Doping asymmetry of superconductivity and coexisting with antiferromagnetism: cuprates and iron-based superconductors

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Work done in collaboration with:

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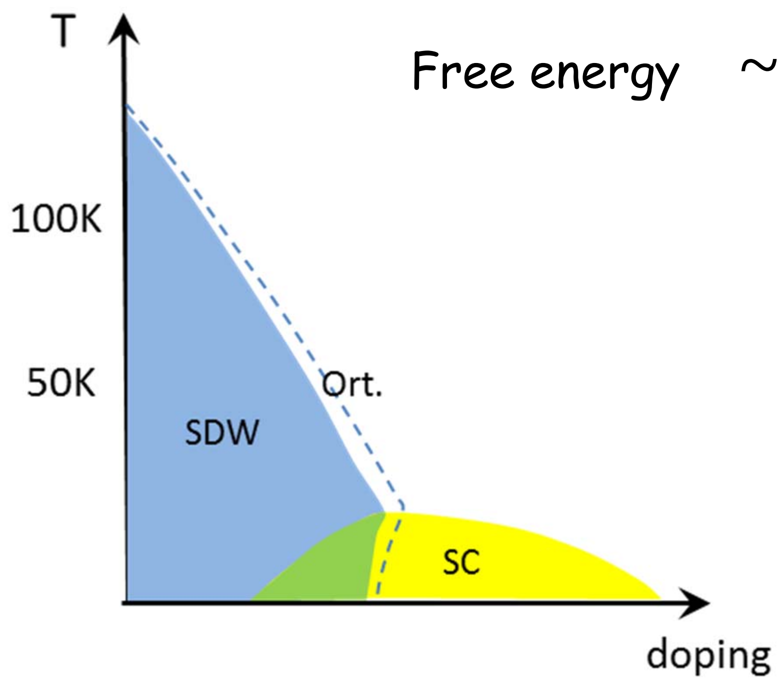
- J. Schmalian @ *KIT Karlsruhe.*

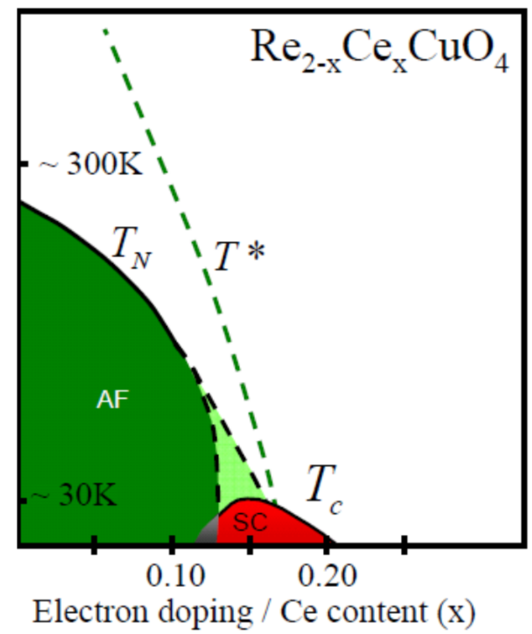
Typical phase diagram for novel superconductors

Commensurate AF order microscopically coexist with unconventional superconductivity



Free energy $\sim \beta\Delta_{SC}^{2}\Delta_{AF}^{2}$

$$\beta < 0$$



disorder, pressure

El-doped cuprates,

N.P. Armitage, P. Fournier, R. Greene, RMP 82 (2010)

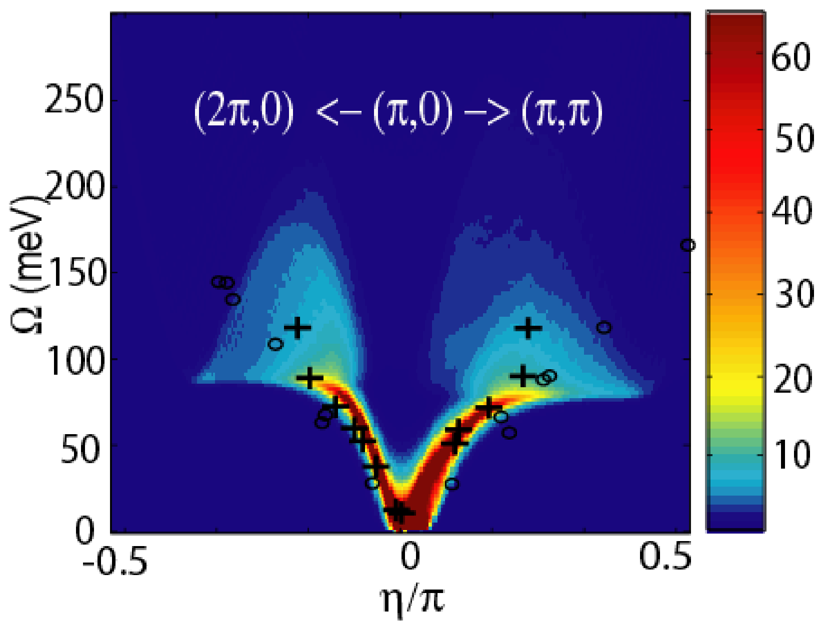
- the same electrons d-electrons participate in the Cooper-pairing and magnetism
- Spin rotational and translational symmetries are broken $\Rightarrow$ consequence for unconventional Cooper-pairing

For s-wave and partially d-wave

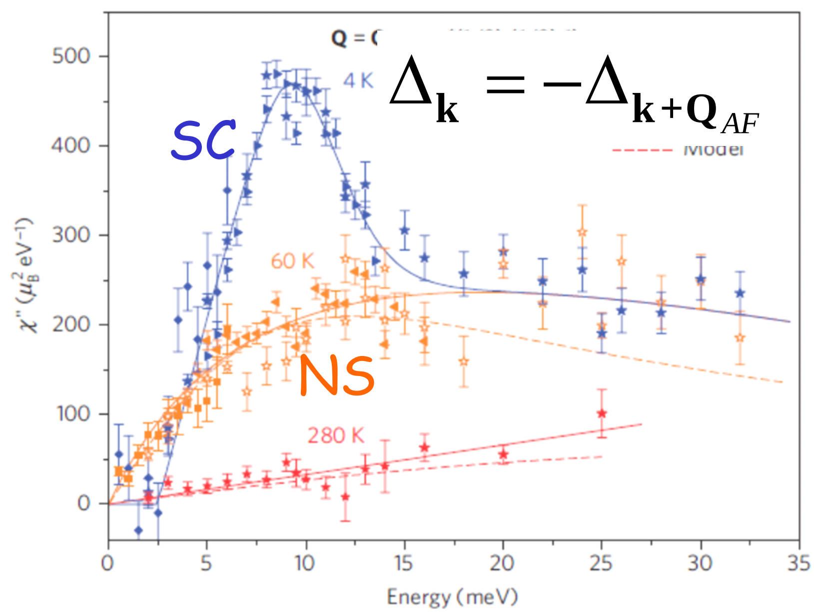
M. Machida, T. Takimoto, Bulaevskii, ...

