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Selection of Magnetic Order and Magnetic Excitations in the SDW State of Iron-based Superconductors

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Selection of magnetic order and magnetic excitations in the metallic SDW state of ferropnictides

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- Introduction
- Peculiarities of the SDW state in the itinerant scenario
- Spin excitations
- Conclusions

Collaborators:

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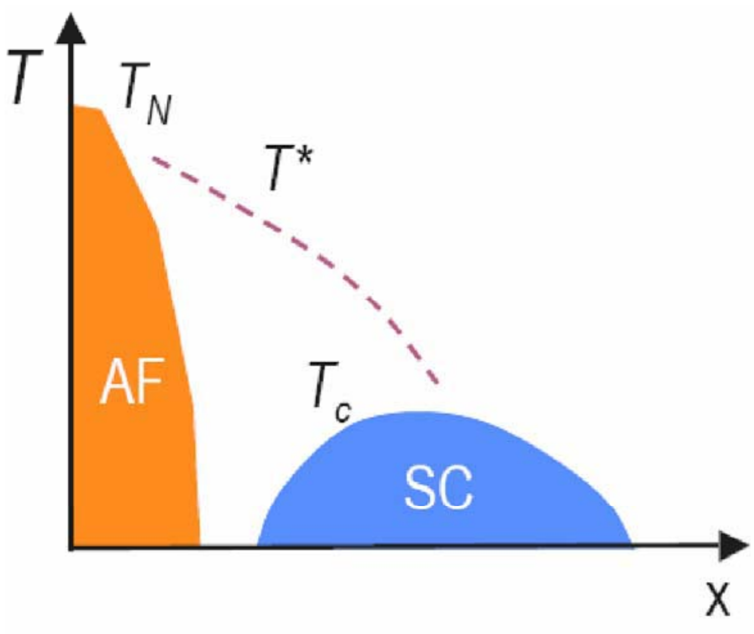
- **A. Akbari, @** *Institut für Theoretische Physik III, Ruhr-Uni Bochum*
- **J. Knolle, R. Moessner, @** *MPI Physik komplexer Systeme, Dresden*

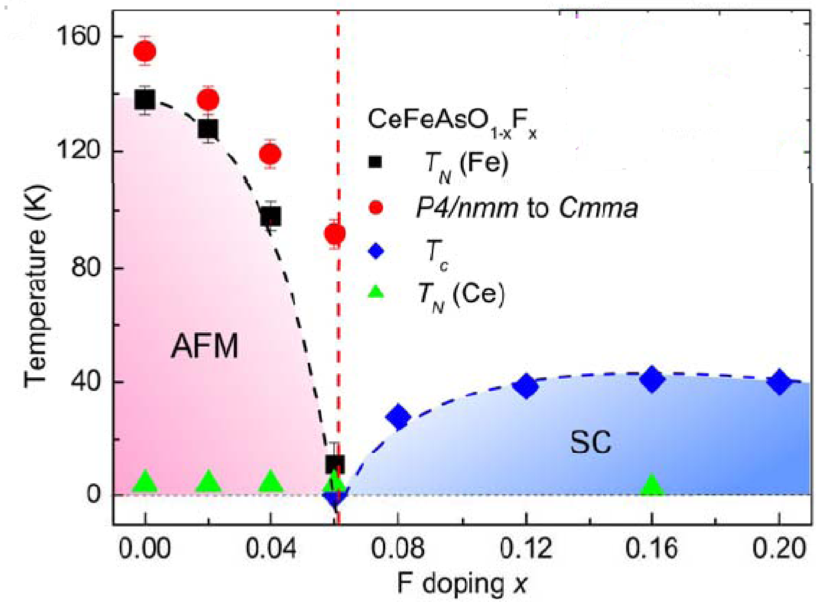
Cu-oxides versus Fe-pnictides

Phase Diagram

Cuprates



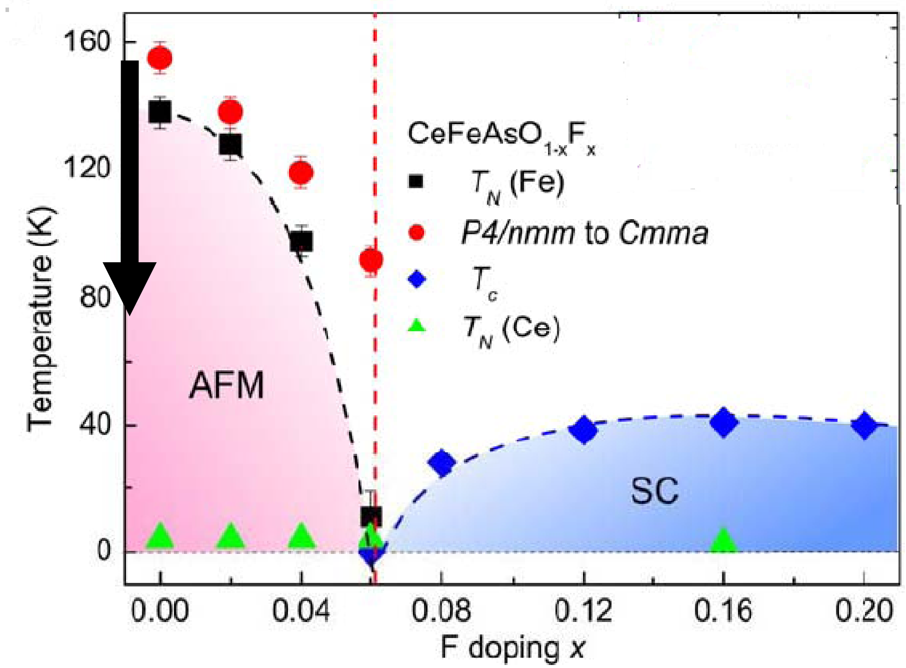
Fe-based superconductors



J. Zhao et al., Nat. Mater. 7, 953 (2008)

- Like CuO_2, phase diagram of FeAs has AFM in proximity to the SC state
- However, unlike CuO_2 all regions of FeAs-phase diagram are metallic

Itinerant approach to the ferropnictides



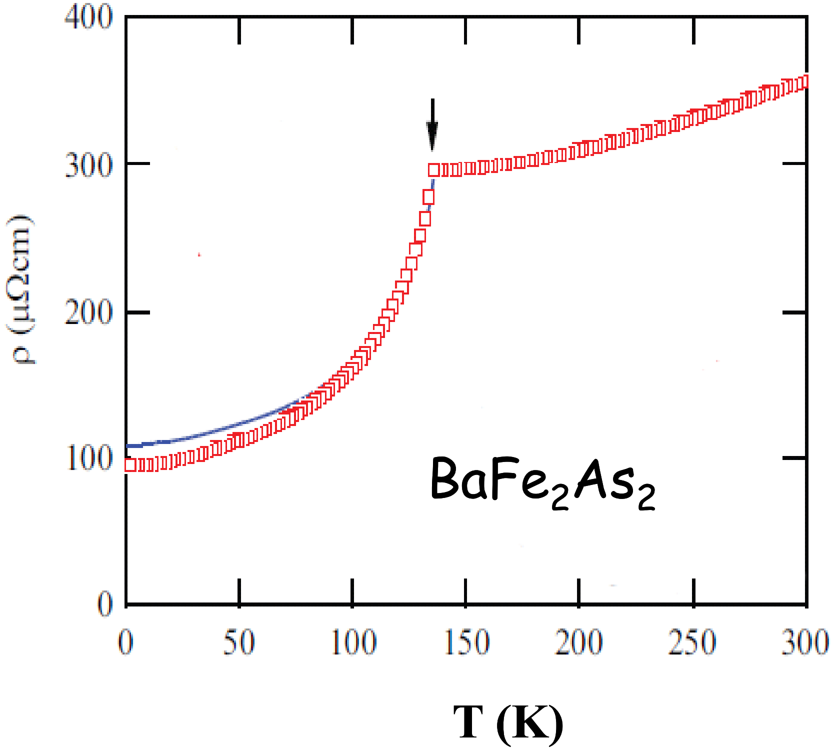
J. Zhao et al., Nat. Mater. 7, 953 (2008)

- **The systems are metals in the normal state**
- **The interactions are smaller than the bandwidth**

AFM state in the itinerant scenario: selection of the magnetic order

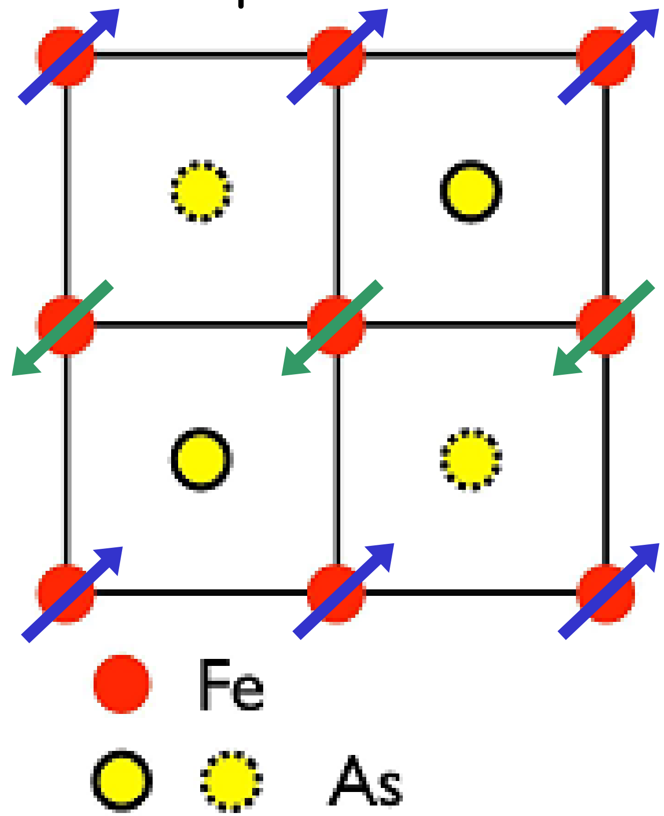
Itinerant approach to ferropnictides

Metallic transport



N. Kurita et al., PRB 79, 214439 (2009)

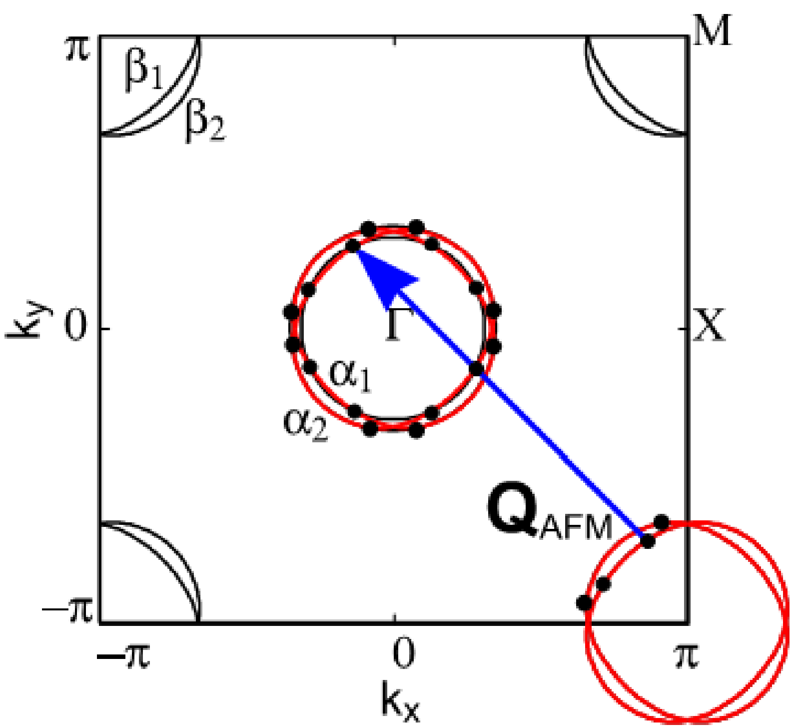
Magnetic order with well-defined spin wave excitations

