2357-5

Innovations in Strongly Correlated Electronic Systems: School and Workshop

6 - 17 August 2012

Interplay between superconductivity, magnetism and nematic order in the iron pnictides - Part I

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Columbia University &

Los Alamos National Laboratory

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US-DOE

NSF (PIRE)

ICAM

ICTP Workshop

Aug 10th, 2012

postdoc positions available!!!

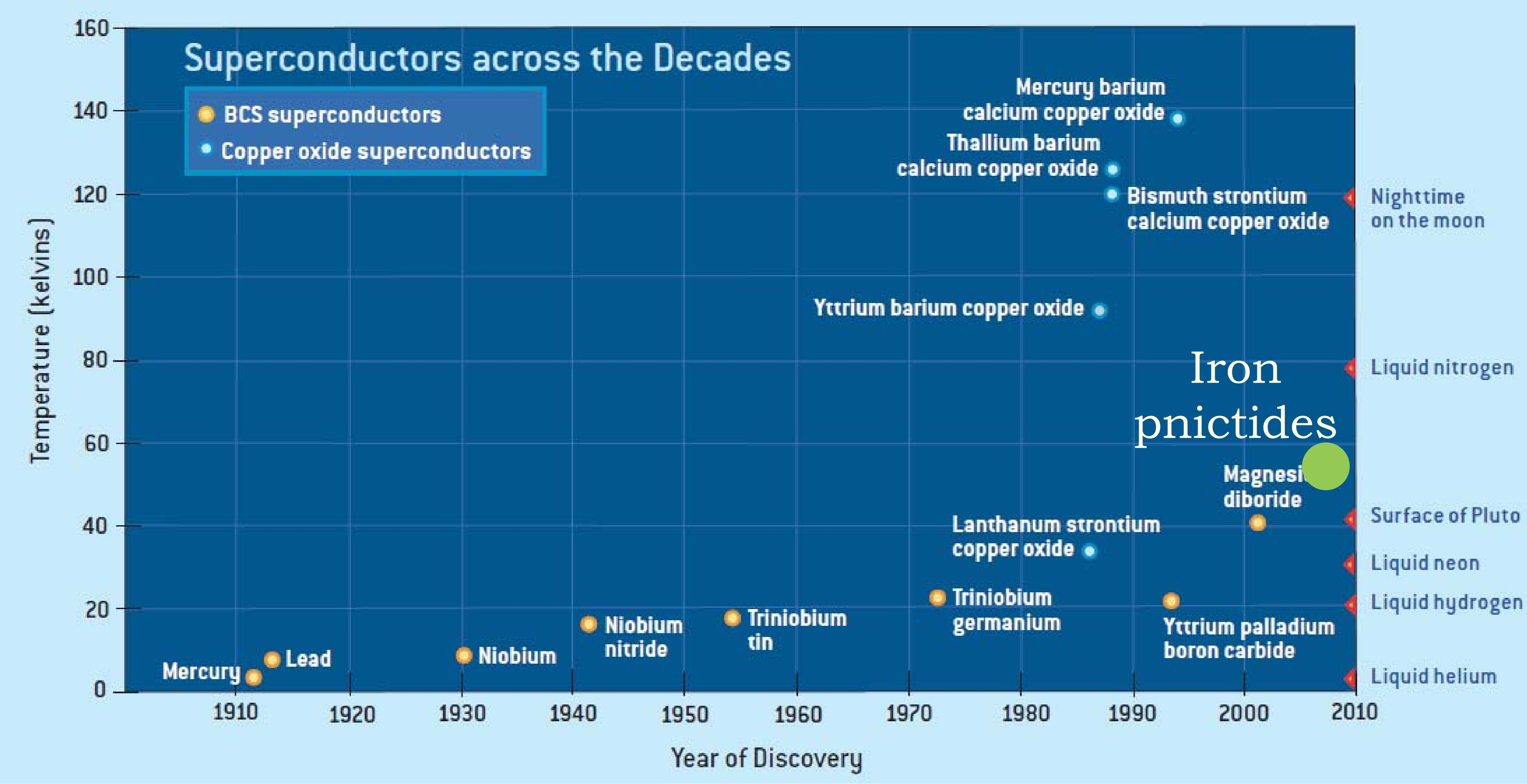
Rafael M. Fernandes

University of Minnesota

Outline

1. **The superconducting state (Lecture I)**
   - *unconventional superconductivity*
2. **The magnetic state (Lectures I & II)**
   - *itinerant or localized?*
3. **The nematic state (Lecture II)**
   - *a new electronic phase that emerges from magnetism and triggers structural and orbital order*
4. **Competing orders (Lecture II)**
   - *competition between SC, magnetism, and nematics*

Superconductivity reaches the iron age!

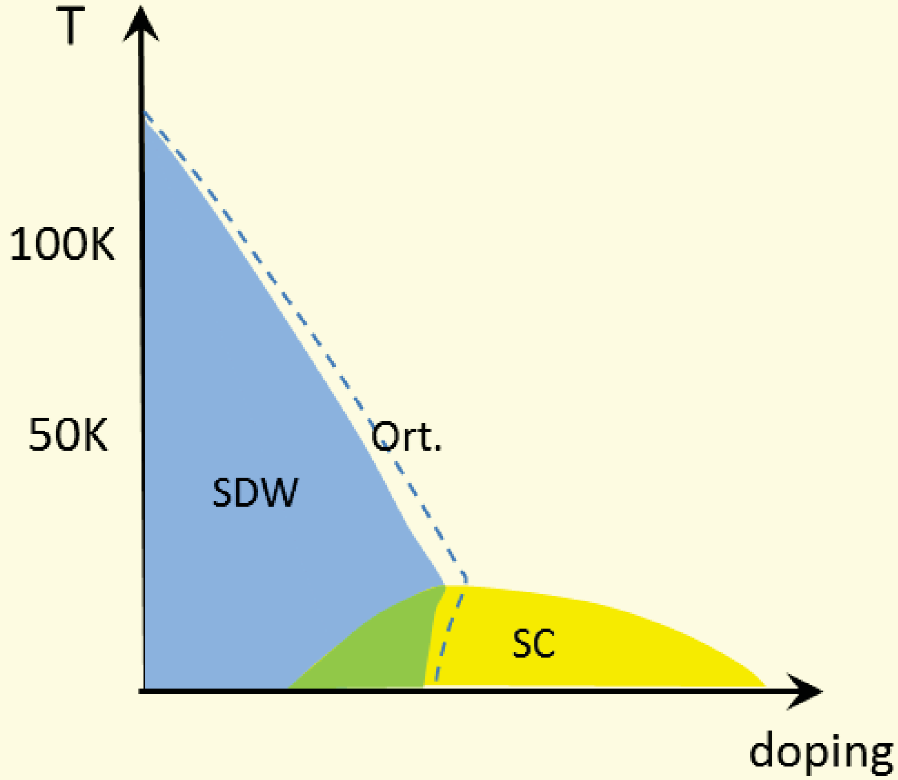


stone age → **copper age** → **iron age**

first high-temperature superconductors since the cuprates!

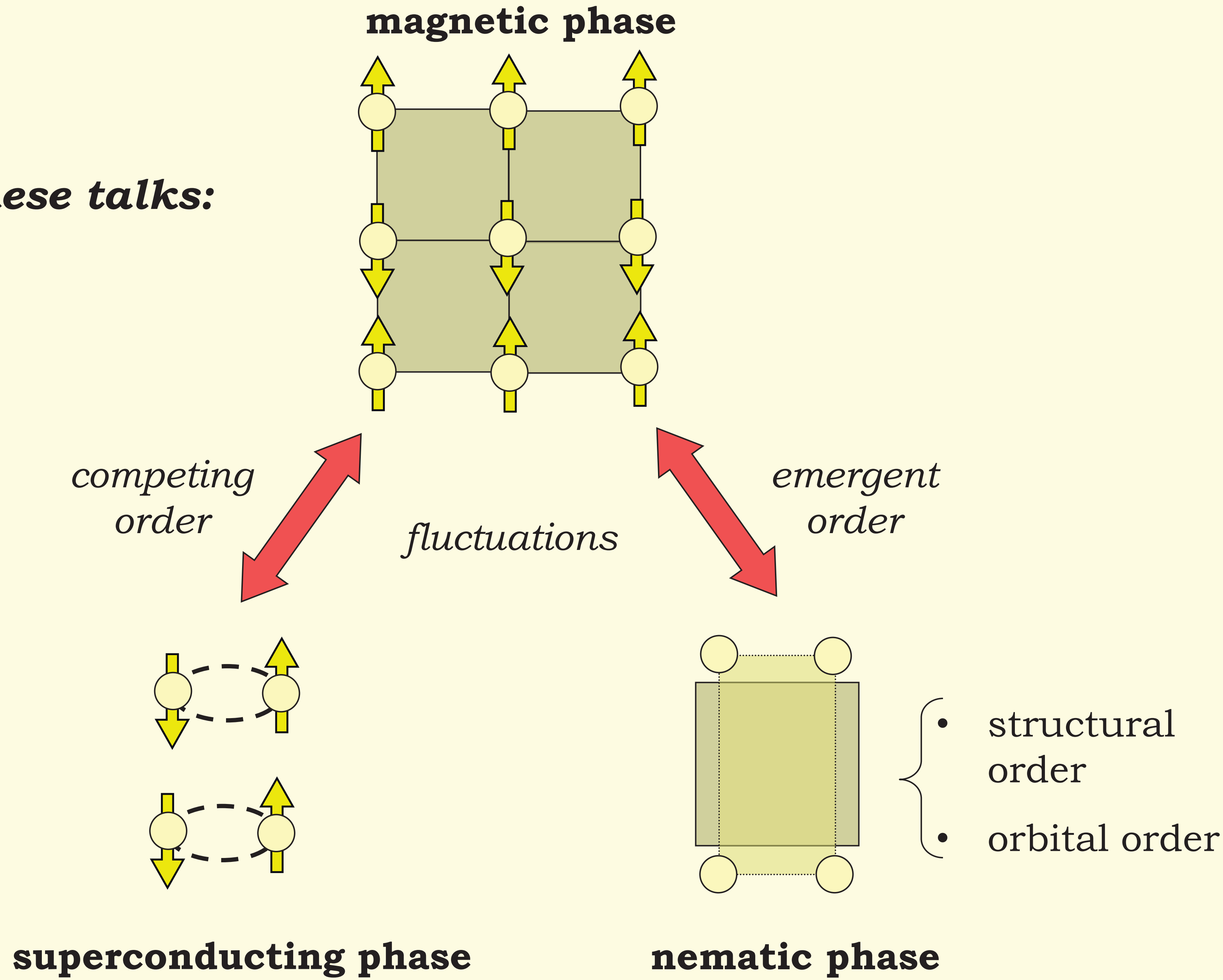
Iron pnictides: typical phase diagram

magnetic, structural, and superconducting order



- How these different ordered states interact with each other?
- Is there a primary degree of freedom?

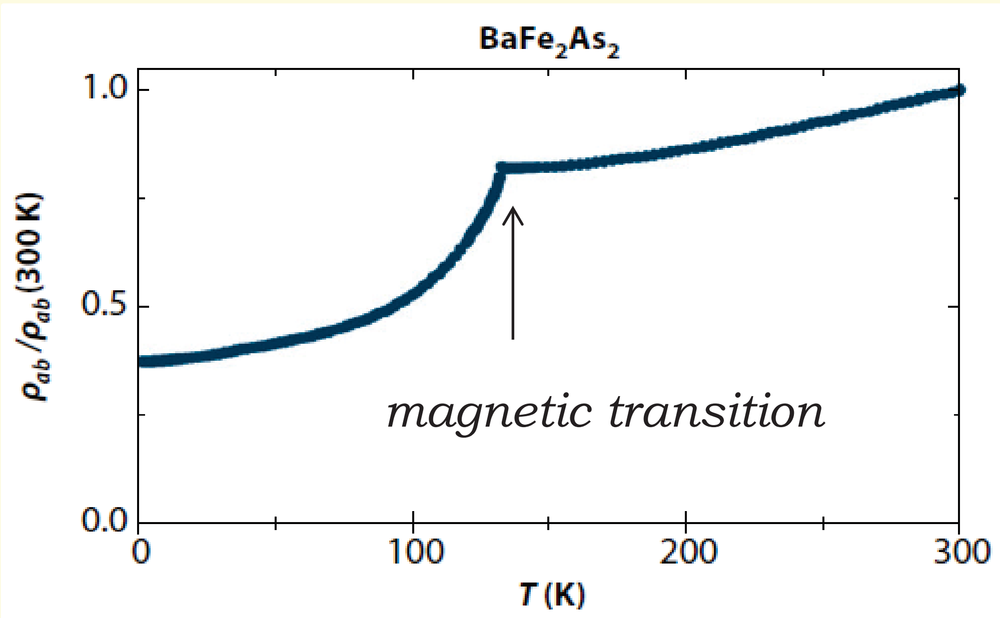
In these talks:



Iron pnictides: multi-band systems

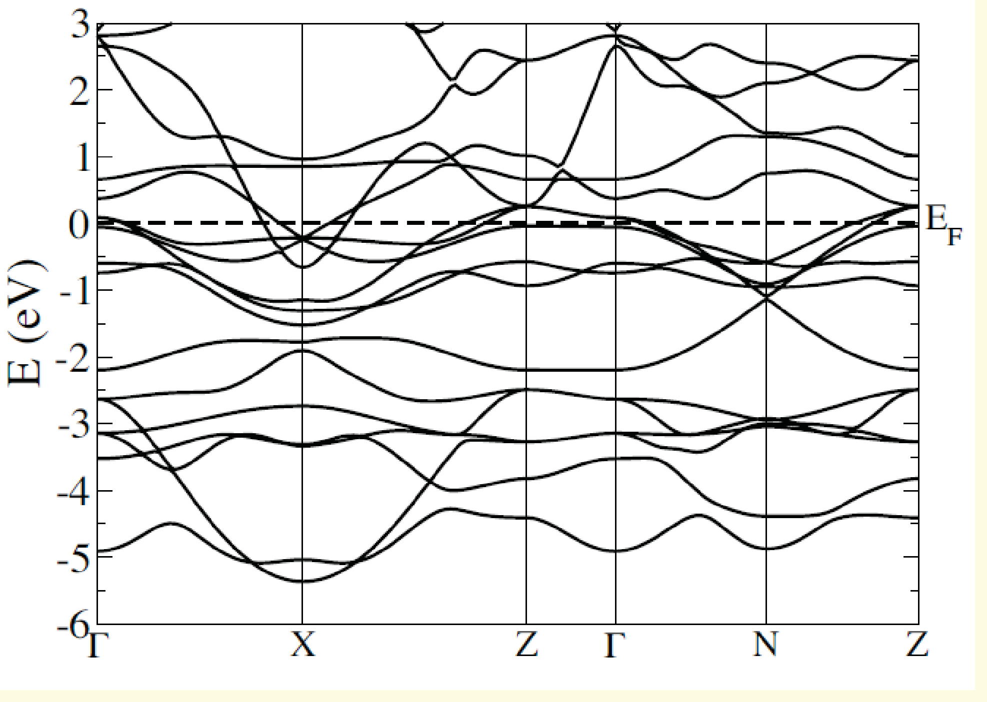
- Parent compounds are metals

- Before adding any interactions, we need to understand the non-interacting properties of the tetragonal phase.

