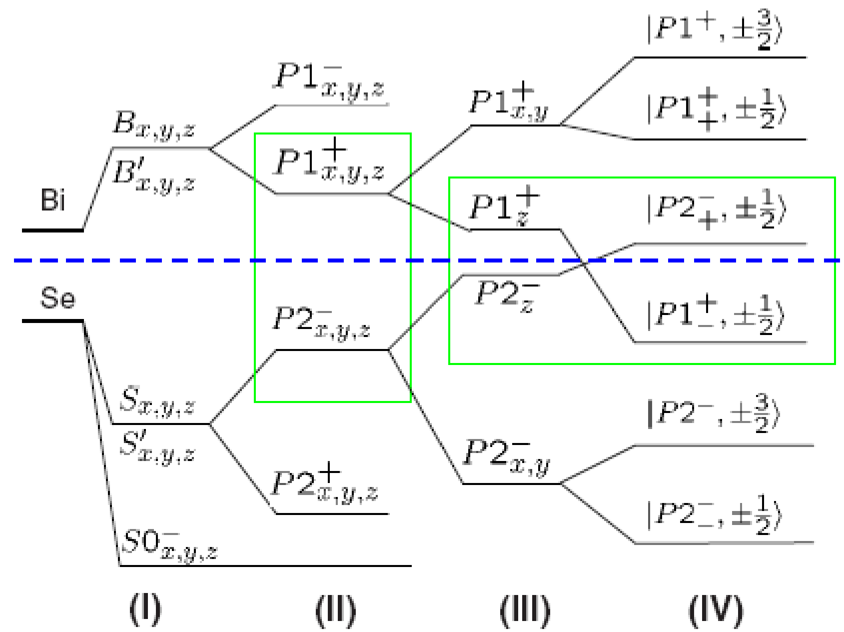
Surface states?

what is the role of the topological insulator state?

Bi2Se3: normal state

(H Zhang et al Nat. Phys. 09; C X Liu et al PRB 10)





D_{3d}

$$D_{3d} = (E, 2C_3, 3U_2) \times P$$

band inversion at k=0 Γ point

$D_{\infty h}$

Model for k ~ 0:

$$H_N = (M_0 + \ldots)\sigma_z + (B_0 + ..)k_z\sigma_y + (A_0 + \ldots)(k_y s_x - k_x s_y)\sigma_x$$

↓

$P1_z^+ \quad P2_z^-$

parity operator: σ_z

Fu and Berg 10:

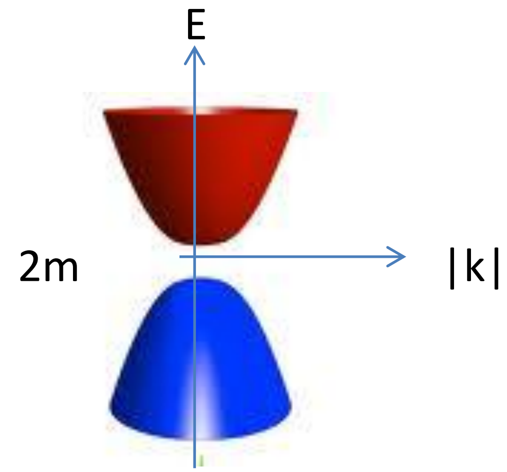
$$H_N(\vec{k}) = m\sigma_x + v_z k_z \sigma_y + v\sigma_z(k_x s_y - k_y s_x)$$

parity operator: σ_x

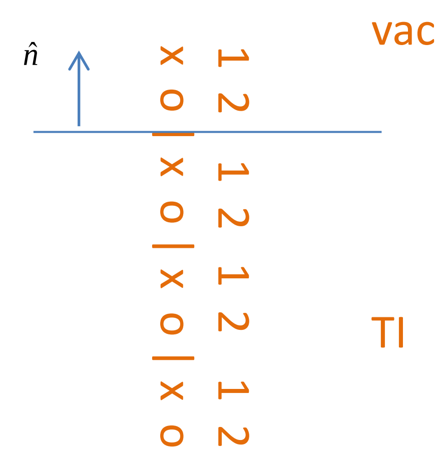
Dirac like Hamiltonian

$$E_k = \pm \varepsilon_k$$

$$\epsilon_{\vec{k}} \;=\; (m^2 + v_z^2 k_z^2 + v^2 k_{\|}^2)^{1/2}$$



$$H_N(\vec{k}) = m\sigma_x + v_z k_z \sigma_y + v\sigma_z(k_x s_y - k_y s_x)$$



Boundary condition

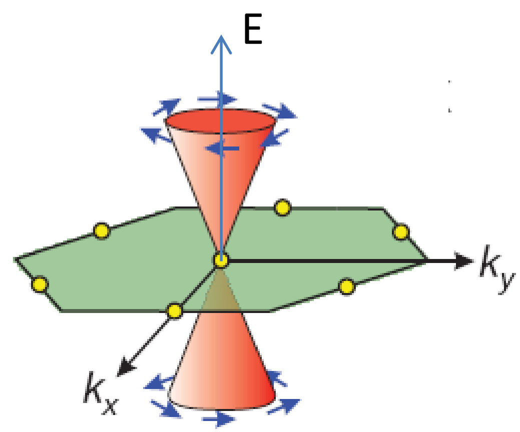
$$< \sigma_z = -1 | \Psi > = 0$$

$$\downarrow$$

2

Surface bound state as Dirac cone if

$$\mathrm{sgn}(m v_z) < 0$$



Positive energy branch along $v\hat{n} \times \vec{k}$

Superconducting state:

Fu and Berg 10: local pairs, investigated phase diagram with local interaction

$$|1\uparrow 1\downarrow>, |1\uparrow 2\downarrow>, ... |1\uparrow 2\uparrow>, |1\downarrow 2\downarrow>$$ (6 total)

