Newly Discovered FeAs-Superconductors: Opportunity and Challenge

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Outline

- Historical Review

- Preliminary Experimental Results
  1. High Tc
  2. SDW at undopped state
  3. Multiband SC
  4. Unconventional SC

- Existing Theories
  1. Band Structure calculations: LDA
  2. Proposed Pairing Symmetry
- Our Minimal Model: two-band, d-wave pairing, SDW

- Our Microscopic Model and Calculations: intra- and inter band SF fluctuations

- Outlook

Brief historical introduction

- 1911: Onnes discovered superconductivity (Noble Prize)
- 1933: Meissner effect (Meissner & Ochsenfeld)
- 1934: A two-fluid model (London brothers)
- 1950: Ginzburg-Landau theory (G-L)

1957: Type-I and type-II Superconductor (Noble Prize)

- 1957: Microscopic theory of conventional superconductivity (BCS) (Noble Prize)
- 1962: Josephson effect (Noble Prize)
- 1986: High-Tc superconductors LaBaCuO (Tc ~ 30K) (Bednorz & MÜller) (Noble Prize)
- 1987: $Y_1Ba_2Cu_3O_7$ (Tc ~ 90K, Wu & Chu)
- 1995-1996: D-wave pairing symmetry
- 2001: MgB_2 (Tc ~40K)
- 2003: $NaCoO_2$ (Tc ~ 5K)
- 2008: Fe-As based high Tc superconductivity (discovered by Hosono and pushed by Chinese physicists)

Microscopic BCS Theory for Conventional Superconductivity

$$H = \sum_{k,\sigma} (\varepsilon_k - \mu) C^{+}_{k\sigma} C_{k\sigma}$$

$$+ \sum_{k,k'} V_{kk'} (C^{+}_{k\uparrow} C^{+}_{-k\downarrow} \left\langle C_{-k\downarrow} C_{k\uparrow} \right\rangle_{k'} + h.c.$$

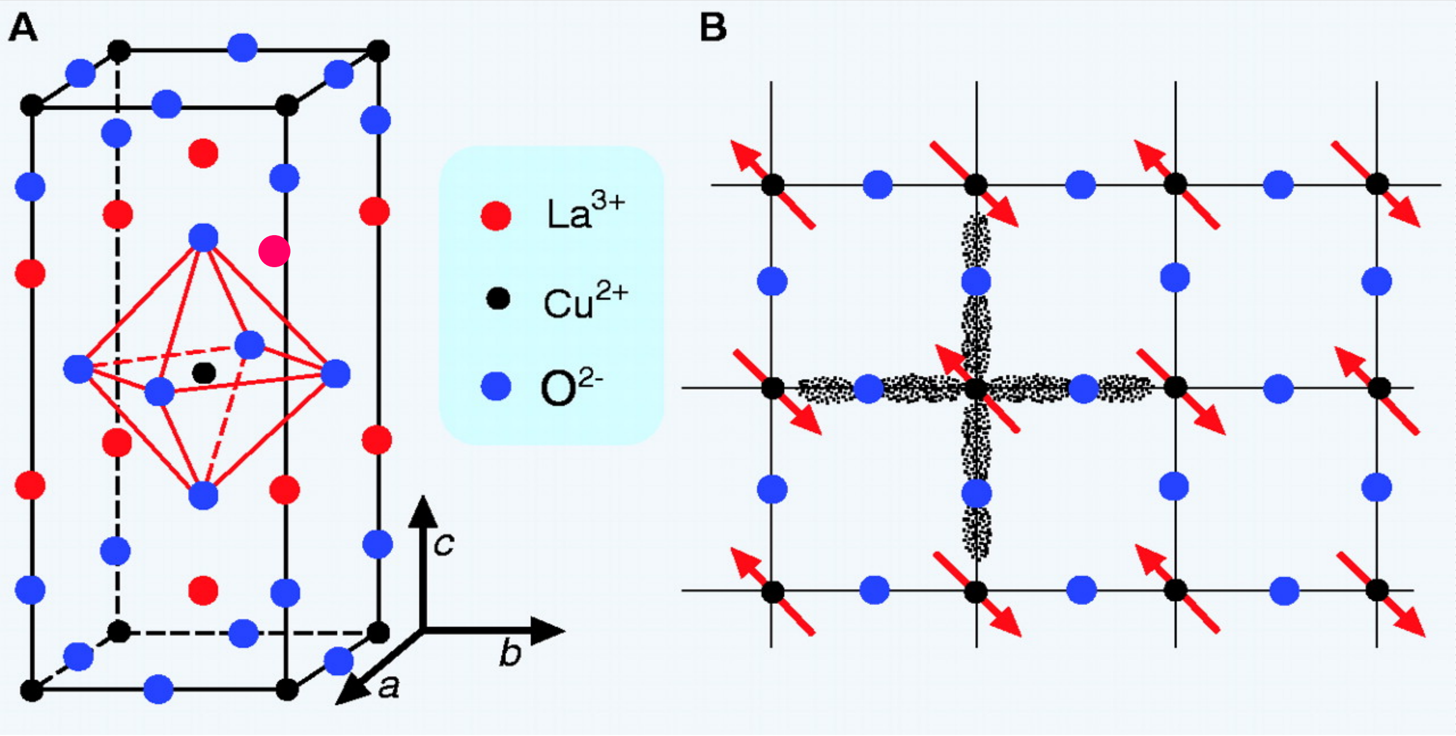
$$- \left\langle C_{-k\downarrow} C_{k\uparrow} \right\rangle_{k}^{*} \left\langle C_{-k'\downarrow} C_{k'\uparrow} \right\rangle_{k'})$$

where

$\left\langle C_{-k\downarrow} C_{k\uparrow} \right\rangle_{k}$ is the Cooper pairing, whose order parameter

$$\Delta = -\sum_{k'} V_{kk'} \left\langle C_{-k'\downarrow} C_{k'\uparrow} \right\rangle_{k'}$$