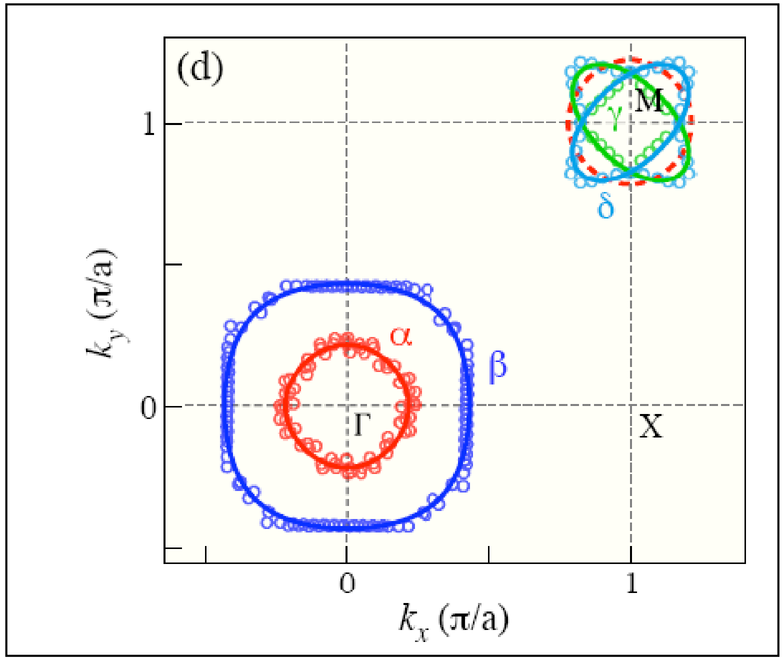


H.-H. Klauss et al., PRL 101, (2008);
Clarina de la Cruz et al., Nature 453 (2008)

Nesting properties

Co and K-doped $BaFe_2As_2$





$$\varepsilon_k^h = -\varepsilon_{k+Q_{AFM}}^e$$

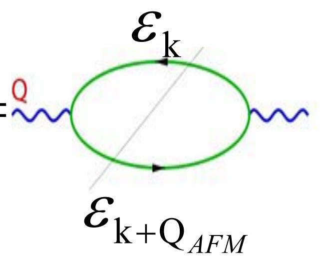
J. Dong et l., I. Mazin et al.,
S. Raghu et al., K. Kuroki et al, …
S. Graser et al., Z. Tesanovic et al.,
M. Korshunov and I. Eremin

ARPES: H. Ding et al., A. Kaminski et al., M.Z.Hasan et al., S. Borisenko et al.,

dHvA: A. Coldea et al., S. Sebastian et al.,

Nesting is a boost for a Q =(π,π) SDW magnetism

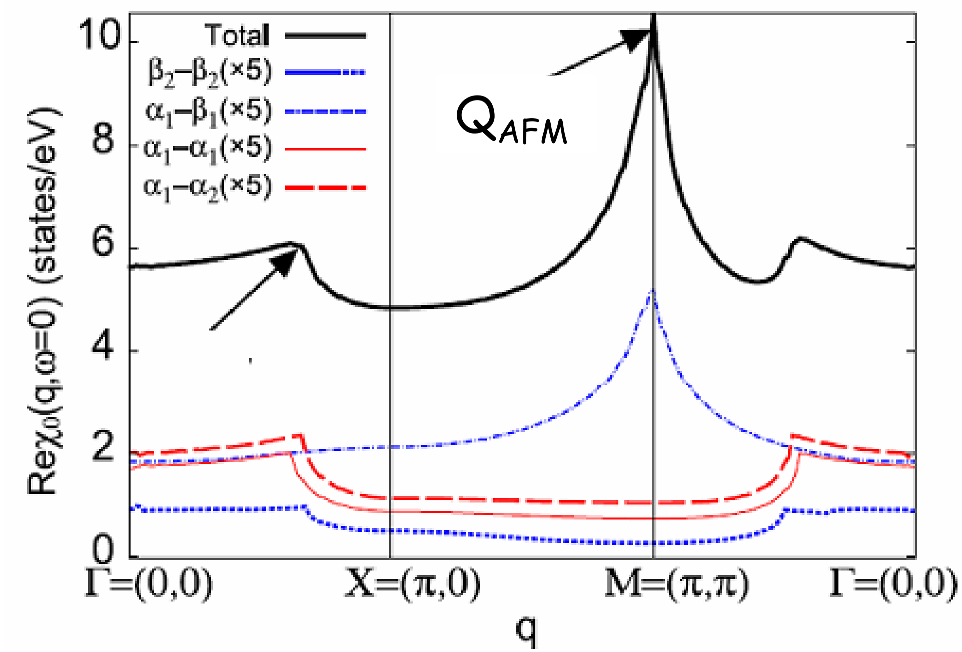
$$\chi(Q_{AFM}) = \frac{\chi_0(Q_{AFM})}{1\text{-}U\,\chi_0(Q_{AFM})} \qquad \chi_0(Q_{AFM}) =$$



$$= \iint_T \frac{d\omega\, d\varepsilon_k}{\omega^2 + \varepsilon_k^2} = \log\frac{E_F}{T}$$

For a perfect nesting, SDW instability occurs already at small U

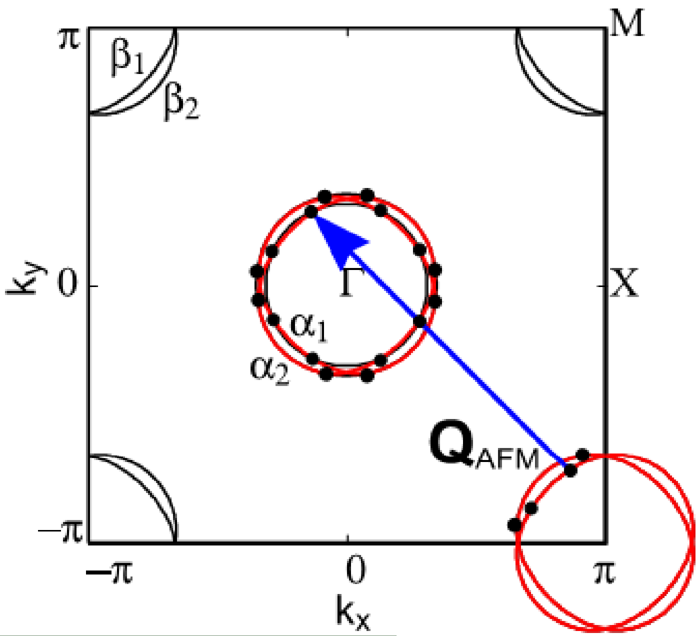
T.M. Rice (for Cr), V. Cvetkovic and Z.Tesanovic, EPL85 (2009)



J. Dong et al., EPL(08); Mazin et al., PRL(08); Eremin, Korshunov, PRB (08)

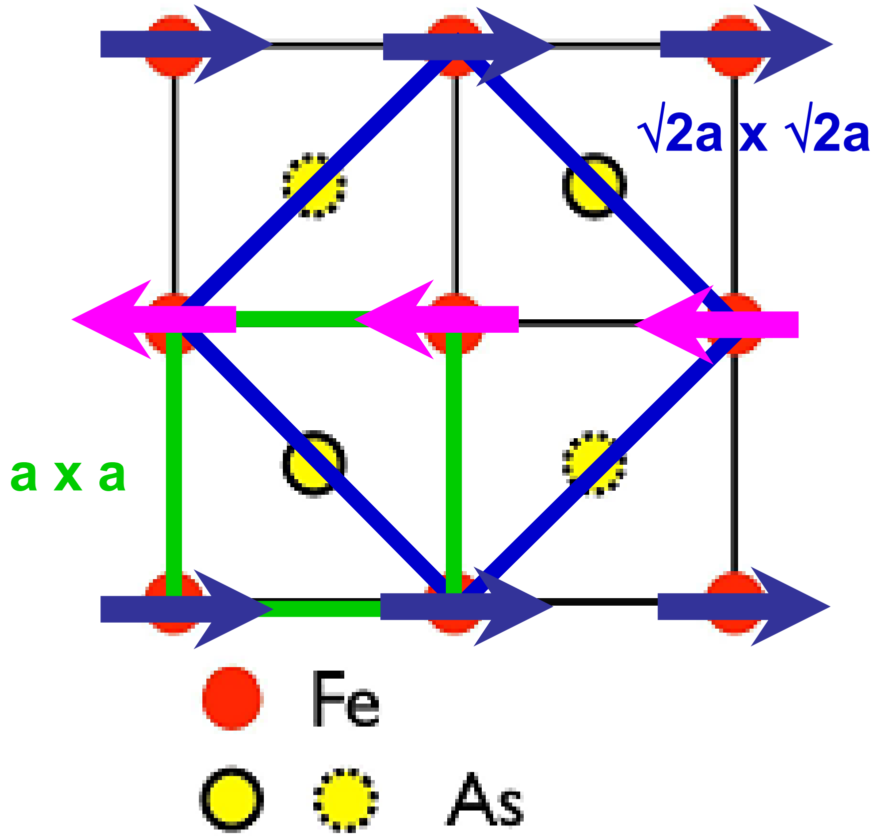
Magnetic structure below T_N

SDW (AF) order with Q=(π,π) for √2a x √2a



$$\varepsilon_k^h = -\varepsilon_{k+Q_{AFM}}^e$$

Lebegue, PRB (07); J. Dong et al., EPL (08), I. Mazin et al. PRL (08), D. J. Singh et al. PRL (08); K. Kuroki et al PRL (08), L. Boeri et al., PRL (08); Tesanovic et al, EPL (08)