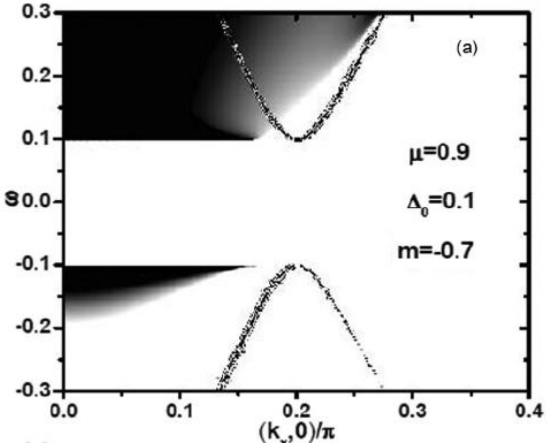
Also noted, different symmetries:

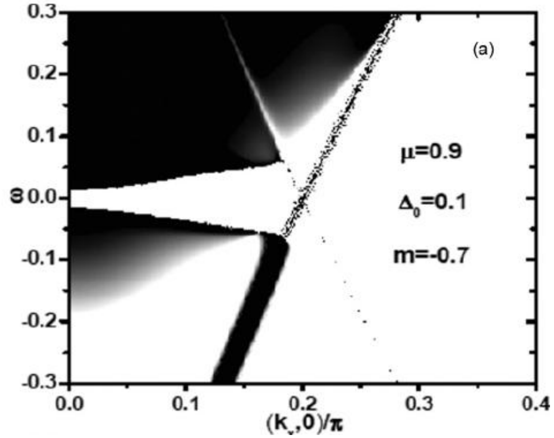
A_{1g}	$\|1\uparrow 1\downarrow> + \|2\uparrow 2\downarrow>$ $\|1\uparrow 2\downarrow> - \|1\downarrow 2\uparrow>$	
A_{1u}	$\|1\uparrow 2\downarrow> + \|1\downarrow 2\uparrow>$	← Fully gapped, topological superconducting state
A_{2u}	$\|1\uparrow 1\downarrow> - \|2\uparrow 2\downarrow>$	
E_u	$\|1\uparrow 2\uparrow>$ $\|1\downarrow 2\downarrow>$	

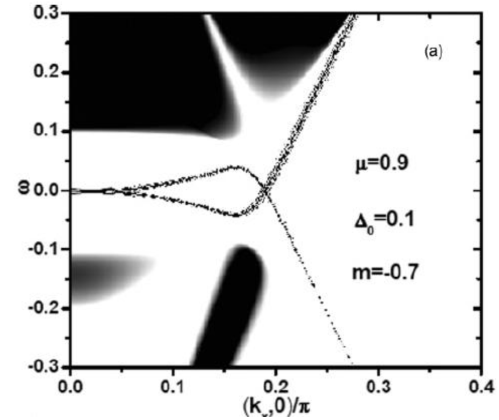
surface bound states investigated, using this picture, by:

Hao and Lee 11,
Sato, Tanaka et al 12
Hsieh and Fu 12
Kamakage et al 12

Hao and Lee 11 :







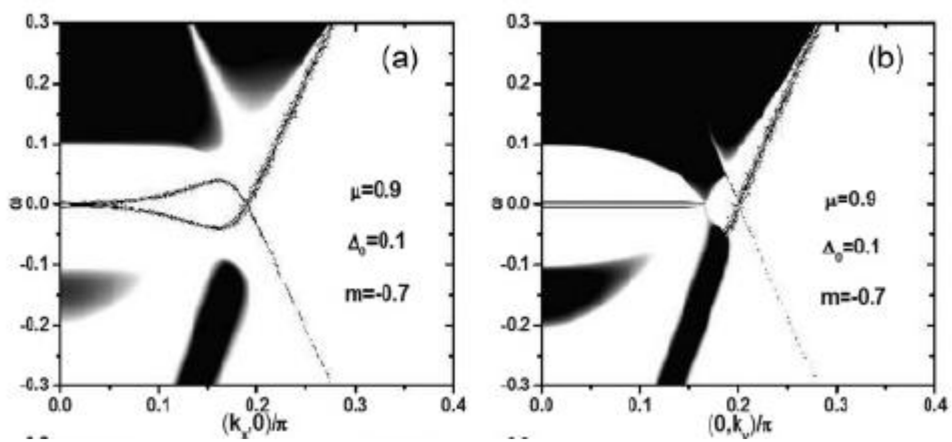
$|1\uparrow 1\downarrow> + |2\uparrow 2\downarrow>$

$|1\uparrow 2\downarrow> - |1\downarrow 2\uparrow>$

$|1\uparrow 2\downarrow> + |1\downarrow 2\uparrow>$

"intrasite opposite spin"

"interorbital odd parity"

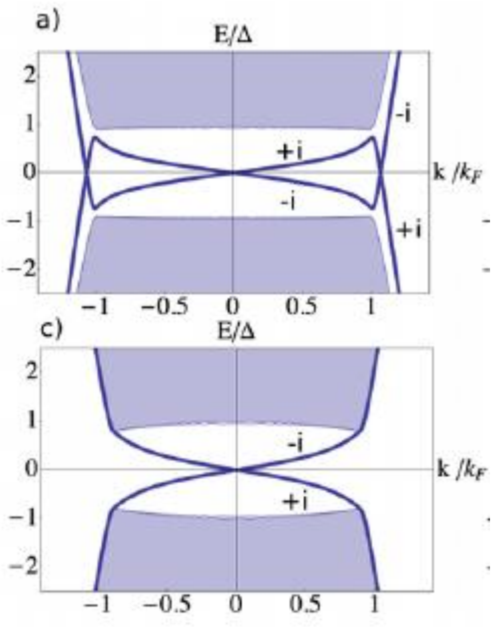


$|1\uparrow 2\uparrow> - |1\downarrow 2\downarrow>$

Hsieh and Fu 12:

