

# Gap Symmetry and Nodal Structure in Fe-based Superconductors



Maxim Khodas

*Collaboration:*

Andrey Chubukov, Univ. of Wisconsin

Sudhakar Pandey, Univ. of Iowa

Phys. Rev. B **86**, 144519 (2012)

Phys. Rev. Lett. **108**, 247003 (2011)

# Outline

## Part I

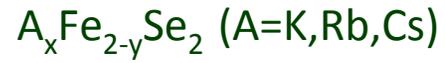
1. Family of iron(Fe)-based superconductors with only electron pockets:  $A_x\text{Fe}_{2-y}\text{Se}_2$ .  $A = \text{K, Rb, Cs}$
2. Pairing symmetry: “s”, “d”, “s+” and “s+i d”

## Part II

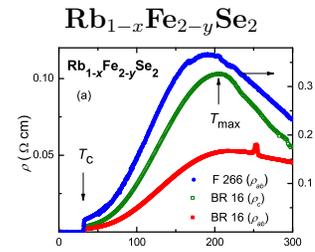
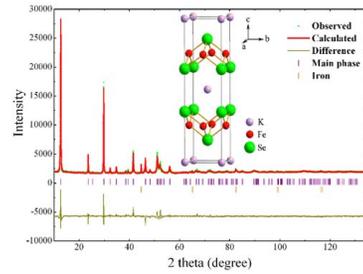
1. Spin Resonance in s+-
2. Role of hybridization and band dispersion

## Part III

1. Raman scattering in s+-



$T_c \simeq 30 - 40\text{K}$



V. Tsurkan, et.al. (2011)

$T_c \approx 32\text{K}$

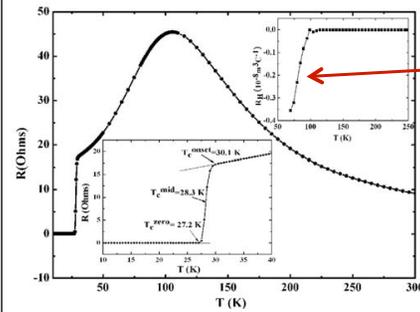
J. Guo et.al.  $\text{K}_x\text{Fe}_2\text{Se}_2$  ( $0 \leq x \leq 1$ )

Isostructural to  $\text{Ba}_x\text{Fe}_2\text{As}_2$  (122)

Intercalation of alkali metal A in between FeSe layers

**"Strongly electron doped" systems,  $A_x\text{Fe}_{2-y}\text{Se}_2$  A= K,Rb,Cs**

Alkali metal A donates electrons to FeSe layers



Negative Hall coefficient

$$R_H < 0$$

electrons

J. Guo et.al.  $\text{K}_x\text{Fe}_2\text{Se}_2$  ( $0 \leq x \leq 1$ )

**"Strongly electron doped" systems,  $A_x\text{Fe}_{2-y}\text{Se}_2$  A= K,Rb,Cs**

**Today's first two talks !**

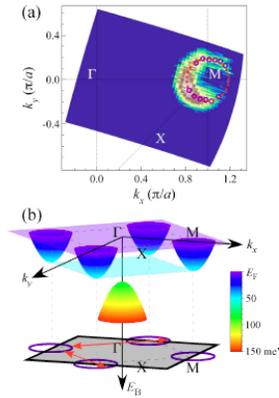
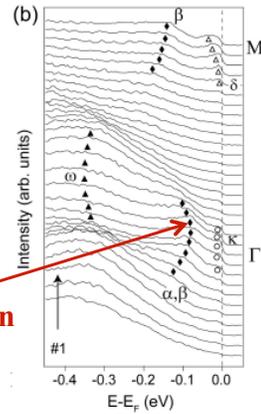
**$T_c \sim 40\text{K}$**

**Only electron FSs are present**

**$\text{KFe}_2\text{Se}_2$**

**hole dispersion**

**Y. Zhang et al**



**Hong Ding et al**

What is the pairing *symmetry* ?

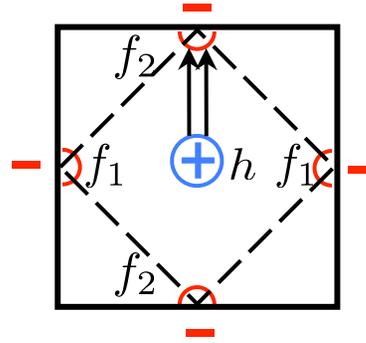
## Pairing: order parameter *symmetry* ?

Look at pnictides with both electron and *hole* pockets

$$\begin{cases} \Delta_h + u\Delta_e \log \frac{\Lambda}{T_c} = 0 \\ \Delta_e + u\Delta_h \log \frac{\Lambda}{T_c} = 0 \end{cases}$$

$$u > 0 \longrightarrow s^\pm$$

$\mathcal{S} \longrightarrow$  Invariant under *crystal* symmetry



**"Strongly electron doped" systems,  $A_x\text{Fe}_{2-y}\text{Se}_2$  A= K,Rb,Cs**

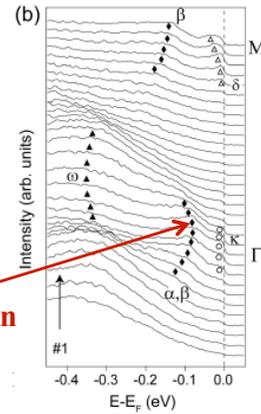
**Today's first two talks !**

**$T_c \sim 40\text{K}$**

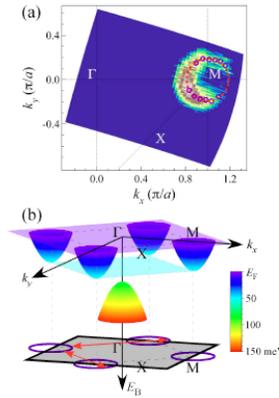
**Only electron FSs are present**

**$\text{KFe}_2\text{Se}_2$**

**hole dispersion**



Y. Zhang et al



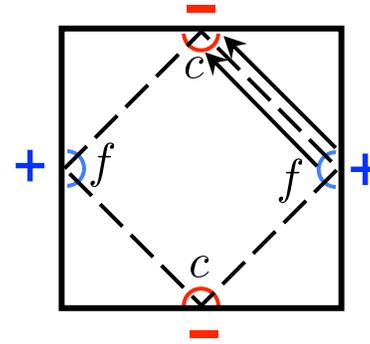
Hong Ding et al

**Hole pockets are gapped –the driving force for s-wave SC is gone**

Can this still work for  $AFe_2Se_2$  ?

Nodeless  $d$  ?

Different from pnictides  
with hole pockets!

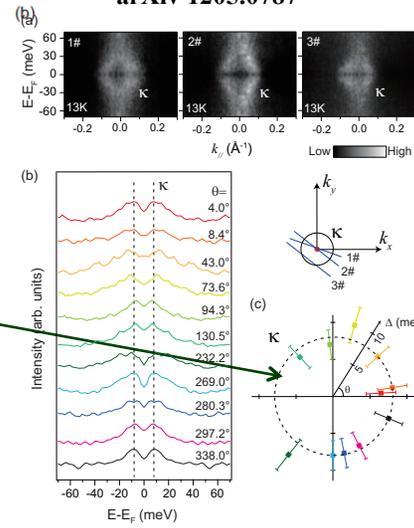
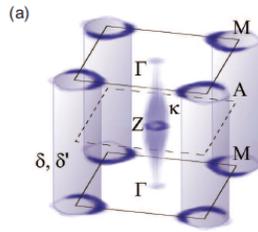
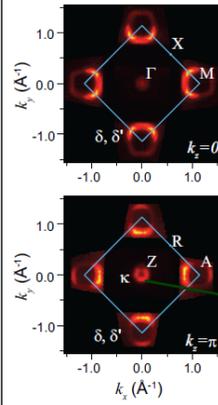


Experiment: ?