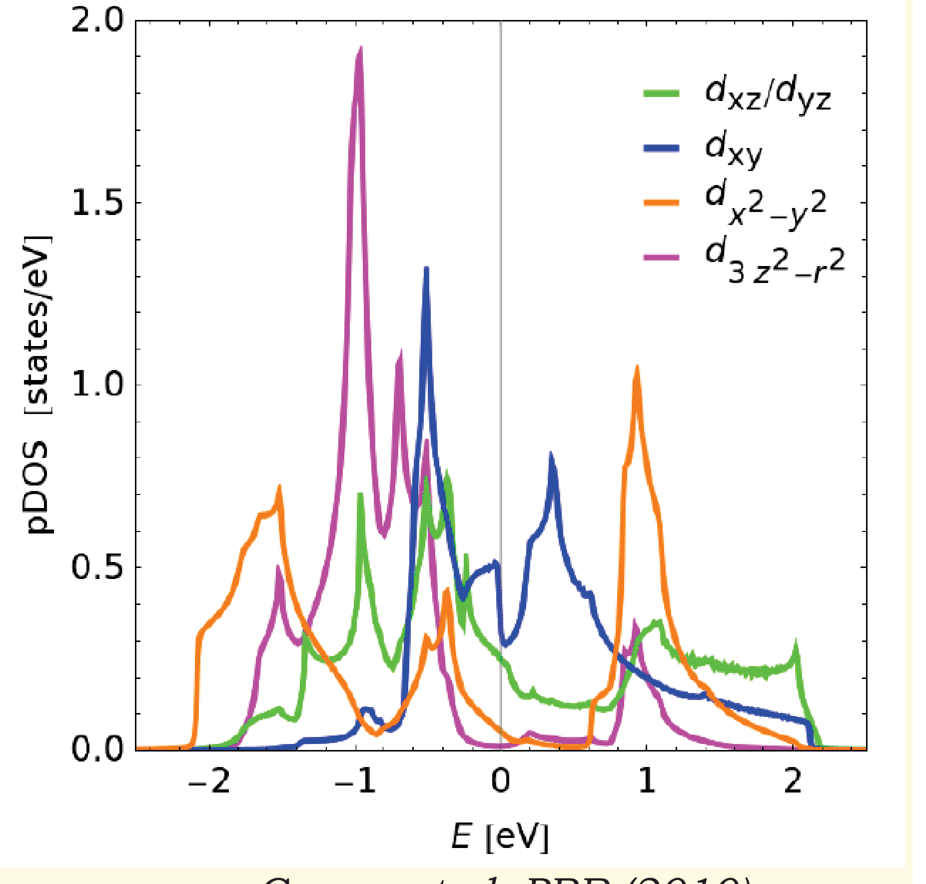


Iron pnictides: band structure

- DFT calculations: Fermi surface has multiple sheets
  - 3d^6 configuration: several orbitals cross the Fermi level



Zhang and Singh, PRB (2009)



Graser et al, PRB (2010)

Iron pnictides: band structure

- DFT calculations: Fermi surface has multiple sheets
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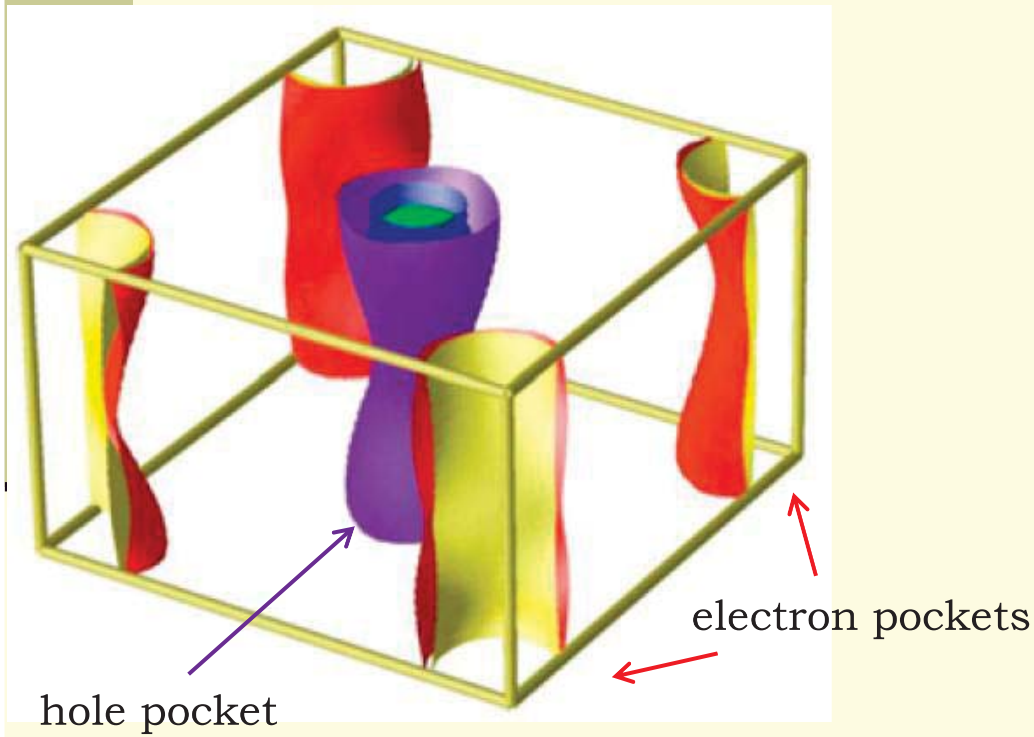
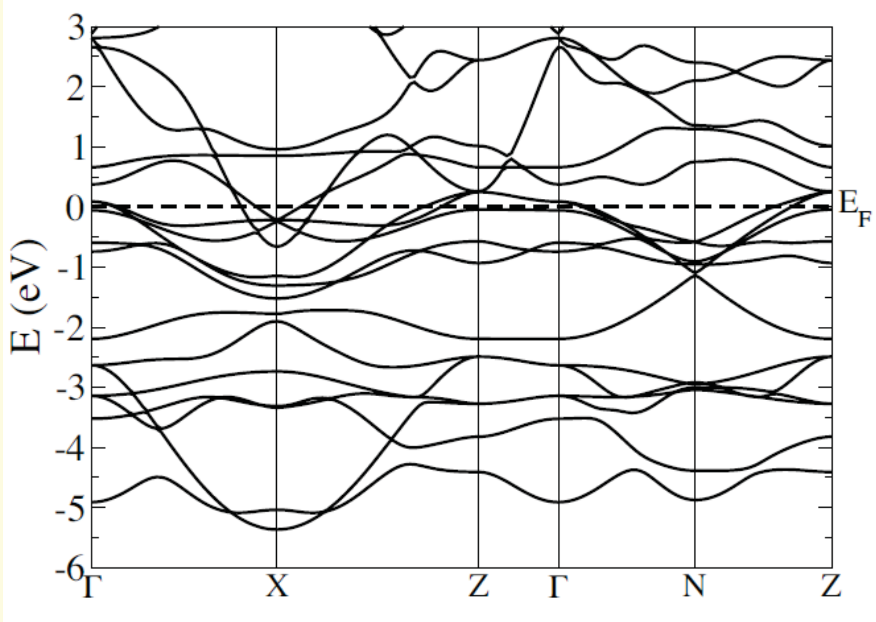


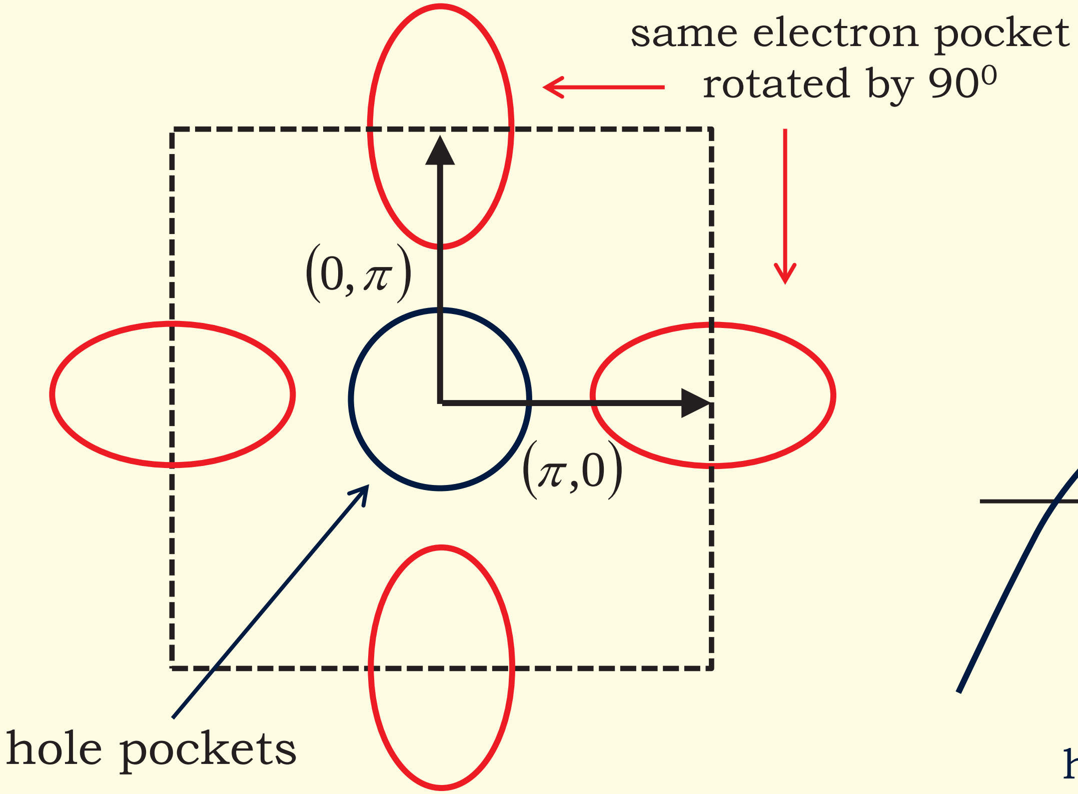


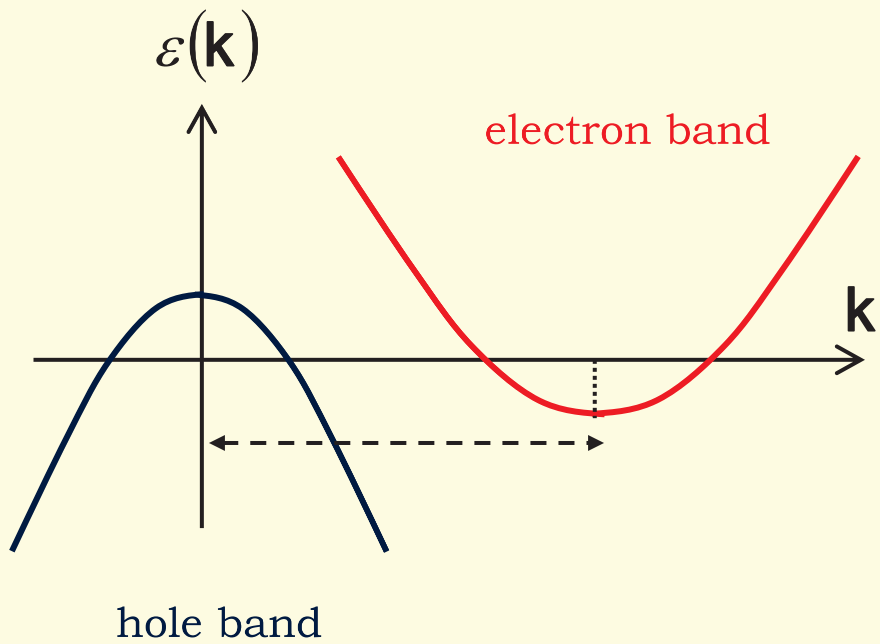
Paglione and Greene, Nature Phys (2010)

Zhang and Singh, PRB (2009)

Iron pnictides: band structure

- A simplified (yet useful) theorist-view of the Fermi surface





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A brief review of BCS superconductivity

- Bardeen, Cooper, and Schrieffer (1957): attractive electron-phonon interaction induces superconductivity