$|1\uparrow 2\downarrow> + |1\downarrow 2\uparrow>$

Topological SC



$\mathrm{sgn}(mv_z) < 0$

$\mathrm{sgn}(mv_z) > 0$

mirror index

Superconductivity with strong spin-orbit

80's: heavy fermions

Anderson, Blount, Rice, ….

if normal state time-reversal and parity symmetric
each k: two degenerate states (pseudospin)
Cooper pairing between pseudospin

pairing wavefunction:

even parity : pseudospin singlet
need only specify momentum dependence (even)

odd parity: pseudospin triplet

$$\begin{pmatrix} -d_x + id_y & d_z \\ d_z & d_x + id_y \end{pmatrix}$$

$\vec{d}(\vec{k})$ spin-vector
k dependent
odd in k

D_{6h}

Yip and Garg 93

complete basis set, up to invariant functions

even

Γ_j	Basis functions
A_{1g}	$1, (k_x^2+k_y^2), k_z^2, \ldots$
A_{2g}	$\mathrm{Im}k_+^6$
B_{1g}	$k_z \mathrm{Im}k_+^3$
B_{2g}	$k_z \mathrm{Re}k_+^3$
E_{1g}	$\begin{bmatrix}\mathrm{Re}\\ \mathrm{Im}\end{bmatrix}: k_z k_+;\ k_z k_-^5$
E_{2g}	$\begin{bmatrix}\mathrm{Re}\\ \mathrm{Im}\end{bmatrix}: k_+^2;\ k_-^4$

odd

Γ_j	Basis functions
A_{1u}	$k_z\hat{\mathbf{z}};\ k_x\hat{\mathbf{x}}+k_y\hat{\mathbf{y}};\ \mathrm{Re}k_+^5\mathbf{r}_+$
A_{2u}	$\mathrm{Im}:\ k_-\mathbf{r}_+;\ k_+^5\mathbf{r}_+;\ k_+^6 k_z\hat{\mathbf{z}}$
B_{1u}	$\mathrm{Im}:\ k_+^3\hat{\mathbf{z}};\ k_+^2 k_z\mathbf{r}_+;\ k_+^4 k_z\mathbf{r}_-$
B_{2u}	$\mathrm{Re}:\ k_+^3\hat{\mathbf{z}};\ k_+^2 k_z\mathbf{r}_+;\ k_+^4 k_z\mathbf{r}_-$
E_{1u}	$\begin{bmatrix}\mathrm{Re}\\ \mathrm{Im}\end{bmatrix}: k_+\hat{\mathbf{z}};\ k_z\mathbf{r}_+;\ k_+^2 k_z\mathbf{r}_-;\ k_-^5\hat{\mathbf{z}};\ k_-^4 k_z\mathbf{r}_-;\ k_-^6 k_z\mathbf{r}_+$
E_{2u}	$\begin{bmatrix}\mathrm{Re}\\ \mathrm{Im}\end{bmatrix}: k_+\mathbf{r}_+;\ k_+^2 k_z\hat{\mathbf{z}};\ k_+^3\mathbf{r}_-;\ k_-^3\mathbf{r}_-;\ k_-^5\mathbf{r}_+;\ k_-^4 k_z\hat{\mathbf{z}}$

$$\hat{r}_\pm = \hat{x} \pm i\hat{y},\ k_\pm = k_x \pm i k_y$$

D_{6h}	E	C_2	$2C_3$	$2C_6$	$3U_2$	$3U_2'$	x P = Parity
D_{3d}	E	~~C_2~~	$2C_3$	~~$2C_6$~~	$3U_2$	~~$3U_2'$~~	

Γ_j	Basis functions
A_{1g}	$1, (k_x^2+k_y^2), k_z^2, \ldots$
A_{2g}	$\mathrm{Im}\, k_+^6$
~~B_{1g}~~	~~$k_z \mathrm{Im}\, k_+^3$~~
~~B_{2g}~~	~~$k_z \mathrm{Re}\, k_+^3$~~
E_{1g}	$\begin{Bmatrix}\mathrm{Re}\\ \mathrm{Im}\end{Bmatrix}: k_z k_+;\ k_z k_-^5$
~~E_{2g}~~	~~$\begin{Bmatrix}\mathrm{Re}\\ \mathrm{Im}\end{Bmatrix}: k_+^2;\ k_-^4$~~

Γ_j	Basis functions
A_{1u}	$k_z\hat{\mathbf{z}};\ k_x\hat{\mathbf{x}}+k_y\hat{\mathbf{y}};\ \mathrm{Re}\, k_+^5 \mathbf{r}_+$
A_{2u}	$\mathrm{Im}:\ k_-\mathbf{r}_+;\ k_+^5\mathbf{r}_+;\ k_+^6 k_z\hat{\mathbf{z}}$
~~B_{1u}~~	~~$\mathrm{Im}:\ k_+^3\hat{\mathbf{z}};\ k_+^2 k_z\mathbf{r}_+;\ k_+^4 k_z\mathbf{r}_-$~~
~~B_{2u}~~	~~$\mathrm{Re}:\ k_+^3\hat{\mathbf{z}};\ k_+^2 k_z\mathbf{r}_+;\ k_+^4 k_z\mathbf{r}_-$~~
E_{1u}	$\begin{Bmatrix}\mathrm{Re}\\ \mathrm{Im}\end{Bmatrix}: k_+\hat{\mathbf{z}};\ k_z\mathbf{r}_+;\ k_+^2 k_z\mathbf{r}_-;\ k_-^5\hat{\mathbf{z}};\ k_-^4 k_z\mathbf{r}_-;\ k_-^6 k_z\mathbf{r}_+$
~~E_{2u}~~	~~$\begin{Bmatrix}\mathrm{Re}\\ \mathrm{Im}\end{Bmatrix}: k_+\mathbf{r}_+;\ k_+^2 k_z\hat{\mathbf{z}};\ k_+^3\mathbf{r}_-;\ k_-^3\mathbf{r}_-;\ k_-^5\mathbf{r}_+;\ k_-^4 k_z\hat{\mathbf{z}}$~~