High-Tc Copper-Oxides

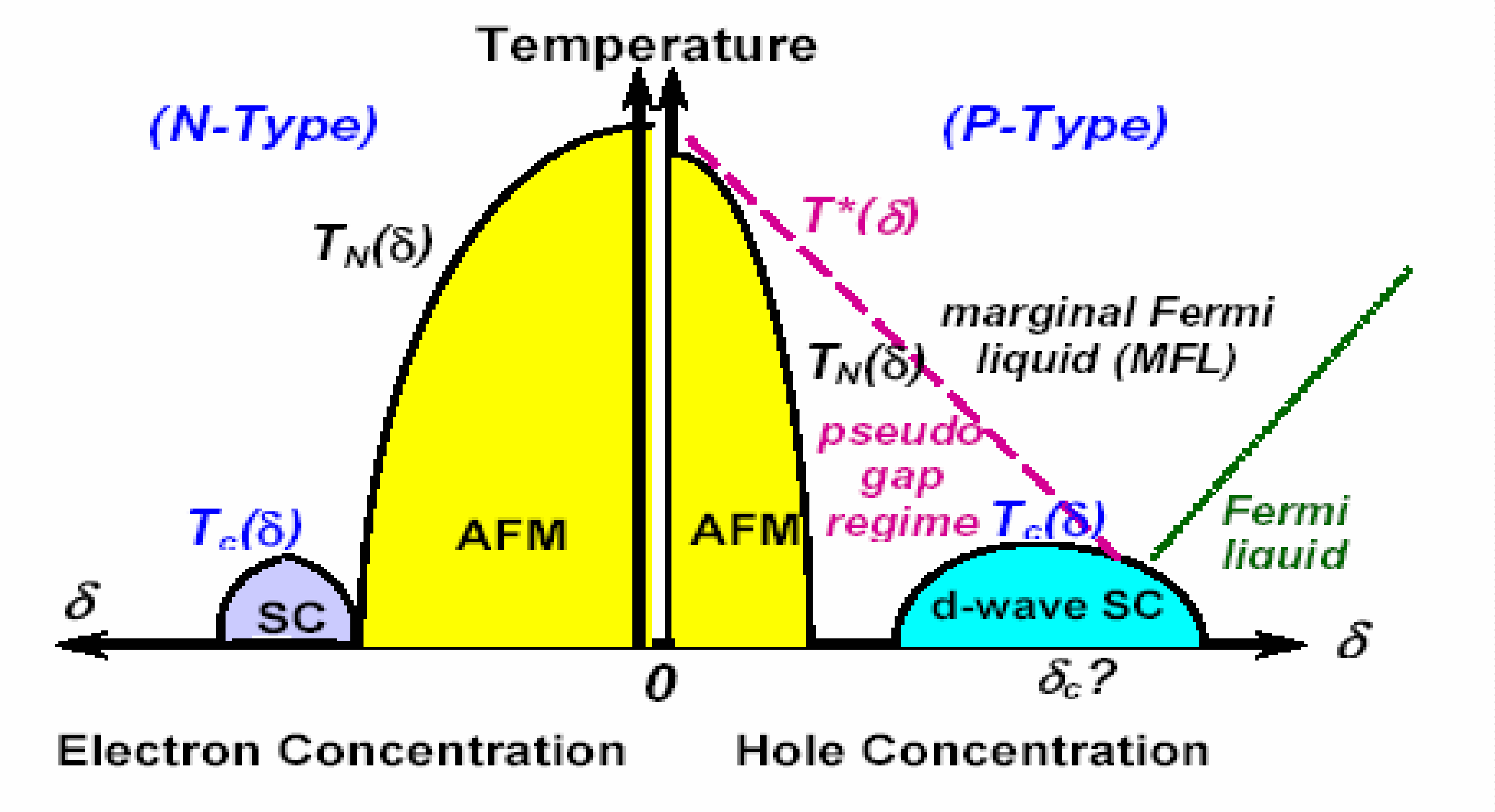


Crystal structure of La_2CuO_4 Schematic of CuO_2 plane

Main Understandings

- Doped Mott Insulators
- Main Physics in CuO_2 Planes
  - Strong electronic correlation
  - AFM spin correlation
- Superconducting state: rather normal; while normal state: abnormal;
- An Acceptable Microscopic theory is still awaited

Schematic Phase Diagram



Fe-As SC: Experimental Results (I)

- Higher Tc

  Electron-doped Materials:

  $LaO_{0.9}F_{0.1}FeAs$ 26K

  $CeO_{1-x}F_xFeAs$ 41K, $SmO_{1-x}F_xFeAs$ 43K

  $PrO_{0.89}F_{0.11}FeAs$ 52K, …$ReFeAsO_{1-x}$ 55K

  Hole-doped Materials:

  $La_{1-x}Sr_xOFeAs$ 25K, etc.

Crystal Structure of LaOFeAsF

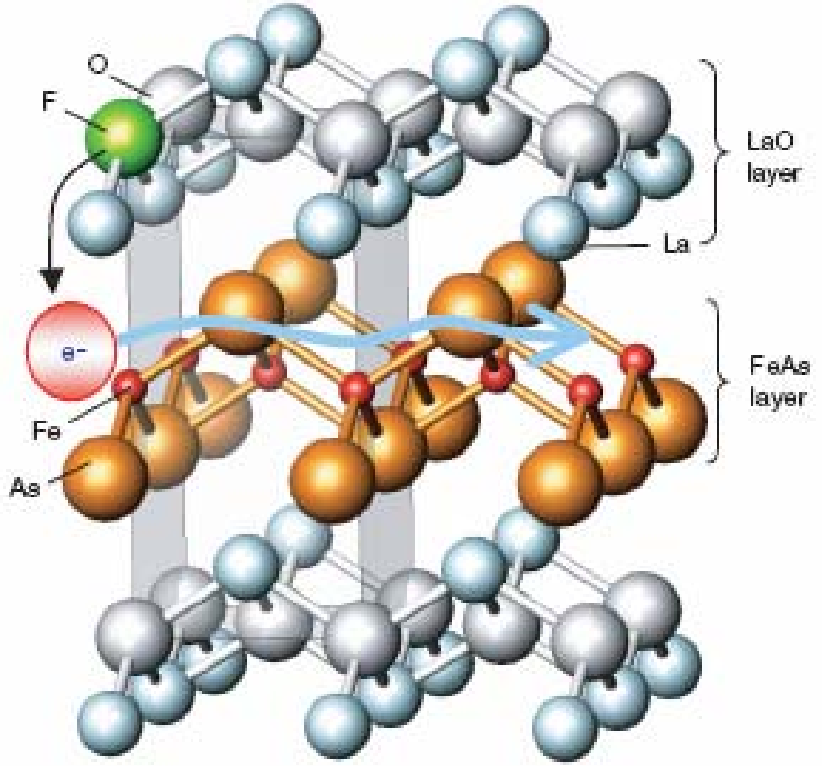
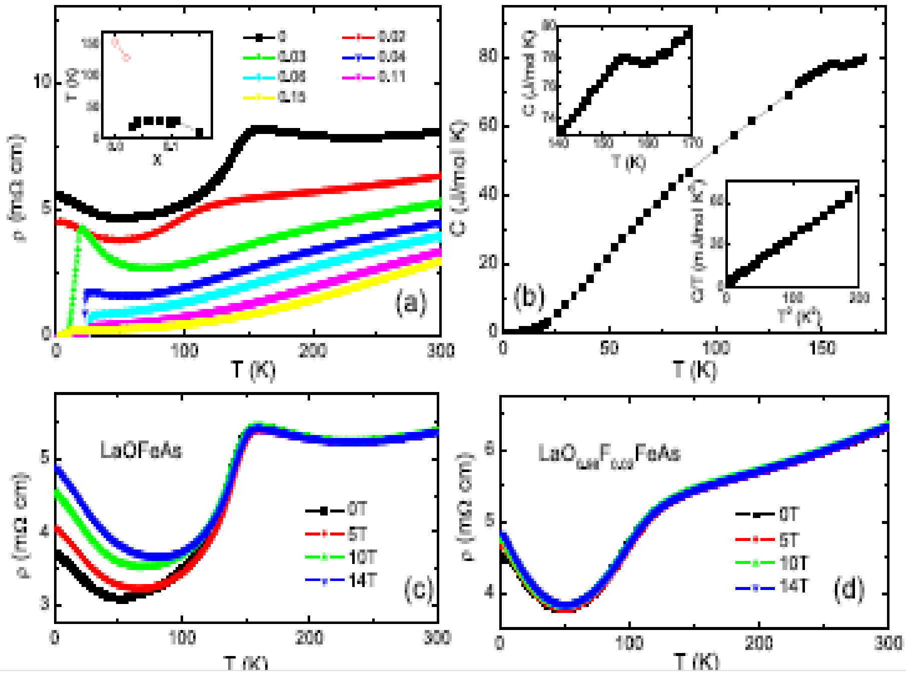