Spin excitations: AF metal ⇒ unconventional SC

AF state:
Goldstone mode at Q_{AF} and spin waves



Unconventional SC state:
Spin resonance at Q_{AF} due phase structure of the SC order parameter



D. Inosov et al., Nature Physics 6, 178 - 181 (2010)

- do the spin resonance and the Goldstone mode coexist at Q_{AF} ?
- both excitations are results of the many-body effects
- consider an itinerant AF order coexisting with unconventional SC

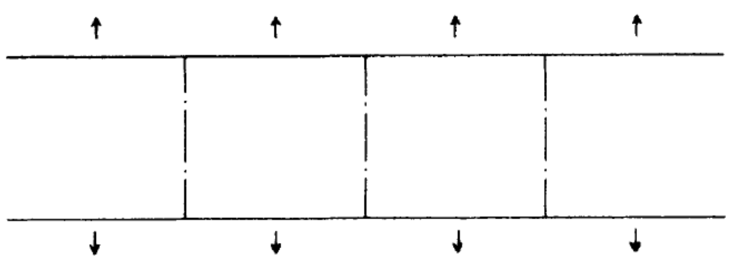
Single-band Hubbard model: a primer

$$H = -t \sum_{\substack{\langle i,j \rangle \\ \alpha}} (c_{i,\alpha}^{\dagger} c_{j,\alpha} + \mathrm{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Assume finite ground state magnetization:

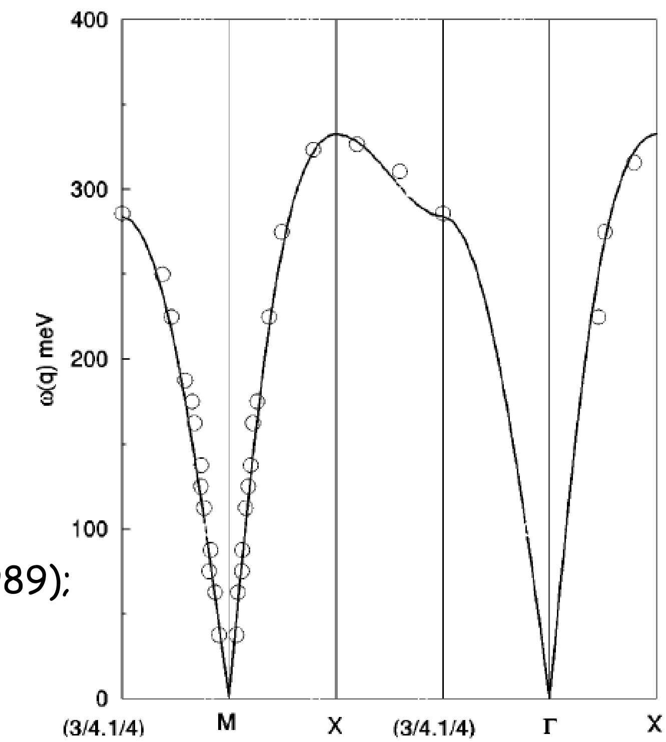
$$\langle \Omega | S_Q^Z | \Omega \rangle \equiv \sum_k \langle \Omega | c_{k+Q,\alpha}^{\dagger} \sigma_{\alpha\alpha'}^{3} c_{k\alpha'} | \Omega \rangle$$

Include transverse fluctuations:



J. R. Schrieffer, X. G. Wen, and S. C. Zhang PRB 39, 11663 (1989);
A. Chubukov and D. Frenkel, PRB 46, 11884 (1992)

Peres, Araujo, PRB 65, (2002)
R. Coldea et al., PRL 86, (2001)



Spin excitations in multiband systems

Spin operator has an additional label s: $$\mathbf{S}_s(\mathbf{q}) = \sum_{\mathbf{k},\sigma,\sigma'} \psi^\dagger_{s\sigma}(\mathbf{k}+\mathbf{q})\frac{\sigma_{\sigma\sigma'}}{2}\psi_{s\sigma'}(\mathbf{k})$$

SDW order Parameters: $$\sigma\Delta_{\nu\nu'} = \sum_{\mathbf{k}} \langle \psi^\dagger_{\nu\sigma}(\mathbf{k})\psi_{\nu'\sigma}(\mathbf{k}+\mathbf{Q})\rangle$$

translational symmetry breaking in the AFM phase:

$$H_{SDW} = \sum_{\mathbf{k}}{}' \hat{\psi}^\dagger_\sigma(\mathbf{k}) \begin{pmatrix} H_0(\mathbf{k}) & \sigma M \\ \sigma M & H_0(\mathbf{k}+\mathbf{Q}) \end{pmatrix} \hat{\psi}_\sigma(\mathbf{k})$$

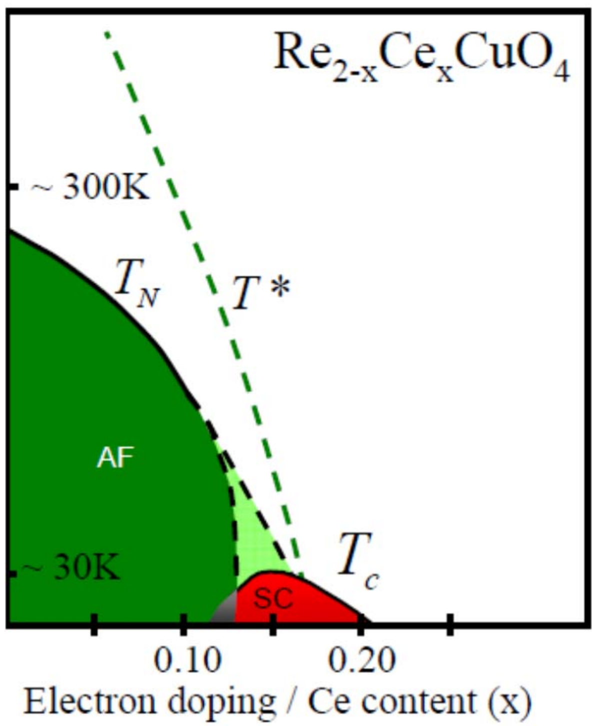
off-diagonal Umklapp components in the AFM state:

$$\hat{\chi}^{\pm}_{spqt} = \begin{pmatrix} \chi^{\pm}_{spqt}(\mathbf{q},\mathbf{q}) & \chi^{\pm}_{spqt}(\mathbf{q},\mathbf{q}+\mathbf{Q}) \\ \chi^{\pm}_{spqt}(\mathbf{q}+\mathbf{Q},\mathbf{q}) & \chi^{\pm}_{spqt}(\mathbf{q}+\mathbf{Q},\mathbf{q}+\mathbf{Q}) \end{pmatrix}$$

$$\chi^{RPA}_{bsta} = \chi^{0}_{bsta} + \chi^{RPA}_{b'sta'} U_{c'b'a'd'} \chi^{0}_{bc'd'a}$$

Mean-field equation coincides with pole condition in $\chi^{+-}(q=Q_{AF},\Omega=0)$

Microscopic coexistence of AF order with $Q_{AF}=(\pi,\pi)$ and d-wave superconductivity: electron-doped cuprates