D_{3d}

even parity		
A_{1g}	1	$\vert 1 \uparrow 1 \downarrow> + \vert 2 \uparrow 2 \downarrow>$
		$\vert 1 \uparrow 2 \downarrow> - \vert 1 \downarrow 2 \uparrow>$
A_{2g}	Im k_+^6	
E_g	Re $k_z k_+$	
	Im	
odd parity		
A_{1u}	$k_z \hat{z}$; $k_x \hat{x} + k_y \hat{y}$	$\vert 1 \uparrow 2 \downarrow> + \vert 1 \downarrow 2 \uparrow>$
A_{2u}	$k_x \hat{y} - k_y \hat{x}$	$\vert 1 \uparrow 1 \downarrow> - \vert 2 \uparrow 2 \downarrow>$
E_u	Re $k_+ \hat{z}$; $k_z \hat{r}_+$; $k_+^2 k_z \hat{r}_-$	$i(\vert 1 \uparrow 2 \uparrow> - \vert 1 \downarrow 2 \downarrow>)$
	Im	$\vert 1 \uparrow 2 \uparrow> + \vert 1 \downarrow 2 \downarrow>$

A_{1u} and E_u: what linear combination?

I: Construct pseudospin basis

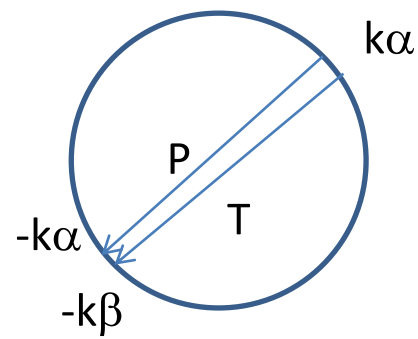
II: project

pseudospins: $\vec{\rho}$ acting on a 2D Hilbert space

(1)

$$
\begin{aligned}
|-\vec{k},\alpha> &= P|\vec{k},\alpha> \\
|-\vec{k},\beta> &= T|\vec{k},\alpha>
\end{aligned}
$$

$$|\vec{k},\beta>= PT|\vec{k},\alpha>$$



(2) $\rho_x(\vec{k}) = |\vec{k}\alpha><\vec{k}\beta| + |\vec{k}\beta><\vec{k}\alpha|$ $\longrightarrow$ $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

α → up

β → down

(ρ_x, ρ_y, ρ_z) like an axial vector (pseudospin)

(1) P and T

$$H_N(\vec{k}) = m\sigma_x + v_z k_z \sigma_y + v\sigma_z(k_x s_y - k_y s_x)$$

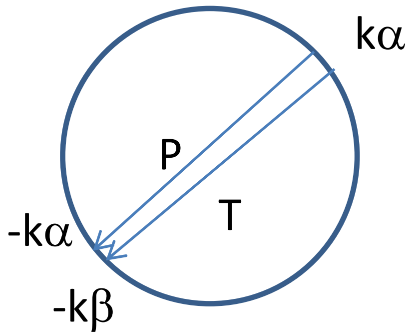
$$|\vec{k}, \alpha' > \equiv \frac{1}{\sqrt{2}N} e^{i\vec{k}\cdot\vec{r}} \begin{pmatrix} E_{\vec{k}} + vk_{\parallel} \\ m + iv_z k_z \end{pmatrix} \begin{pmatrix} 1 \\ ie^{i\phi_{\vec{k}}} \end{pmatrix}$$

$$|\hat{s} = \hat{z} \times \hat{k} > = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ ie^{i\phi_{\vec{k}}} \end{pmatrix}$$

orbital spin

(on half of fermi surface)

others defined by P and T



(2) $\vec{\rho}$ axial vector (proper rotational properties)

unitary transformation

$$|\vec{k},\alpha\rangle = \frac{e^{-i\alpha_{\vec{k}}/2}}{\sqrt{2}}(|\vec{k},\alpha'\rangle - i\,e^{i(\phi_{\vec{k}}+\alpha_{\vec{k}})}|\vec{k},\beta'\rangle)$$

$$e^{-i\alpha_{\vec{k}}} = (\mathrm{sgn}E_{\vec{k}})\frac{m - i\,v_z k_z}{\left(m^2 + v_z^2 k_z^2\right)^{1/2}}$$

the rest by P and T

$$|\vec{k},\beta\rangle = \frac{e^{i\alpha_{\vec{k}}/2}}{\sqrt{2}}(|\vec{k},\beta'\rangle - i\,e^{-i(\phi_{\vec{k}}+\alpha_{\vec{k}})}|\vec{k},\alpha'\rangle)$$

Projection:

even parity		
A_{1g}	1	$\|1\uparrow 1\downarrow> + \|2\uparrow 2\downarrow>$
		$\|1\uparrow 2\downarrow> - \|1\downarrow 2\uparrow>$
A_{2g}	Im k_+^6	
E_g	Re $k_z k_+$	
	Im	
odd parity		
A_{1u}	$k_z\hat{z};\ k_x\hat{x} + k_y\hat{y}$	$\|1\uparrow 2\downarrow> + \|1\downarrow 2\uparrow>$
A_{2u}	$k_x\hat{y} - k_y\hat{x}$	$\|1\uparrow 1\downarrow> - \|2\uparrow 2\downarrow>$
E_u	Re $k_+\hat{z};\ k_z\hat{r}_+;\ k_+^2 k_z\hat{r}_-$	$i(\|1\uparrow 2\uparrow> - \|1\downarrow 2\downarrow>)$
	Im	$\|1\uparrow 2\uparrow> + \|1\downarrow 2\downarrow>$