John
Bardeen

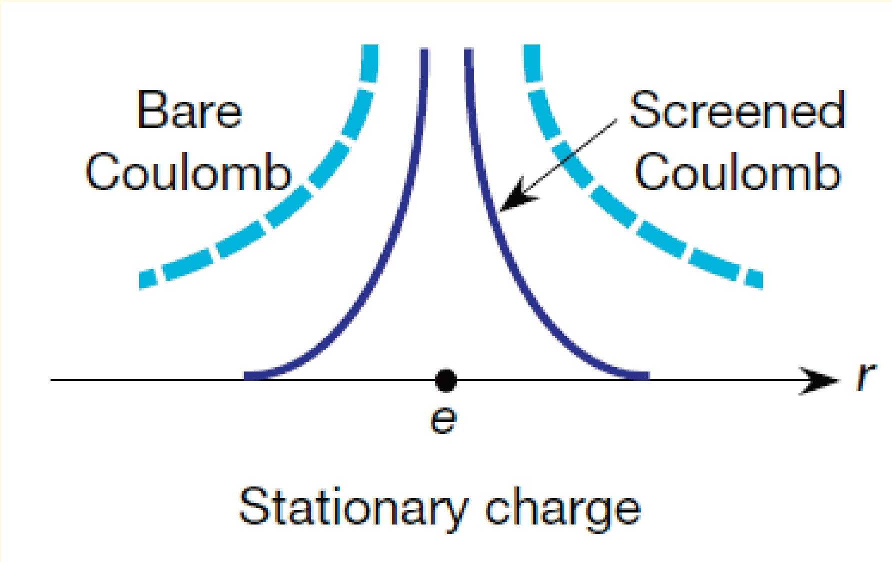
Leon
Cooper

Robert
Schrieffer

Nobel Prize
1972

A brief review of BCS superconductivity

- Bardeen, Cooper, and Schrieffer (1957): attractive electron-phonon interaction induces superconductivity
  - interaction is repulsive at **r**=0, t=0 (Coulomb repulsion)

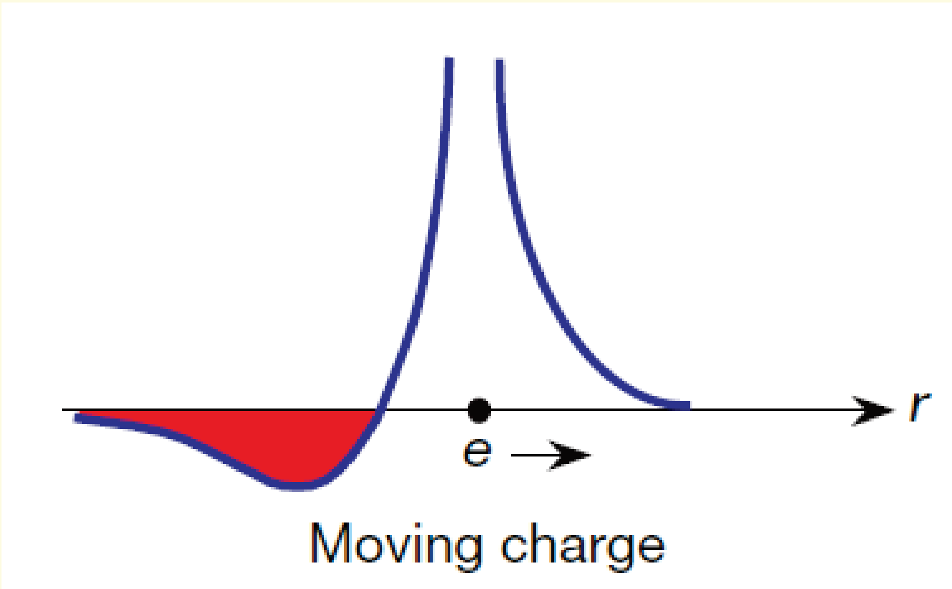


$V > 0 \Rightarrow$ repulsion

figures from Monthoux, Pines, and Lonzarich, Nature (2010)

A brief review of BCS superconductivity

- Bardeen, Cooper, and Schrieffer (1957): attractive electron-phonon interaction induces superconductivity
    - as the particle moves, it polarizes the lattice, leaving an attractive interaction at **r**=0, t>0



$V < 0 \Rightarrow$ attraction

figures from Monthoux, Pines, and Lonzarich, Nature (2010)

A brief review of BCS superconductivity

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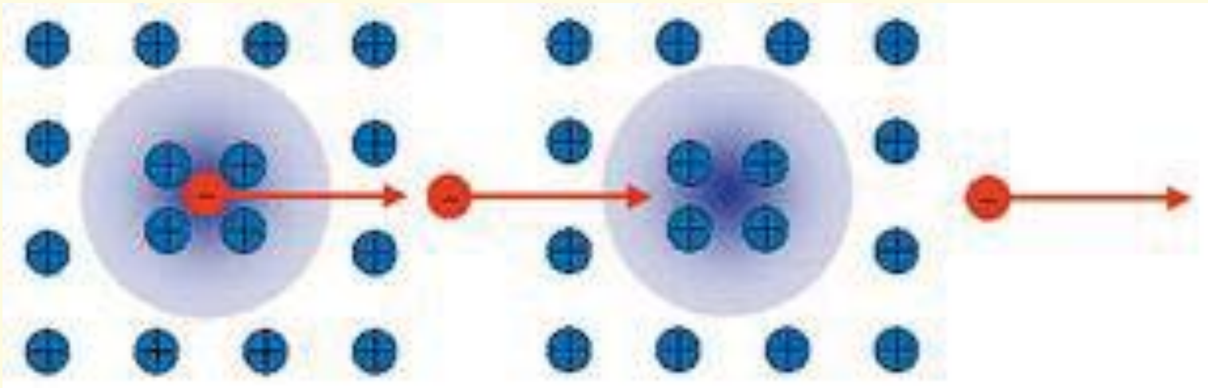
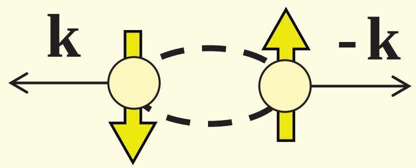


A brief review of BCS superconductivity

- Bardeen, Cooper, and Schrieffer (1957): attractive electron-phonon interaction induces superconductivity
  - bound state: Cooper pairs



New quantum ground state characterized by coherent Cooper pairs

$$T_c = 1.13\,\omega_D \exp\left(-\frac{1}{V\rho_F}\right)$$

Coupling constant can be calculated from first-principles, but NOT T_c...

A brief review of BCS superconductivity

- Bardeen, Cooper, and Schrieffer (1957): attractive electron-phonon interaction induces superconductivity

  - Let’s look a bit more at technical points…

A brief review of BCS superconductivity

- Bardeen, Cooper, and Schrieffer (1957): attractive electron-phonon interaction induces superconductivity

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} \frac{V_{\mathbf{k}-\mathbf{k}'}\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \tanh\left(\frac{E_{\mathbf{k}'}}{2T}\right)$$

$$1 = \lambda \int_0^{\omega_D} \frac{d\varepsilon}{\sqrt{\varepsilon^2 + \Delta^2}} \tanh\left(\frac{\sqrt{\varepsilon^2 + \Delta^2}}{2T}\right)$$

A brief review of BCS superconductivity

- Bardeen, Cooper, and Schrieffer (1957): attractive electron-phonon interaction induces superconductivity
  - linearizing the equation close to T_c

$$1 = \lambda \int_0^{\omega_D} \frac{d\varepsilon}{\varepsilon} \tanh\left(\frac{\varepsilon}{2T_c}\right)$$

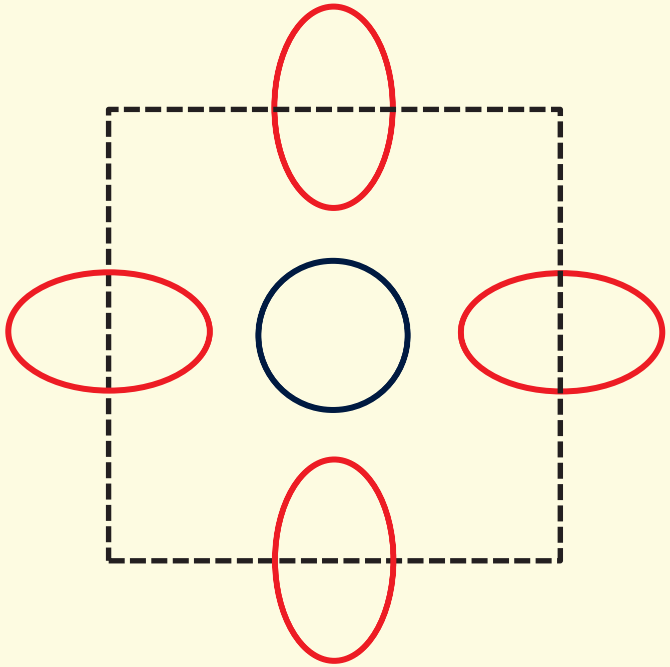
$$T_c = \left(\frac{2\mathrm{e}^{\gamma}}{\pi}\right) \omega_D \, \mathrm{e}^{-1/\lambda}$$

Are the iron pnictides electron-phonon superconductors?

- First-principle calculations of the electron-phonon interaction predict a maximum T_c of 0.8K

  Boeri et al, PRL (2008)

- Before studying other sources of pairing, let's review the possible symmetries of the SC state in a tetragonal system



Symmetry of the superconducting state

- In general, the symmetry of the superconducting state is a subgroup of the symmetry of the normal state

$$X \times R \times T \times U(1)$$

crystal lattice — rotations — time reversal

- ➢ U(1) gauge symmetry is **always broken**
- ➢ in conventional (electron-phonon) superconductors, usually no other symmetry is broken
- ➢ in unconventional superconductors, besides U(1), other symmetries can be broken as well

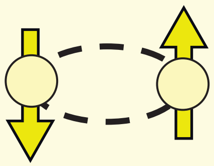
Symmetry of the superconducting state

- In general, the symmetry of the superconducting state is a subgroup of the symmetry of the normal state

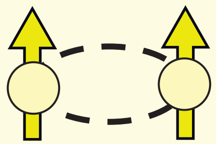
$$X \times R \times T \times U(1)$$

crystal lattice — rotations — time reversal

> ➢ in crystals with inversion symmetry, two possible spin states:



singlet
(anti-symmetric)



triplet
(symmetric)

Symmetry of the superconducting state

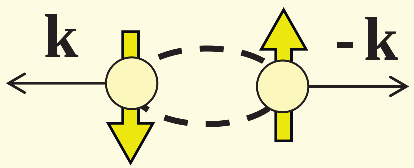
- The total wave-function must be anti-symmetric with respect to the exchange of two electrons

$$X \times R \times T \times U(1)$$

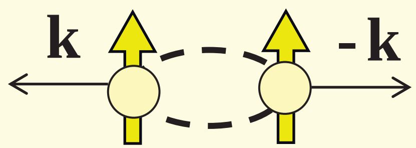
crystal lattice

rotations

time reversal



singlet
(anti-symmetric)



triplet
(symmetric)

Cooper pair wave-function

$$\Psi(-\mathbf{k}) = \Psi(\mathbf{k})$$

even parity
(s-wave, d-wave…)

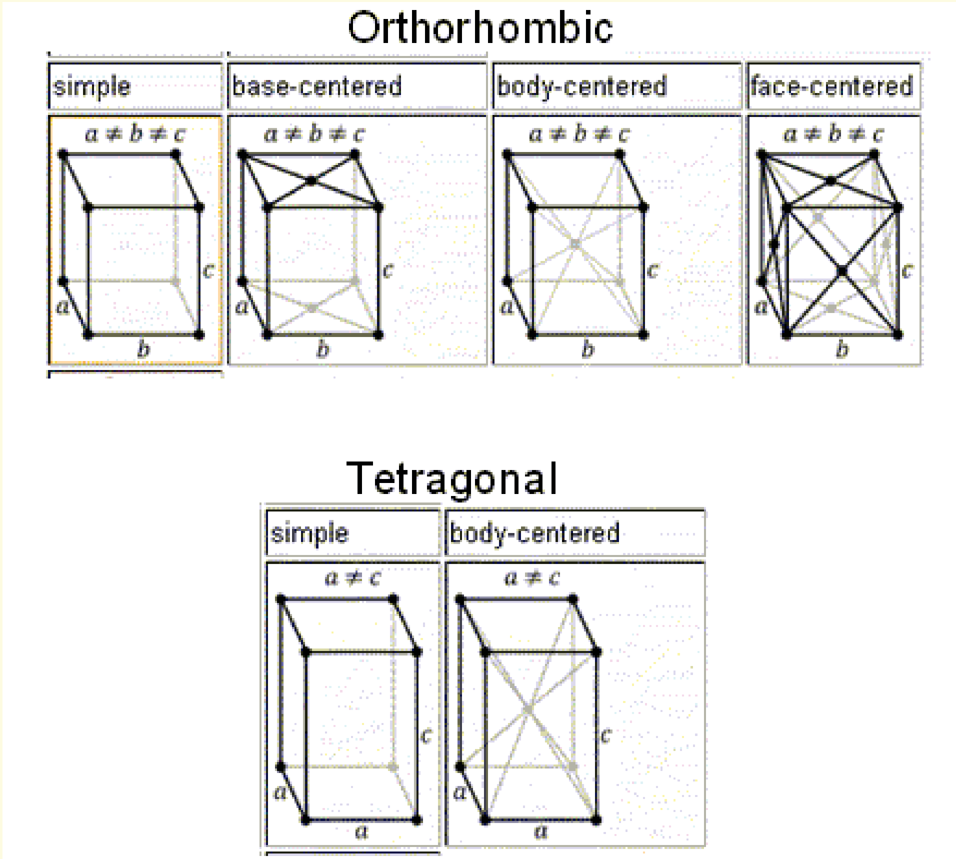
$$\Psi(-\mathbf{k}) = -\Psi(\mathbf{k})$$

odd parity
(p-wave, f-wave…)

Symmetry of the superconducting state

- The possible shapes of the wave-function depend on the irreducible representations of the crystal point group

consider the simple case of a tetragonal lattice



we will restrict our analysis to a ***singlet state*** with ***no time-reversal symmetry breaking*** and ***2 dimensions***

Symmetry of the superconducting state

- Possible symmetries of the Cooper-pair wave-function in the tetragonal lattice

Wave-function name	Group-theoretic notation, T_j	Residual symmetry	Basis function	Nodes
s wave	A_{1g}	$D_{4h}\times \mathrm{T}$	$1,(x^2+y^2),z^2$	none
g	A_{2g}	$D_4[C_4]\times C_i\times \mathrm{T}$	$xy(x^2-y^2)$	line
$d_{x^2-y^2}$	B_{1g}	$D_4[D_2]\times C_i\times \mathrm{T}$	x^2-y^2	line
d_{xy}	B_{2g}	$D_4[D_2']\times C_i\times \mathrm{T}$	xy	line