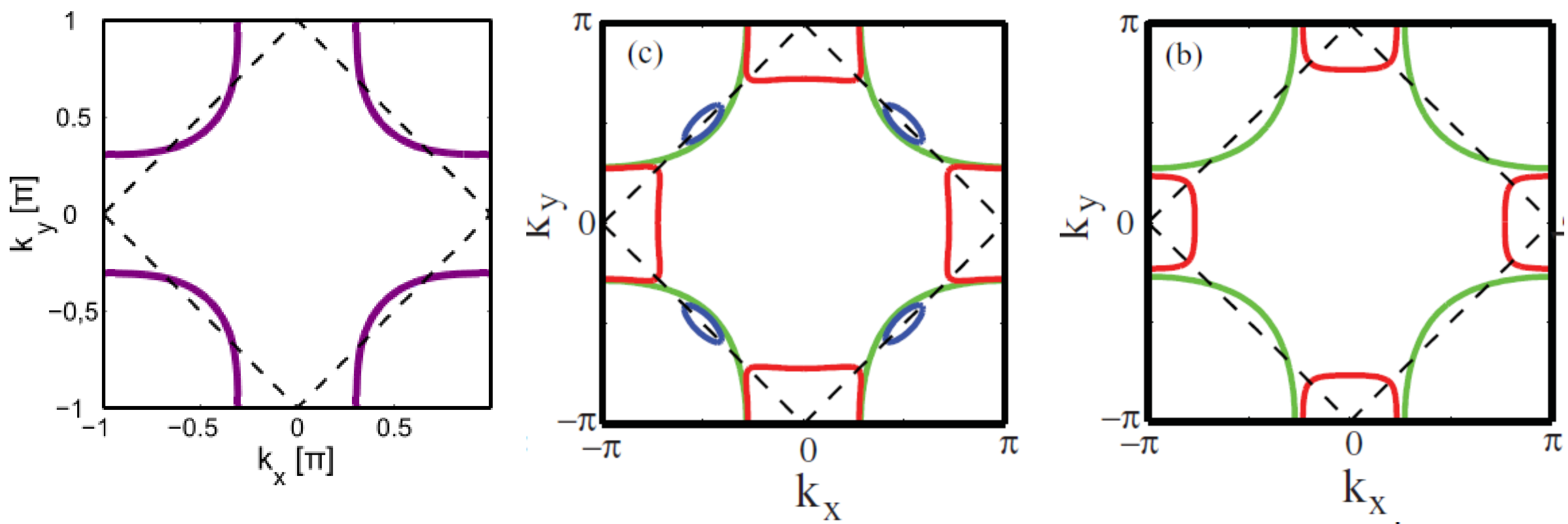


Commensurate SDW state – electronic structure

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \sum_{\mathbf{k},\mathbf{k}',\sigma} U c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}+\mathbf{Q}\sigma} c^{\dagger}_{\mathbf{k}'+\mathbf{Q}\bar{\sigma}} c_{\mathbf{k}'\bar{\sigma}}$$

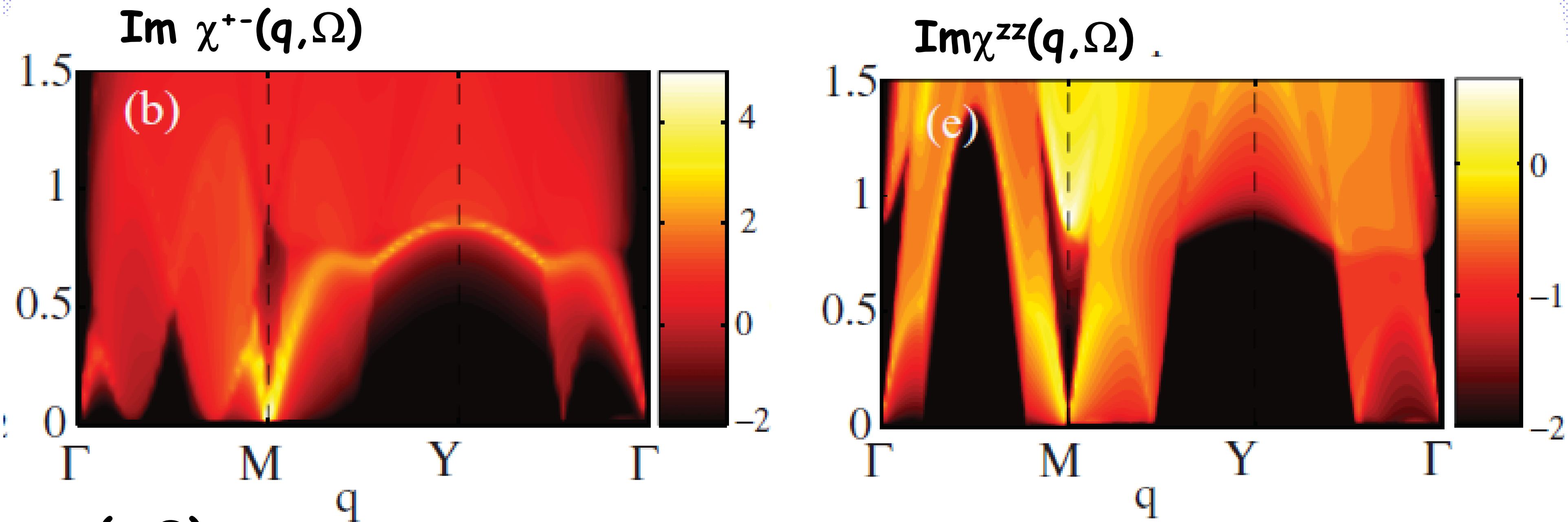
$$W_0 = U/2 \sum_{\mathbf{k},\sigma} \langle c^{\dagger}_{\mathbf{k}+\mathbf{Q},\sigma} c_{\mathbf{k},\sigma} \rangle \mathrm{sgn}\sigma$$

increasing SDW order



$$E^{\alpha,\beta}_{\mathbf{k}} = \varepsilon^{+}_{\mathbf{k}} \pm \sqrt{\left(\varepsilon^{-}_{\mathbf{k}}\right)^2 + W_0^2} \qquad u^2_{\mathbf{k}}, v^2_{\mathbf{k}} = \frac{1}{2}\left[1 \pm \frac{\varepsilon^{-}_{\mathbf{k}}}{\sqrt{\left(\varepsilon^{-}_{\mathbf{k}}\right)^2 + W_0^2}}\right]$$

Spin excitations in AF state: transverse χ^{+-} and longitudinal χ^{zz} channels, n=1.11



$\chi^{+-}(q,\Omega)$ W. Rowe, J. Knolle, I. Eremin, and P. J. Hirschfeld, PRB 86, 134513 (2012)

- the excitations are **the spin waves with damping**
- the damping away from Q_{AF} is due electron and hole pockets
- **the Goldstone mode is preserved** (the coupling between conduction electrons and spin excitations vanishes for Q_{AF})

$\chi^{zz}(q,\Omega)$

- the excitations **are gapped up to twice SDW gap** at Q_{AF}
- away from Q_{AF} the excitations are the **Stoner continuum due to electron and hole pockets**

SDW state – Cooper-pairing instability, $T_{SDW} > T_c$

$$\sum_{\mathbf{k},\mathbf{p},\mathbf{q},\sigma} V_{\mathbf{q}}\, c^{\dagger}_{\mathbf{k}+\mathbf{q}\sigma} c^{\dagger}_{\mathbf{p}-\mathbf{q}\bar{\sigma}} c_{\mathbf{p}\sigma} c_{\mathbf{k}\bar{\sigma}}$$