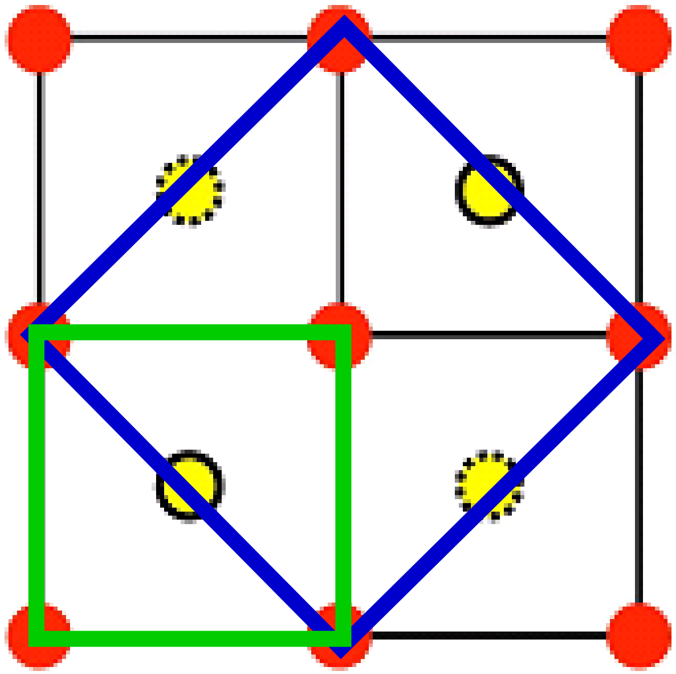


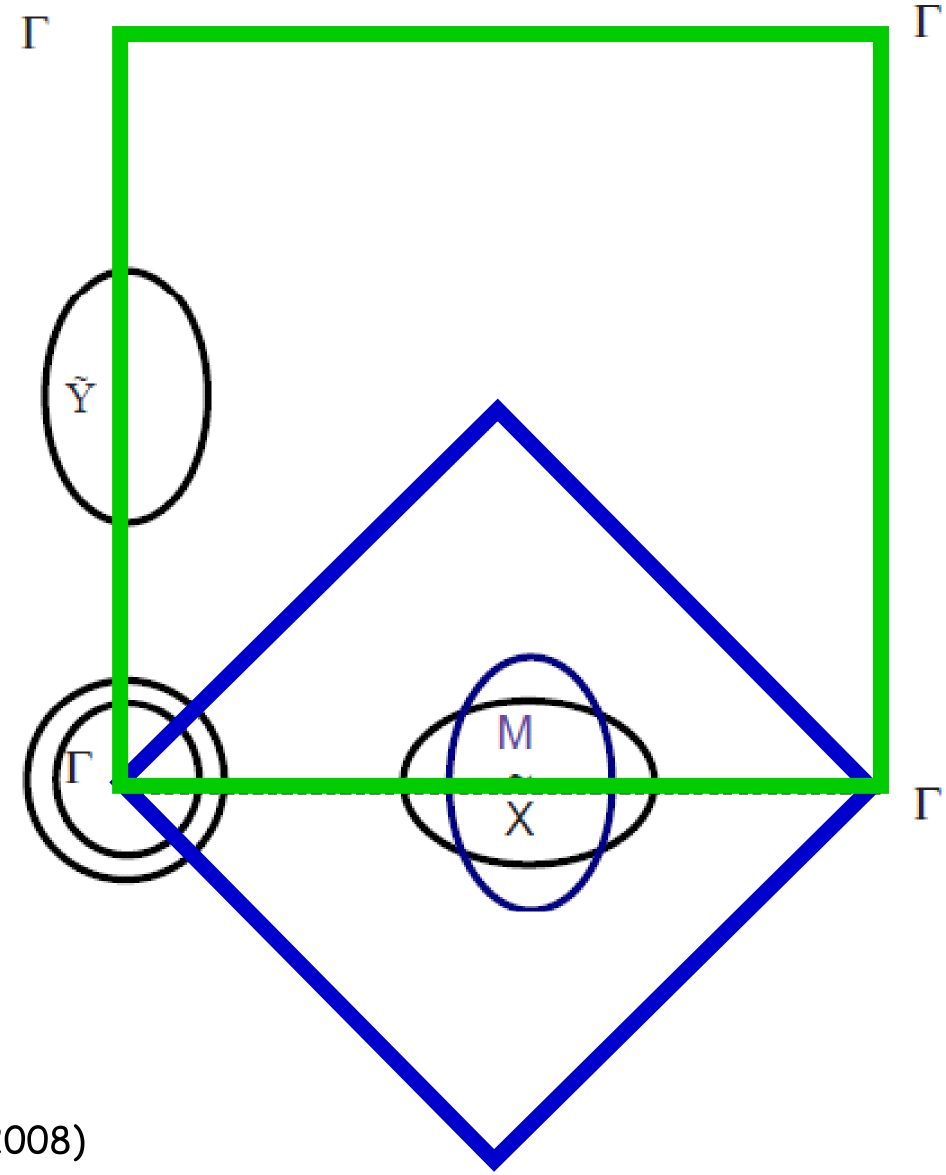
NS: C. de la Cruz et al., Nature 453, 899 (2008); J. Zhao et al., Nat. Mater. (2008); A. Goldman et al., Phys. Rev. B 78 (2008)

How to understand metallic Q'=(0,π) SDW state for a x a ?

The order can be understood from the localized J_1-J_2 model for $J_2>0.5J_1$:
P. Chandra, P. Coleman and A.I. Larkin, PRL64 (1990); Q. Si and E. Abrahams, PRL(2008); C. Xu, M. Mller, and S. Sachdev, PRB(2008); G.S. Uhrig, M. Holt, J. Oitmaa, O.P. Sushkov, and R.R.P. Singh, PRB (2009).

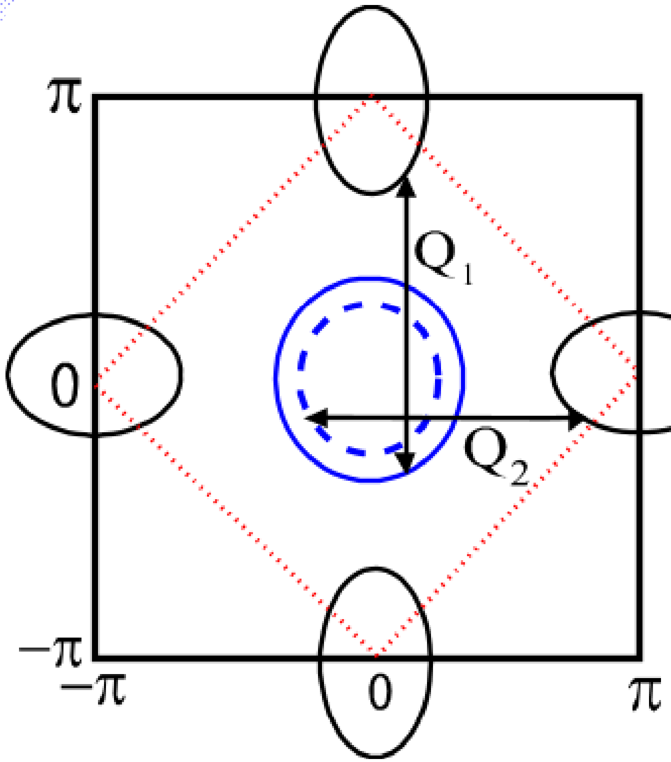
Unfolded Brillouin Zone

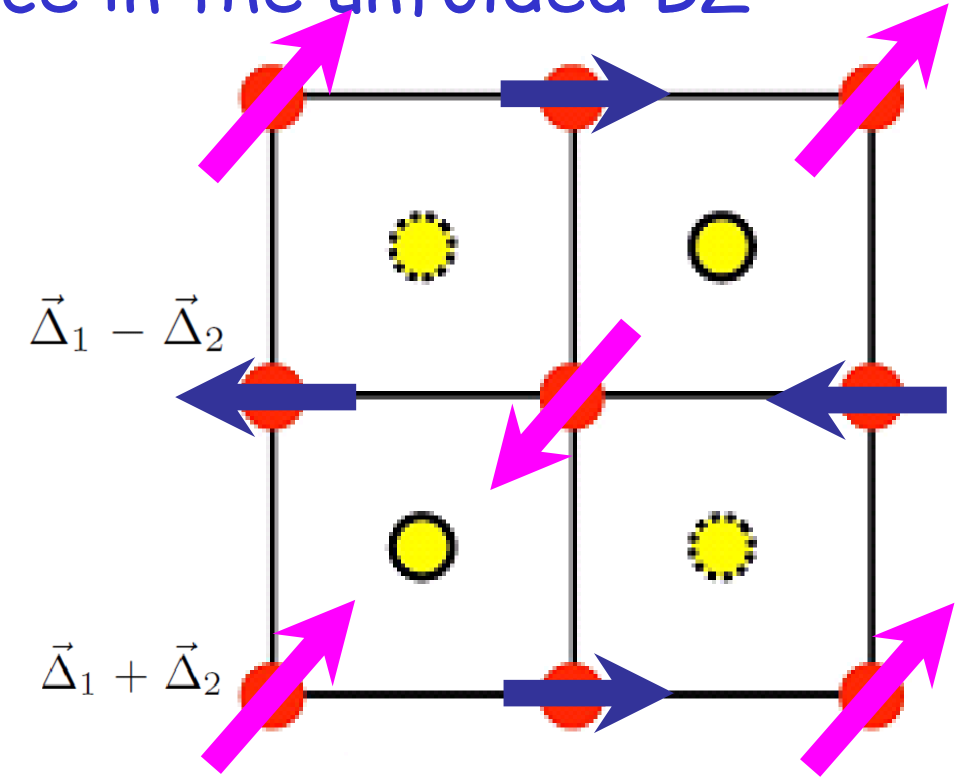




I. Mazin et al., Phys. Rev. Lett. 101, 057003 (2008)

Fermi surface in the unfolded BZ





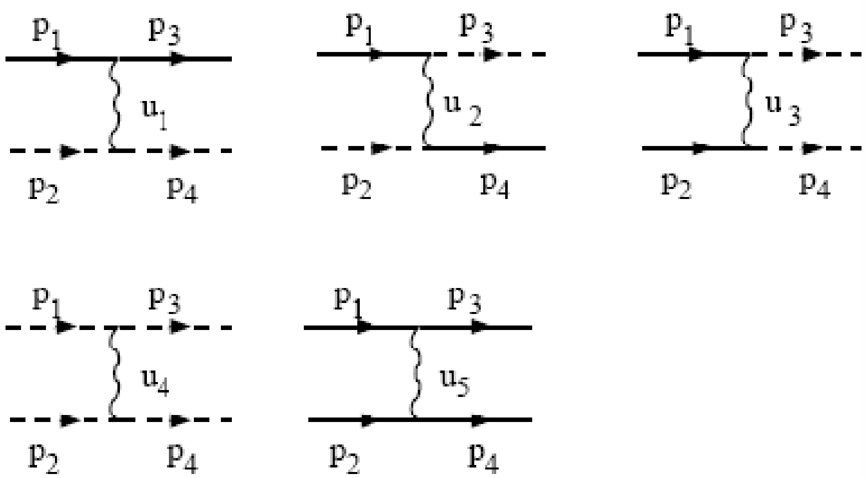
- two nesting wave vectors $\mathbf{Q_1}$=(0,π) and $\mathbf{Q_2}$=(π,0)