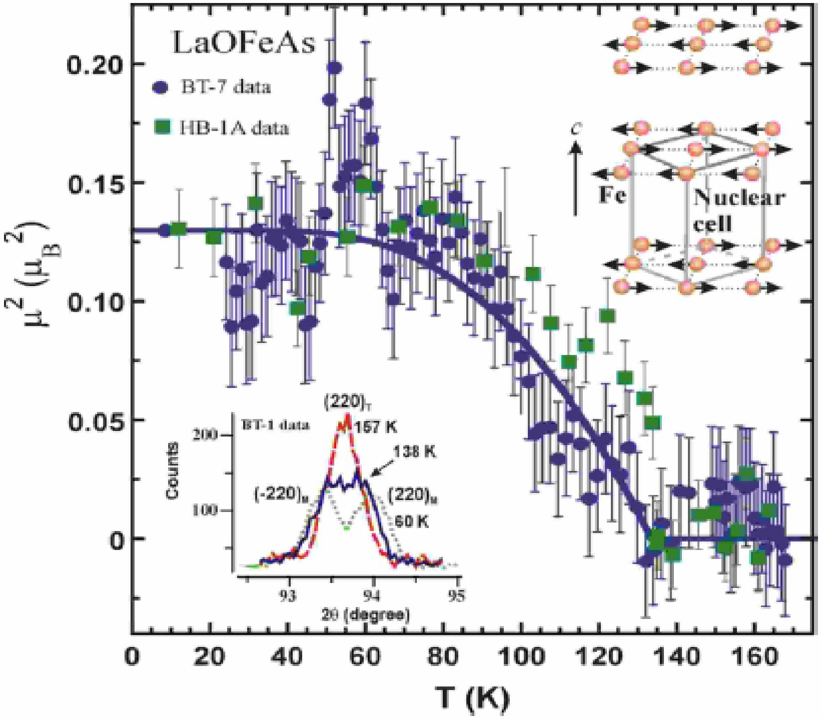
Figure 1 | Schematic crystal structure of LaOFeAs. Electron carriers generated by F-doping into oxygen sites are injected into FeAs metallic layers as a result of the large energy offset between these two layers. We note that the carrier doping layer is spatially separated from the conduction layer.

Experimental Results (II)