– effectively two-band superconductor, umklapp processes have to be treated with care $\left\langle c^{\dagger}_{k\uparrow} c^{\dagger}_{-k-Q\downarrow} \right\rangle$

$$\langle \alpha^{\dagger}_{\mathbf{k},\uparrow} \alpha^{\dagger}_{-\mathbf{k},\downarrow} \rangle \qquad \langle \beta^{\dagger}_{\mathbf{k},\uparrow} \beta^{\dagger}_{-\mathbf{k},\downarrow} \rangle$$

$$\boxed{\begin{aligned} \Delta^{\alpha}_{\mathbf{k}} &= -\sum_{\mathbf{p}\in RBZ} \left[L^{\alpha\alpha}_{\mathbf{k},\mathbf{p}} \frac{\Delta^{\alpha}_{\mathbf{p}}}{2\Omega^{\alpha}_{\mathbf{p}}} + L^{\alpha\beta}_{\mathbf{k},\mathbf{p}} \frac{\Delta^{\beta}_{\mathbf{p}}}{2\Omega^{\beta}_{\mathbf{p}}} \right] \\ \Delta^{\beta}_{\mathbf{k}} &= -\sum_{\mathbf{p}\in RBZ} \left[L^{\beta\alpha}_{\mathbf{k},\mathbf{p}} \frac{\Delta^{\alpha}_{\mathbf{p}}}{2\Omega^{\alpha}_{\mathbf{p}}} + L^{\beta\beta}_{\mathbf{k},\mathbf{p}} \frac{\Delta^{\beta}_{\mathbf{p}}}{2\Omega^{\beta}_{\mathbf{p}}} \right] \end{aligned}}$$

-$L_{k,p}$ coefficients depend on the SDW matrix elements

-The stable coexistence is only for SC with d-wave symmetry

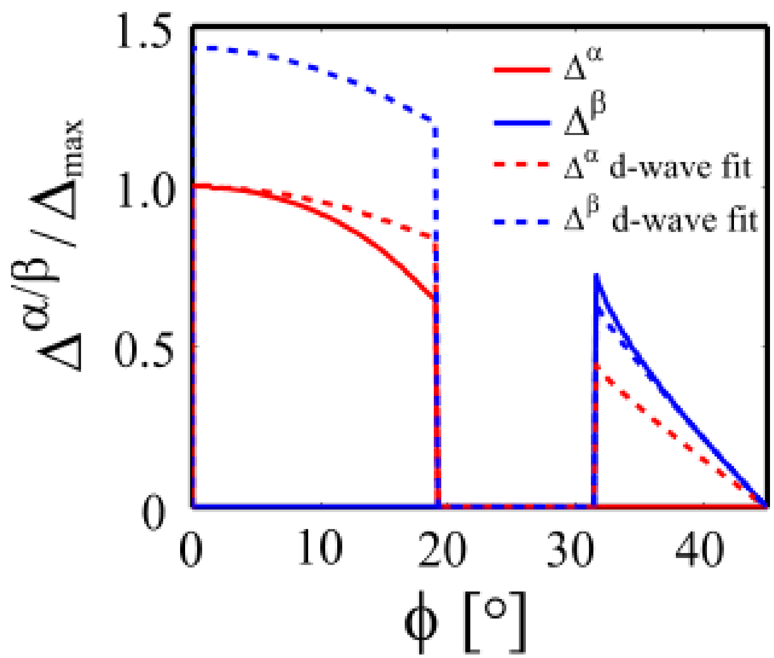
AF background: angular dependence of the sc gap [d-wave]

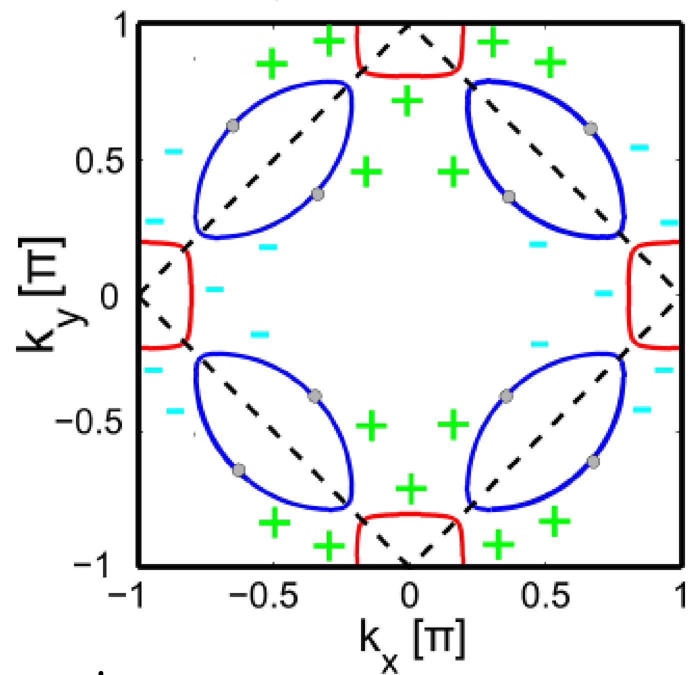
the solution of the gap equation is factorizable

J.-P. Ismer, I. Eremin, E. Rossi, D.K. Morr, and G. Blumberg, PRL 105, 037003 (2010)

$$\Delta_{\mathbf{k}}^{\gamma} = \varphi_{\mathbf{k}}(\Delta_0^{\gamma} + u_{\mathbf{k}} v_{\mathbf{k}} \Delta_1^{\gamma})$$

$$\varphi_{\mathbf{k}} = \cos k_x - \cos k_y \qquad u_{\mathbf{k}} v_{\mathbf{k}} = \frac{W_0}{2\sqrt{(\varepsilon_{\mathbf{k}}^-)^2 + W_0^2}}$$

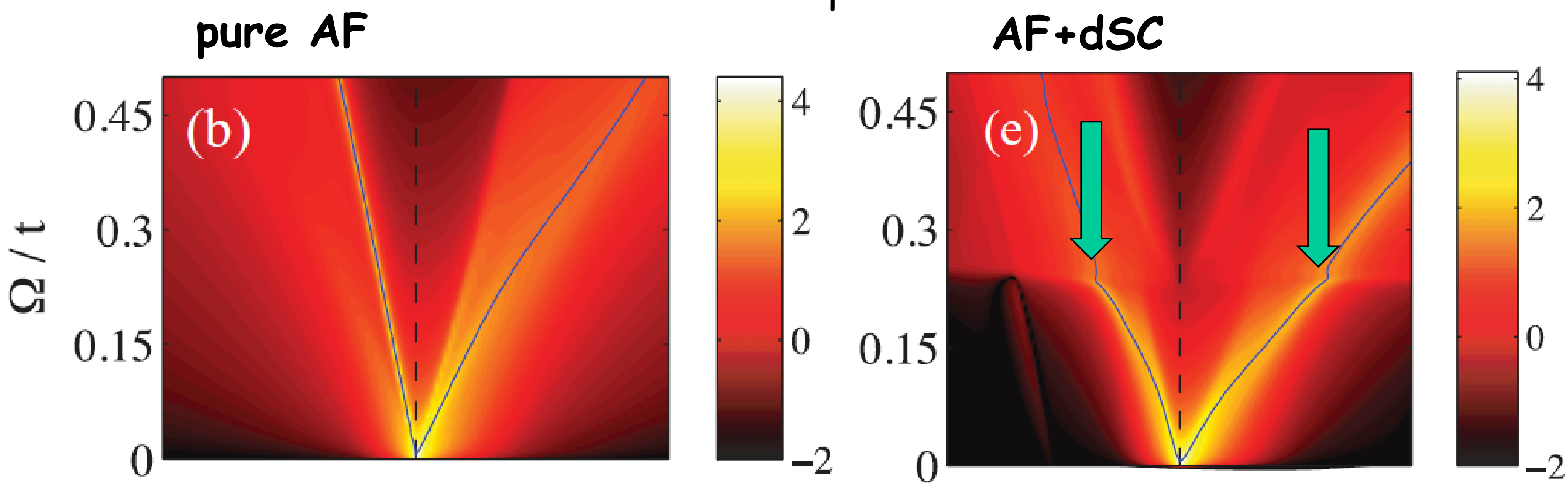




- overall the d-wave symmetry is preserved
- the effect of SDW is an inclusion of higher harmonics **(umklapp terms)**