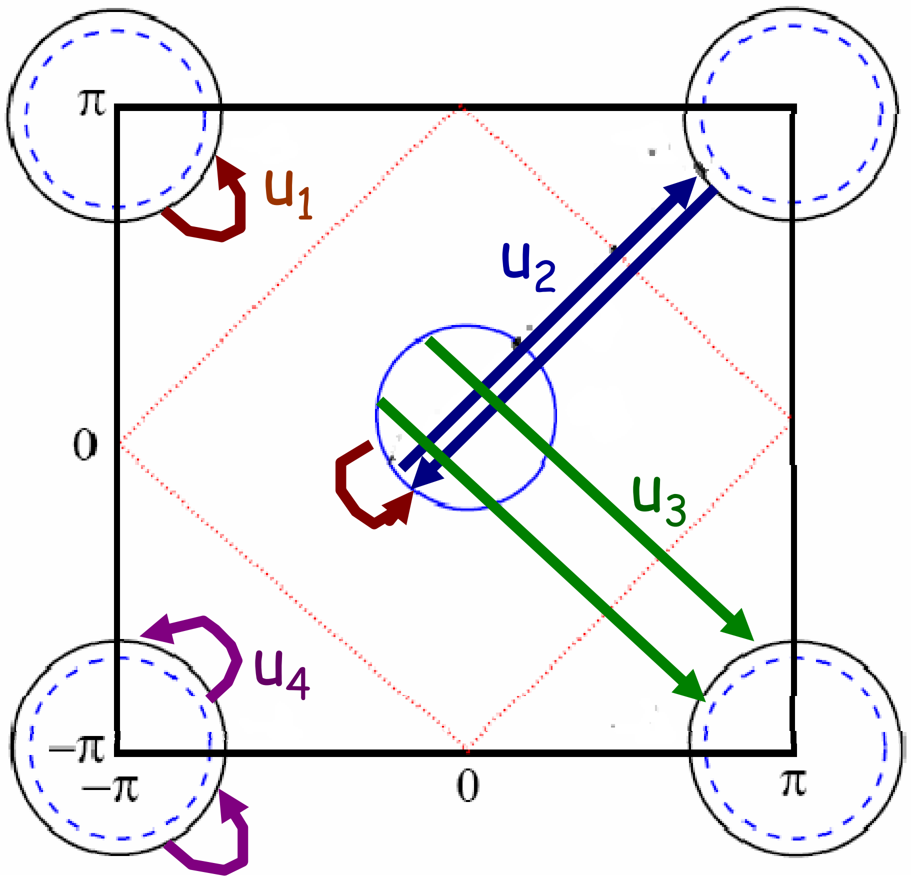
- two vector SDW order parameters

$$\vec{S}(\mathbf{R}) = \vec{\Delta}_1 e^{i\mathbf{Q}_1\mathbf{R}} + \vec{\Delta}_2 e^{i\mathbf{Q}_2\mathbf{R}}$$

- two sublattice order parameters $\vec{\Delta}_1 + \vec{\Delta}_2 \quad \vec{\Delta}_1 - \vec{\Delta}_2$

Two-band model and Fermi-liquid interactions

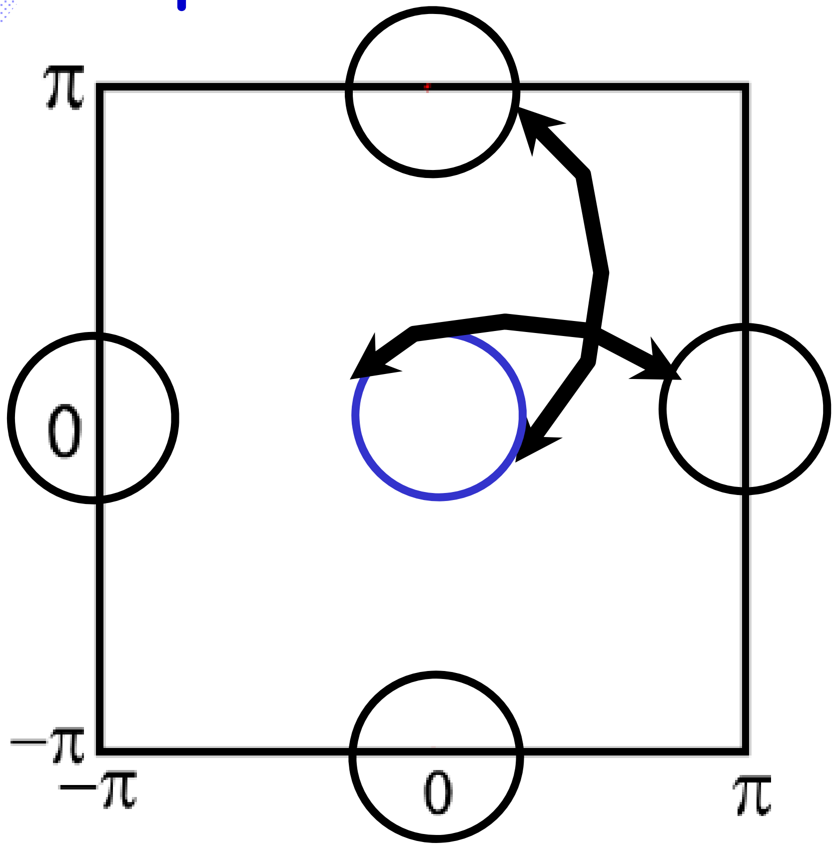


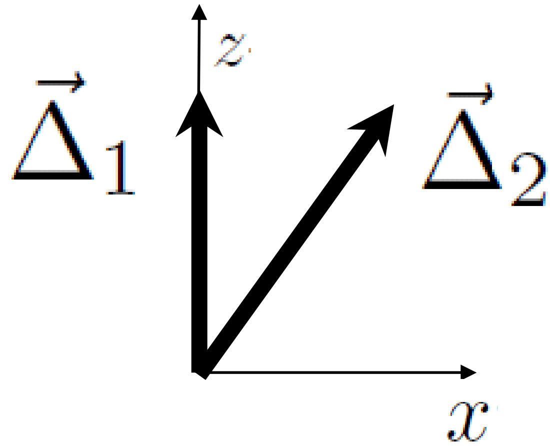


$$u_4 = u_5$$

Chubukov, Efremov, and Eremin, Phys. Rev. B 78 (2008)

Simplest model to solve: 1 hole and 2 electron pockets

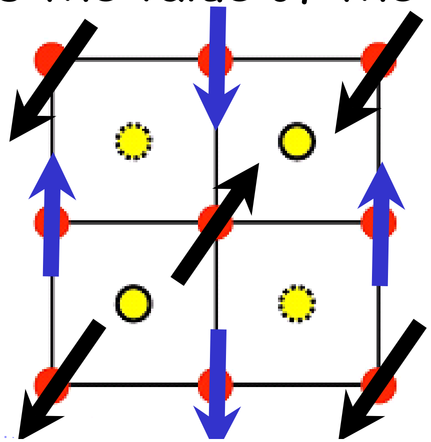




$$1 = \frac{(U_1 + U_3)}{2N} \sum_{\mathbf{p}} \frac{1}{\sqrt{(\varepsilon_{\mathbf{p}}^{-})^2 + \Delta^2}}$$

$$\Delta^2 = \vec{\Delta}_1^2 + \vec{\Delta}_2^2$$

- sets the value of the total order parameter but does not specify $\vec{\Delta}_1$ or $\vec{\Delta}_2$

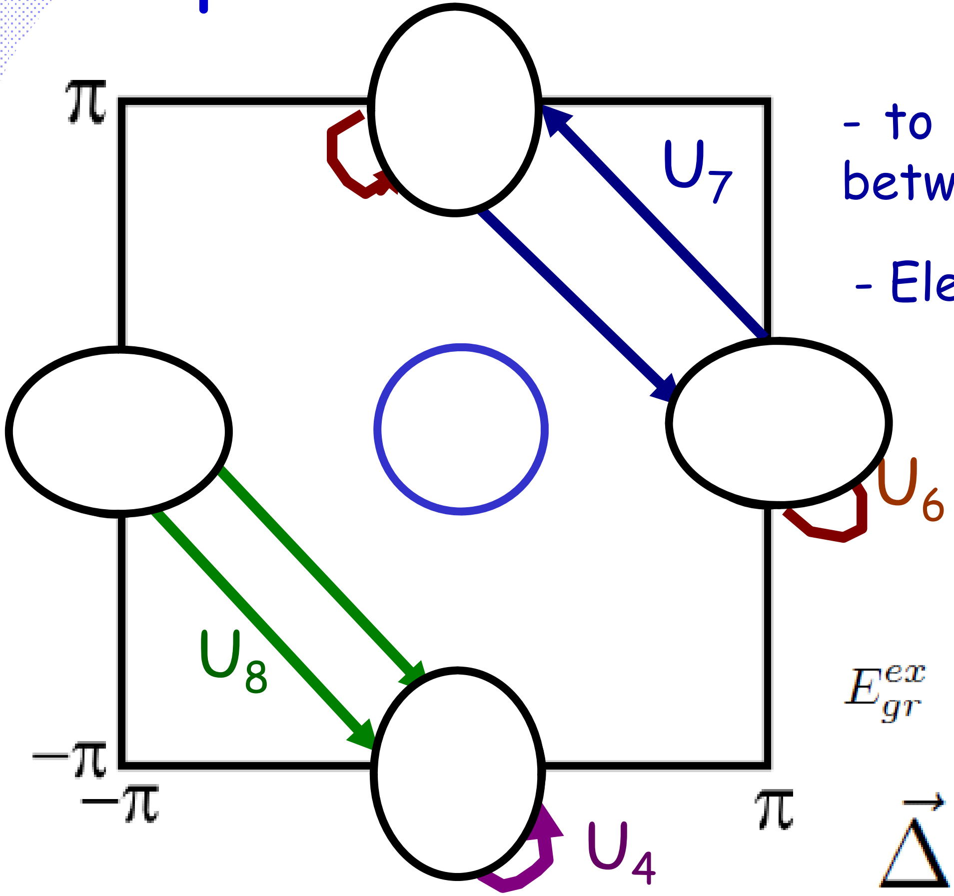


- the ground state degeneracy is even larger than in the J_1-J_2 model of localized spins