→ 1 x

→ $(m/\mu)\times$

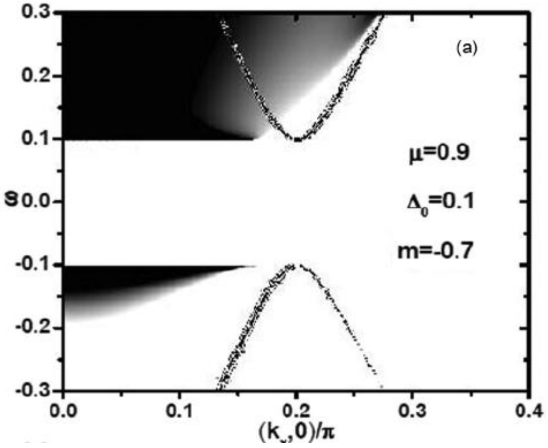
$$\sum_{\vec{k}}' \left[|\vec{k}\alpha, -\vec{k}\beta> - |\vec{k}\beta, -\vec{k}\alpha> \right]$$

→ see later

$$i\sum_{\vec{k}}' \left[\frac{v(k_x - ik_y)}{E_{\vec{k}}} |\vec{k}\alpha, -\vec{k}\alpha> + \frac{v(k_x + ik_y)}{E_{\vec{k}}} |\vec{k}\beta, -\vec{k}\beta> \right]$$

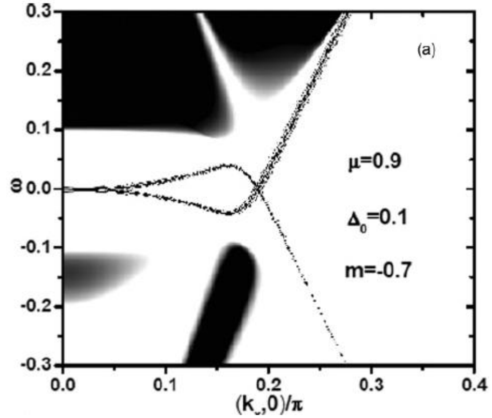
$$\vec{d}(\vec{k}) = \Delta_{2u} \frac{v(k_x\hat{y} - k_y\hat{x})}{\mu}$$

(planar)



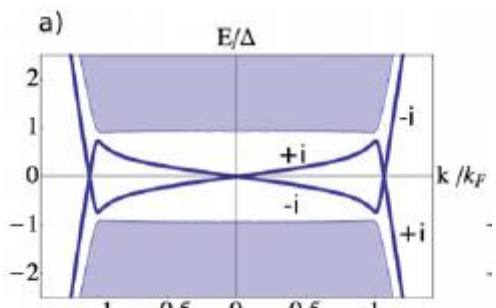
$|1\uparrow 1\downarrow> + |2\uparrow 2\downarrow>$

s-wave, A_{1g}

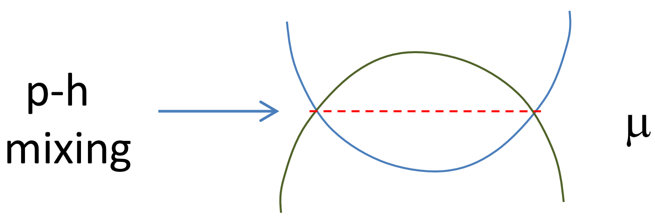


$|1\uparrow 2\downarrow> + |1\downarrow 2\uparrow>$

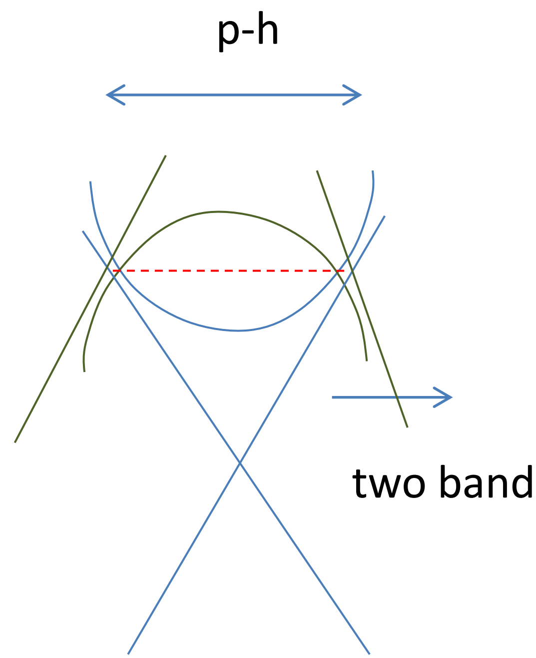
A_{1u}



normal state trivial
(or single band)



normal state TI :



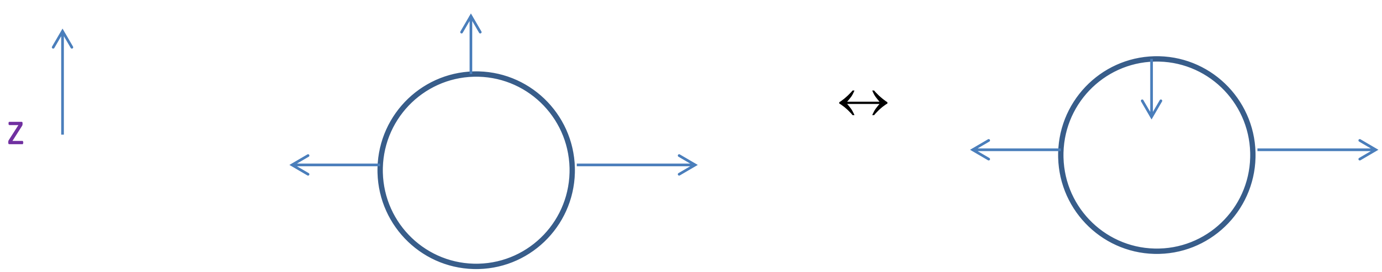
A_{1u} $|1\uparrow 2\downarrow> + |1\downarrow 2\uparrow>$

$$d_{x,y} = \Delta_{1u} \frac{m}{|\mu|} \frac{v k_{x,y}}{(m^2 + v_z^2 k_z^2)^{1/2}}$$