Spin excitations in the coexistence AF+dSC state
transverse channel

Goldstone mode is preserved $\Rightarrow$ no gauge fluctuations, no coupling to the vector potential



W. Rowe, J. Knolle, I. Eremin, and P. J. Hirschfeld, PRB 86, 134513 (2012)

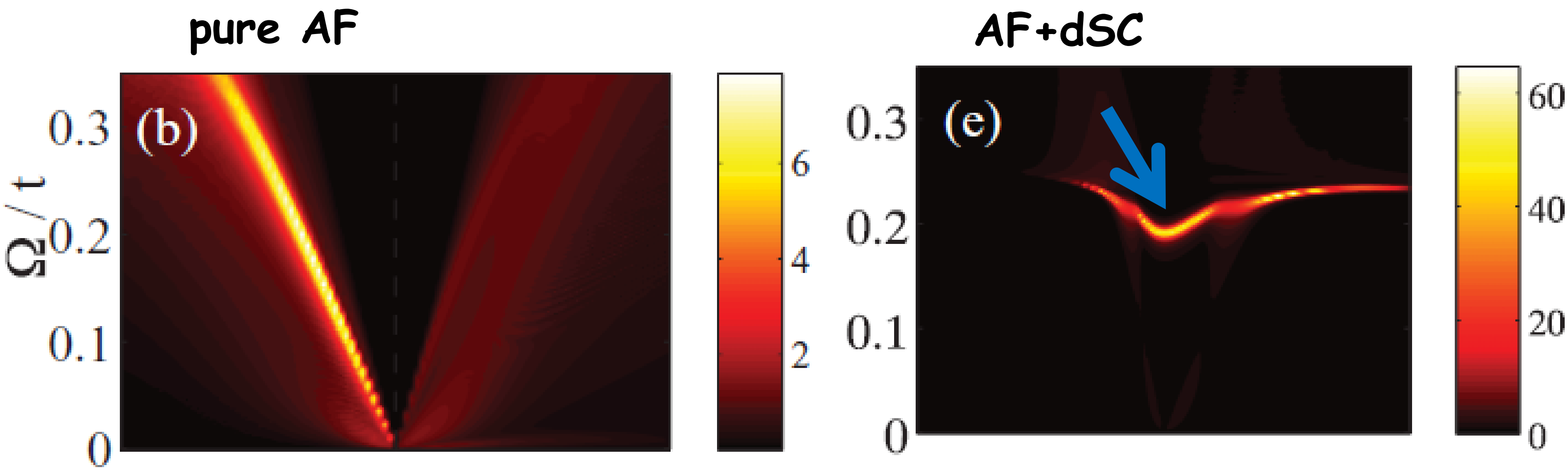
- correction to the spin wave velocity $\Omega \sim c(q-Q_{AF})$, $c \sim O(\Delta_0^2)$

- additional interaction with Stoner continuum around $2\Delta_0$

The transverse excitations are still mainly determined by AF prder

Spin excitations in the coexistence AF+dSC state
longitudinal channel

Spin resonance due to d-wave symmetry of the superconducting gap

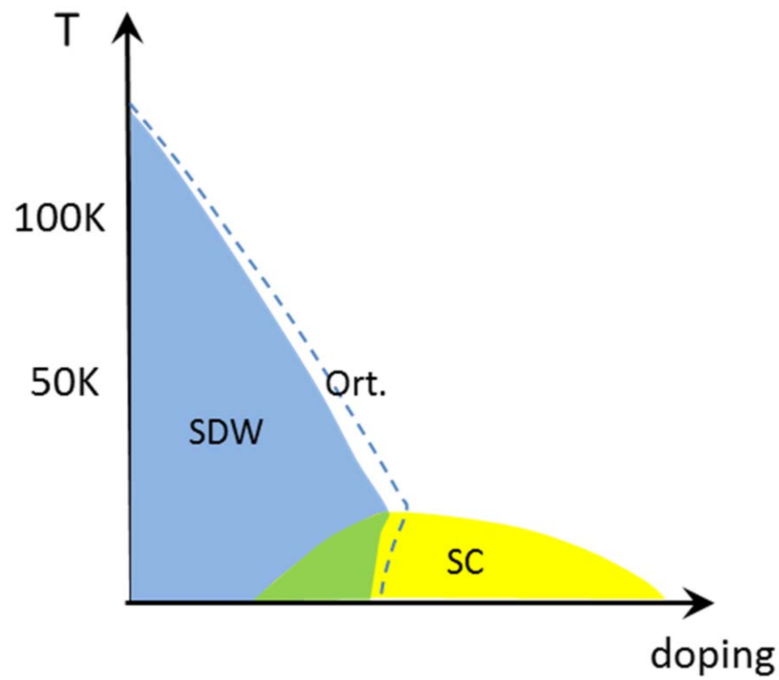


W. Rowe, J. Knolle, I. Eremin, and P. J. Hirschfeld, PRB 86, 134513 (2012)

- true spin resonance forms below $2\Delta_0$ $\quad \Delta_{\mathbf{k}} = -\Delta_{\mathbf{k}+\mathbf{Q}_{AF}}$

- the longitudinal excitations in the AF+dSC state are determined by d-wave superconductivity

Microscopic coexistence of stripe AF order, $Q_{AF}=(\pi,0)$ and s^{+-}-wave SC: iron-based superconductors



Selection of the $(\pi,0)$ order: two scenarios

1) **orbital ordering** induces the structural transition, T_s

renormalization of the magnetic exchange constants

AFM transition at a lower temperature, T_N

F. Krüger et al., PRB 79 (2009);
W. G. Yin, C. C. Lee, and W. Ku, PRL 105 (2010)

2) Magnetic **order parameter manifold** $O(3) \times \mathrm{Z}_2$

Ising Z_2 variable orders prior to rotational O(3) or together due to ellipticity of the electron pocketes

$$\sigma = \left\langle \vec{M}_1 \cdot \vec{M}_2 \right\rangle = \left\langle \vec{\Delta}_1^2 - \vec{\Delta}_2^2 \right\rangle$$

P. Chandra, P. Coleman, and A.I. Larkin, PRL 64 (1990).
C. Xu, M. Müller, and S. Sachdev, PRB 78 (2008).
R. M. Fernandes et al., PRL 105 (2010).
I.Eremin and A.V. Chubukov, PRB 81 (2010)
A. Yaresko et al., PRB 79, (2009)