Today's first two talks !

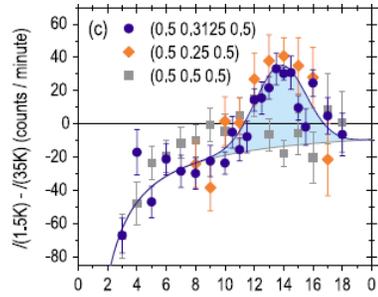
Very recent ARPES

Feng's group  
arXiv 1205.0787



No nodal gap,  
inconsistent with d-wave

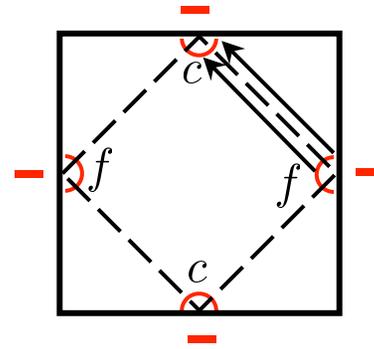
# What about regular s-wave?



**Spin resonance**  
**below  $T_c$**  Inosov et al



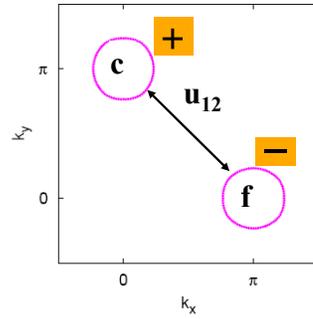
Requires sign changing order parameter



**There is a third possibility**  
**“another s<sup>+</sup>-”**

**Consistent with both ARPES and neutrons**

### Let's go back to d-wave reasoning



Suppose FSs are circles  
(must be identical circles)

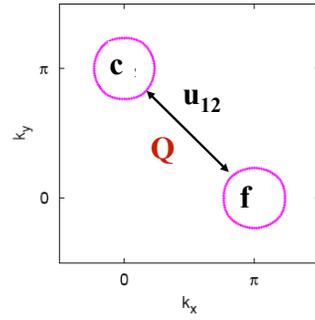
d-wave:  $\Delta_c = -\Delta_f$

$$\Delta_c = \langle c_{\uparrow}^{\dagger} c_{\downarrow}^{\dagger} \rangle, \quad \Delta_f = \langle f_{\uparrow}^{\dagger} f_{\downarrow}^{\dagger} \rangle$$

$$T_c : 1 = u_{12} \chi_{pp}(0)$$

$$\chi_{pp}(0) = \text{diagram} = \iint_{\uparrow} \frac{d\omega d\varepsilon_k}{\omega^2 + \varepsilon_k^2} = \log \frac{E_F}{T} \quad \text{Cooper logarithm}$$

And what if we consider inter-pocket pairing ?



**s-wave**

Singlet

$$\langle c_{\uparrow}^{\dagger} f_{\downarrow}^{\dagger} \rangle = \Delta = \langle f_{\uparrow}^{\dagger} c_{\downarrow}^{\dagger} \rangle$$

$$T_c : 1 = u_{12} \chi_{pp}(Q)$$

$$\chi_{pp}(Q) = \text{diagram} = \iint_{\uparrow} \frac{d\omega d\epsilon_k}{\omega^2 + \epsilon_k^2} = \log \frac{E_F}{T} \quad \text{Cooper logarithm}$$

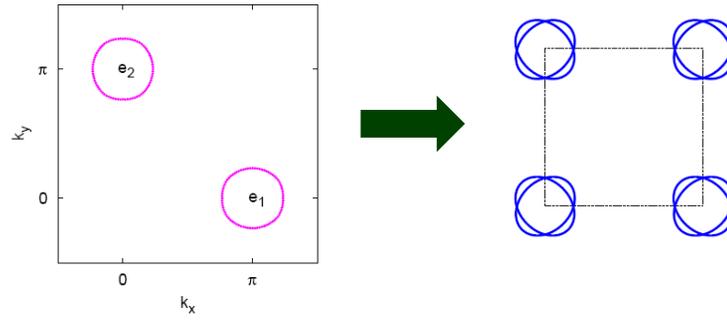
**Exactly the same result as for plus-minus gap**

**d-wave and s-wave pairing states are completely degenerate for circular electron pockets**

Not essential:

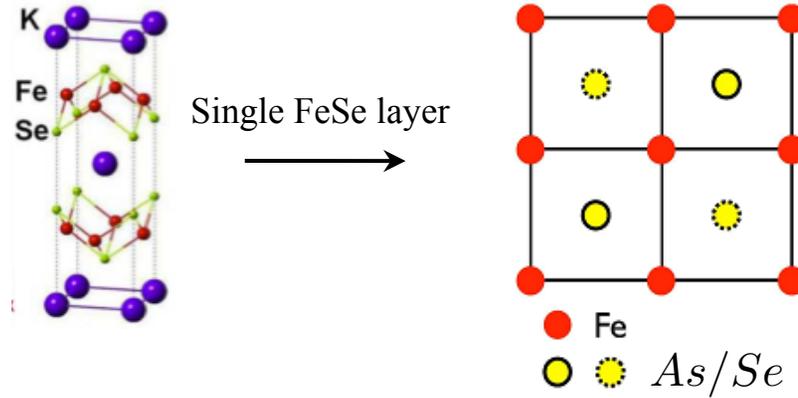
Additional symmetry:  $O(2)$  Rotations in  $(c, f)$  orbital space

### Experimental picture: folded Brillouin zone

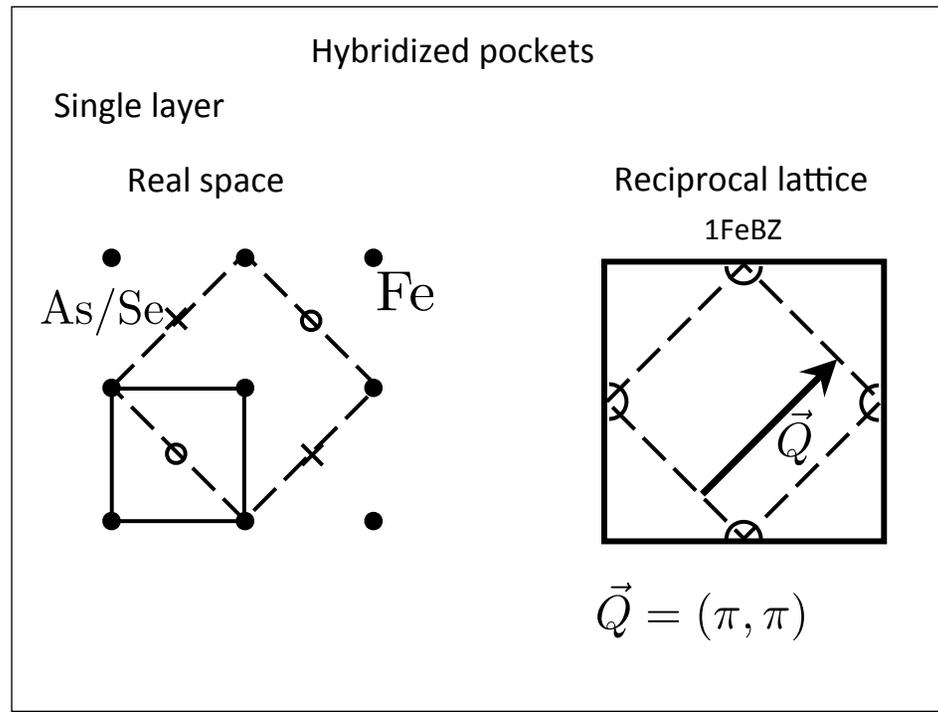


## Hybridization

**Folding: pnictogen/chalcogen is above or below Fe plane**



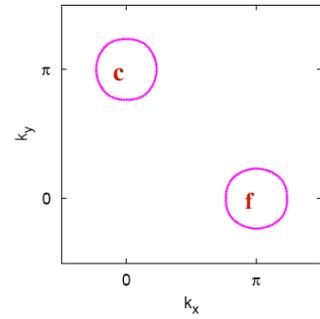
**Two non-equivalent positions of Fe – unit cell has 2 Fe atoms**