$$d_z = \Delta_{1u} (\mathrm{sgn}\mu) \frac{v_z k_z}{(m^2 + v_z^2 k_z^2)^{1/2}}$$

$$\frac{d_{\|}}{d_z} = \frac{m}{\mu} \frac{v k_{\|}}{v_z k_z}$$

depends on $\mathrm{sgn}(m v_z)$



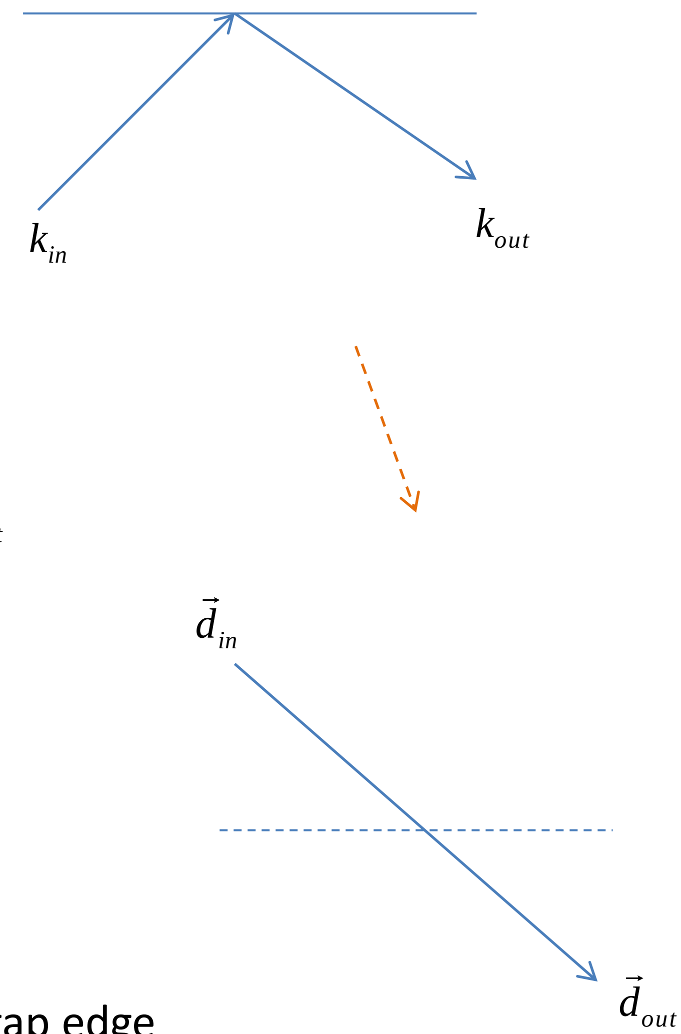
cf. Balian Werthamer state

$\vec{d} \,//\, \vec{k}$

surface state: Dirac cone

Surface states

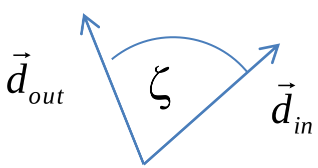
(single band picture):



odd parity $\vec{d}(\vec{k})$

$$\begin{pmatrix} -d_x + id_y & d_z \\ d_z & d_x + id_y \end{pmatrix} \qquad \vec{d}_{in} \neq \vec{d}_{out}$$

Choose quantization axes along $\vec{d}_{in} \times \vec{d}_{out}$



$$\begin{pmatrix} -d_{x'_s} + id_{y'_s} & 0 \\ 0 & d_{x'_s} + id_{y'_s} \end{pmatrix}$$

phase difference $\chi = \mp\zeta$

($\chi=0$ if glancing incidence) E → gap edge

positive branch along $(\mathrm{sgn}\mu)\vec{d}_{\rm in} \times \vec{d}_{\rm out}$

E > 0 branch:

Normal state

$v\hat{n} \times \vec{k}$ if TI

Superconducting state

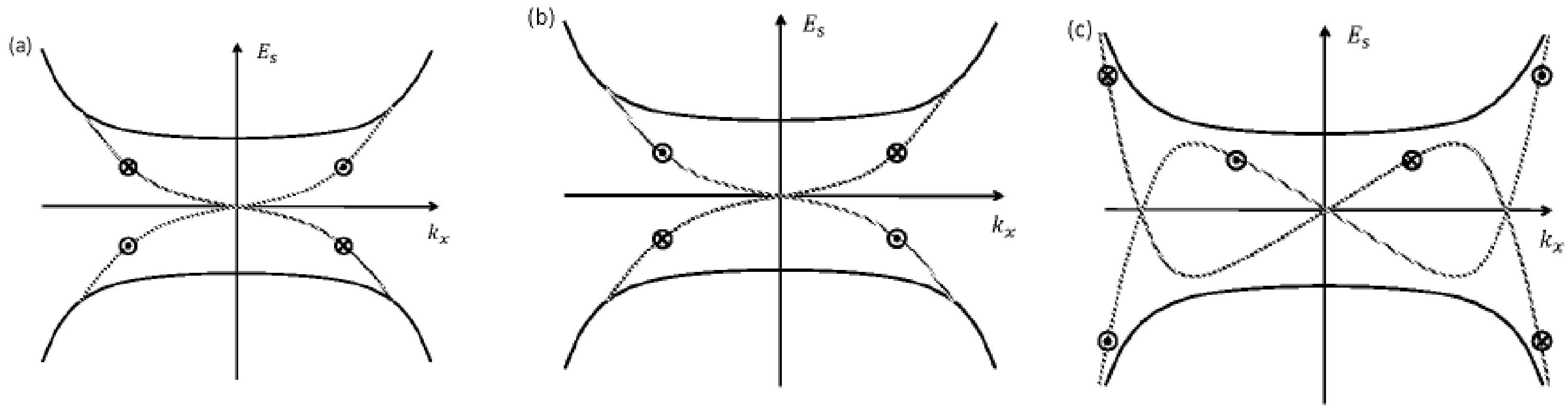
$(\mathrm{sgn}\mu)\vec{d}_{\mathrm{in}} \times \vec{d}_{\mathrm{out}}$