Kirtley and Tsuei, RMP (2000)

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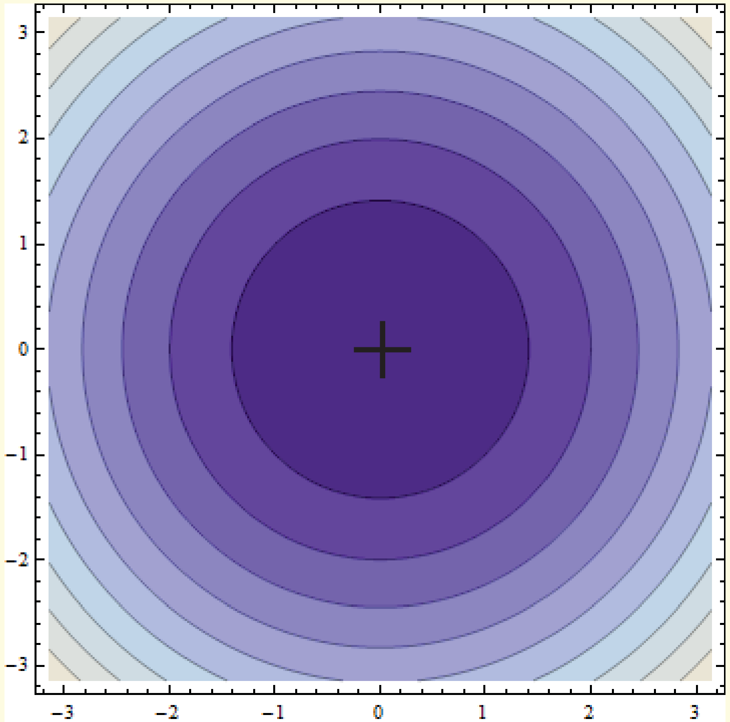
Contour plot of the wave-functions in the first Brillouin zone



gap is constant around a spherical Fermi surface

does not change sign under a 90⁰ rotation

usual state of conventional superconductors

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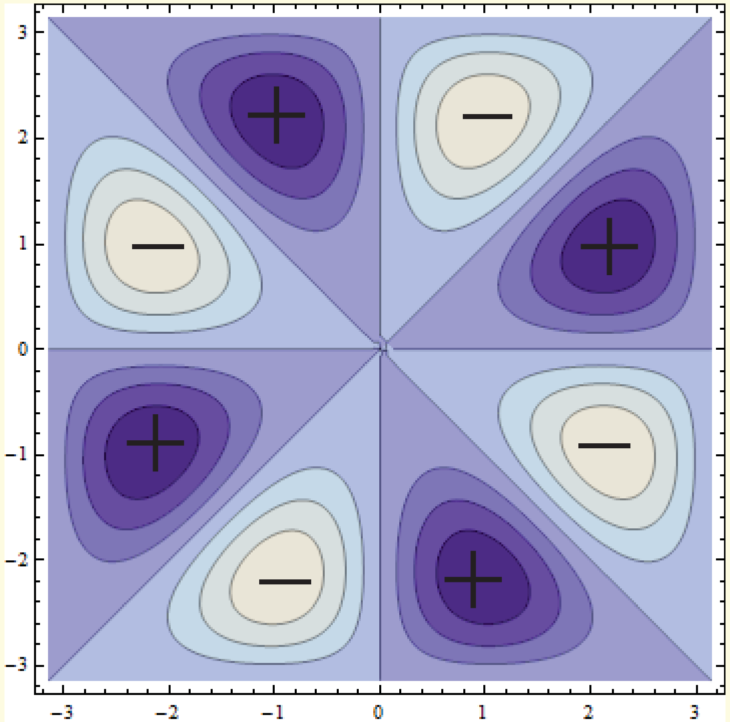

gap changes sign around a spherical Fermi surface

does not change sign under a 90⁰ rotation

4 line nodes (zeros of the gap)

Wave-function name	Group-theoretic notation, T_j	Residual symmetry	Basis function	Nodes
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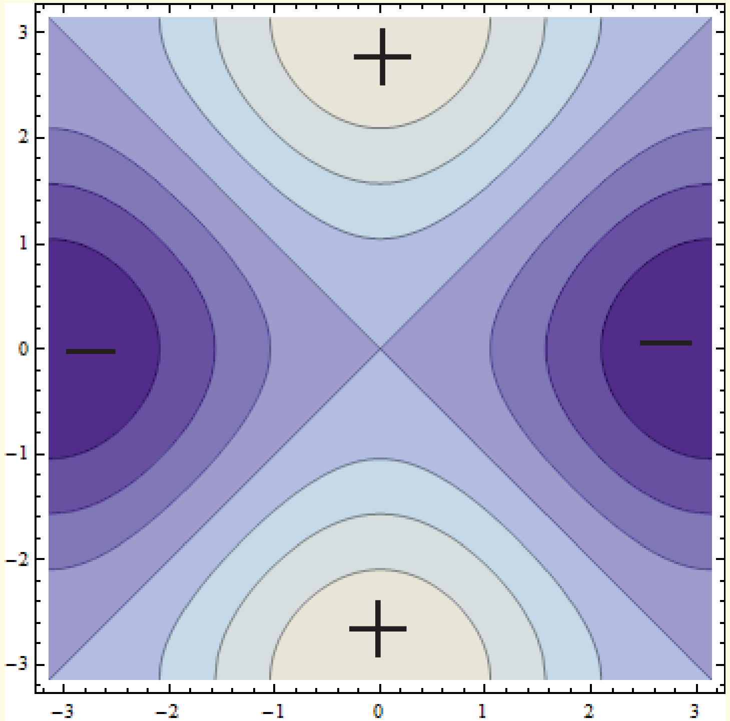

gap changes sign around a spherical Fermi surface

does not change sign under a 180⁰ rotation

2 diagonal line nodes (zeros of the gap)

Wave-function name	Group-theoretic notation, T_j	Residual symmetry	Basis function	Nodes
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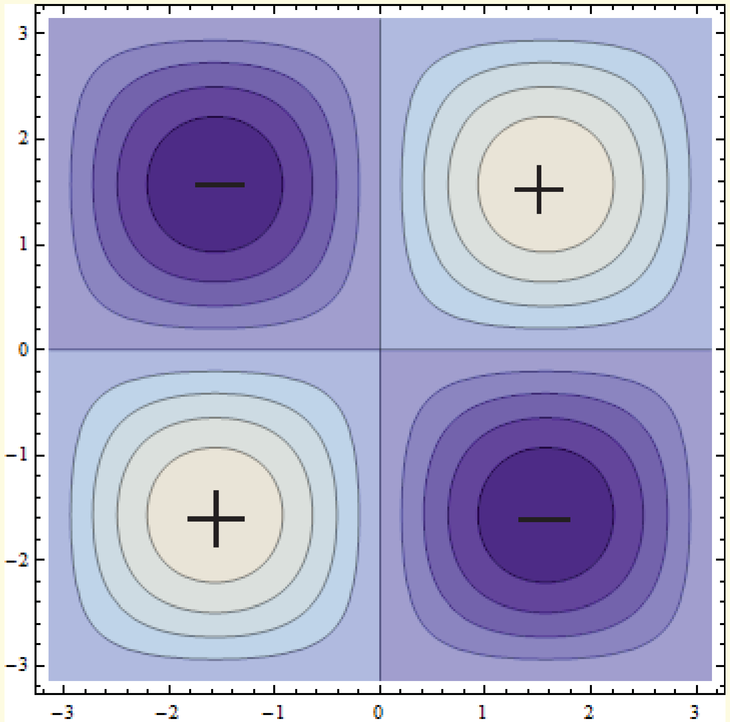

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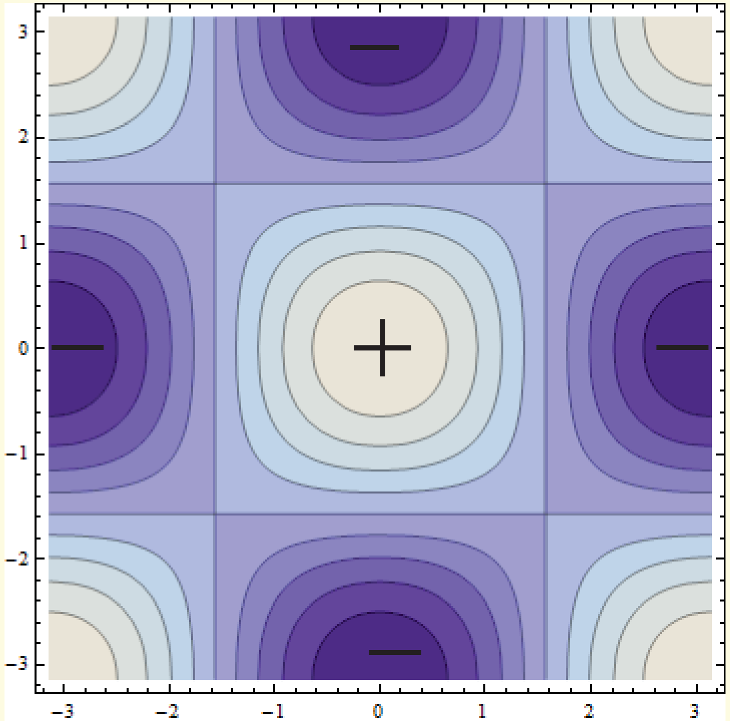

gap function of the A_{1g} representation can also have line nodes not fixed by symmetry

extended s-wave

Wave-function name	Group-theoretic notation, T_j	Residual symmetry	Basis function	Nodes
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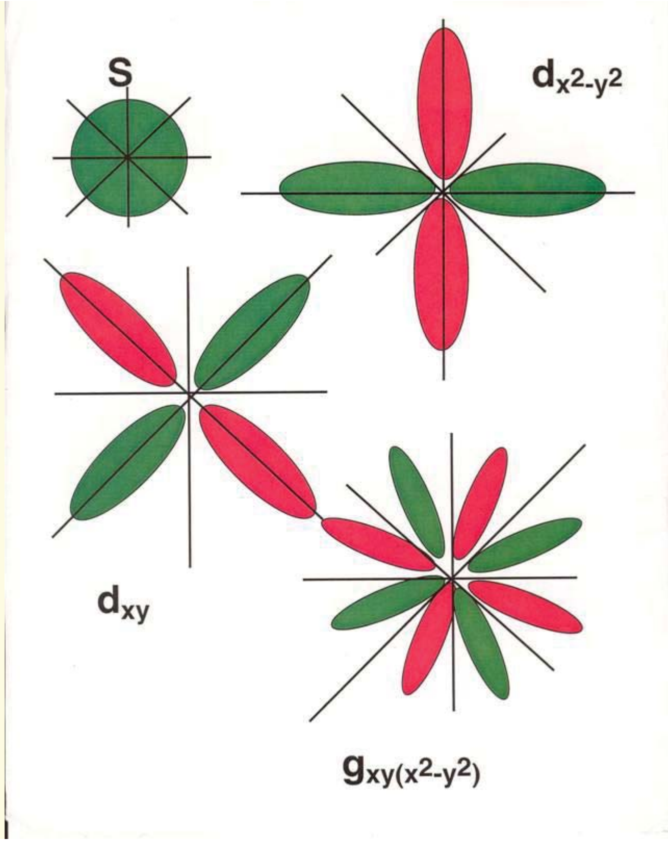
$d_{x^2-y^2}$	B_{1g}	$D_4[D_2]\times C_i\times T$	x^2-y^2	line
d_{xy}	B_{2g}	$D_4[D_2']\times C_i\times T$	xy	line



why would the gap function vanish in some regions of the Brillouin zone?

Repulsive interactions!

Superconductivity due to repulsive interactions

- Several approaches: (non-extensive list)
  - RVB theory: slave-boson, Gutzwiller projection, variational Monte Carlo

    Anderson, Science (1987)

  - Recent numerical solutions of the Hubbard model (DMFT)

    cf. Tremblay's talk

  - Pairing mediated by spin fluctuations

    Berk and Schrieffer, PRL (1966)

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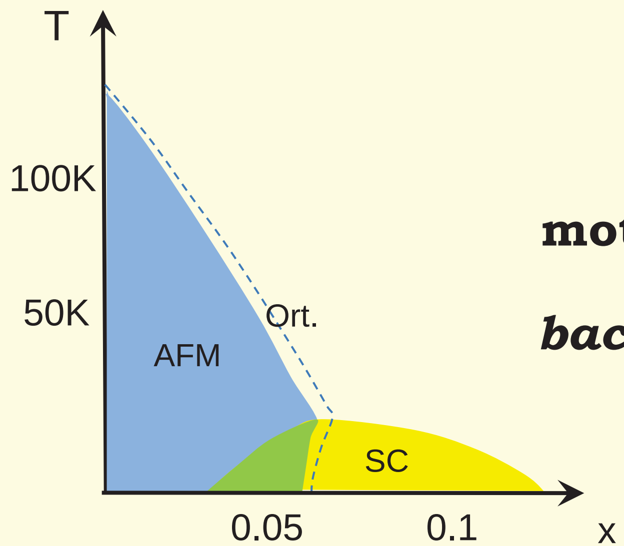


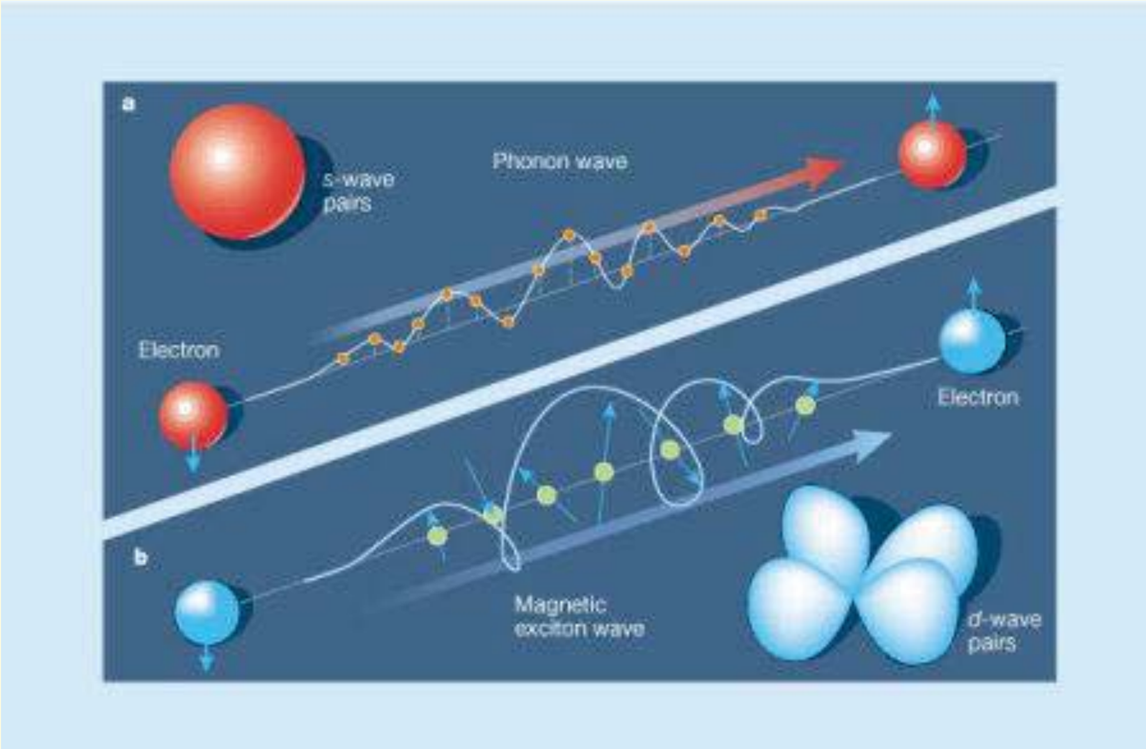
motivation: proximity to a magnetic instability

back to the blackboard...