- SDW in the normal state



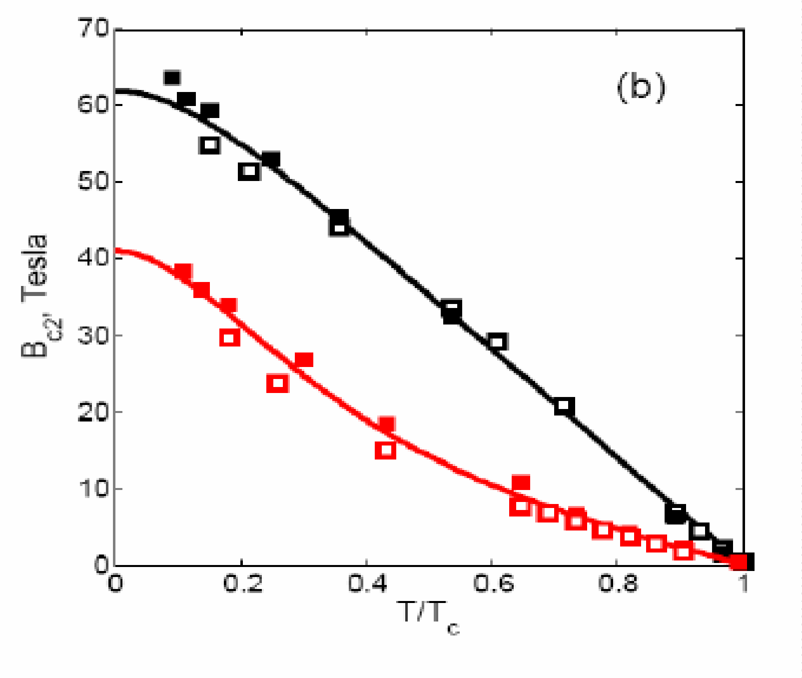
Reflective Optical Spectroscopy



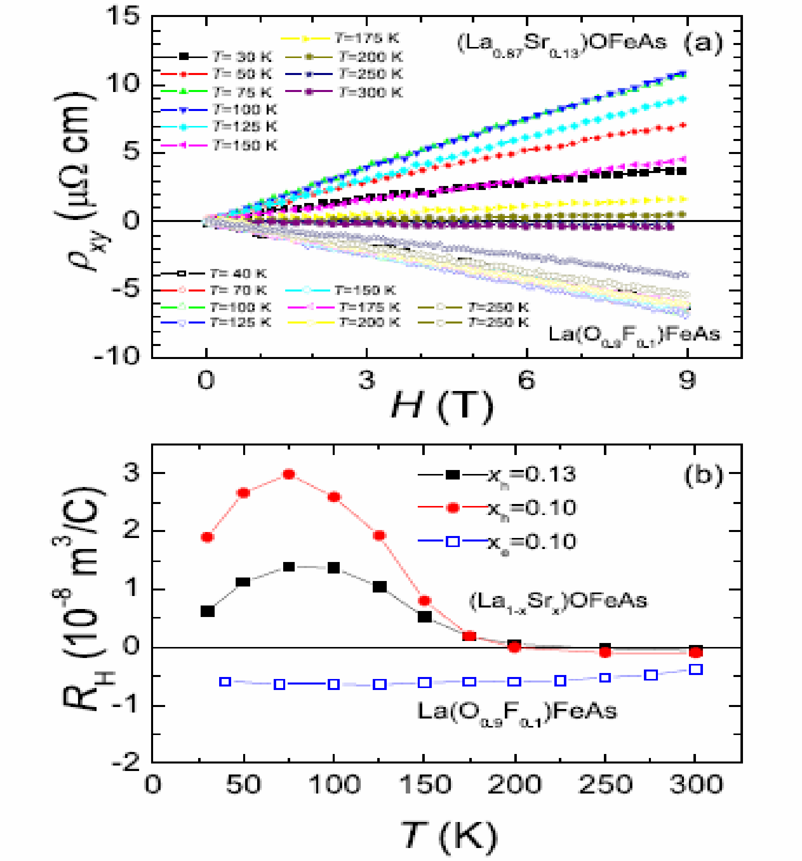
Neutron scattering data

Experimental Results (III)

- ☐ Multiband Effect



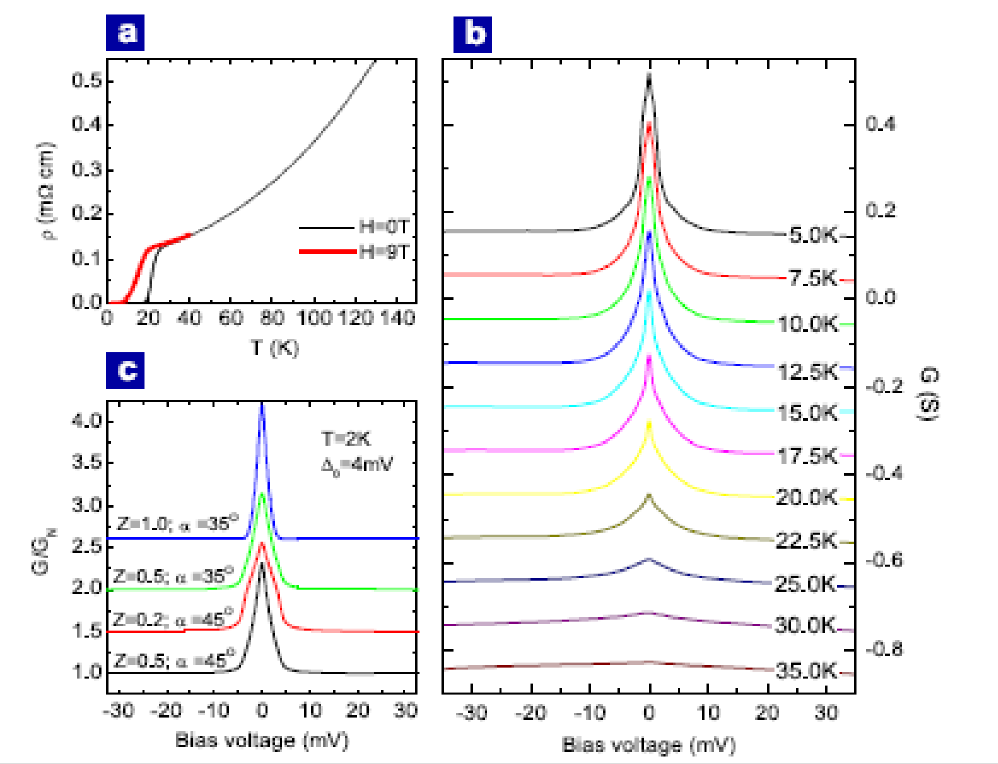
The lines corresponds to Bc2(T) calculated from the two-gap theory.

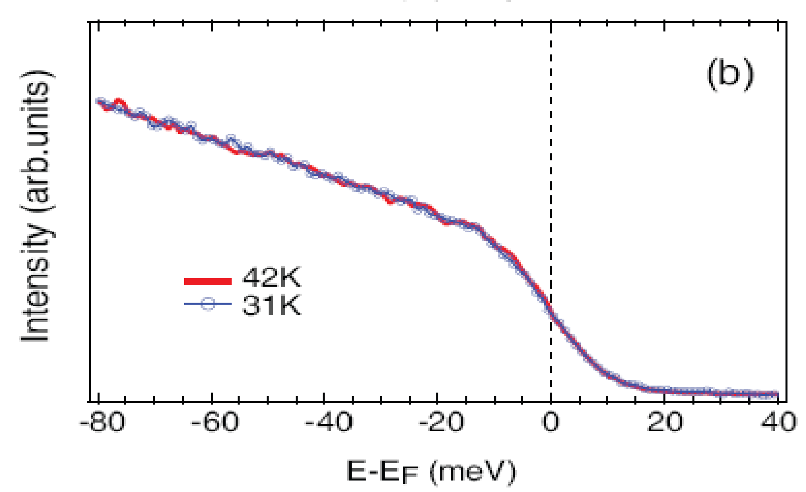


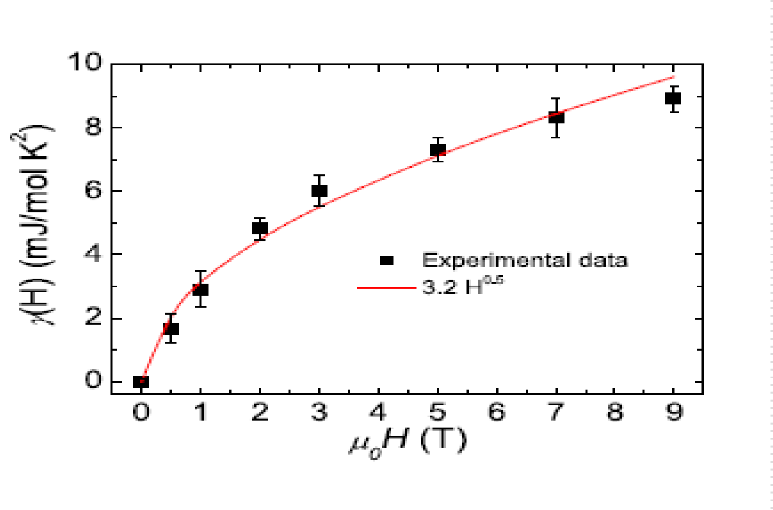
Temperature dependence of Hall resistivity was observed which may suggest a strong multiband effect in the electron-doped and hole-doped samples.