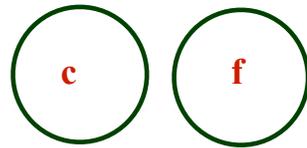
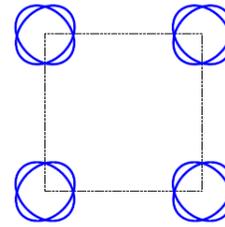
I wish to introduce a standard terminology from the outset to avoid confusion

**A simple picture of folding – a shift of the position of the FSs**

**unfolded zone**

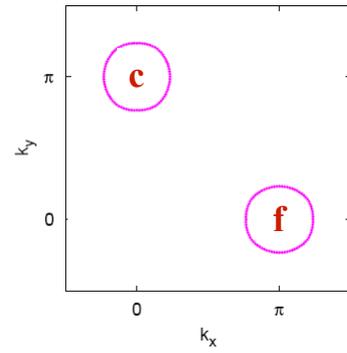


**folded zone**

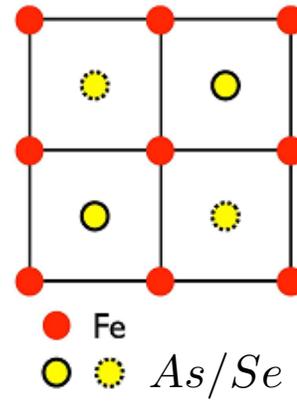


Inter-pocket and intra-pocket pairing are degenerate

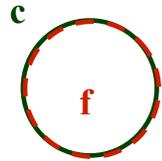
**In reality, the transformation from folded to unfolded zone is not only a position shift – there is also a hybridization between electron pockets**



$$H_{hybr} = \lambda(c_k^\dagger f_{k+Q} + f_{k+Q}^\dagger c_k)$$



$$H_{hybr} = \lambda(c_k^\dagger f_{k+Q} + f_{k+Q}^\dagger c_k)$$



**no hybridization**

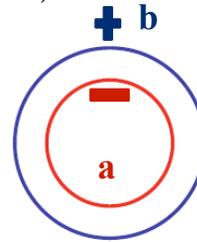
$$\langle c_{\uparrow}^\dagger c_{\downarrow}^\dagger \rangle = \Delta = \langle f_{\uparrow}^\dagger f_{\downarrow}^\dagger \rangle$$

**d - wave**

$$\langle c_{\uparrow}^\dagger f_{\downarrow}^\dagger \rangle = \Delta = \langle f_{\uparrow}^\dagger c_{\downarrow}^\dagger \rangle$$

**s - wave**

**s-wave is inter-pocket pairing in terms of original fermions**



**s<sup>+</sup> gap**

$$a = (c + f)/\sqrt{2}$$

$$b = (c - f)/\sqrt{2}$$

**hybridization**

$$\langle a_{\uparrow}^\dagger a_{\downarrow}^\dagger \rangle = \Delta = -\langle b_{\uparrow}^\dagger b_{\downarrow}^\dagger \rangle$$

**s - wave**

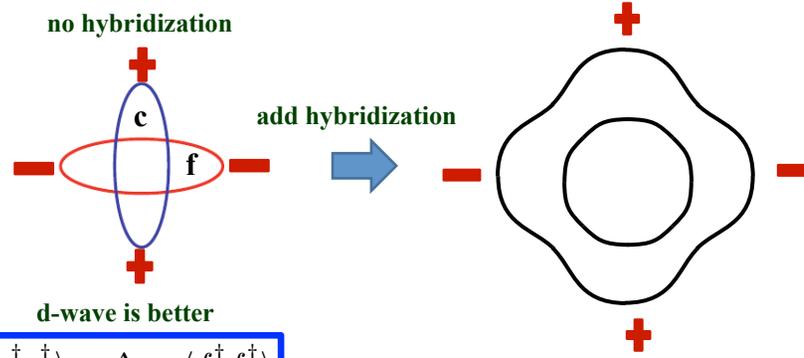


$$\langle a_{\uparrow}^\dagger b_{\downarrow}^\dagger \rangle = \Delta = \langle b_{\uparrow}^\dagger a_{\downarrow}^\dagger \rangle$$

**d - wave**

**d-wave is inter-pocket pairing in terms of hybridized fermions**

A situation is somewhat different when  
electron pockets are ellipses



d-wave is better

$$\langle c_{\uparrow}^{\dagger} c_{\downarrow}^{\dagger} \rangle = \Delta = \langle f_{\uparrow}^{\dagger} f_{\downarrow}^{\dagger} \rangle$$

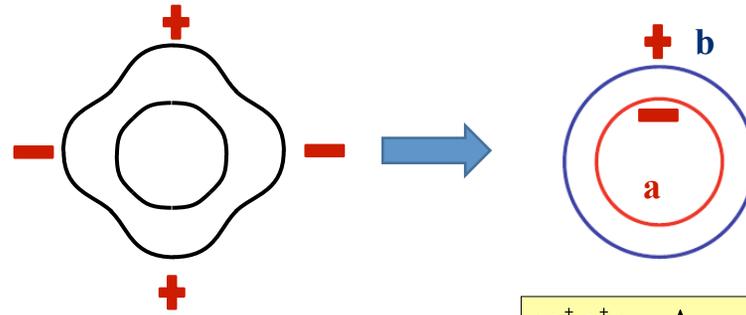
**d - wave**

$$\langle c_{\uparrow}^{\dagger} f_{\downarrow}^{\dagger} \rangle = \Delta = \langle f_{\uparrow}^{\dagger} c_{\downarrow}^{\dagger} \rangle$$

**s - wave**

for small hybridization,  
d-wave is still better.  
This is a conventional,  
d-wave

Let's increase hybridization further



Eventually s-wave  
wins

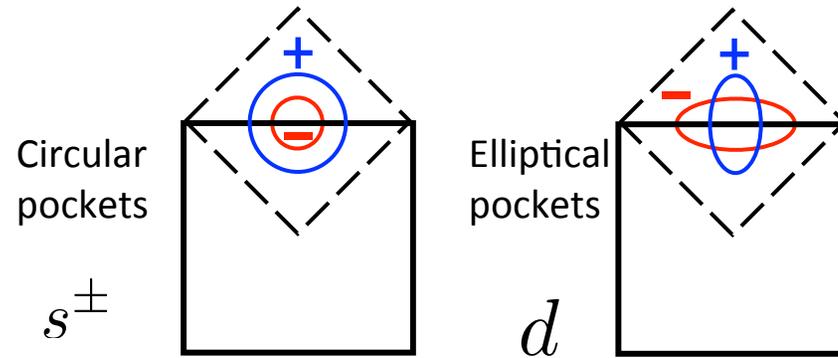
$$\langle a_{\uparrow}^{\dagger} a_{\downarrow}^{\dagger} \rangle = \Delta = -\langle b_{\uparrow}^{\dagger} b_{\downarrow}^{\dagger} \rangle$$

s-wave

$$\langle a_{\uparrow}^{\dagger} b_{\downarrow}^{\dagger} \rangle = \Delta = \langle b_{\uparrow}^{\dagger} a_{\downarrow}^{\dagger} \rangle$$

d-wave

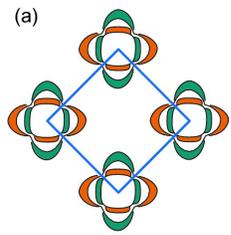
# The effect of hybridization for different pocket configuration