Superconductivity mediated by spin fluctuations

- Effective interaction in the singlet channel:

$$V_{\text{pair}} \propto \chi_s(\mathbf{r})$$



spin fluctuations are the glue

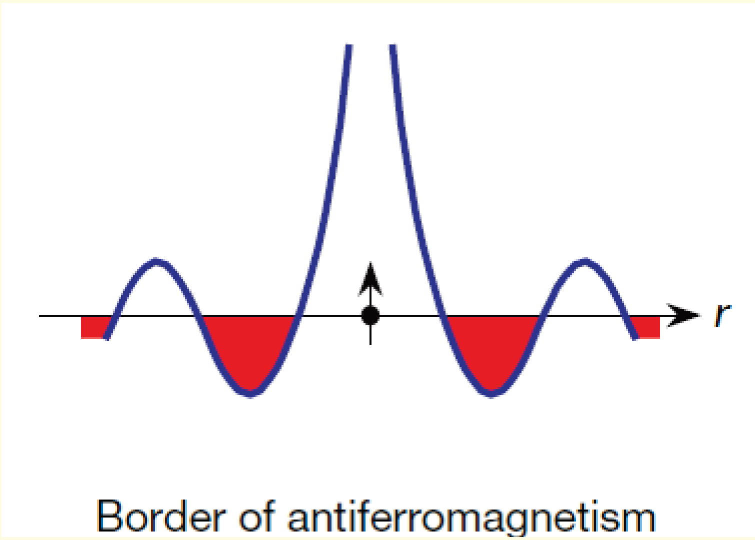
purely electronic mechanism

Superconductivity mediated by spin fluctuations

- Effective interaction in the singlet channel:

$$V_{\text{pair}} \propto \chi_s(\mathbf{r})$$

  - for an antiferromagnetic instability, $\chi_s(\mathbf{r})$ is maximum and positive at the origin, but oscillates



regions of attractive and repulsive interaction

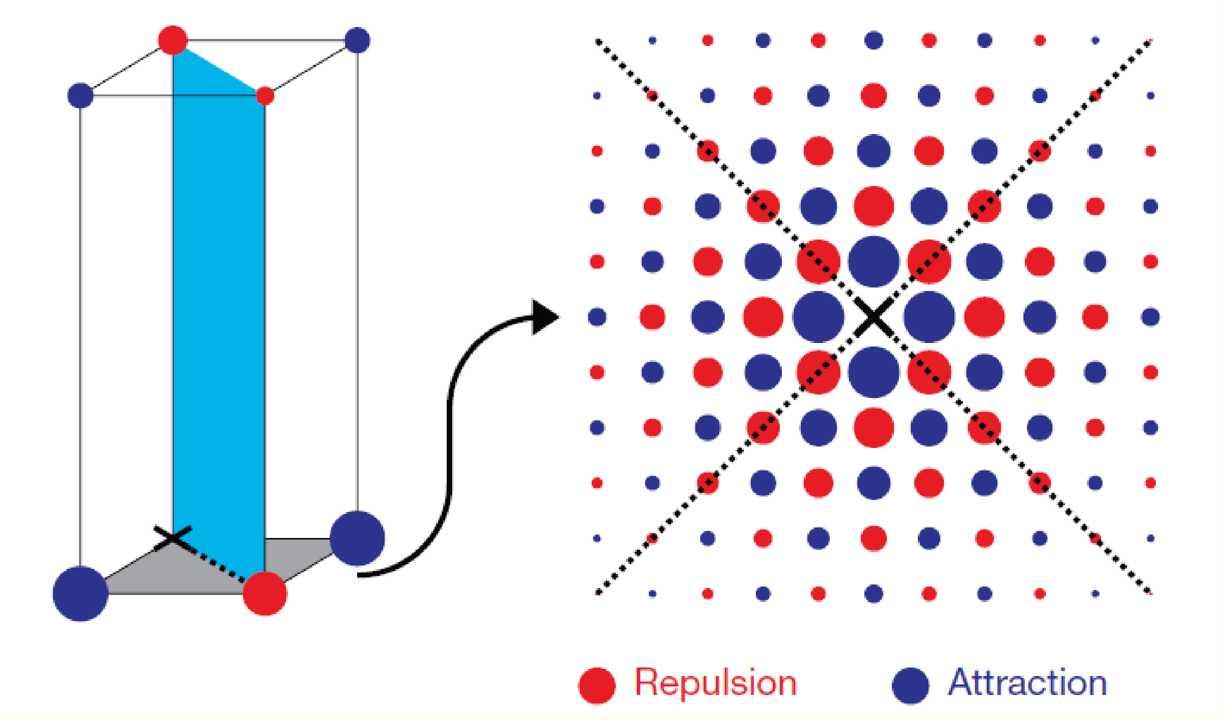
Cooper-pair wave-function changes in space to match the attractive regions

figure from Monthoux, Pines, and Lonzarich, Nature (2010)

Spin-fluctuations mechanism

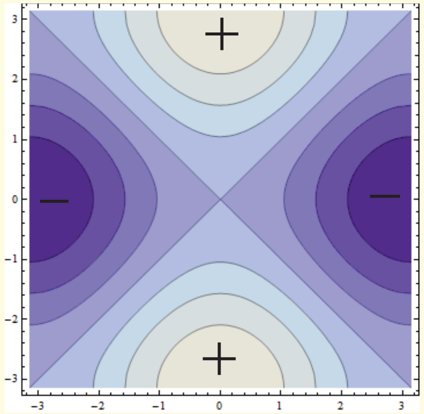
- Antiferromagnetic susceptibility in single-band tetragonal system: real space

$$V_{\text{pair}} \propto \chi_s(\mathbf{r})$$



gap would benefit by vanishing at the diagonals

$d_{x^2-y^2}$ - wave



Spin-fluctuations mechanism

- Problem simplifies if we look in **momentum-space**

$$V_{\mathbf{k}-\mathbf{k}'} \approx \chi_s(\mathbf{Q})\delta_{\mathbf{k}-\mathbf{k}',\mathbf{Q}}$$

a well-defined repulsive interaction in momentum-space

magnetic ordering vector

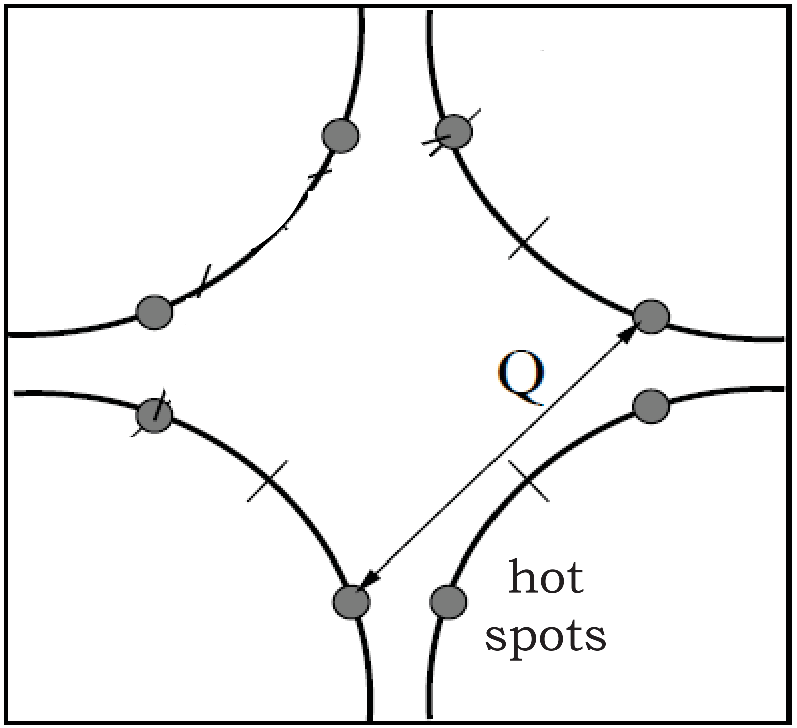
Spin-fluctuations mechanism

- Problem simplifies if we look in **momentum-space**

$$V_{\mathbf{k}-\mathbf{k}'} \approx \chi_s(\mathbf{Q})\delta_{\mathbf{k}-\mathbf{k}',\mathbf{Q}}$$

a repulsive interaction strongly peaked in momentum-space

typical Fermi surface for the cuprates



Chubukov, Pines, Schmalian (2002)

BCS-like gap equation:

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} \frac{V_{\mathbf{k}-\mathbf{k}'}\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \tanh\left(\frac{E_{\mathbf{k}'}}{2T}\right)$$

with $E_{\mathbf{k}} = \sqrt{\varepsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2} > 0$

Spin-fluctuations mechanism

- Problem simplifies if we look in **momentum-space**

$$V_{\mathbf{k}-\mathbf{k}'} \approx \chi_s(\mathbf{Q})\,\delta_{\mathbf{k}-\mathbf{k}',\mathbf{Q}}$$

a repulsive interaction strongly peaked in momentum-space

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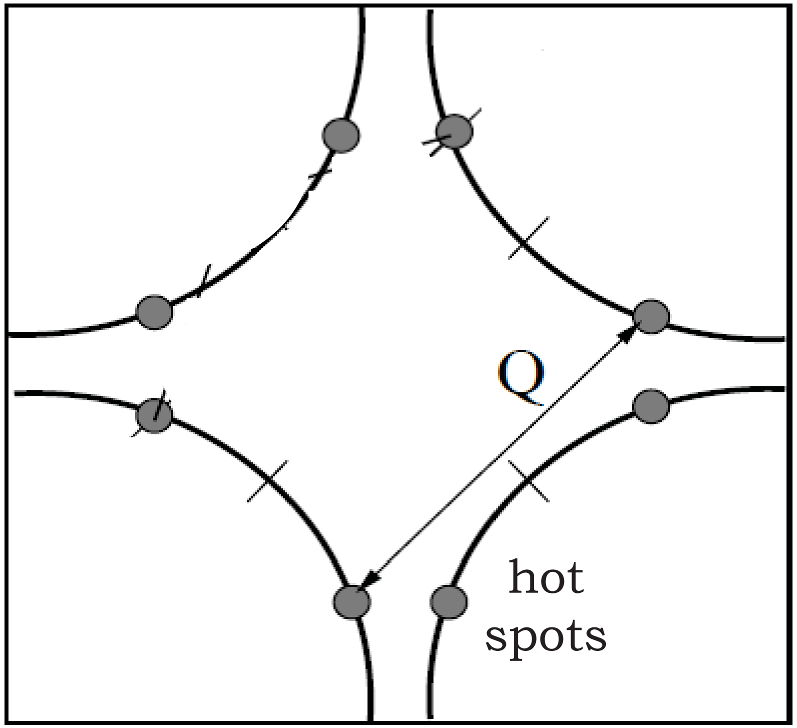


Chubukov, Pines, Schmalian (2002)

BCS-like gap equation:

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} \underbrace{\frac{V_{\mathbf{k}\text{-}\mathbf{k}'}\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \tanh\left(\frac{E_{\mathbf{k}'}}{2T}\right)}$$

the main contribution to the momentum sum comes from: $\mathbf{k}' \approx \mathbf{k} + \mathbf{Q}$