Experimental Results (IV)

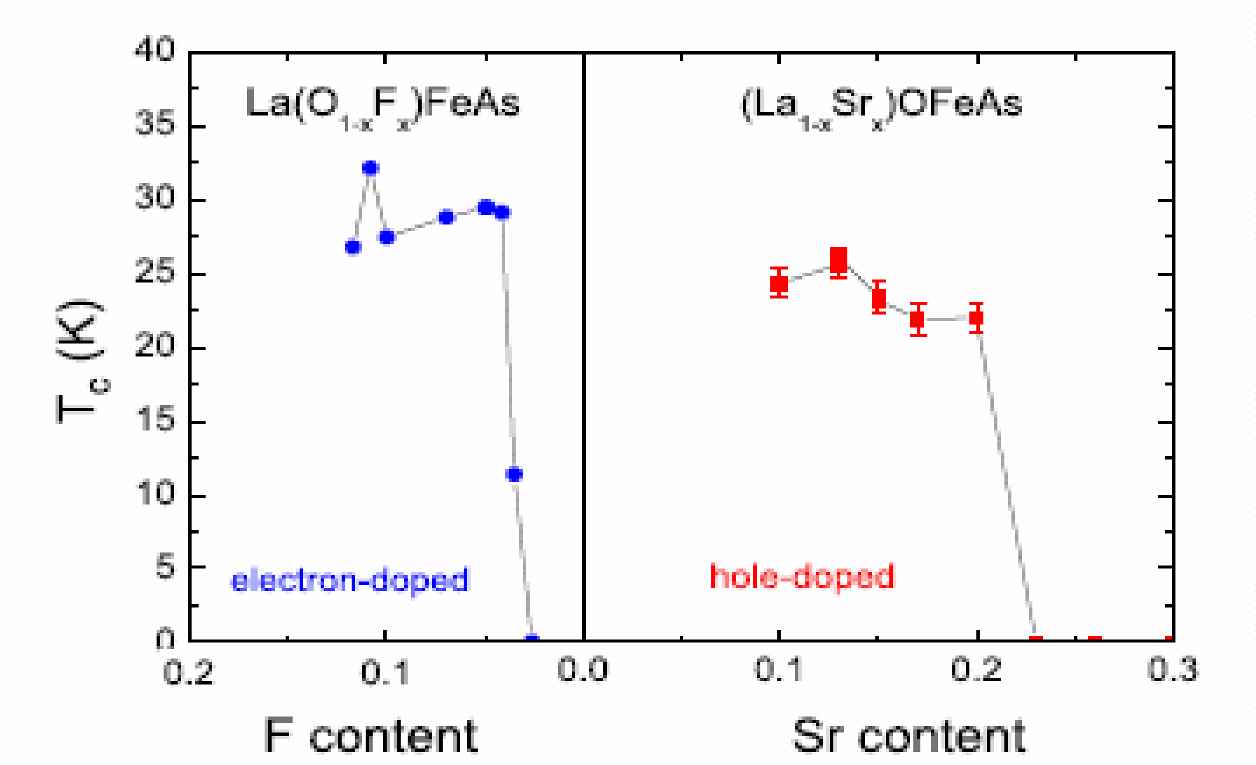
- Unconventional SC



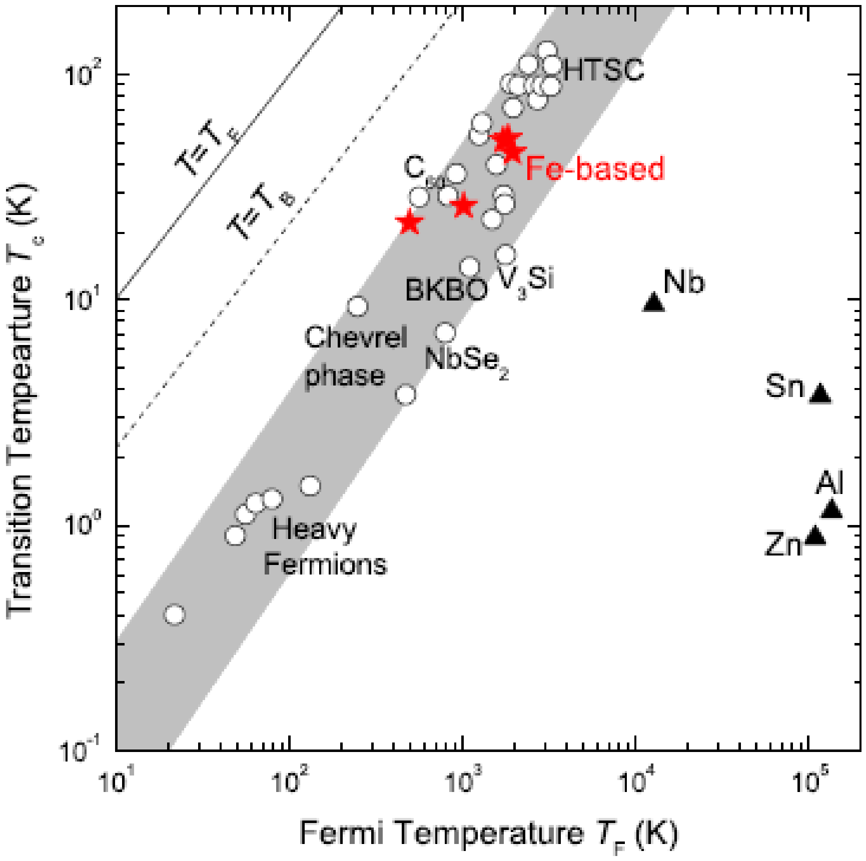




- Symmetric Phase Diagram (Electron-doping vs hole-doping)