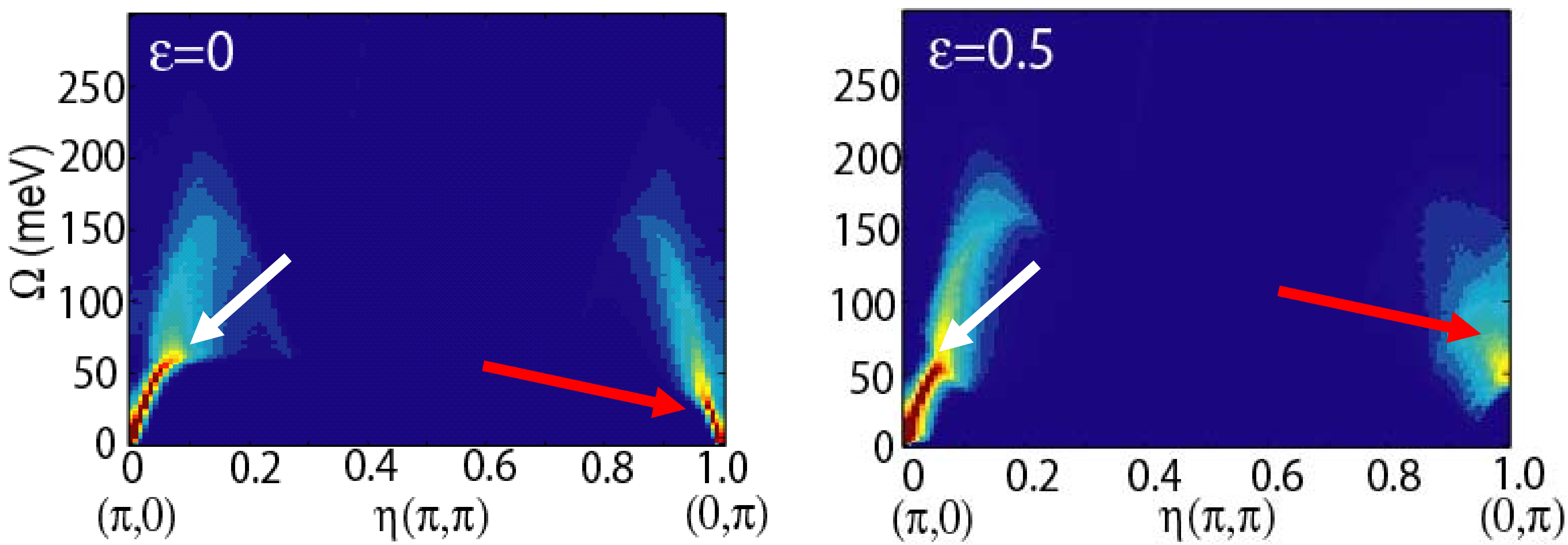
Transverse spin excitations in the AF phase

off-diagonal Umklapp components in the AFM state:

$$\hat{\chi}^{\pm}_{spqt} = \begin{pmatrix} \chi^{\pm}_{spqt}(\mathbf{q},\mathbf{q}) & \chi^{\pm}_{spqt}(\mathbf{q},\mathbf{q}+\mathbf{Q}) \\ \chi^{\pm}_{spqt}(\mathbf{q}+\mathbf{Q},\mathbf{q}) & \chi^{\pm}_{spqt}(\mathbf{q}+\mathbf{Q},\mathbf{q}+\mathbf{Q}) \end{pmatrix}$$

$$\chi^{RPA}_{bsta} = \chi^{0}_{bsta} + \chi^{RPA}_{b'sta'} U_{c'b'a'd'} \chi^{0}_{bc'd'a}$$

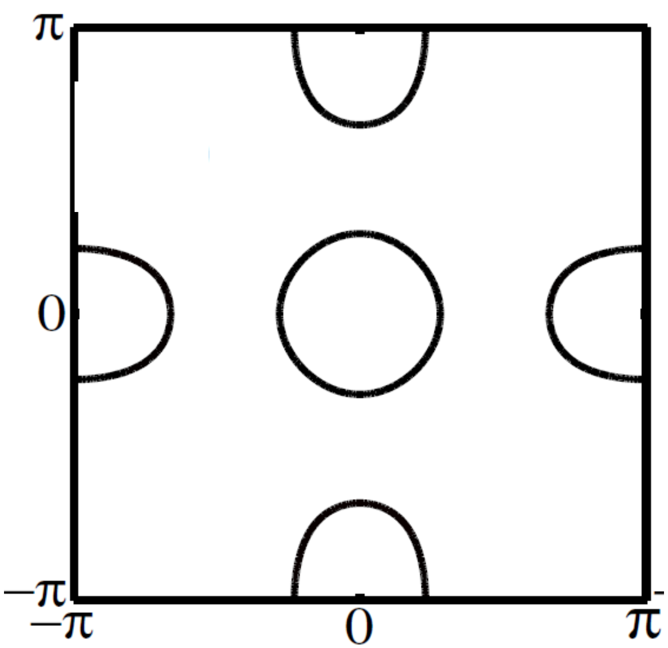
J. R. Schrieffer, X. G. Wen, and S. C. Zhang PRB 39 (1989)
P. Brydon and C. Timm, PRB 80 (2009)
J. Knolle, I. Eremin, A. Chubukov, and R. Moessner PRB 81 (2010)



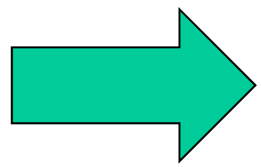
- well-defined spin waves around Q_1
- finite ellipticity ⇒ Q_2 -mode is gapped

S^{+-} Superconductivity on the background of AF (stripe) phase

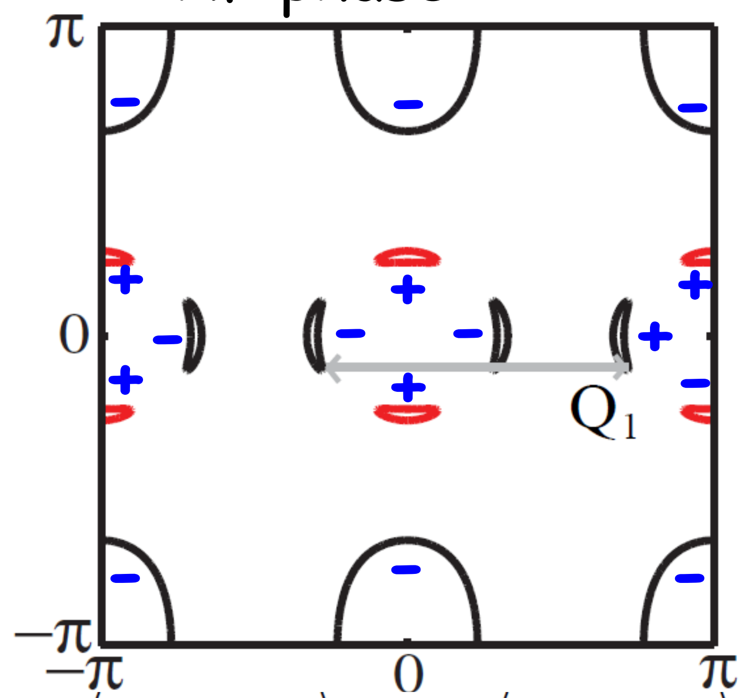
Paramagnetic phase



- Folding along Q_1 momentum



AF phase



$$\Delta_{\mathbf{k}}^{\alpha} = -u_{\mathbf{k}}^2\Delta_1 - v_{\mathbf{k}}^2\Delta_2$$

$$\Delta_{\mathbf{k}}^{\beta} = v_{\mathbf{k}}^2\Delta_1 + u_{\mathbf{k}}^2\Delta_2$$

$$\Delta_2 = +\frac{u_{sc}}{2}\sum_{\mathbf{p}}\left\{u_{\mathbf{p}}^2\left\langle \alpha_{\mathbf{p}\uparrow}^{\dagger}\alpha_{-\mathbf{p}\downarrow}^{\dagger}\right\rangle + v_{\mathbf{p}}^2\left\langle \beta_{\mathbf{p}\uparrow}^{\dagger}\beta_{-\mathbf{p}\downarrow}^{\dagger}\right\rangle\right\}$$

$$\Delta_1 = -\frac{u_{sc}}{2}\sum_{\mathbf{p}}\left\{v_{\mathbf{p}}^2\left\langle \alpha_{\mathbf{p}\uparrow}^{\dagger}\alpha_{-\mathbf{p}\downarrow}^{\dagger}\right\rangle + u_{\mathbf{p}}^2\left\langle \beta_{\mathbf{p}\uparrow}^{\dagger}\beta_{-\mathbf{p}\downarrow}^{\dagger}\right\rangle\right\}$$