O(6) degeneracy [5 Goldstone modes]

(0, π) or (π,0) are two of many possibilities

Simplest model to solve: 1 hole and 2 electron pockets



- to add the interaction (density-density) between electron pockets

- Electron pockets are elliptic, ε

Positive ∝ $(m_x - m_y)^2$

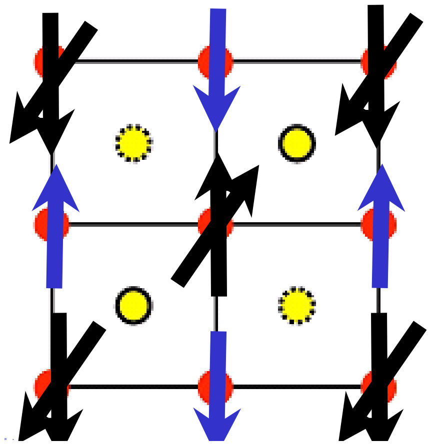
$$E_{gr}^{ellipt} = C|\vec{\Delta}_1|^2|\vec{\Delta}_2|^2$$

< 0

$$E_{gr}^{ex} = 2A^2 \left[(U_6 + U_8 - U_7 - U_4)\right] \frac{|\vec{\Delta}_1|^2|\vec{\Delta}_2|^2}{\Delta^4}$$

$\vec{\Delta}_1 = 0$ or $\vec{\Delta}_2 = 0$

I. Eremin and A.V. Chubukov, PRB 81, 024511 (2010)



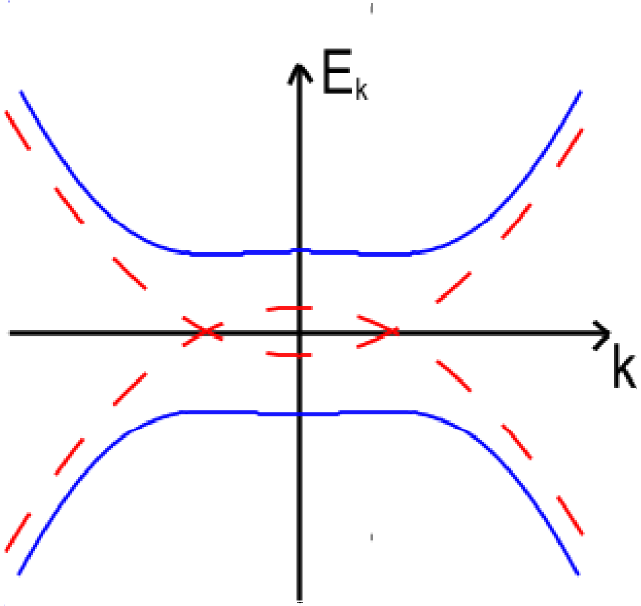
(0, π) or (π,0) is selected !

- no need for quantum fluctuations in itinerant picture [within 'ab-initio' J.J.Pulikkotil et al., arXiv:0809.0283; A. Yaresko et al., PRB 79, (2009)]

- charge fluctuations are crucial

SDW state: electronic structure

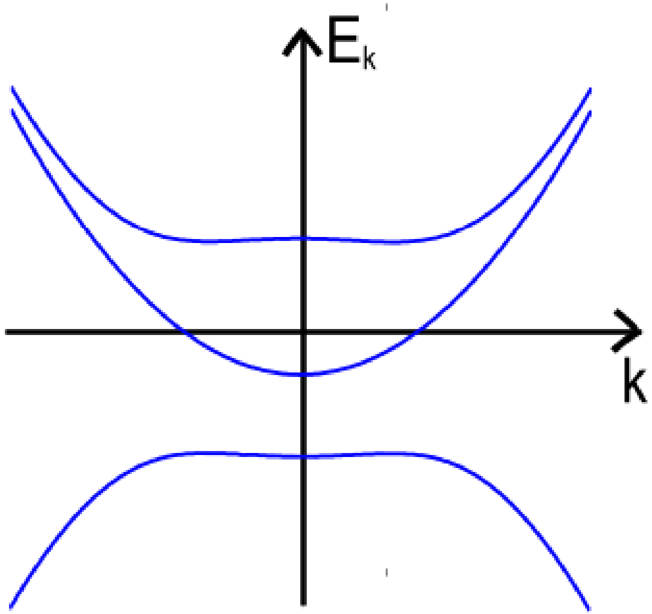
usual SDW



$$E_{\mathbf{p}} = \pm\sqrt{(\varepsilon_{\mathbf{p}})^2 + |\Delta|^2}$$

-insulator

Metallic SDW state in pnictides

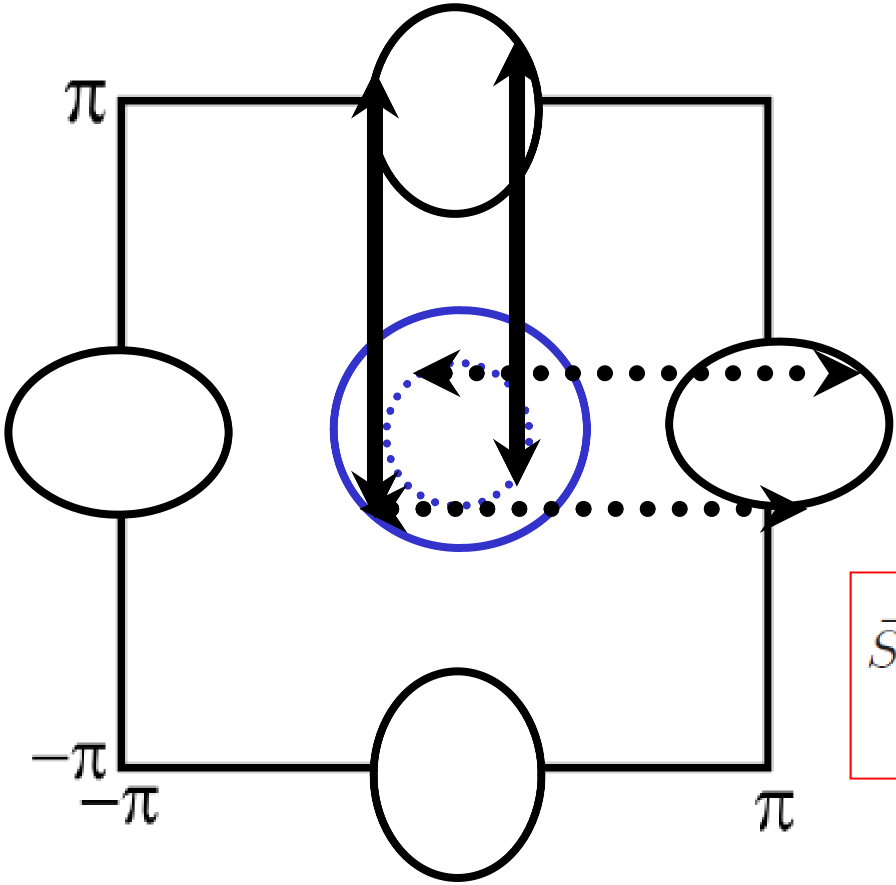


$$E_{\mathbf{p}} = \pm\sqrt{(\varepsilon_{\mathbf{p}})^2 + |\Delta|^2} \qquad \varepsilon^{\beta}_{\mathbf{p}}$$

one of the combination of the electron pockets will decouple from SDW

Metal even for complete nesting !

Inclusion of the 4 hole pocket



$$\vec{\Delta}_{11} = \Delta_1^z = -U_{SDW}^{\{1\}} \sum_{\mathbf{p}} \langle \alpha^\dagger_{1\mathbf{p}\uparrow} \beta_{1\mathbf{p}\uparrow} \rangle$$

$$\vec{\Delta}_{12} = \Delta_1^x = -U_{SDW}^{\{1\}} \sum_{\mathbf{p}} \langle \alpha^\dagger_{1\mathbf{p}\uparrow} \beta_{2\mathbf{p}\downarrow} \rangle$$

$$\vec{\Delta}_{21} = \Delta_2^z = -U_{SDW}^{\{2\}} \sum_{\mathbf{p}} \langle \alpha^\dagger_{2\mathbf{p}\uparrow} \beta_{1\mathbf{p}\uparrow} \rangle$$

$$\vec{\Delta}_{22} = \Delta_2^x = -U_{SDW}^{\{2\}} \sum_{\mathbf{p}} \langle \alpha^\dagger_{2\mathbf{p}\uparrow} \beta_{2\mathbf{p}\downarrow} \rangle$$

$$\begin{aligned} \vec{S}(\mathbf{R}) \;\propto\; & \vec{n}_z \left(\Delta_1 \cos\theta - \Delta_2 \sin\theta\right) e^{i\mathbf{Q}_1\mathbf{R}} \\ & + \vec{n}_x \left(\Delta_1 \sin\theta + \Delta_2 \cos\theta\right) e^{i\mathbf{Q}_2\mathbf{R}} \end{aligned}$$

$$\tan\,\theta = \Delta_1/\Delta_2 \text{ or } \tan\,\theta = -\Delta_2/\Delta_1$$

Correction to the ground state energy: $E_{gr}(\theta) = E_0 + E_1 \sin^2(2\theta)$

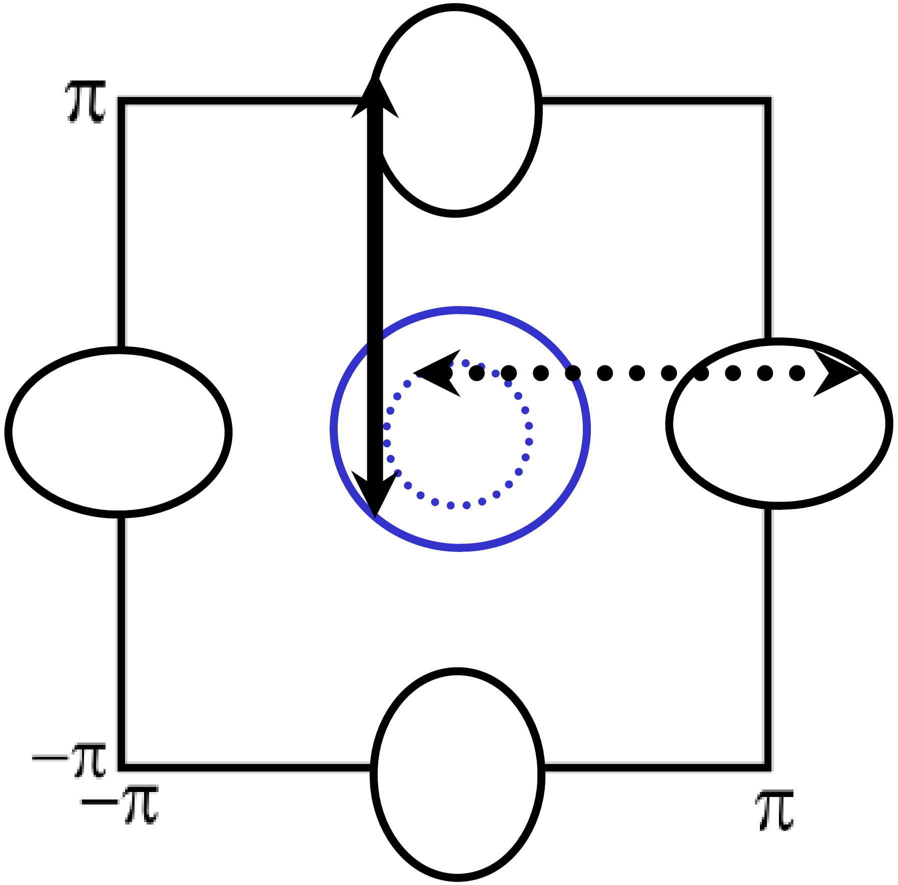
The selected ground state is not the observed (0,π) state