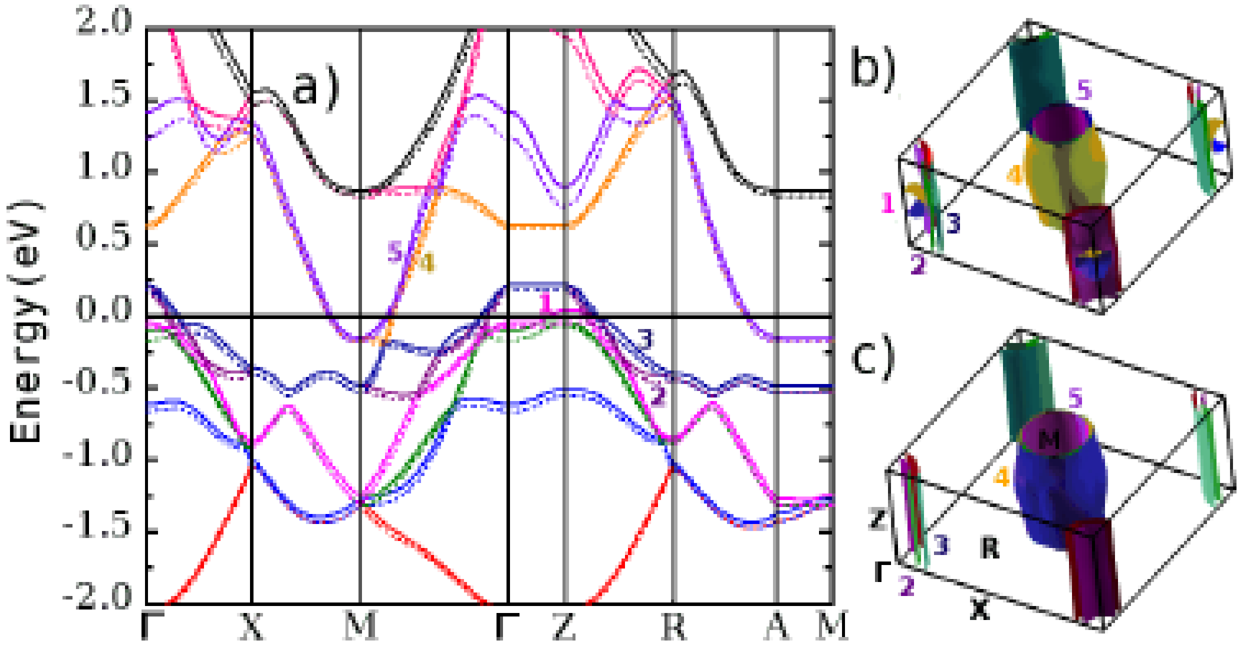
Tc vs TF_of unconventional superconductors (grey region)



Band Structure Calculations (LDA, DMFT)

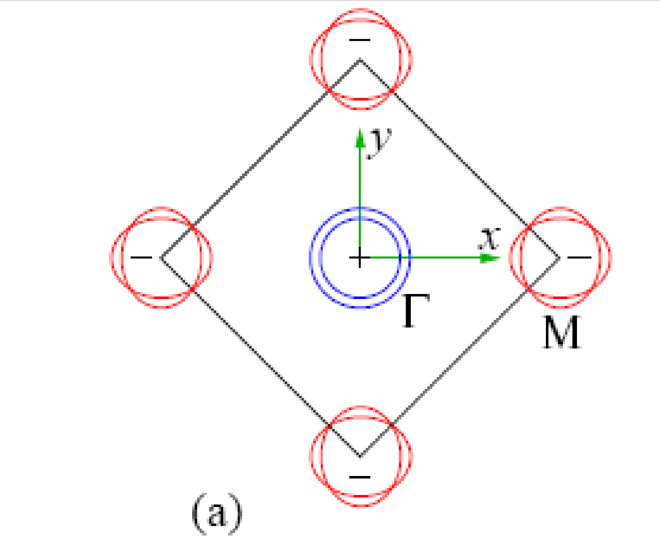
- LDA (nonmagnetic structures)

F-doping). The Fermi energy sets to zero.



Proposed Pairing Symmetry

- Extended s-wave
- Spin-triplet p-wave
- Spin-triplet orbit-singlet s-wave



Extended s-wave:
FS pockets located around Γ and around M, SC order parameters on the two sets of the FSs have the opposite signs.

Our Work and Main Findings

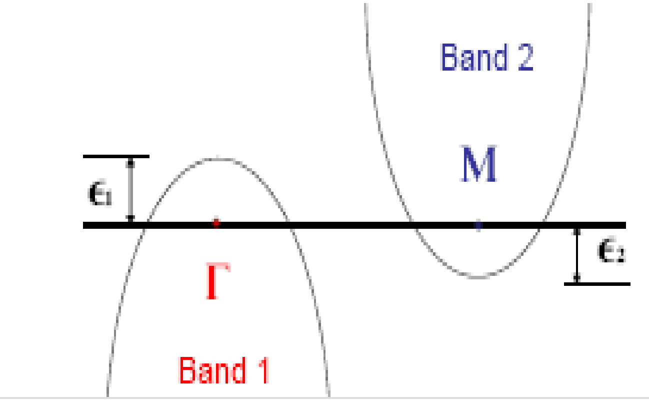
(1) Han, Chen, Wang, EPL 82, 37007 (2008); arXiv: 0803.4346
(2) Yao, Li, Wang, arXiv: 0804.4166 (2008)

- The normal state has an SDW order ($Q=(\pi, \pi)$), while upon the charge carrier doping the SDW order drops rapidly and the SC order emerges
- due to the two-band (electron and hole) SC nature of the material, Tc as a function of the effective doping density shows a nearly symmetric electron-hole doping dependence
- two-band superconducting state exhibits a d-wave symmetry (SDW fluctuations)
- Fluctuation-exchange approach on a microscopic two-band model yields quantitative results, supporting strongly our simple effective two-band model

Our Minimal Model

- 2-band BCS d-wave pairing + intraband Hubbard interaction

$$
\begin{aligned}
H = & \sum_{k\sigma} \xi_{1k} c^{+}_{k\sigma} c_{k\sigma} + \sum_{k\sigma} \xi_{2k} d^{+}_{k\sigma} d_{k\sigma} + U_{eff} \sum_{i\sigma} n_{1i\sigma} n_{2i\bar{\sigma}} \\
& + \sum_{kk'} V^{11}_{kk'} c^{+}_{k'\uparrow} c^{+}_{-k'\downarrow} c_{-k\uparrow} c_{k\downarrow} + \sum_{kk'} V^{22}_{kk'} d^{+}_{k'\uparrow} d^{+}_{-k'\downarrow} d_{-k\uparrow} d_{k\downarrow} \\
& + \sum_{kk'} (V^{12}_{kk'} c^{+}_{k'\uparrow} c^{+}_{-k'\downarrow} d_{-k\uparrow} d_{k\downarrow} + h.c.)
\end{aligned}
$$