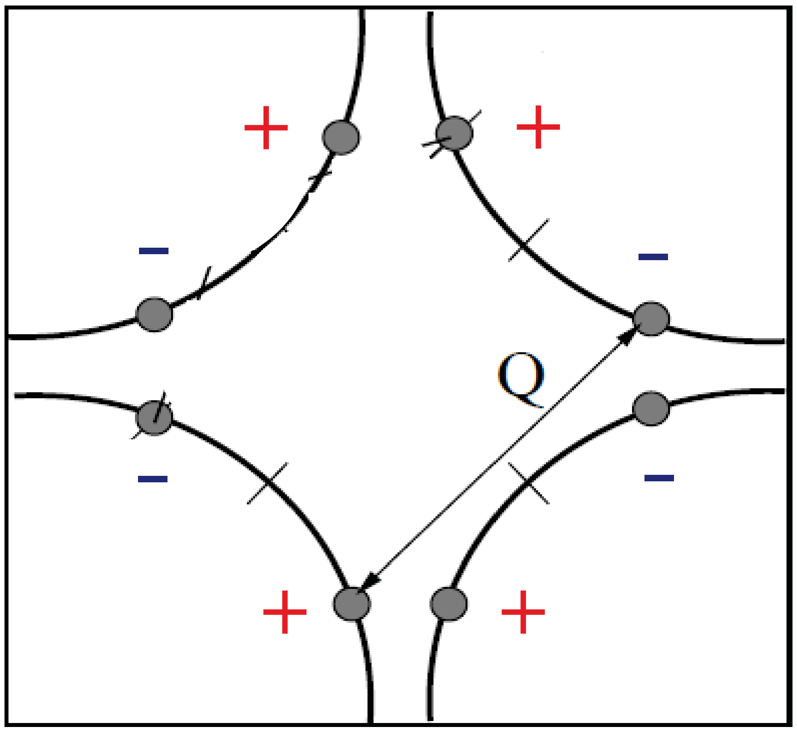
Spin-fluctuations mechanism

- Problem simplifies if we look in **momentum-space**

$$V_{\mathbf{k}-\mathbf{k}'} \approx \chi_s(\mathbf{Q})\,\delta_{\mathbf{k}-\mathbf{k}',\mathbf{Q}}$$

a repulsive interaction strongly peaked in momentum-space

typical Fermi surface for the cuprates



Chubukov, Pines, Schmalian (2002)

BCS-like gap equation:

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} \frac{V_{\mathbf{k}\text{-}\mathbf{k}'}\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \tanh\left(\frac{E_{\mathbf{k}'}}{2T}\right)$$

since $\chi_s(\mathbf{Q}) > 0$ *, it must follow:*

$$\operatorname{sign}\Delta_{\mathbf{k}} = -\operatorname{sign}\Delta_{\mathbf{k}+\mathbf{Q}}$$

$$\Rightarrow\ d_{x^2-y^2}\text{ - wave}$$

Spin-fluctuations mechanism: iron pnictides

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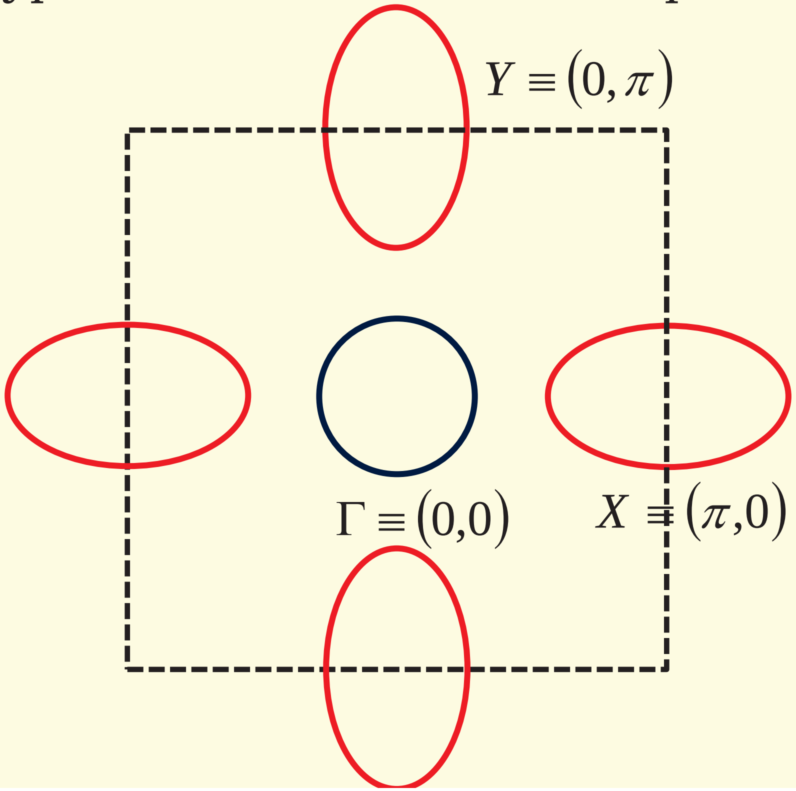
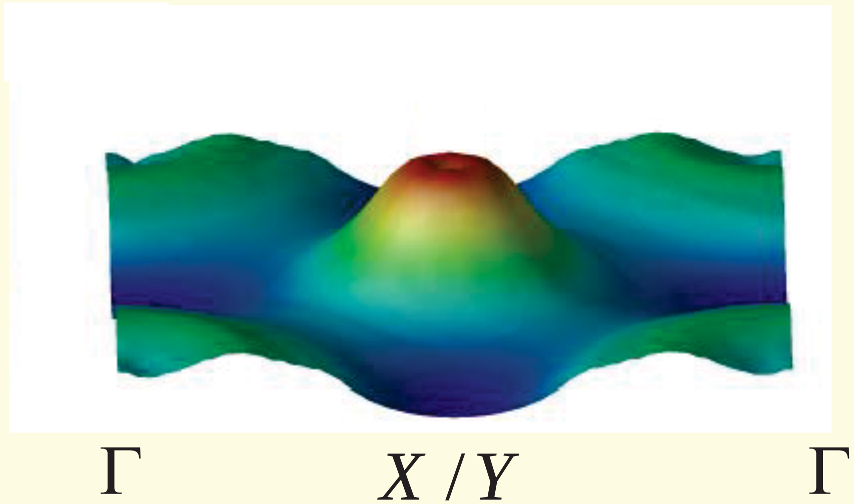
typical Fermi surface for the pnictides



magnetic susceptibility



Mazin et al, PRL (2008)

Spin-fluctuations mechanism: iron pnictides

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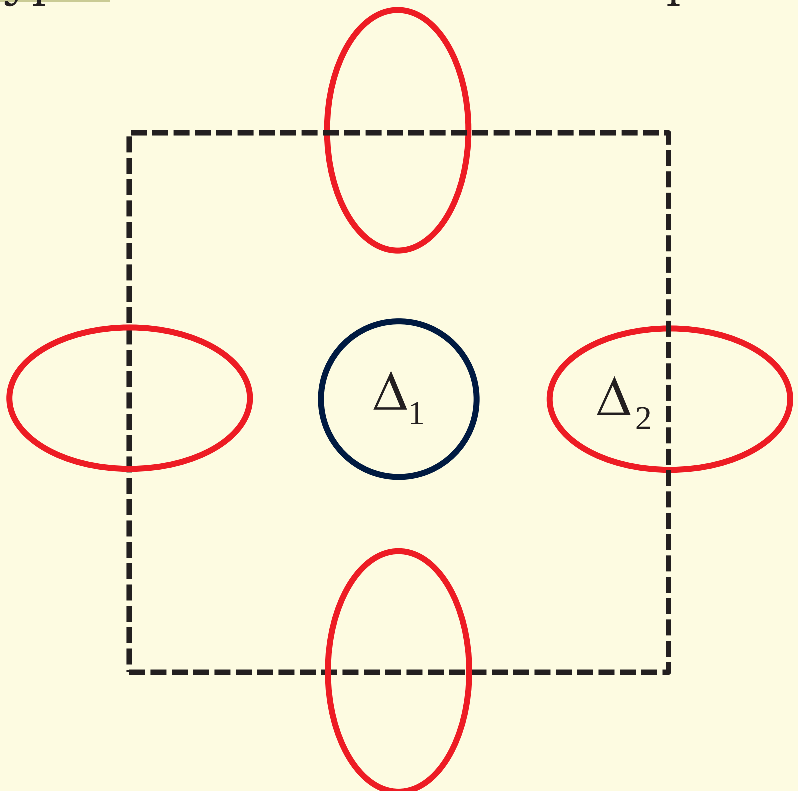


BCS-like gap equation

$$\begin{cases} \Delta_1 = -V\Delta_2 \sum_{\mathbf{k}} \frac{1}{2E_{2,\mathbf{k}}} \tanh\left(\frac{E_{2,\mathbf{k}}}{2T}\right) \\ \Delta_2 = -V\Delta_1 \sum_{\mathbf{k}} \frac{1}{2E_{1,\mathbf{k}}} \tanh\left(\frac{E_{1,\mathbf{k}}}{2T}\right) \end{cases}$$

with $E_{i,\mathbf{k}} = \sqrt{\varepsilon_{i,\mathbf{k}}^2 + \Delta_i^2} > 0$

Spin-fluctuations mechanism: iron pnictides

- Linearized gap equations (close to T_c)

$$\begin{pmatrix}\Delta_1 \\ \Delta_2\end{pmatrix}\begin{pmatrix}0 & -V \\ -V & 0\end{pmatrix} = \frac{1}{\rho_F \ln\left(W/T_c\right)}\begin{pmatrix}\Delta_1 \\ \Delta_2\end{pmatrix}$$

two solutions: $T_c = W e^{-\frac{1}{\lambda\rho}}$

$$\boxed{\begin{pmatrix}\Delta_1 \\ \Delta_2\end{pmatrix} \propto \begin{pmatrix}+1 \\ +1\end{pmatrix} \qquad \lambda = -V}$$

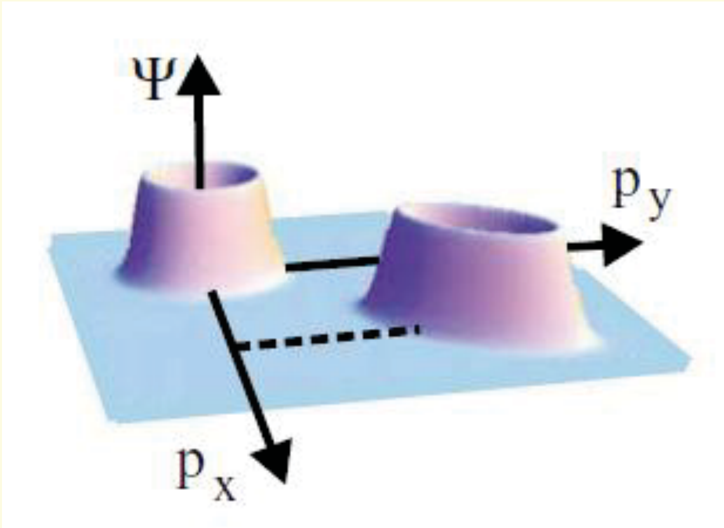
$$\begin{pmatrix}\Delta_1 \\ \Delta_2\end{pmatrix} \propto \begin{pmatrix}+1 \\ -1\end{pmatrix} \qquad \lambda = V$$

Spin-fluctuations mechanism: iron pnictides

- Pairing due to conventional attractive electron-phonon interaction (enhanced by charge/orbital fluctuations)

$$V < 0$$

$\boxed{s^{++}\ \textbf{state}}$



Kontani & Onari, PRL (2010)

Spin-fluctuations mechanism: iron pnictides

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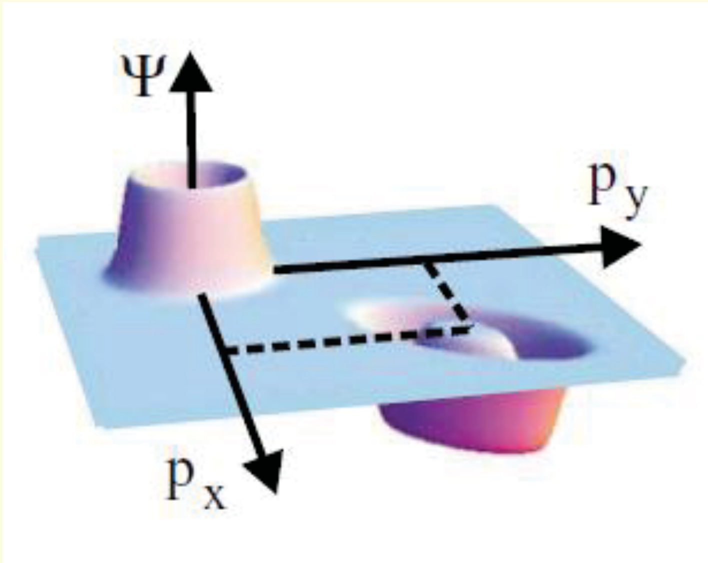
Spin-fluctuations mechanism: iron pnictides

- Pairing due to purely repulsive electronic interaction (enhanced by spin fluctuations)

$$V > 0$$

$\boxed{s^{+-}\ \textbf{state}}$



Mazin et al, PRL (2008)
Kuroki et al, PRL (2008)
Chubukov et al, PRB (2008)
Cvetkovic et al, EPL (2009)
Wang et al, PRL (2009)
Sknepnek et al, PRB (2009)
Graser et al, NJP (2009)