Z. Tesanovic, private communication

I. Eremin and A.V. Chubukov, PRB 81, 024511 (2010)

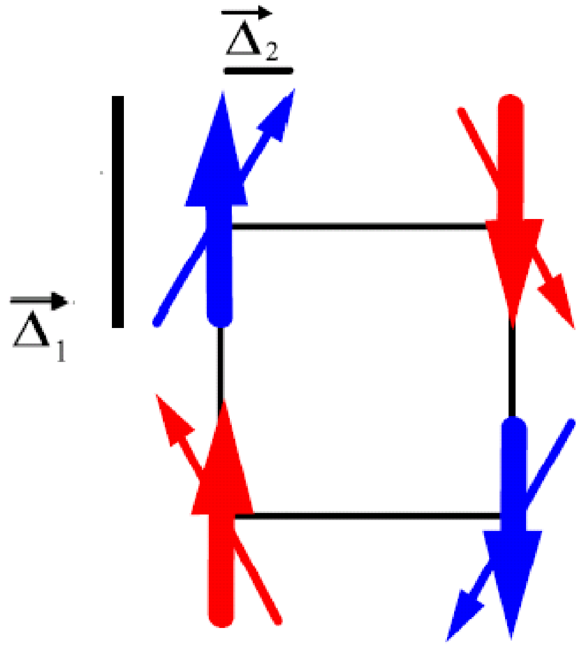
Inclusion of the 4 hole pocket

Assume (0,π) SDW order is settled; new hole pocket can only form (π,0) SDW order with remnant (ungapped) combination of the electron pocket



- even the interactions might be similar the second (π,0) SDW component will appear only for U=Ucr due to difference in masses

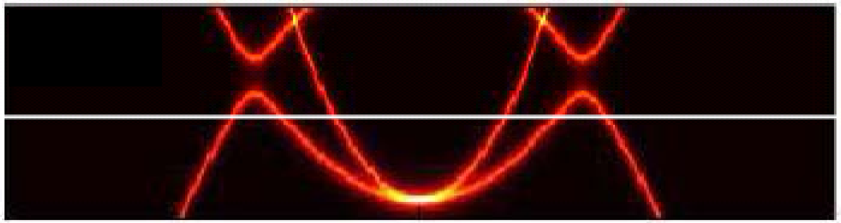
- for U>Ucr stripe order will be distorted



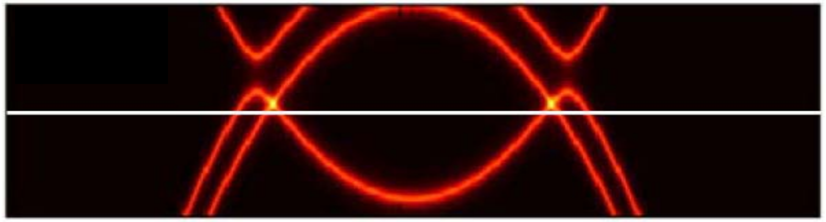
There is no continuous evolution of the metallic (π,0) state for U⇒∞

SDW state: electronic structure in the folded BZ

(π,π) and (0,0) points in the folded BZ are not equivalent

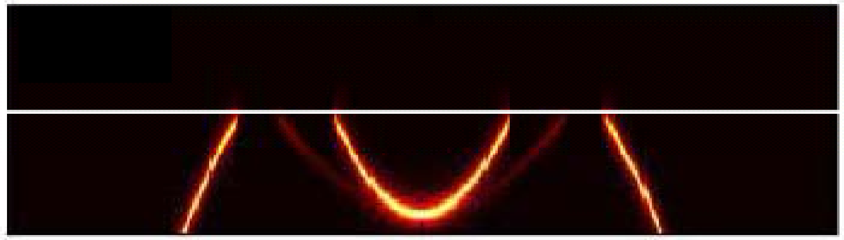


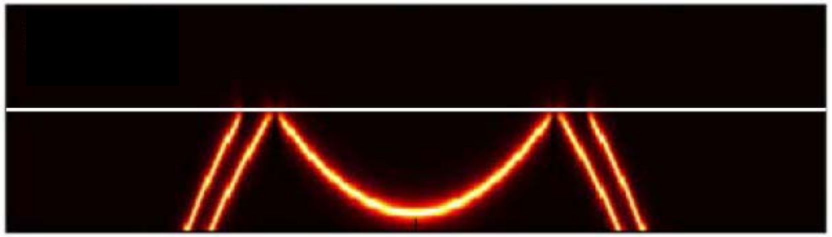
E_F



(π,π) (0,0)

ARPES: f(E)xIm G

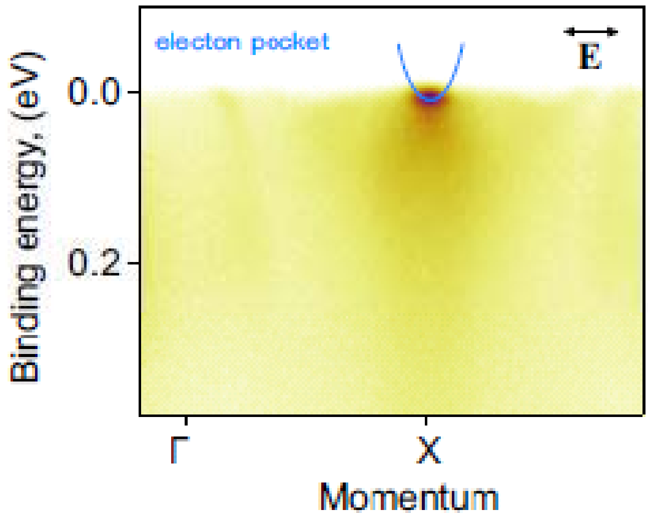


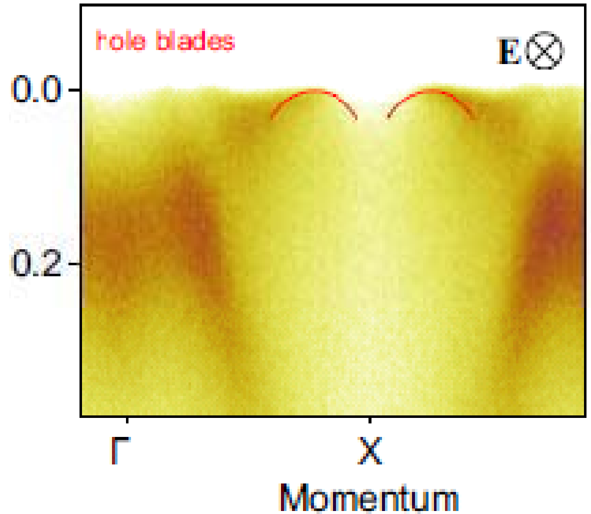


(π,π) (0,0)