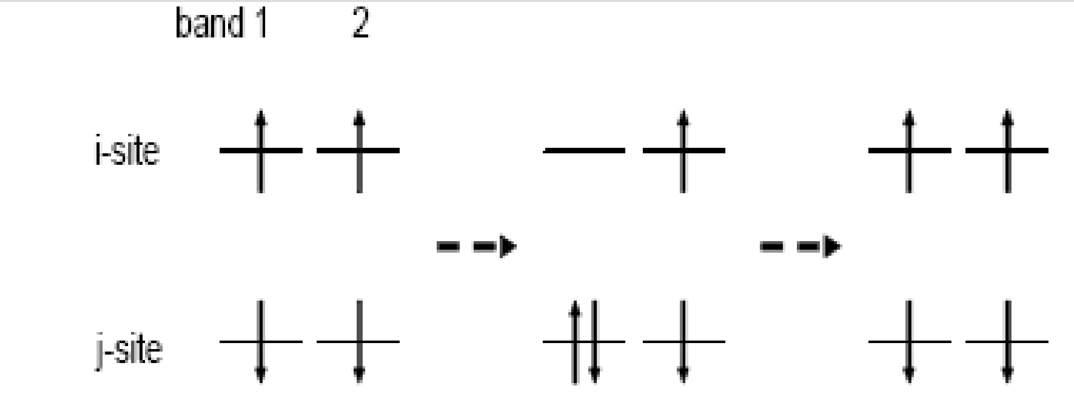
$$DOS : \rho_{1,2} = 1/(4\pi t_{1,2}), W_{h,e} = 1/\rho_{1,2}$$

$$n_h^0 = 2\rho_1 \varepsilon_0^{(1)}, n_e^0 = 2\rho_2 \varepsilon_0^{(2)}$$

Double-degenerated with each for one Fe-sublattice

Origin of the SC Pairing

$$H_i = U\sum_{l\sigma} n_{il\sigma} n_{il\bar{\sigma}} + U'\sum_{\sigma\sigma'} n_{i1\sigma} n_{i2\sigma'} + J_H \vec{\sigma}_{i1} \bullet \vec{\sigma}_{i2}$$



→ Intraband AF fluctuation → Intraband d-wave SC

Origin of SDW Order

- Condensate of bound electron-hole pairs “excitons”

$$1 = U_{eff}\chi_0^{12}(Q), \chi_0^{12}(Q) = -\sum_k \frac{f(\xi_{1k}) - f(\xi_{2k+Q})}{\xi_{1k} - \xi_{2k+Q}}$$

To obtain a simple analytical formula of T_{SDW} , we set $m_1=m_2$ and $\varepsilon_1=\varepsilon_2=\varepsilon_0$, where the prefect nesting With $Q=(\pi,\pi)$ between the two bands occurs at the undoped case ($\mu=0$).

$$\frac{T_{SDW}}{W} \approx \frac{2e^{\gamma}}{\pi}\sqrt{\frac{\varepsilon_0}{W}(1-\frac{\varepsilon_0}{W})}e^{-(Ueff/W)^{-1}} e^{-1.71(\frac{W}{8T_{SDW}}x)^2}, \gamma \approx 0.577$$

SDW State

- Below T_{SDW}, the SDW ordering emerges, SDW order parameter is defined as

$$\Delta_{SDW} = U_{eff} \sum_{k} \langle c_{k\uparrow} d^{+}_{k+Q\downarrow} \rangle$$

$$1 = -U_{eff} \sum_{k} \frac{f(\eta_{2k} + \Omega_k) - f(\eta_{2k} - \Omega_k)}{2\Omega_k},$$

$$\Omega_k = \sqrt{\eta_{1k}^2 + \Delta_{SDW}^2}, \eta_{1k} = (\xi_{1k} - \xi_{2k+Q})/2, \eta_{2k} = (\xi_{1k} + \xi_{2k+Q})/2$$

SDW State

- Counterpart of Cooper electron-electron pair

$$2\Delta_{SDW} / T_{SDW} \approx 3.53 (BCS.result)$$

According to optical conductivity spectra,

$$2\Delta_{SDW}(8K) \approx 350 cm^{-1} = 504K, T_{SDW} \approx 150K$$

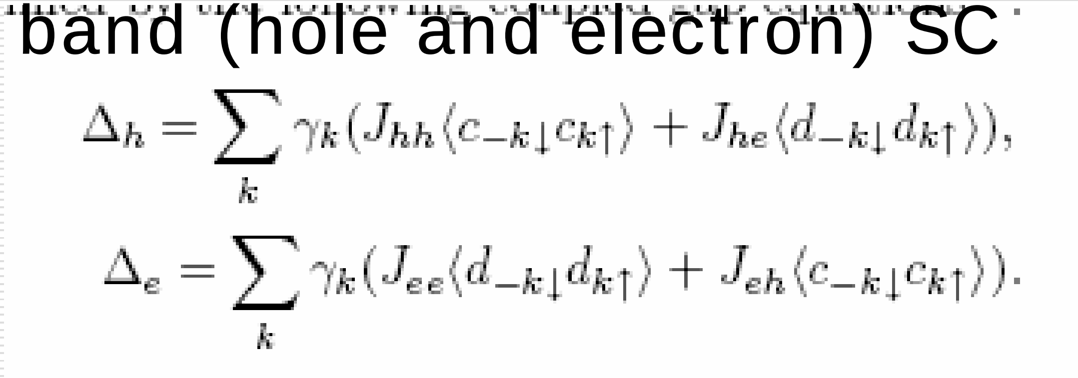
$$so..2\Delta_{SDW}(8K) / T_{SDW} \approx 3.4$$

The AF moment/Fe is estimated ~0.31, (exp. ~0.36) ;

T_{SDW} decreases with the shrinkage of lattice.