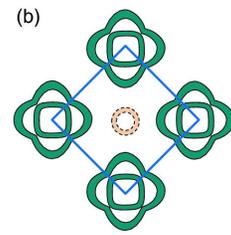
I. Mazin, PRB (2011)

Competition: hybridization vs. ellipticity

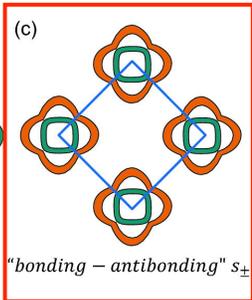
Qualitative argument



*"quasi - nodeless" d*

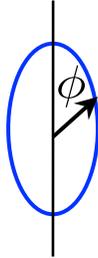


*"incipient"  $s_{\pm}$*



*"bonding - antibonding"  $s_{\pm}$*

### Hybridization vs. ellipticity (cont)



$$v_F(\phi) = v_F(1 + a \cos 2\phi)$$

$$k_F(\phi) = k_F(1 + \boxed{b} \cos 2\phi)$$

Anisotropy parameter

} Small

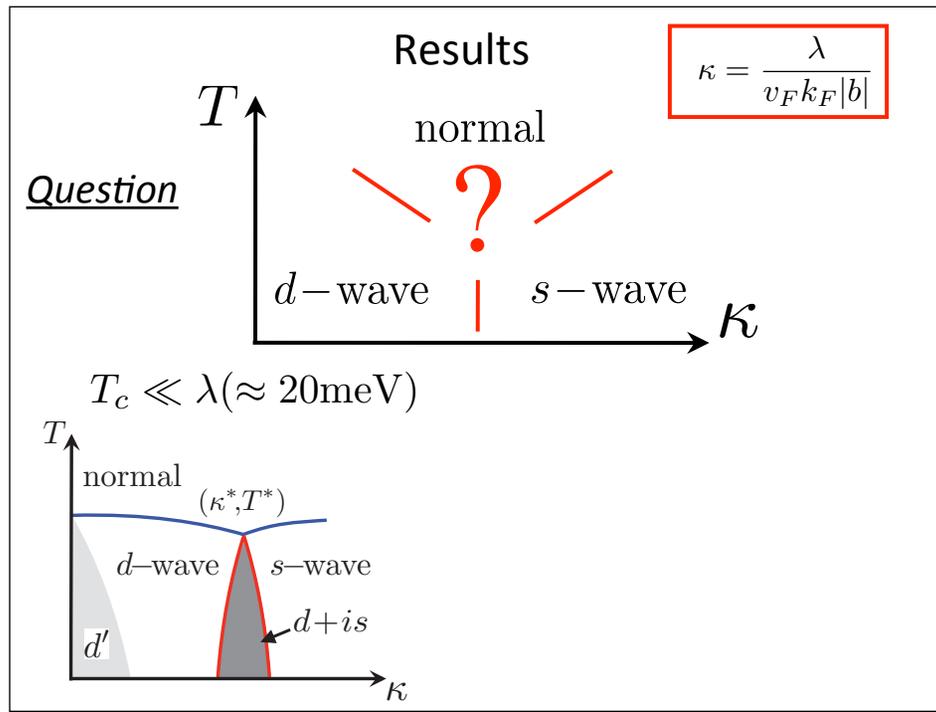
$$\frac{\lambda}{v_F k_F}$$

Dimensionless hybridization

$$\kappa = \frac{\text{hybridization}}{\text{ellipticity}}$$

$$\kappa = \frac{\lambda}{v_F k_F |b|}$$

→ Can be anything

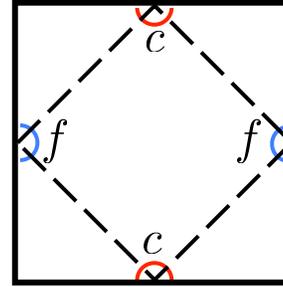


Model: *quadratic* part



Two electron pockets:

$c$   $f$



+ hybridization

$$H_2 = \sum_{\vec{k}} \epsilon_{\vec{k}}^c c_{\vec{k}}^\dagger c_{\vec{k}} + \sum_{\vec{k}} \epsilon_{\vec{k}}^f f_{\vec{k}}^\dagger f_{\vec{k}} + \sum_{\vec{k}} \lambda \left[ c_{\vec{k}}^\dagger f_{\vec{k}} + f_{\vec{k}}^\dagger c_{\vec{k}} \right]$$

## Model (cont): interaction

$$H_1 = u_1 \sum_k \left[ c_{\sigma}^{\dagger} f_{\sigma'}^{\dagger} f_{\sigma'} c_{\sigma} + f_{\sigma}^{\dagger} c_{\sigma'}^{\dagger} c_{\sigma'} f_{\sigma} \right]$$



$$H_2 = u_2 \sum_k \left[ c_{\sigma}^{\dagger} f_{\sigma'}^{\dagger} c_{\sigma'} f_{\sigma} + f_{\sigma}^{\dagger} c_{\sigma'}^{\dagger} f_{\sigma'} c_{\sigma} \right]$$



$$H_3 = u_3 \sum_k \left[ c_{\sigma}^{\dagger} c_{\sigma'}^{\dagger} f_{\sigma'} f_{\sigma} + f_{\sigma}^{\dagger} f_{\sigma'}^{\dagger} c_{\sigma'} c_{\sigma} \right]$$



$$H_4 = u_4 \sum_k \left[ c_{\sigma}^{\dagger} c_{\sigma'}^{\dagger} c_{\sigma'} c_{\sigma} + f_{\sigma}^{\dagger} f_{\sigma'}^{\dagger} f_{\sigma'} f_{\sigma} \right]$$



### Interaction: microscopics

$$H = \frac{U}{2}n^2 + 2JS^2 \longrightarrow \begin{aligned} n &= c_\alpha^\dagger c_\alpha + f_\alpha^\dagger f_\alpha \\ \mathbf{S} &= \frac{1}{2}(c_\alpha^\dagger c_\beta + f_\alpha^\dagger f_\beta)\sigma_{\alpha\beta} \end{aligned}$$

$\downarrow$ 
 $\downarrow$ 
 $SU(2)$

Hubbard                  Hund

Additional symmetry:  $O(2)$       Rotations in  $(c, f)$  orbital space

$$H = \frac{U}{2}n^2 + 2JS^2 + \frac{J'}{2}\tilde{n}^2 \quad \tilde{n} = c_\alpha^\dagger f_\alpha - f_\alpha^\dagger c_\alpha$$

$$O(2) \longrightarrow \boxed{u_4 - u_3 = u_1 + u_2 = U - 3J - J'}$$

A.F. Kemper, T.A. Maier, S. Graser, H-P. Cheng, P.J. Hirschfeld and D.J. Scalapino,  
New J. Phys. 12, 073030(2010).