Spin-fluctuations mechanism: iron pnictides

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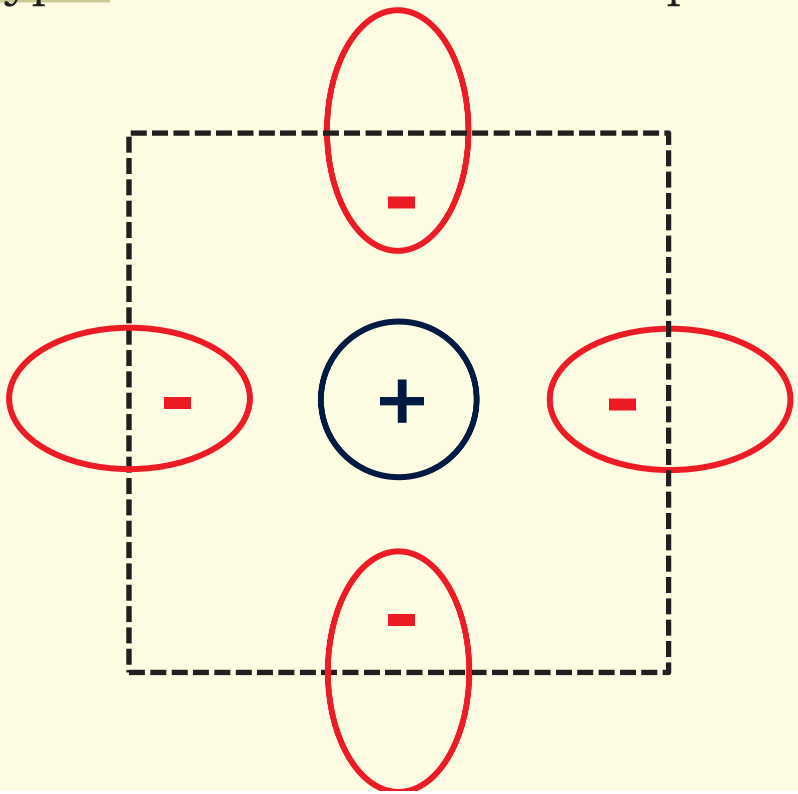
a repulsive interaction strongly peaked in momentum-space

typical Fermi surface for the pnictides



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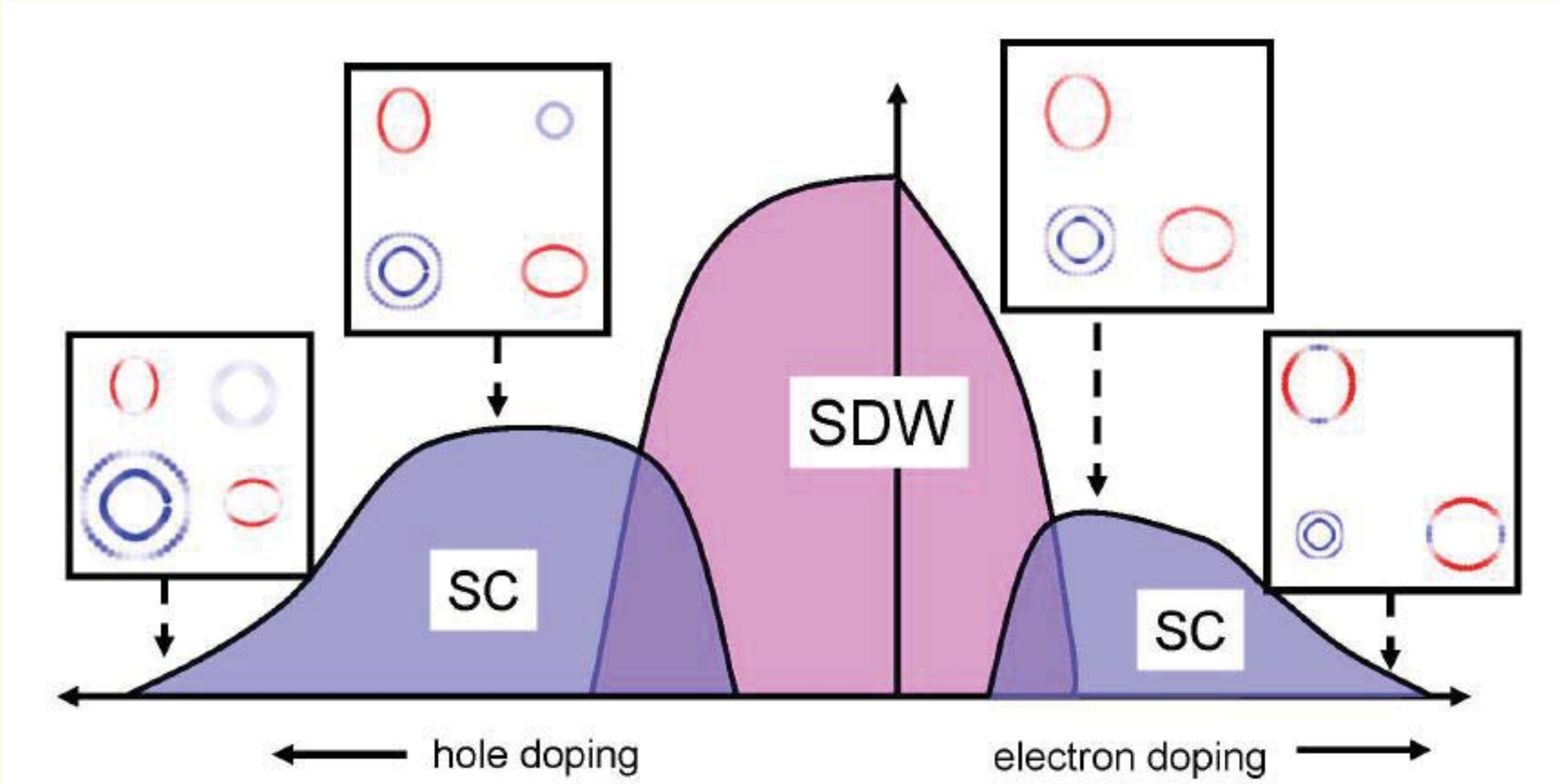
with $E_{i,\mathbf{k}} = \sqrt{\varepsilon_{i,\mathbf{k}}^2 + \Delta_i^2} > 0$

- The presence of intra-band repulsion can lead to accidental nodes (i.e. not enforced by symmetry)

- RPA, RG, FLEX, and fRG calculations give an s^{+-} state, but also show that a d-wave state may happen for certain dopings



Hirschfeld et al, RPP (2011)

How to probe spin fluctuations experimentally?

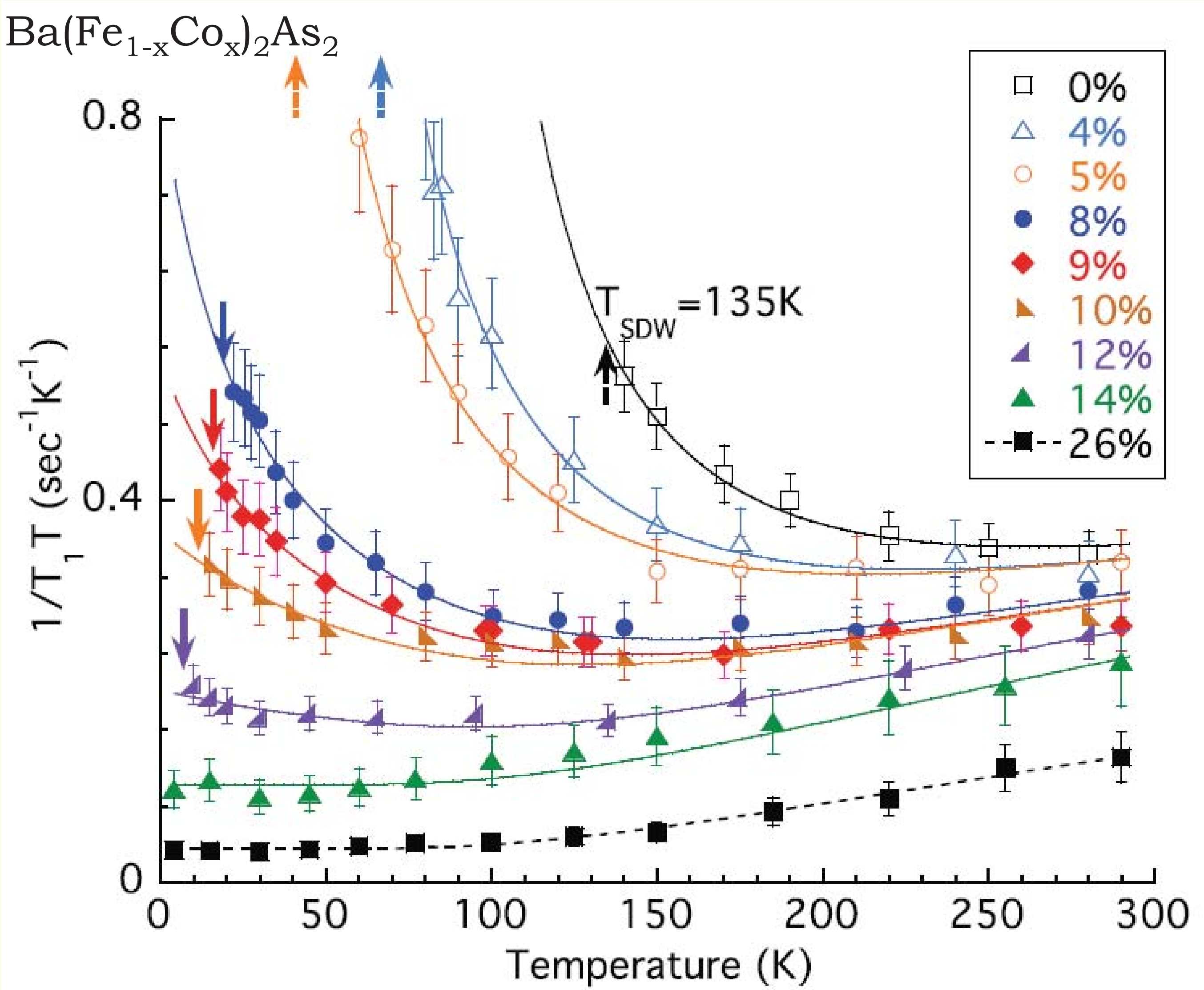
- Nuclear magnetic resonance (NMR): measures the momentum-integrated dynamic magnetic susceptibility
  - *spin-lattice relaxation rate*

$$\frac{1}{T_1} \propto T \lim_{\omega \to 0} \sum_{\mathbf{q}} \frac{\operatorname{Im} \chi(\mathbf{q}, \omega)}{\omega}$$

➢ *for a two-dimensional metal near an AFM transition:*

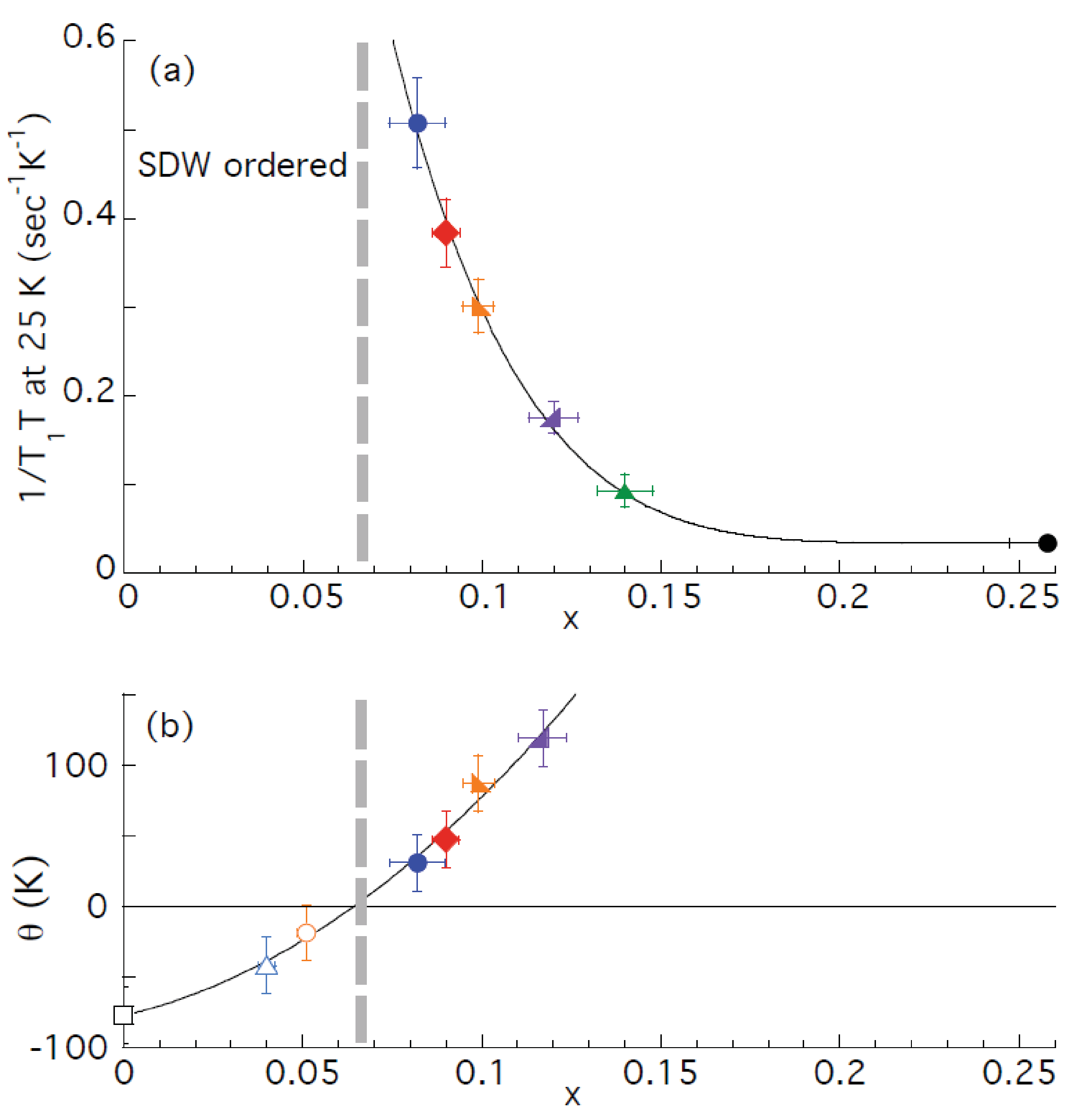
$$\frac{1}{T_1 T} \propto \frac{1}{T+\theta}$$

$$\theta \approx -T_{AFM}$$



Ning et al, PRL (2008)

- *for a two-dimensional metal near an AFM transition:* $$\frac{1}{T_1T} \propto \frac{1}{T+\theta}$$