- no additional nodal structure of the sc gap

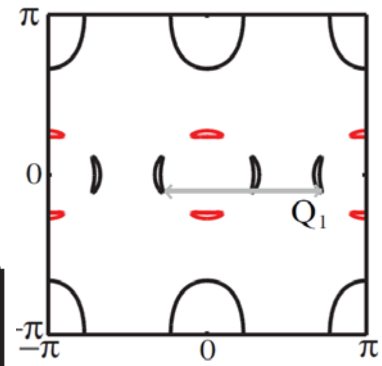
D. Parker, et al. PRB80 (2009); A.B.Vorontsov et al, PRB81 (2010); R. M. Fernandes et al., PRB82 (2010).

- sequential unitary transformations allowed only for coexistent s^{+-} and AF phase

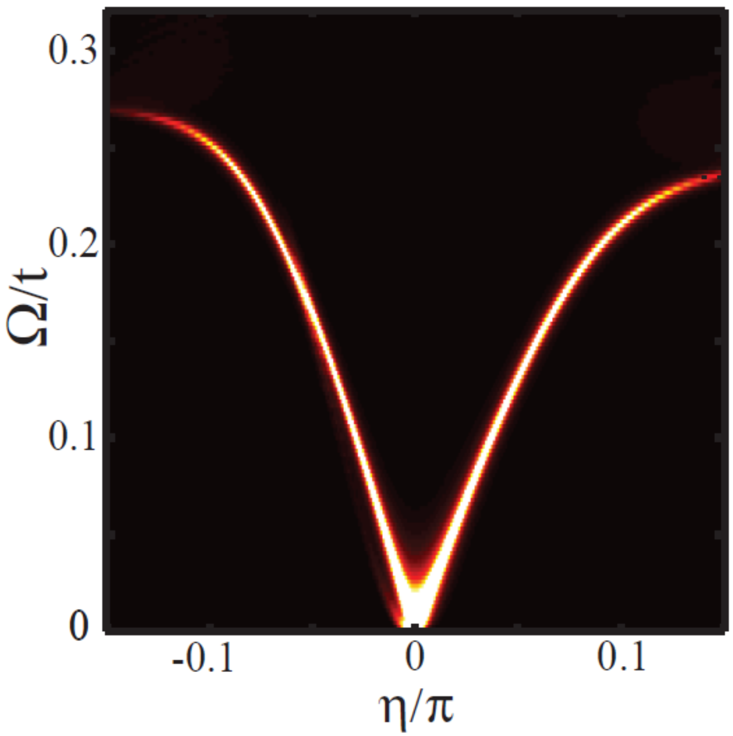
J. Knolle, I. Eremin, J. Schmalian, and R. Moessner, PRB84 (2011)

Transverese spin excitations in the coexistence phase: Q_1

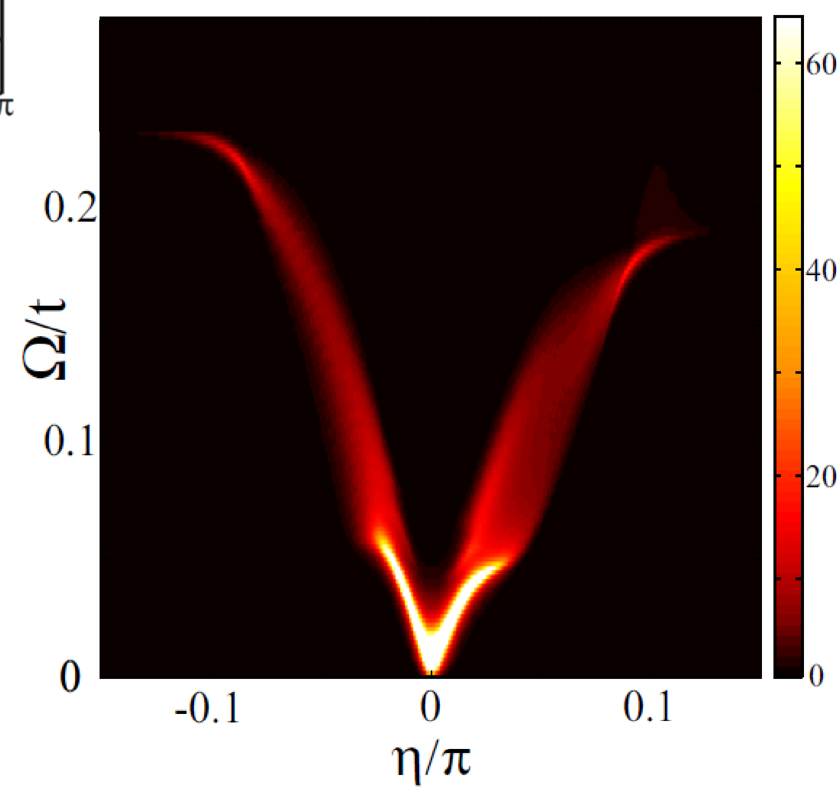
Condition for Goldstone mode at Q_1 coincides with MF equation for AF order



AF phase



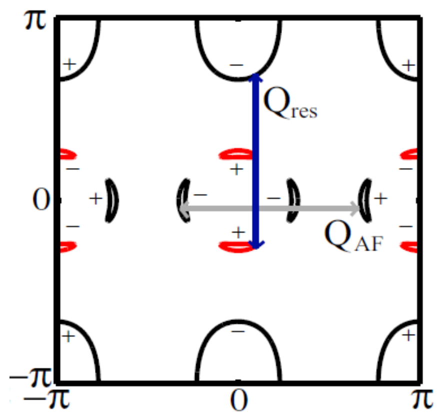
AF+SC phase



-The excitations at Q_1 are still determined by the AF order

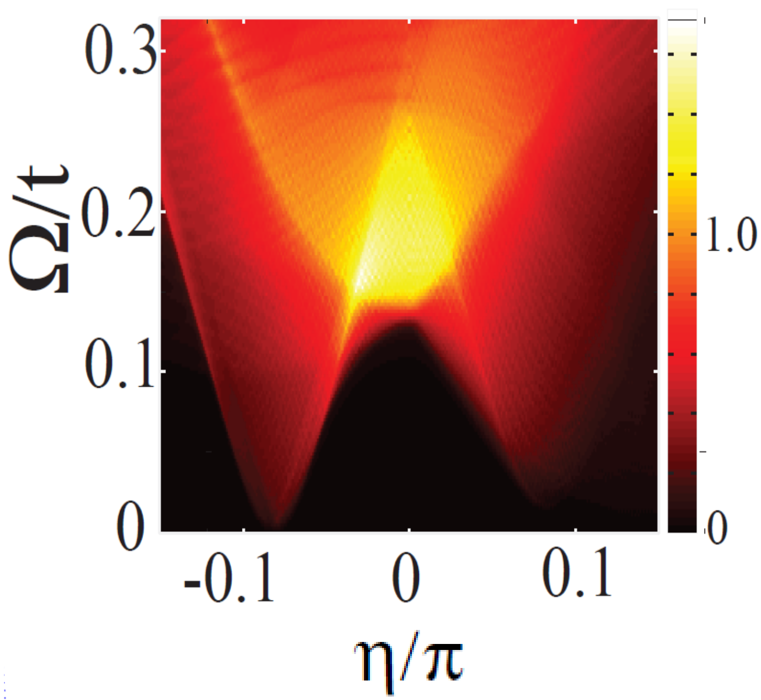
- effectively 'larger' damping, additional log singularity at 2Δ