## Phase diagram

Ginzburg-Landau functional  
two order parameters

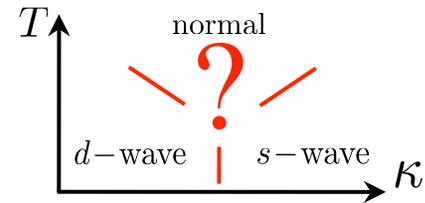
$\Delta_s$  s-wave

$\Delta_d$  d-wave

~~$\Delta_d^* \Delta_s$~~  ← symmetry

$$F_{GL} = A_s |\Delta_s|^2 + A_d |\Delta_d|^2 + \frac{B_s}{2} |\Delta_s|^4 + \frac{B_d}{2} |\Delta_d|^4$$

$$+ C |\Delta_s|^2 |\Delta_d|^2 + \frac{E}{2} [(\Delta_s \Delta_d^*)^2 + (\Delta_s^* \Delta_d)^2]$$

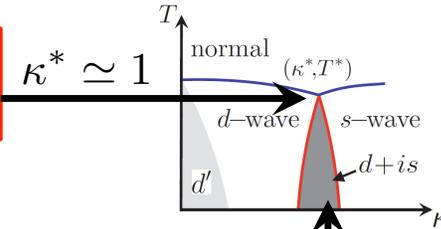


## Ginzburg-Landau functional treatment (cont)

$$F_{GL} = A_s |\Delta_s|^2 + A_d |\Delta_d|^2 + \frac{B_s}{2} |\Delta_s|^4 + \frac{B_d}{2} |\Delta_d|^4 + C |\Delta_s|^2 |\Delta_d|^2 + \frac{E}{2} [(\Delta_s \Delta_d^*)^2 + (\Delta_s^* \Delta_d)^2]$$

Tetracritical point:

$$A_s(\kappa^*, T^*) = A_d(\kappa^*, T^*)$$



$$\lambda \gg T_c$$



$$B_s = B_d = B = \frac{10}{3} E$$

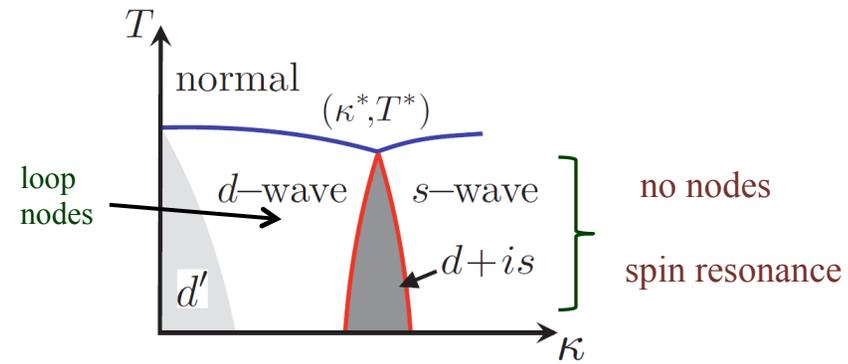
$$C = 2E$$

$$\text{B+E > C} \rightarrow s + id$$

## Conclusions:

The pairing between electron pockets **MUST** include inter-pocket pairing on equal footing with intra-pocket pairing

Talk by Jiangping Hu



## Part II

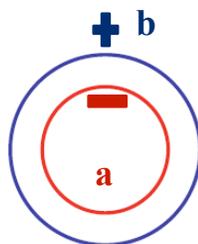
### Spin resonance in “s+” state

# Spin resonance in “s+−” state

d-wave,  
extended s-wave

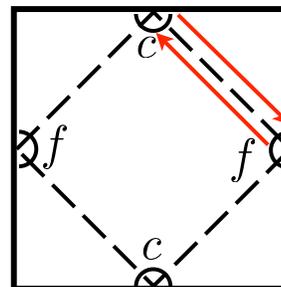
T.A. Maier, S. Graser, P.J. Hirschfeld, D.J. Scalapino  
PRB **83**,100515 (2011);

T.A. Maier, P.J. Hirschfeld, D.J. Scalapino  
PRB **86**,094514 (2012);



$$a = (c + f)/\sqrt{2}$$

$$b = (c - f)/\sqrt{2}$$



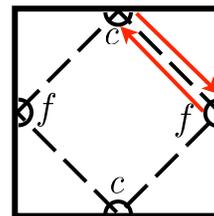
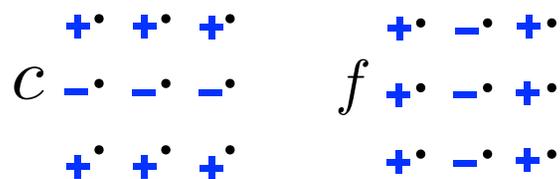
Bonding



Anti-bonding ??

Real space (I.Mazin)

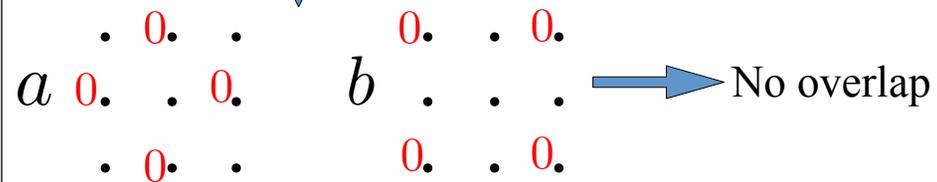
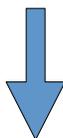
Fe