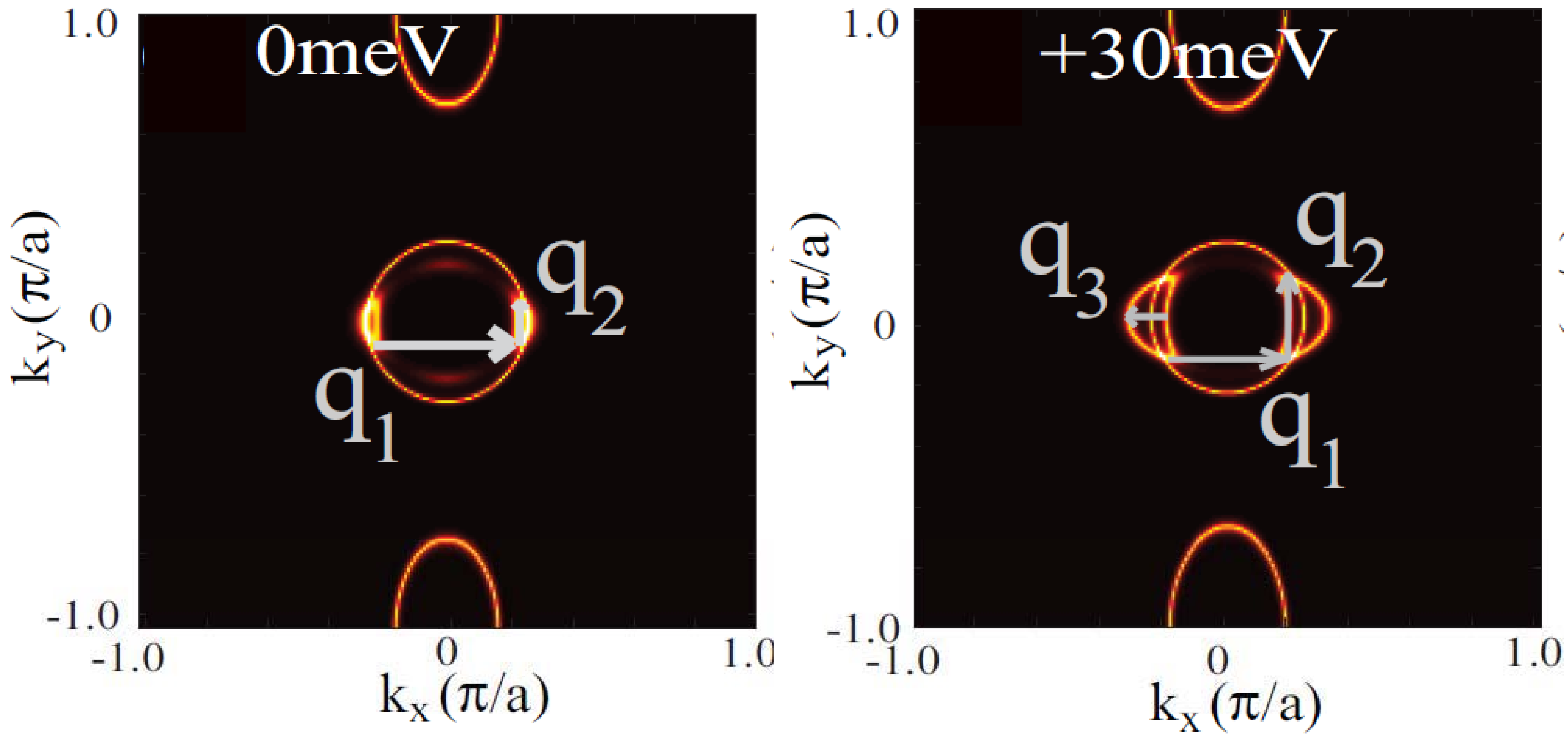
ARPES data

V. Zabolotnyy et al., Nature (2009)





Anisotropy of the SDW ⇒ Spectral Density

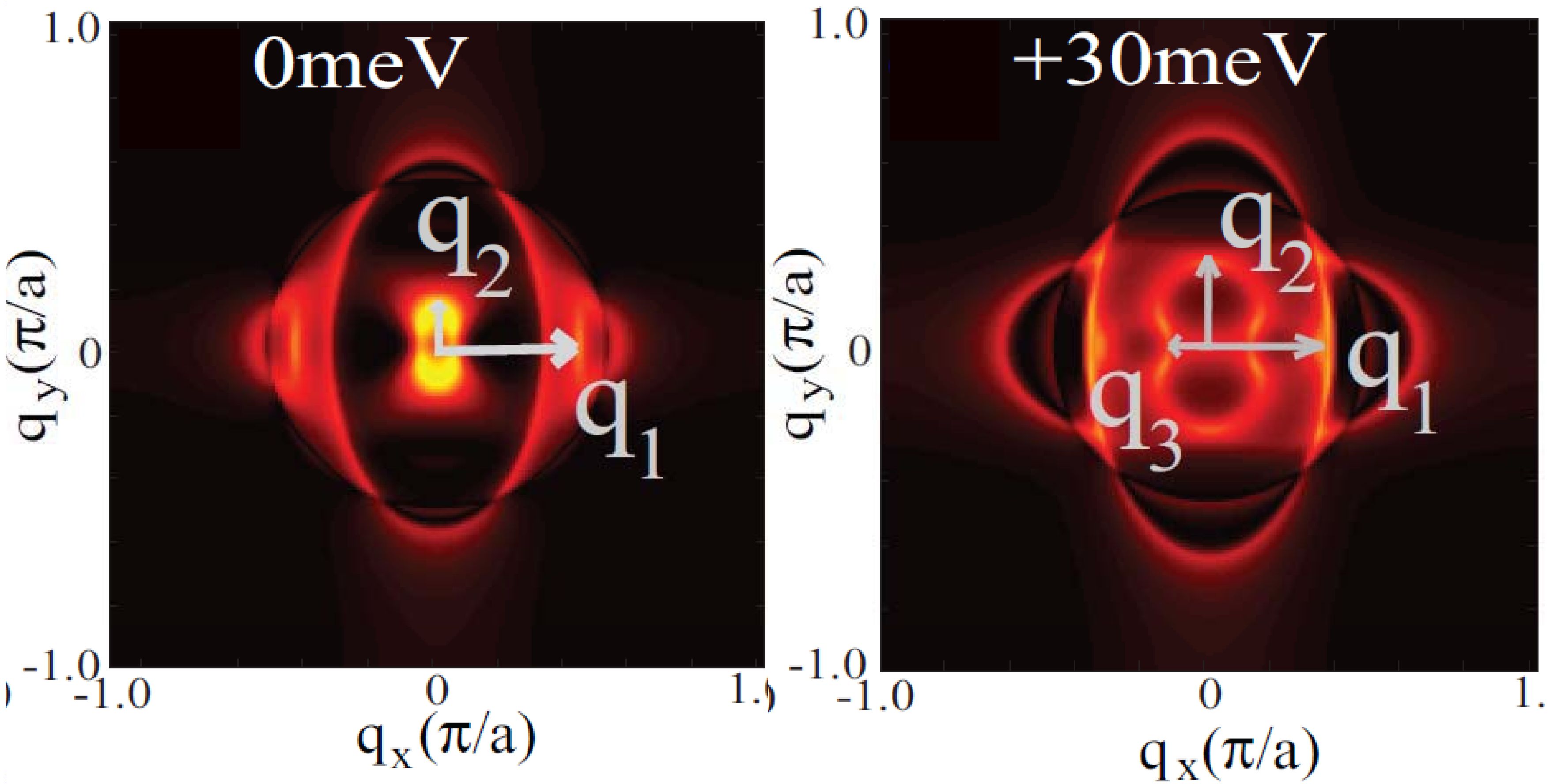


electronic anisotropy due to remnant pockets in the SDW $(0,\pi)$ order

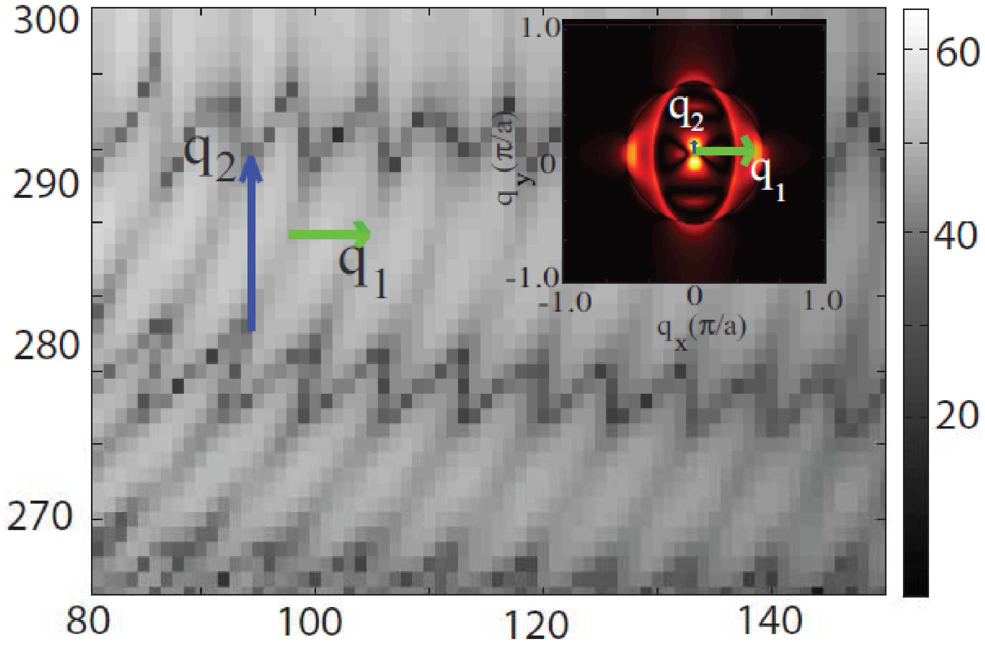
Anisotropy of the SDW ⇒ quasiparticle interference

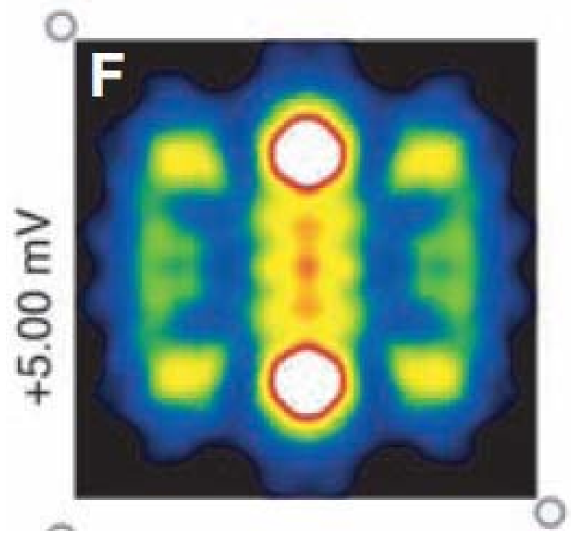
Impurity induced interference

$$G_\sigma(\mathbf{k},\mathbf{k}',\omega_n) = G_{0\sigma}(\mathbf{k},\omega_n)[\delta_{\mathbf{k},\mathbf{k}'} + t_\sigma(\mathbf{k},\mathbf{k}',\omega_n)G_{0\sigma}(\mathbf{k}',\omega_n)]$$



Anisotropy of the SDW ⇒ Quasiparticle interference





Exp: Chuang et al., Science 327, 181 (2010)

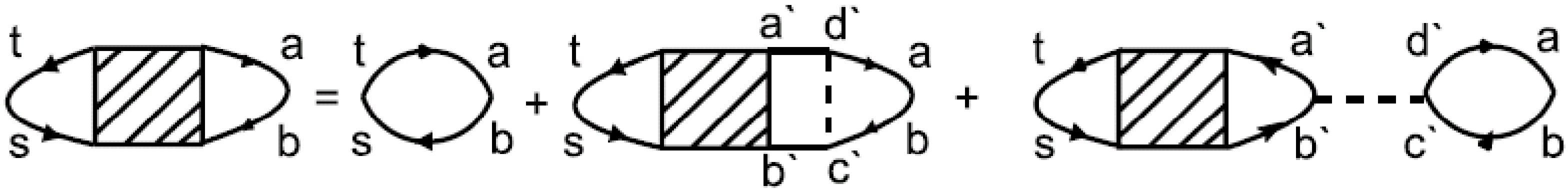
J. Knolle, I. Eremin, A. Akbari, and R. Moessner, Phys. Rev. Lett. 104 (2010)

- Presence of small remnant pockets ⇒ small magnetic moments

- Impurities act as pinning centers ⇒ inhomogeneity is more visible

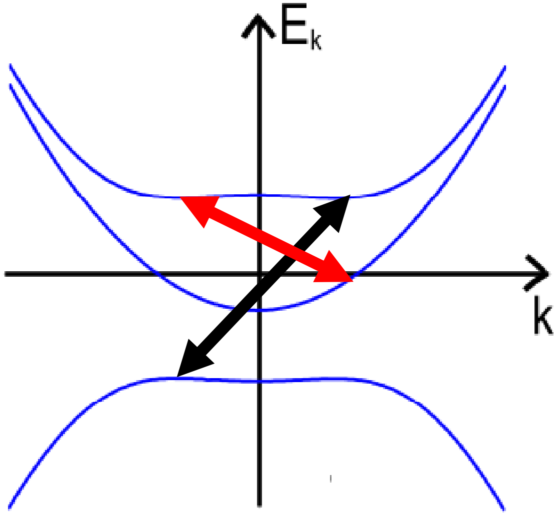
AFM state in the itinerant scenario: magnetic excitations