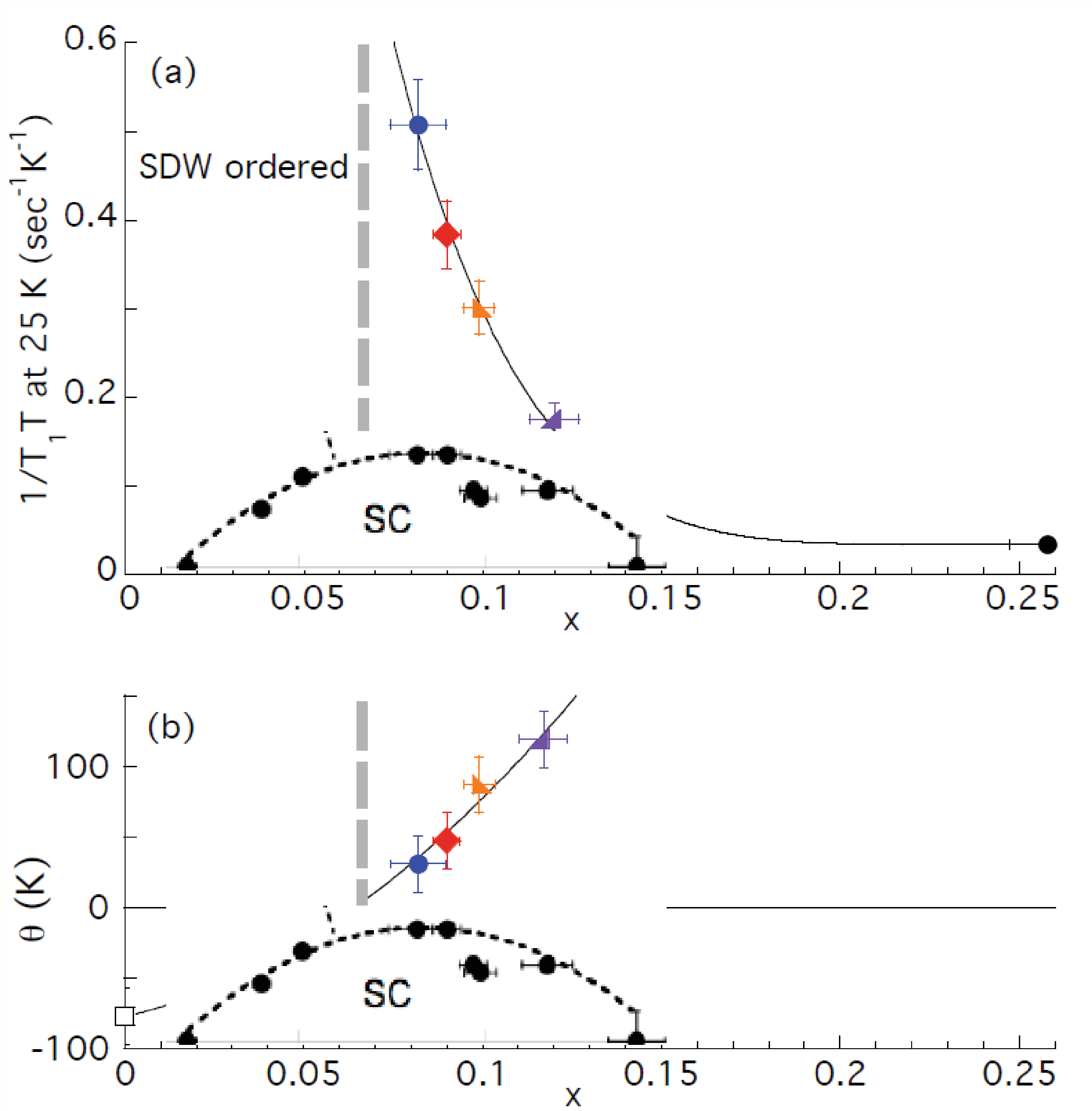


$\theta < 0$: magnetic order

$\theta > 0$: magnetic fluctuations

Ning et al, PRL (2008)

➢ *for a two-dimensional metal near an AFM transition:* $\dfrac{1}{T_1 T} \propto \dfrac{1}{T+\theta}$



$\theta < 0$: magnetic order

$\theta > 0$: magnetic fluctuations

Ning et al, PRL (2008)

How to probe spin fluctuations experimentally?

- Inelastic neutron scattering (INS): directly measurement of the spin-spin correlation function
  - *cross section for the scattered neutrons:*

$$I(\mathbf{q},\omega) \propto \frac{\operatorname{Im}\chi(\mathbf{q},\omega)}{\omega}$$

How to probe spin fluctuations experimentally?

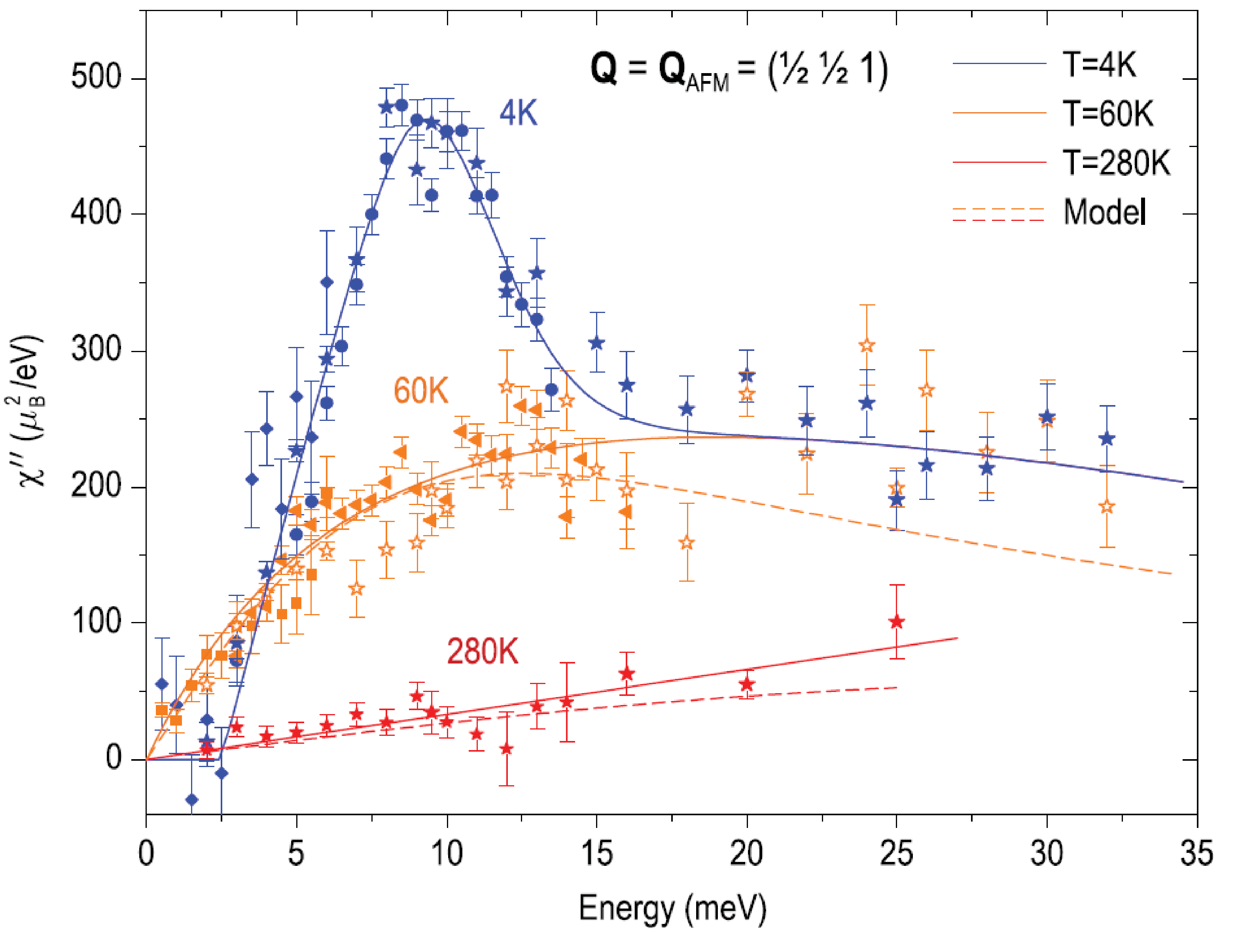
- Inelastic neutron scattering (INS): directly measurement of the spin-spin correlation function
  - *near a metallic AFM transition:*

$$I(\mathbf{q},\omega) \propto \frac{1}{\left(\xi^2 |\mathbf{q}-\mathbf{Q}|^2 + 1\right)^2 + \omega^2 \Gamma^2}$$

width in momentum space gives the magnetic correlation length

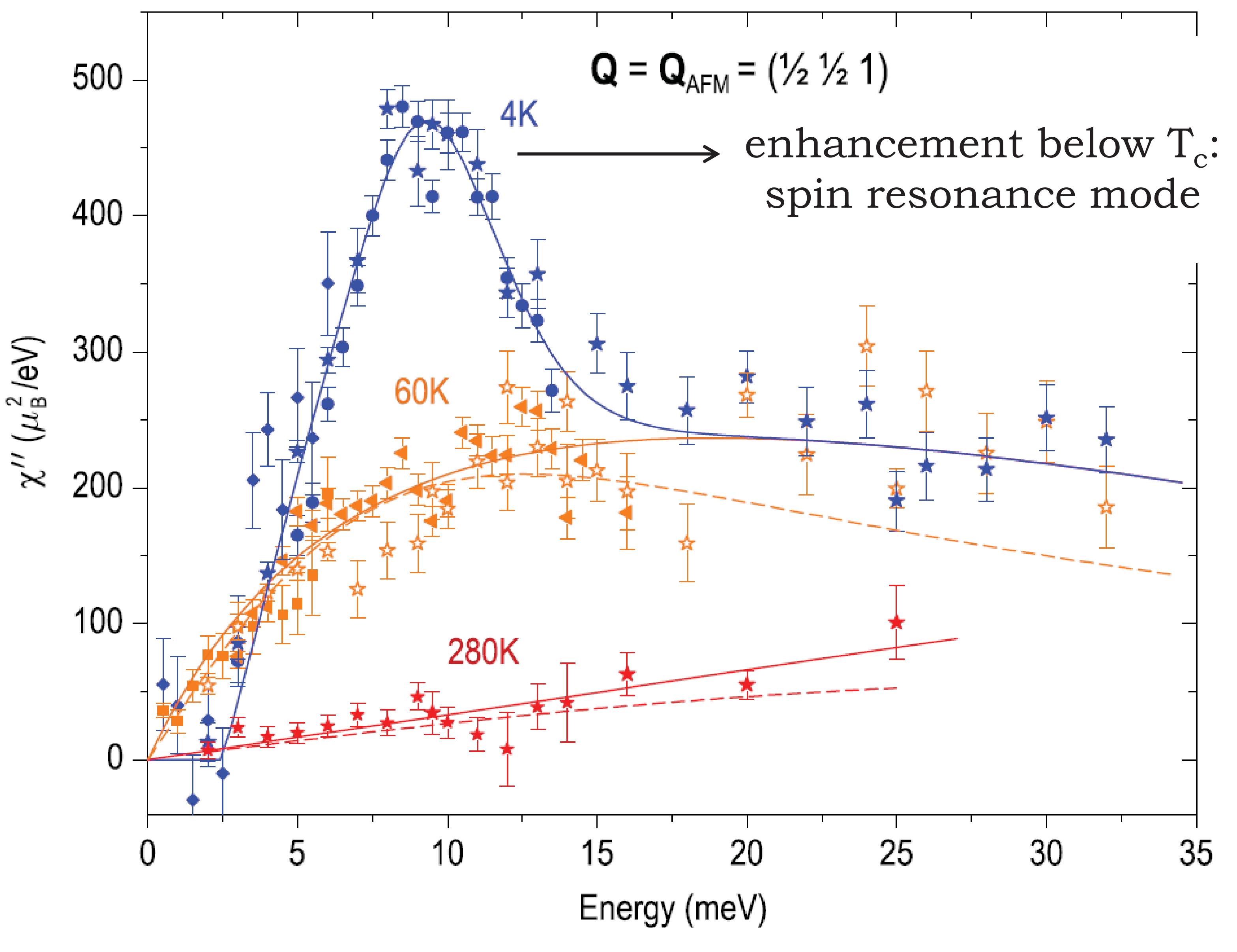
width in energy space gives the Landau damping

$T_c = 25K$ $Ba(Fe_{1-x}Co_x)_2As_2$



Inosov et al, Nature Phys (2009)

$T_c = 25K$ $Ba(Fe_{1-x}Co_x)_2As_2$



Inosov et al, Nature Phys (2009)

How to probe spin fluctuations experimentally?

- Resonance mode is an indirect consequence that the SC gap changes sign across the Fermi surface

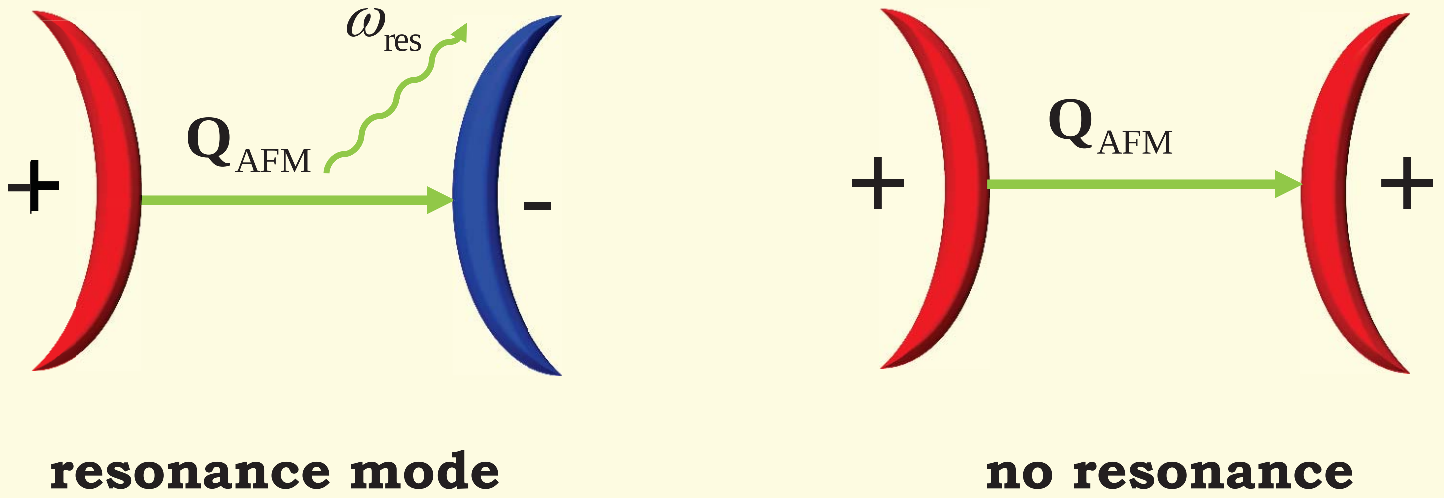


figure from Schmalian, Physik Journal (2011)