$$a = (c + f)/\sqrt{2}$$

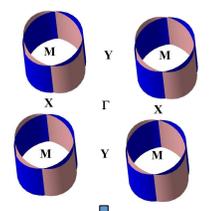
$$b = (c - f)/\sqrt{2}$$

Hybridization

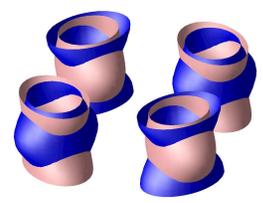


$k_z$  dispersion

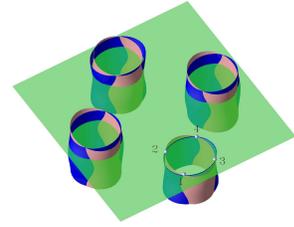
A) weak



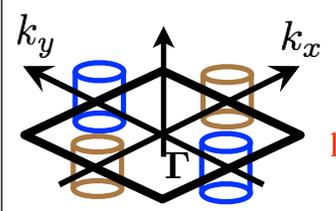
B) strong



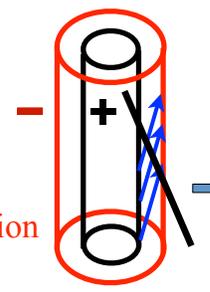
C) moderate



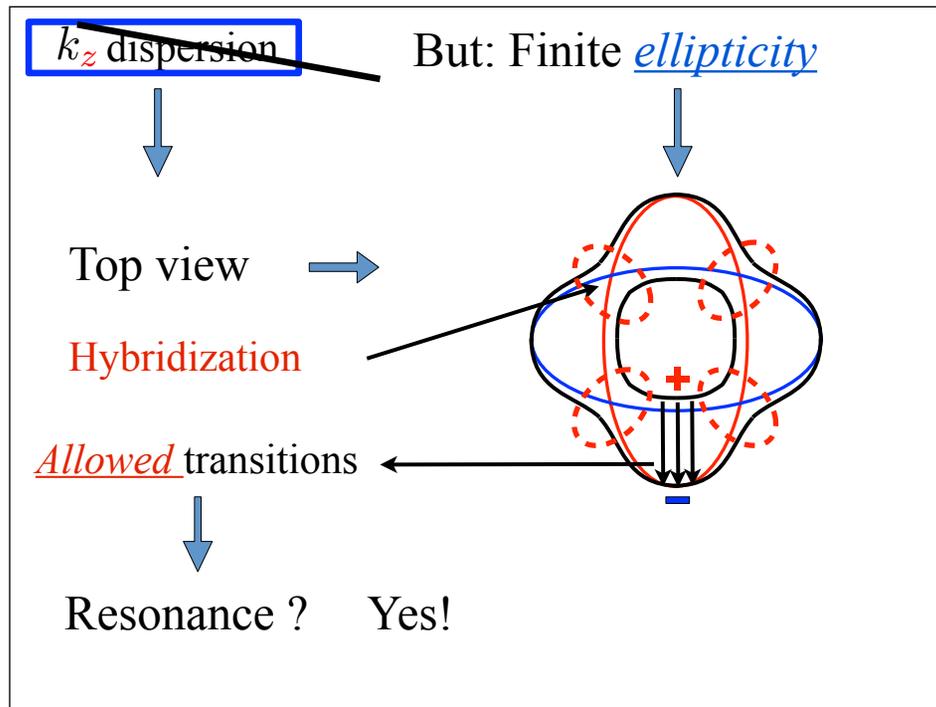
cylinders



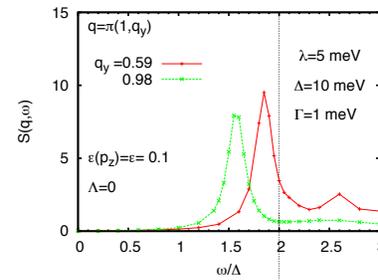
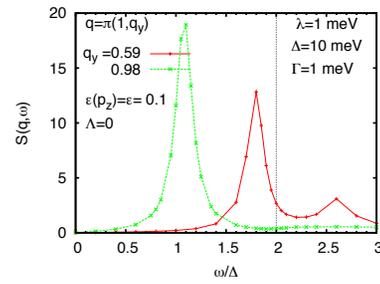
hybridization



No resonance

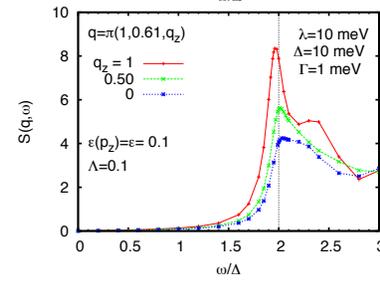
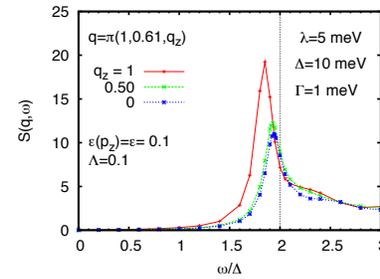
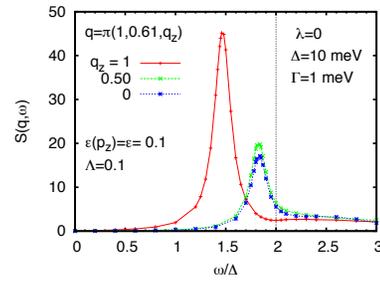


### Numerics: (Magnetically stable normal state)



- Resonance survives the hybridization
- Hybridization suppresses the resonance
- ``Touching'' condition is intact

# Numerics (cont): add weak $k_z$ dispersion



- Resonance
- Band dispersion → Resonance dispersion
- Hybridization suppresses dispersion

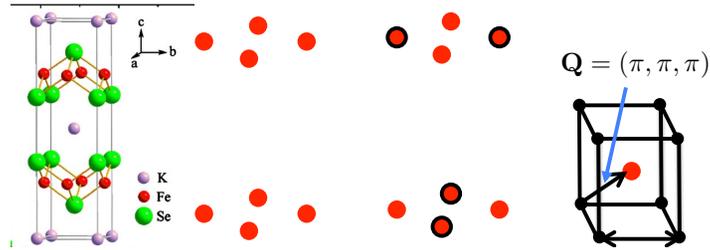
## Part II (cont)

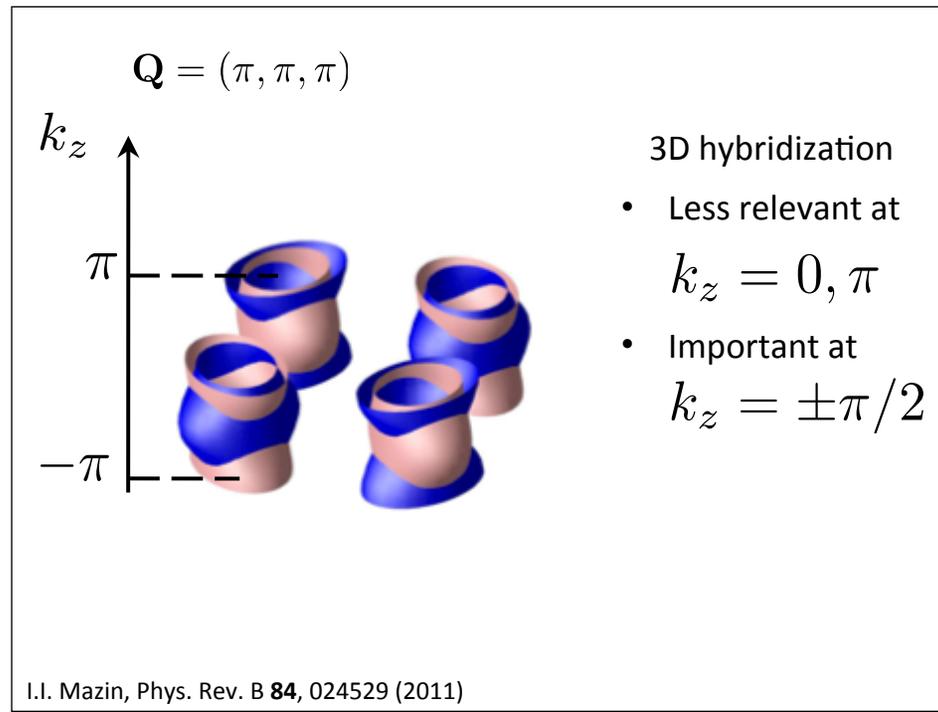
**Spin resonance in “s+<sup>-</sup>” state**  
**strong dispersion**