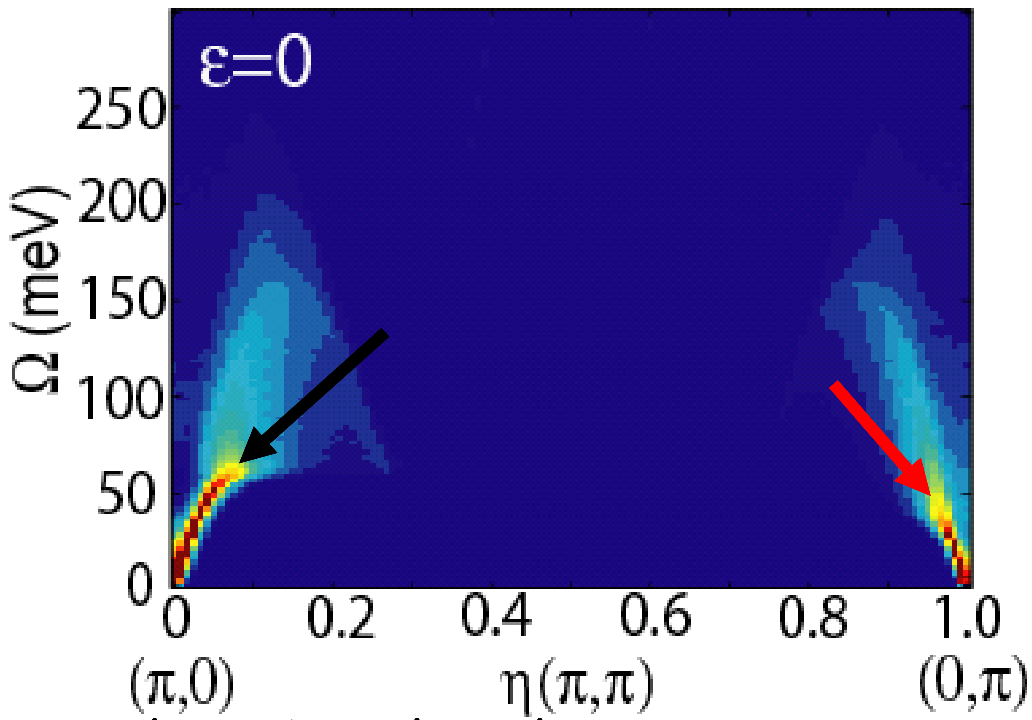
Transverse spin susceptibility ⇒ spin waves



$$[\chi^{st}_{ba}]_{RPA} = \chi^{st}_{ba} + [\chi^{st}_{b'a'}]_{RPA} U^{b'a'}_{c'd'} \chi^{c'd'}_{ba}$$

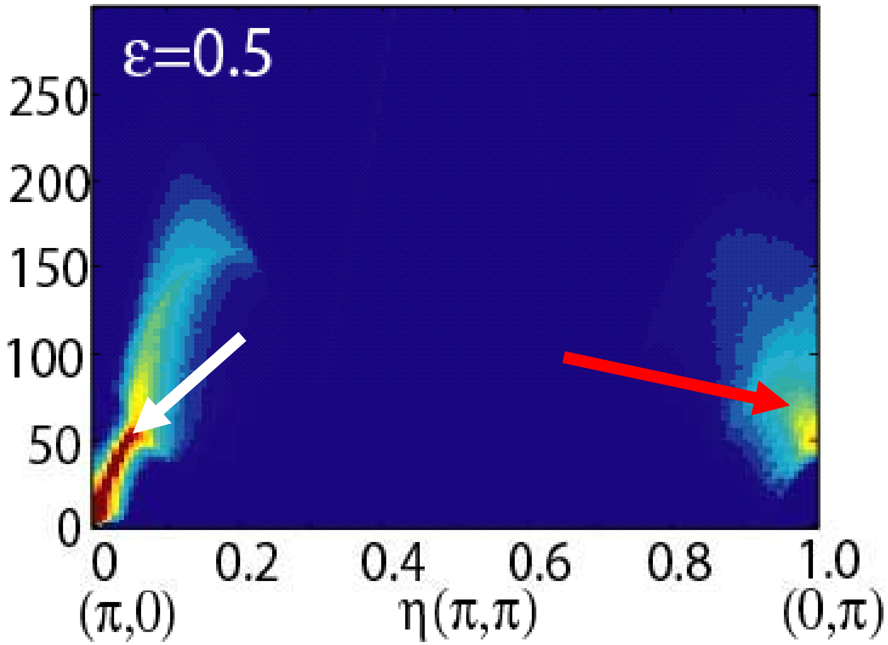
Complete nesting

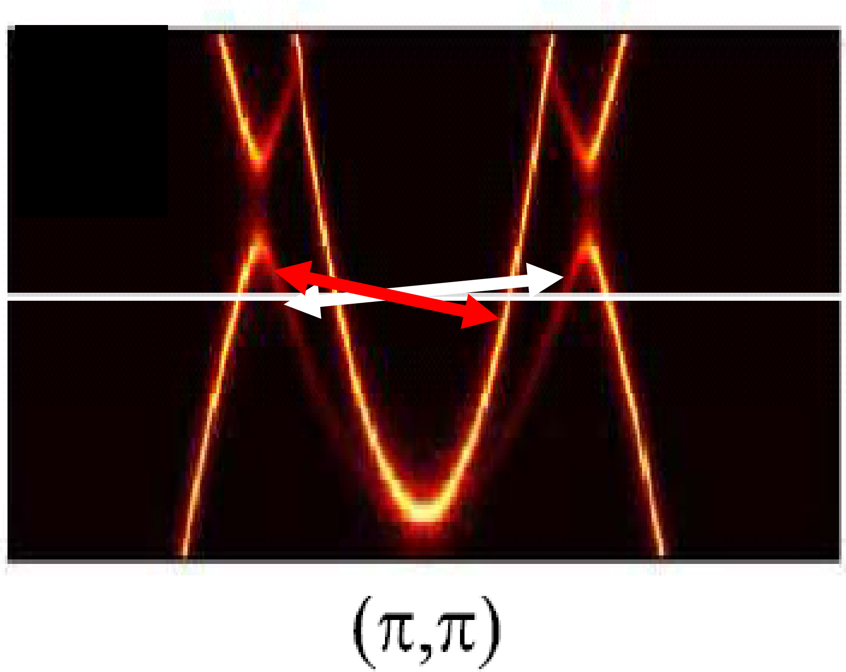




- continuum is gapped, no Landau damping
- Goldstone modes at Q_1 and Q_2

Transverse spin susceptibility ⇒ ellipticity

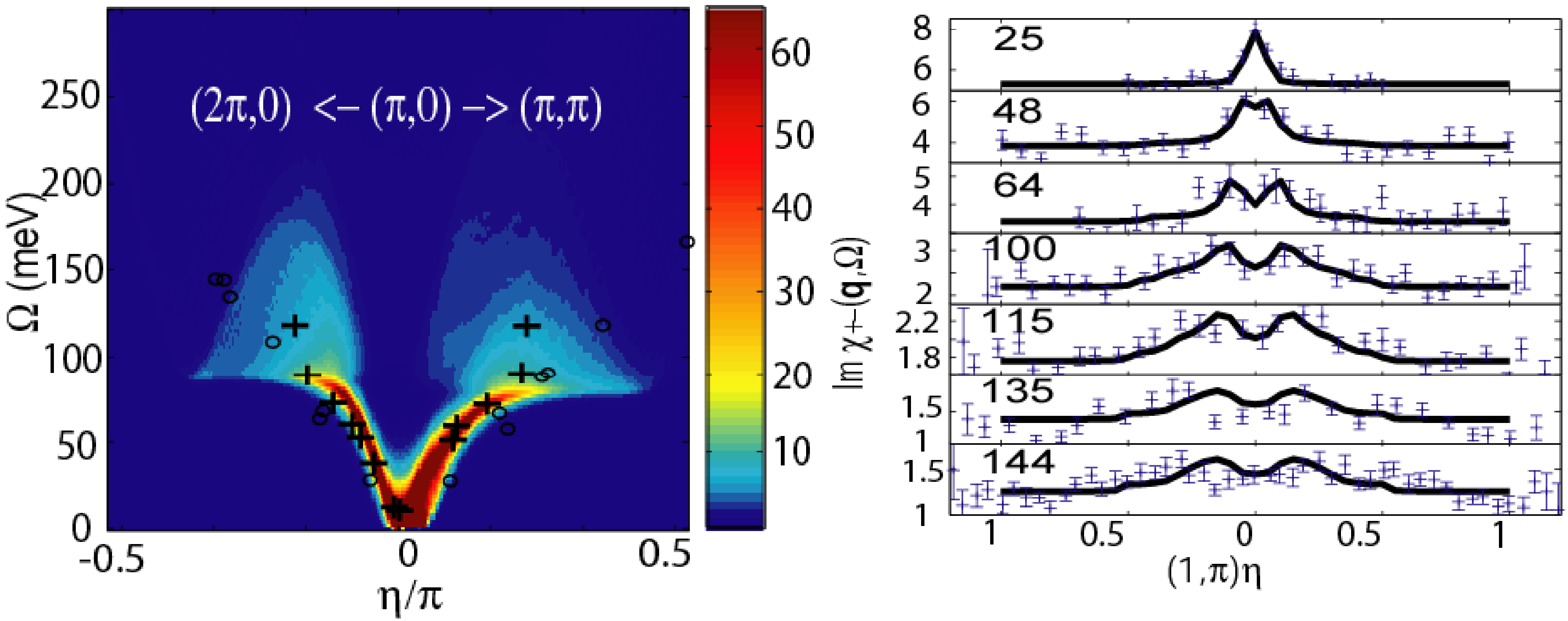




- finite continuum, Landau damping
- well-defined spin waves around Q_1
- paramagnons around Q_2

Spin waves ⇒ Comparison to experiment

Exp. J. Zhao et al., Nature Phys. 5, 555 (2009); S. O. Diallo et al., Phys. Rev. Lett. 102 187206 (2009)



- only one out of two elliptic pockets is involved in SDW
  ⇒ anisotropic spin wave velocity along x and y directions (30%)

- even above ~90meV there are well-defined peaks in the q-cuts for a given Ω

Theory: J. Knolle, I. Eremin, A.V. Chubukov, and R. Moessner, PRB 81, 140506(R) (2010)

Conclusions

Itinerant approach to ferropnictides:

Peculiarities of the AFM state in the itinerant scenario

- metallic AFM state with $(0,\pi)$ or $(\pi, 0)$ order is stabilized by the ellipticity of the electron pockets and e-e interaction at (π,π)

-well-defined spin wave excitations with anisotropic spin wave velocities; strong anisotropy along x and y direction

-AFM state is always a metal with more FS crossing than in the normal state; in the folded BZ (0,0) and (π, π) are not equivalent

- no correspondence to the J1-J2 model in strong coupling limit