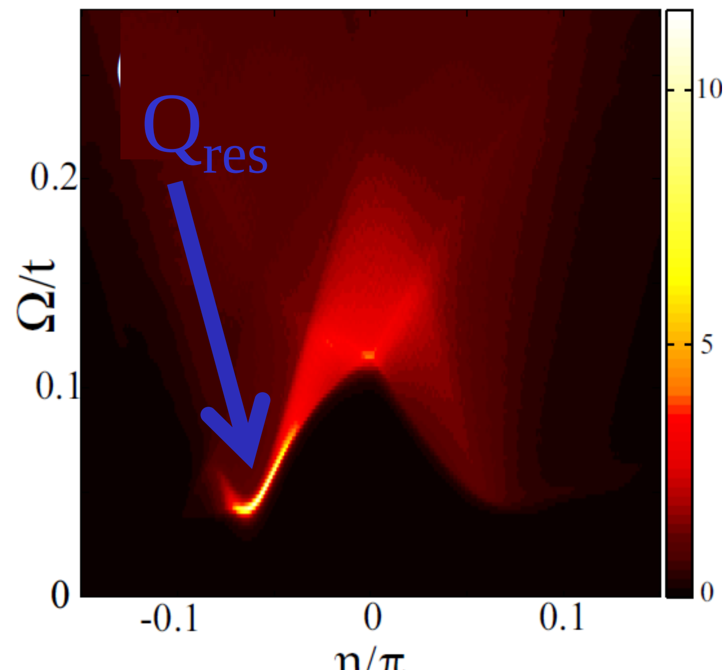
Transverese spin excitations in the coexistence phase: Q_2



AF phase

AF+SC phase





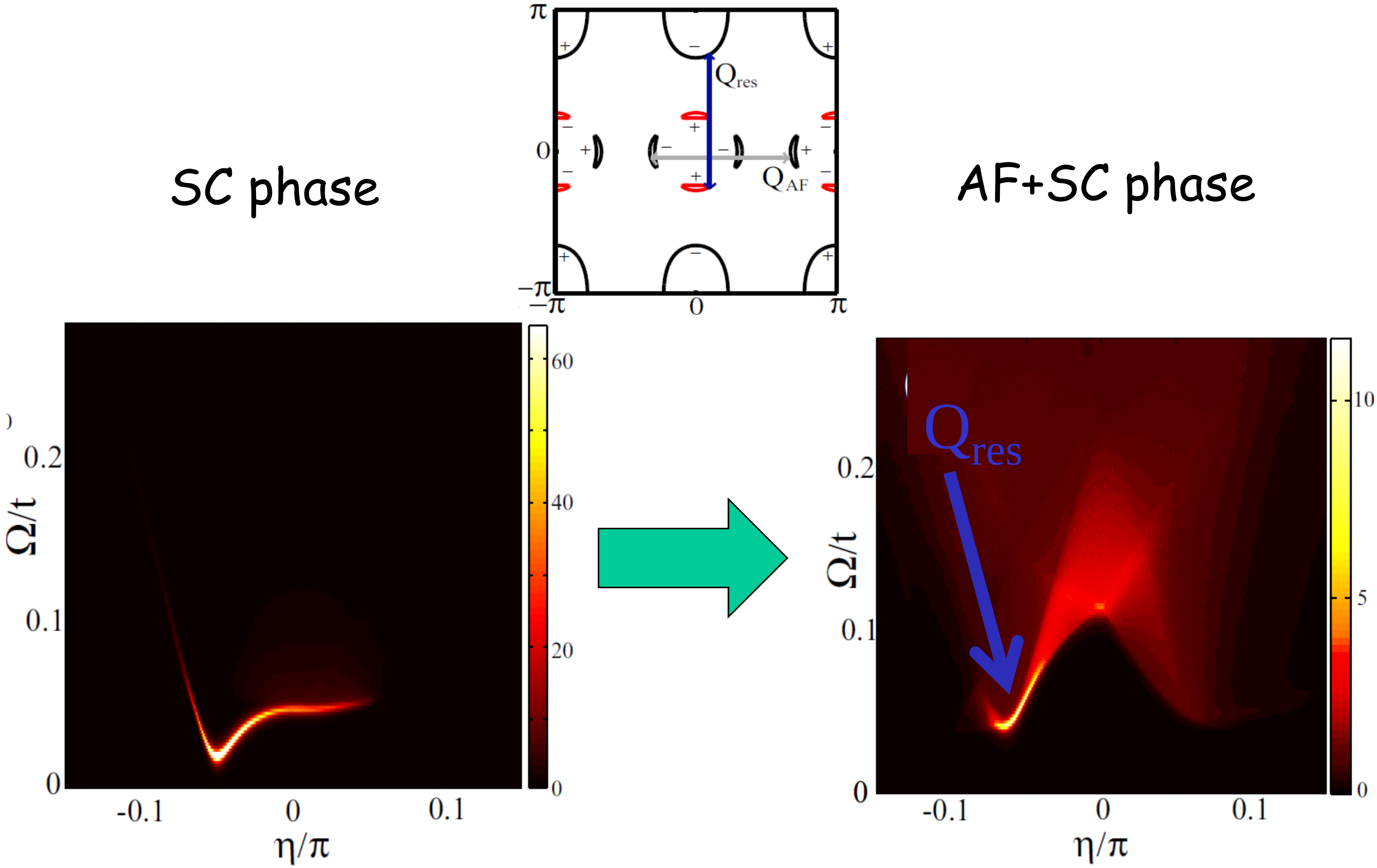
J. Knolle, I. Eremin, J. Schmalian, and R. Moessner,
PRB 84, 180510(R) (2011)

-The excitations at Q_2 acquire smaller gap
- there is a resonant excitation at incommensurate Q_{res}

Transverese spin excitations in the coexistence phase: Q_2

SC phase

AF+SC phase



SC tends to restore the high-symmetry point of the magnetic Hamiltonian

Conclusions

Coexistence of AF and unconventional superconductivity

(π,π) AF order and d-wave SC

-transverse excitations are excitations of the AF state (Goldstone mode and spin waves) **but** modified due to SC

-Longitudinal excitations originate from the SC state: **true dispersive spin resonance** at Q_{AF}

$(\pi,0)$ AF order and unconventional s^{+-}-wave SC

-**The transverse excitations are separated in the Q-space**

- the excitations around the "failed" ordering wave vector Q_2 become resonant at energies $\Omega_{res} < 2\Delta$ (mostly determined by SC order).

- the excitations around the AF ordering wave vector Q_1 are dominated by the AF order and are weakly affected by SC

J.-P. Ismer, I. Eremin, E. Rossi, D.K. Morr, and G. Blumberg, Phys. Rev. Lett. 105, 037003 (2010)
J. Knolle, I. Eremin, J. Schmalian, and R. Moessner, PRB 84, 180510(R) (2011)
W. Rowe, J. Knolle, I. Eremin, and P. J. Hirschfeld, Phys. Rev. B 86, 134513 (2012)