122-material

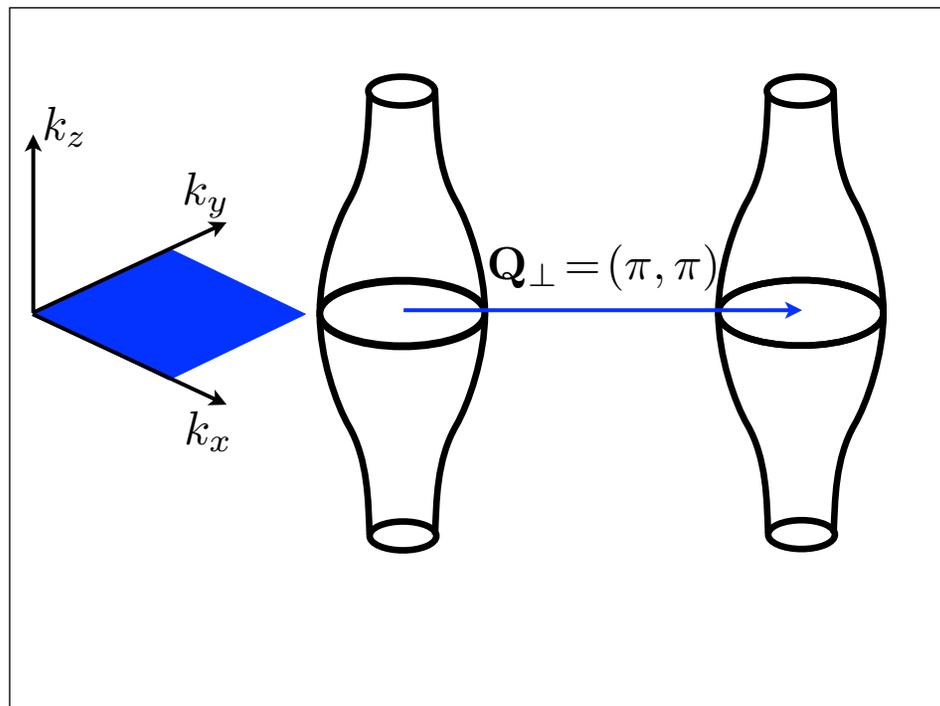
$$Q = (\pi, \pi, \pi)$$

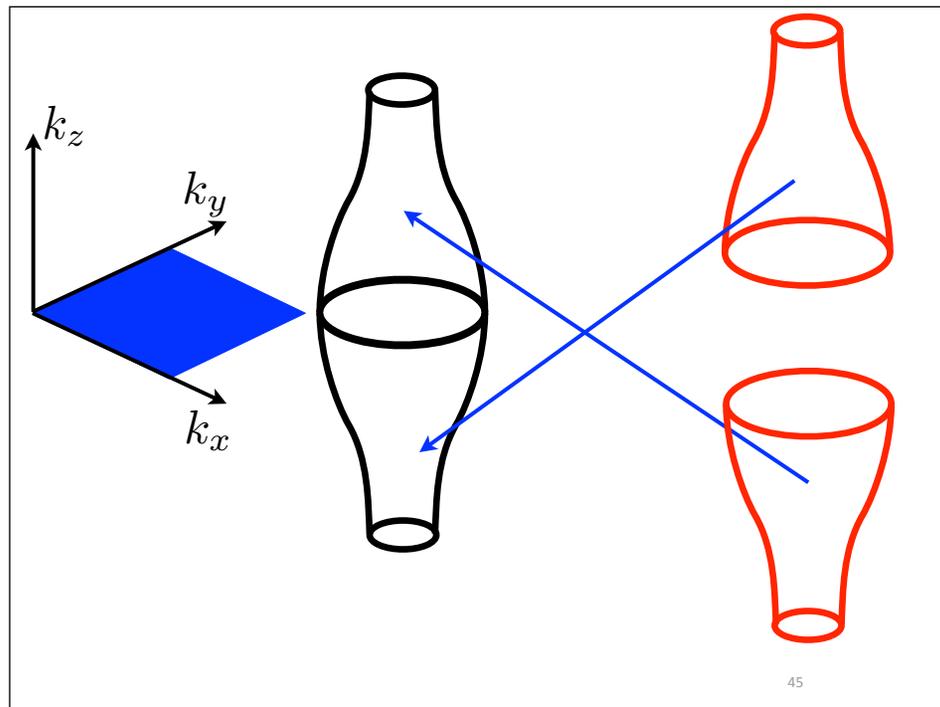
Simple cubic  $\rightarrow$  FCC (rock salt)  $\rightarrow$  BCC reciprocal lattice

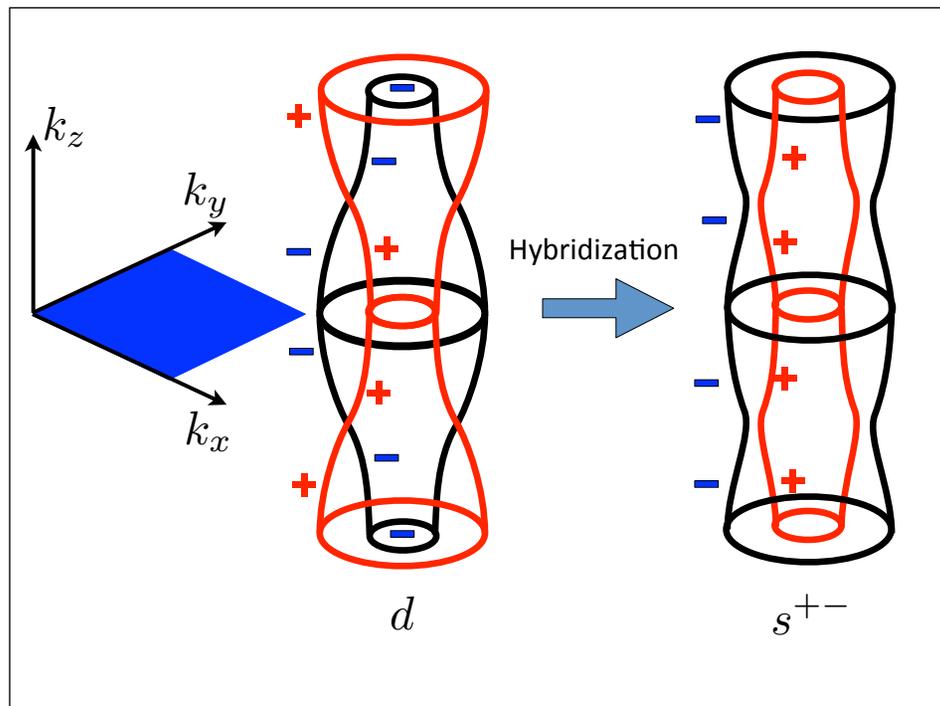


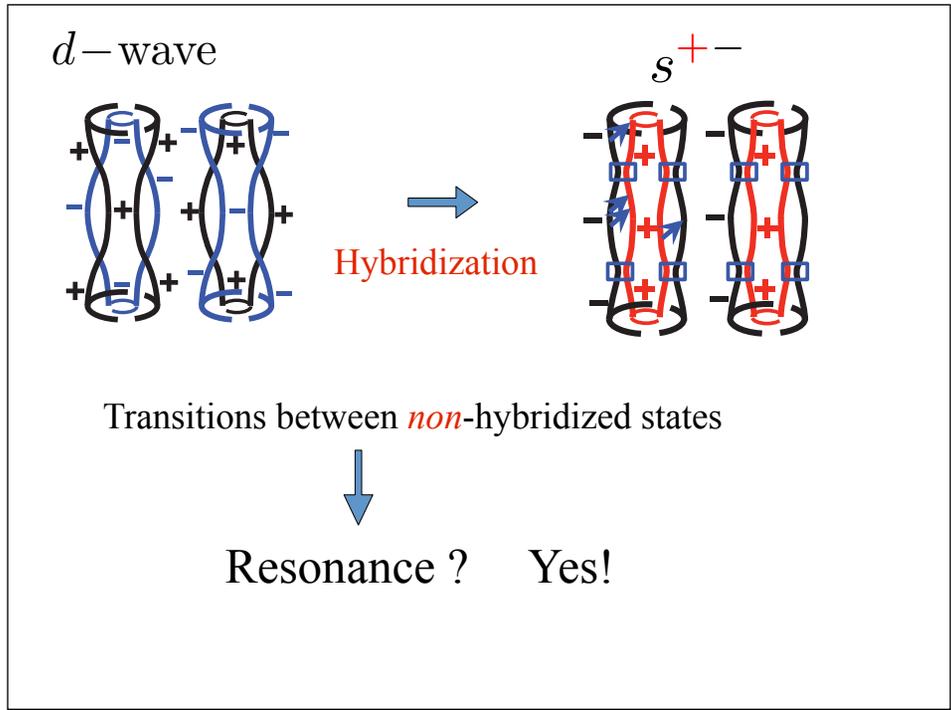


When those 3D pockets cross



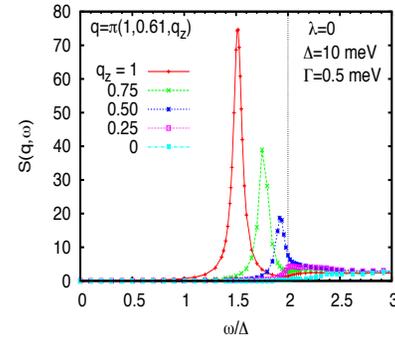
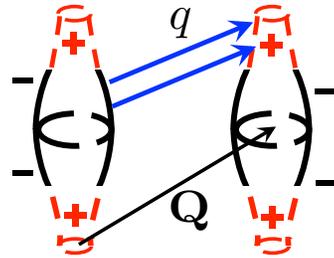
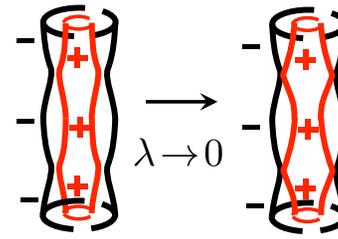