A_{1u} E_u $\propto \mathrm{sgn}(mv_z) v\hat{n} \times \vec{k}_{in}$

follows from $\frac{d_{\|}}{d_z} = \frac{m}{\mu} \frac{vk_{\|}}{v_z k_z}$

A_{1u}

v < 0



$\mathrm{sgn}(m v_z) > 0$

single band
or
two band

$\mathrm{sgn}(m v_z) < 0$

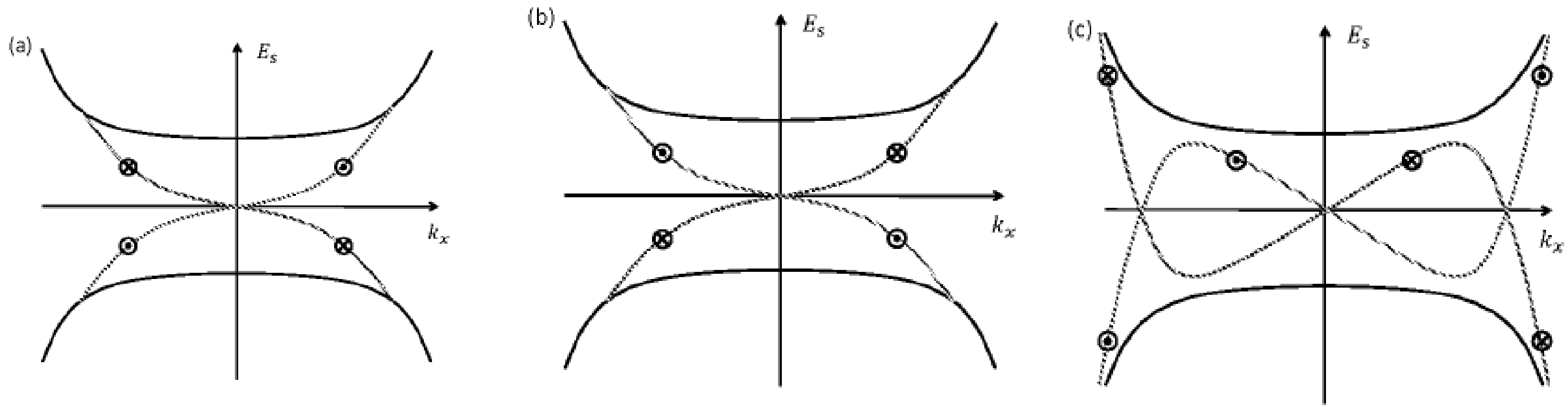
single band

$\mathrm{sgn}(m v_z) < 0$

two band

A_{1u}

v < 0



$\mathrm{sgn}(mv_z) > 0$	$\mathrm{sgn}(mv_z) < 0$	$\mathrm{sgn}(mv_z) < 0$
single band or two band	single band	two band

$|k_{//}| < k_F$ determined by superconducting order parameter

$|k_{//}| > k_F$ determined by normal state topology

Q: Anomalous dispersion an indicator of TI ?

NO: only d(k) on the Fermi surface matters

$$H_N = (m_0 + C\,k^2 + \ldots)\sigma_x + (v_z + ..)k_z\sigma_y + (v_0 + \ldots)(k_x s_y - k_y s_x)\sigma_z$$

↑ ↑

opp signs

$$\frac{d_\parallel}{d_z} = \frac{m}{\mu}\frac{v k_\parallel}{v_z k_z}$$

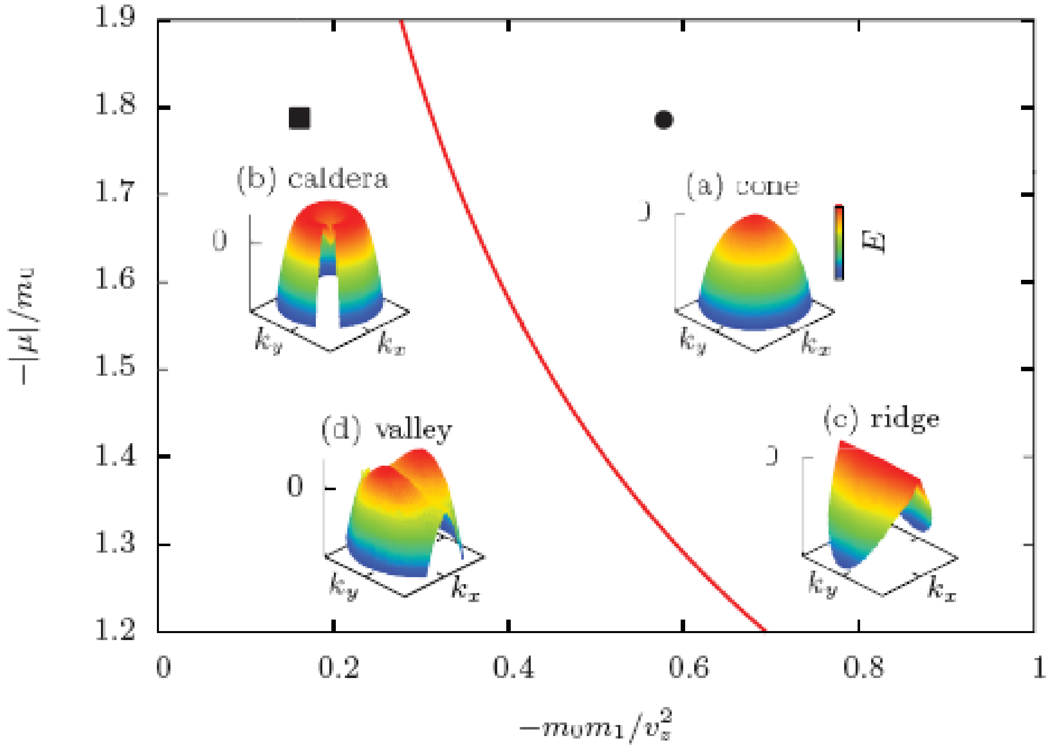
$m \to m_0 + Ck^2$

k on Fermi surface

can change from anomalous to ordinary for increasing C or $|\mu|$

Yamakage et al 12

$$m = m_0 + m_1 k_z^2$$



A_{1u}

$|1\uparrow 2\downarrow\rangle + |1\downarrow 2\uparrow\rangle$

E_u

$|1\uparrow 2\uparrow\rangle - |1\downarrow 2\downarrow\rangle$

Summary:

pseudospin basis

bulk order parameters

orbital/spin → pseudospin basis

anomalous dispersions related to peculiar d(k)

the dispersion for $k < k_F$

purely property of the superconducting order parameter

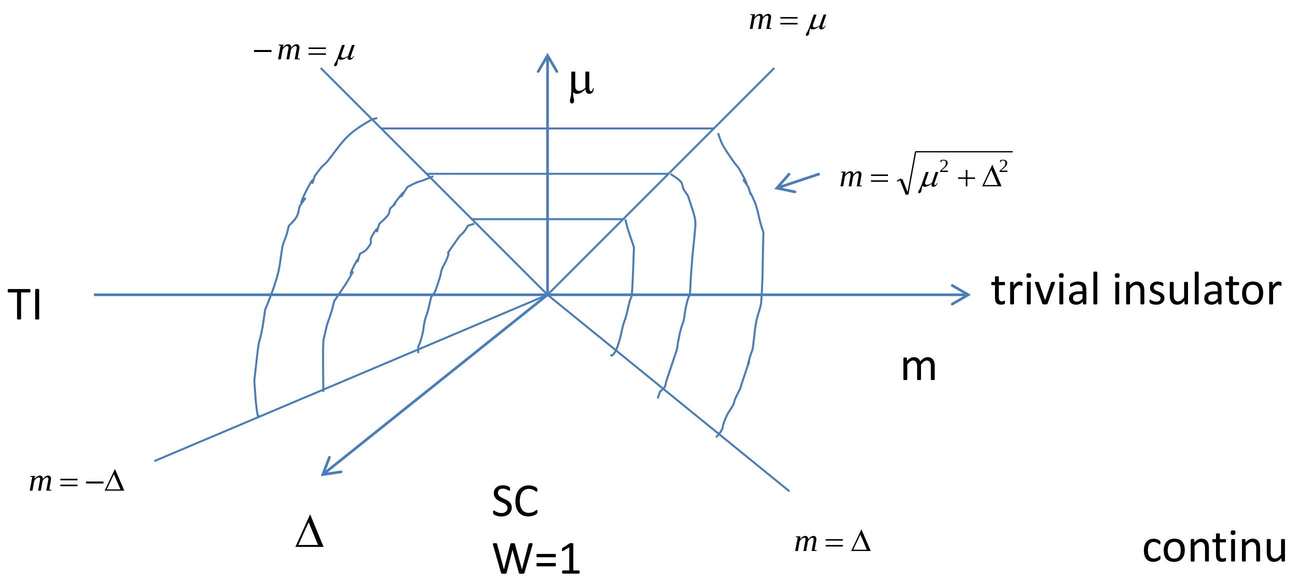
dispersion at $k > k_F$: normal state property

except duplication due to particle-hole

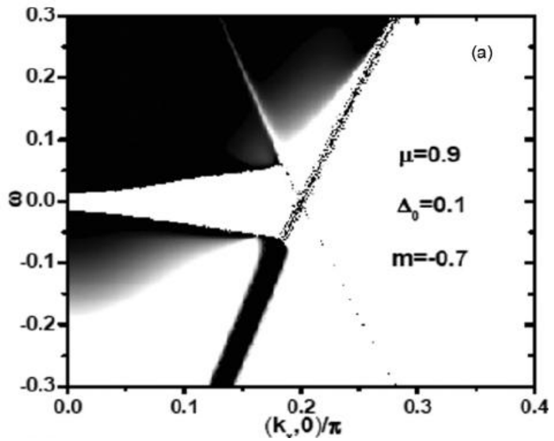
Single band picture:

m = 0, line nodes on equator $d_{x,y} = 0$ $d_z \propto k_z$

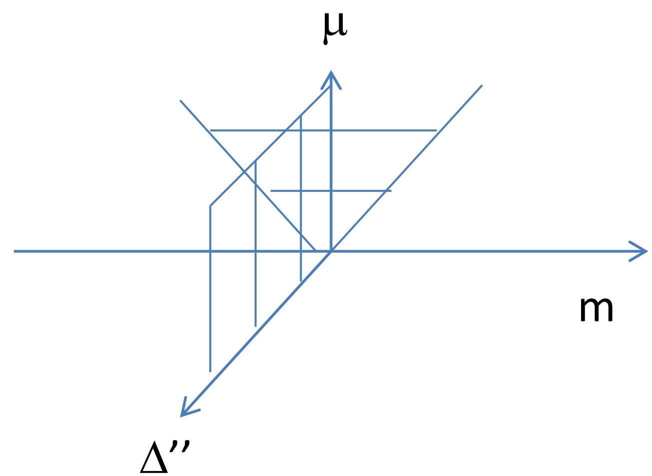
full two band:



continuous at m=0
if $\Delta \neq 0$



$$(m/\mu)\times \sum\nolimits_{\vec{k}}' \left[|\vec{k}\alpha, -\vec{k}\beta> - |\vec{k}\beta, -\vec{k}\alpha> \right]$$



A''_{1g} $|1\uparrow 2\downarrow> - |1\downarrow 2\uparrow>$

but can be smoothly connected if include

$$|1\uparrow 1\downarrow> + |2\uparrow 2\downarrow>$$