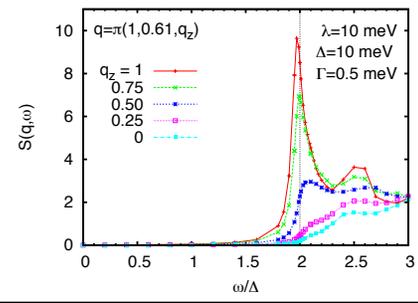
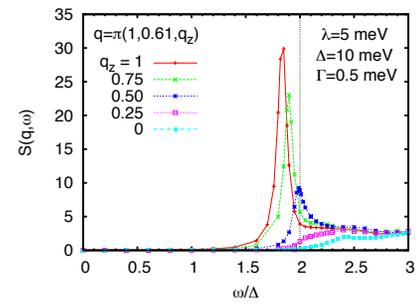


1) Take a limit  $\lambda \rightarrow 0$

2) Unfold (not necessary)

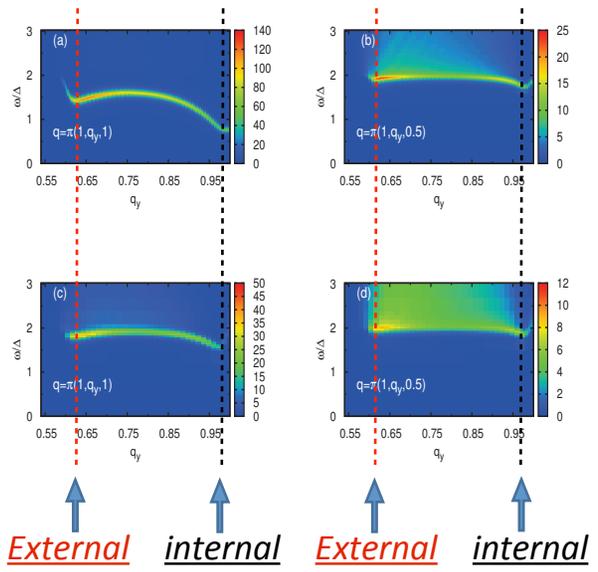


# Turn on hybridization



# Dependence on *transversal* $q$ -components

“Touching”  
conditions



## Part II

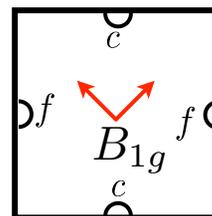
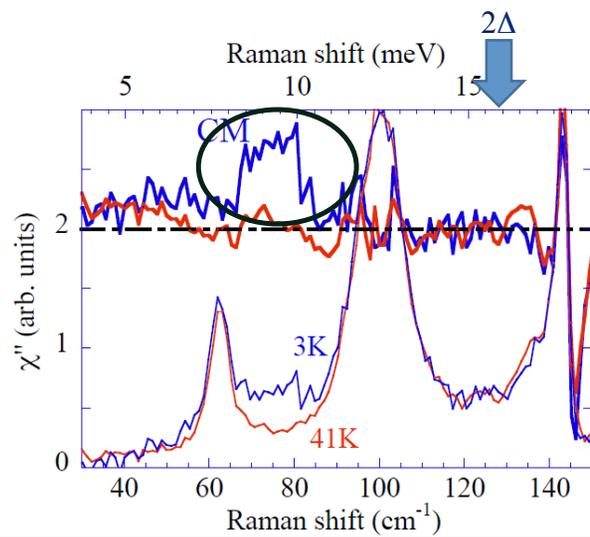
### Conclusions:

- (1) Spin resonance is consistent with  $S^{+-}$
- (2) Band dispersion  $\longleftrightarrow$  Resonance dispersion

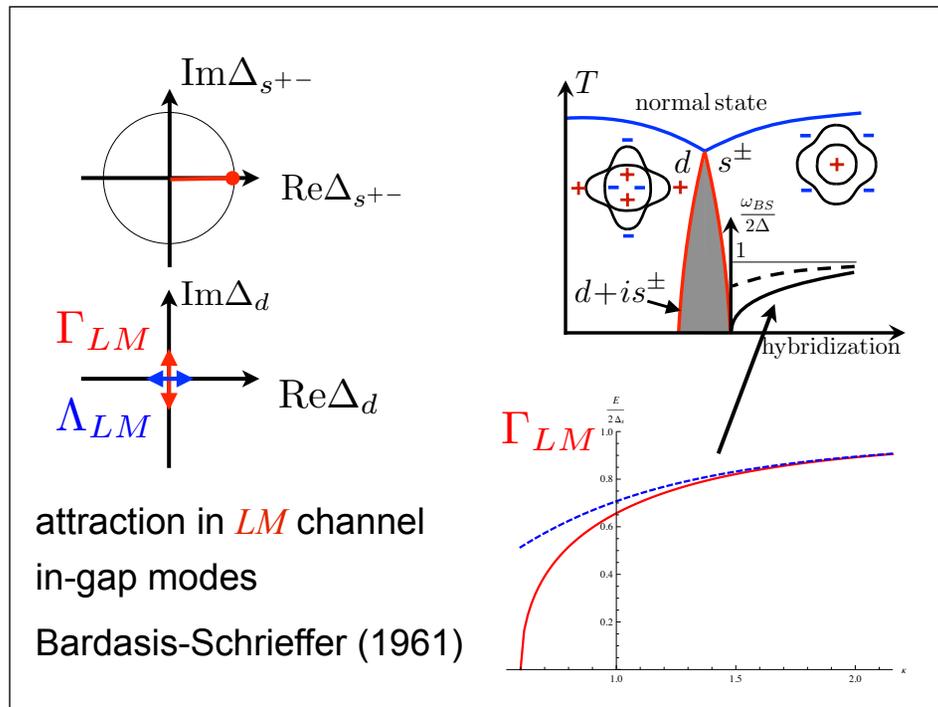
## Part III

### **Raman spectroscopy in “s+” state**

Data from Girsh Blumberg

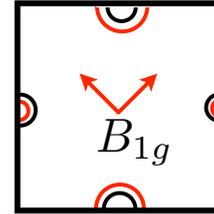


Girsh Blumberg,  
unpublished



$$[\text{density, phase}]_- = i$$

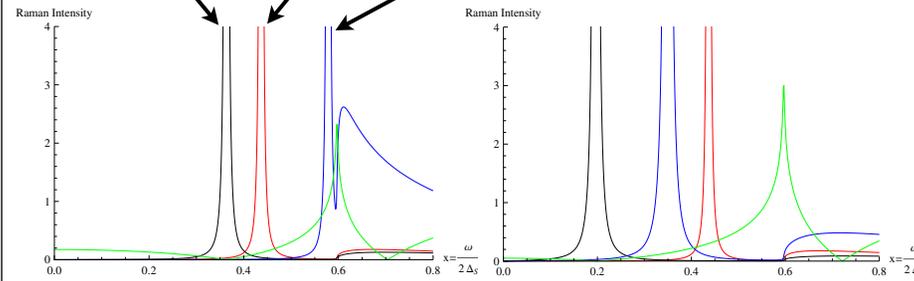
Coupling is strong: 1 *in-gap* mode  
 neutral mode: No Coulomb



Raman peak

Bardasis-Schrieffer,  $\Gamma_d$

Nematic charge exciton (needs attraction)



## Part III

### Conclusions:

- (1) Raman in  $S^{+-}$   $\Rightarrow$  d-wave excitations
- (2) Proximity to s+i d, charge fluctuations  $\Rightarrow$  stronger signal