SC State

- Two band (hole and electron) SC



$$\Delta_h = \sum_k \gamma_k \left(J_{hh}\langle c_{-k\downarrow} c_{k\uparrow}\rangle + J_{he}\langle d_{-k\downarrow} d_{k\uparrow}\rangle\right),$$

$$\Delta_e = \sum_k \gamma_k \left(J_{ee}\langle d_{-k\downarrow} d_{k\uparrow}\rangle + J_{eh}\langle c_{-k\downarrow} c_{k\uparrow}\rangle\right).$$

At Tc, we have linearized gap equation,

$$\begin{pmatrix} J_{hh}K_1 & J_{he}K_2 \\ J_{eh}K_1 & J_{ee}K_2 \end{pmatrix}\begin{pmatrix} \Delta_h \\ \Delta_e \end{pmatrix} = \begin{pmatrix} \Delta_h \\ \Delta_e \end{pmatrix}, K_{1,2} = \sum_k \frac{\tanh(\xi_{1,2k}/2T_c)}{2\xi_{1,2k}}\gamma_k^2$$

Non-zero solution, for Tc

$$\det\begin{pmatrix} J_{hh}K_1 - 1 & J_{he}K_2 \\ J_{eh}K_1 & J_{ee}K_2 - 1 \end{pmatrix} = 0$$

SC State

- General case: $J_{ee}, J_{hh} > 0$, $J_{ee}J_{hh}$‡$J_{eh}J_{he} > 0$.

$$\breve{J}_{hh}=J_{hh}/W_h, \breve{J}_{ee}=J_{ee}/W_e, \breve{J}_{eh}^2=(J_{eh}J_{he})/W_eW_h, \breve{J}\breve{J}=\breve{J}_{eh}\breve{J}_{he}-\breve{J}_{ee}\breve{J}_{hh}$$

We obtain,

$$\frac{T_c}{\sqrt{W_eW_h}}=\frac{e^{\gamma}}{\pi}[n_en_h(2-n_e)(2-n_h)]^{1/4}e^{-\frac{1}{\lambda_{eff}}}, where$$

$$\frac{1}{\lambda_{eff}}=\{[(\frac{1}{4}\breve{J}\breve{J}\ln\frac{n_e(2-n_e)W_e^2}{n_h(2-n_h)W_h^2}+\frac{\breve{J}_{hh}-\breve{J}_{ee}}{2})^2+\breve{J}_{eh}\breve{J}_{he}]^{1/2}-\frac{1}{2}(\breve{J}_{hh}+\breve{J}_{ee})\}/\breve{J}\breve{J}$$

SC State

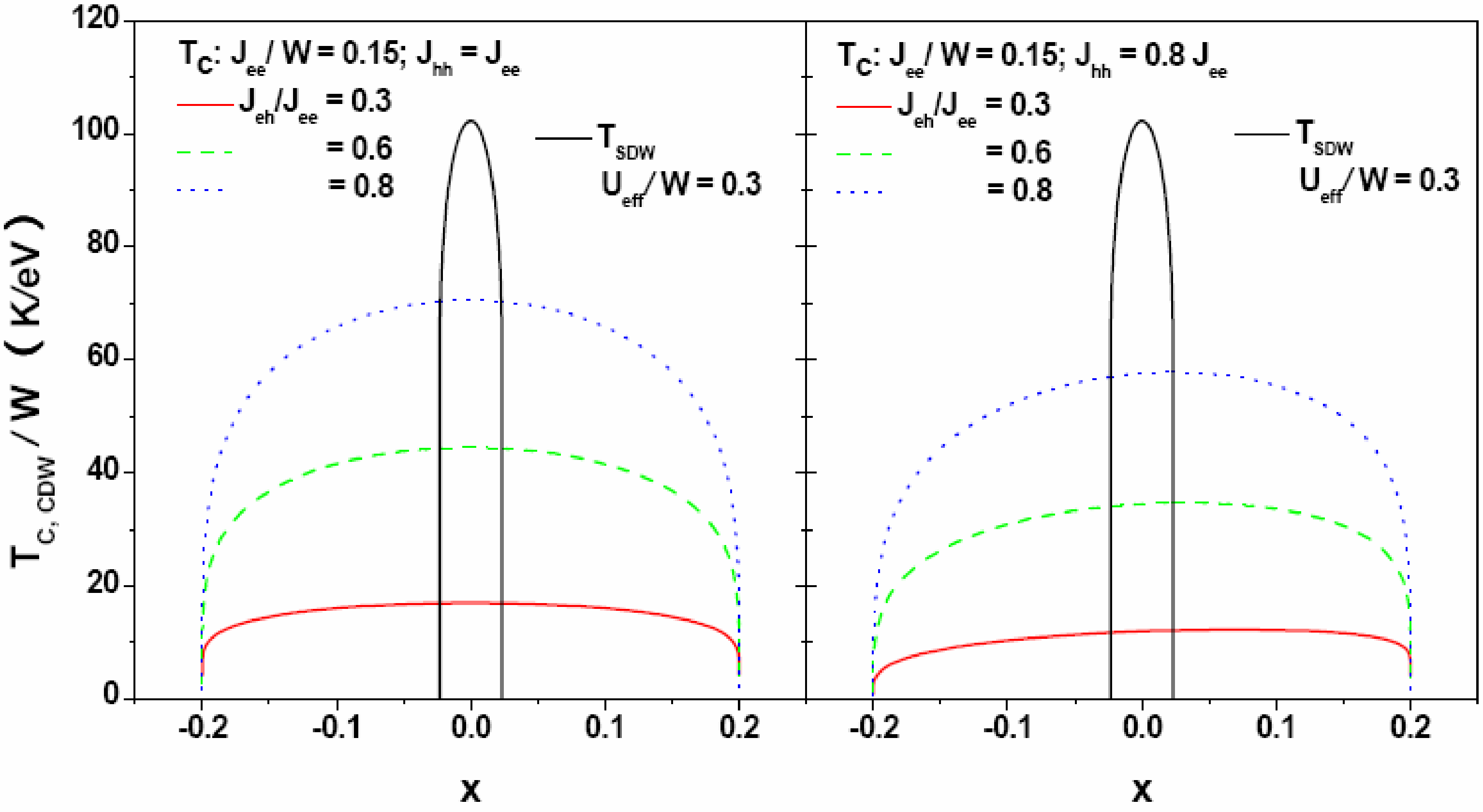
- Special case: $J_{eh}J_{he}=J_{ee}J_{hh}$.

$$\frac{T_c}{\sqrt{W_eW_h}}=\frac{e^{\gamma}}{\pi}\left(\sqrt{\frac{W_e}{W_h}}\right)^{\frac{\breve{J}_{ee}-\breve{J}_{hh}}{\breve{J}_{ee}+\breve{J}_{hh}}}\left[\sqrt{n_e(2-n_e)}\right]^{\frac{\breve{J}_{ee}}{\breve{J}_{ee}+\breve{J}_{hh}}}\left[\sqrt{n_h(2-n_h)}\right]^{\frac{\breve{J}_{hh}}{\breve{J}_{ee}+\breve{J}_{hh}}}e^{-\frac{1}{\breve{J}_{ee}+\breve{J}_{hh}}}$$

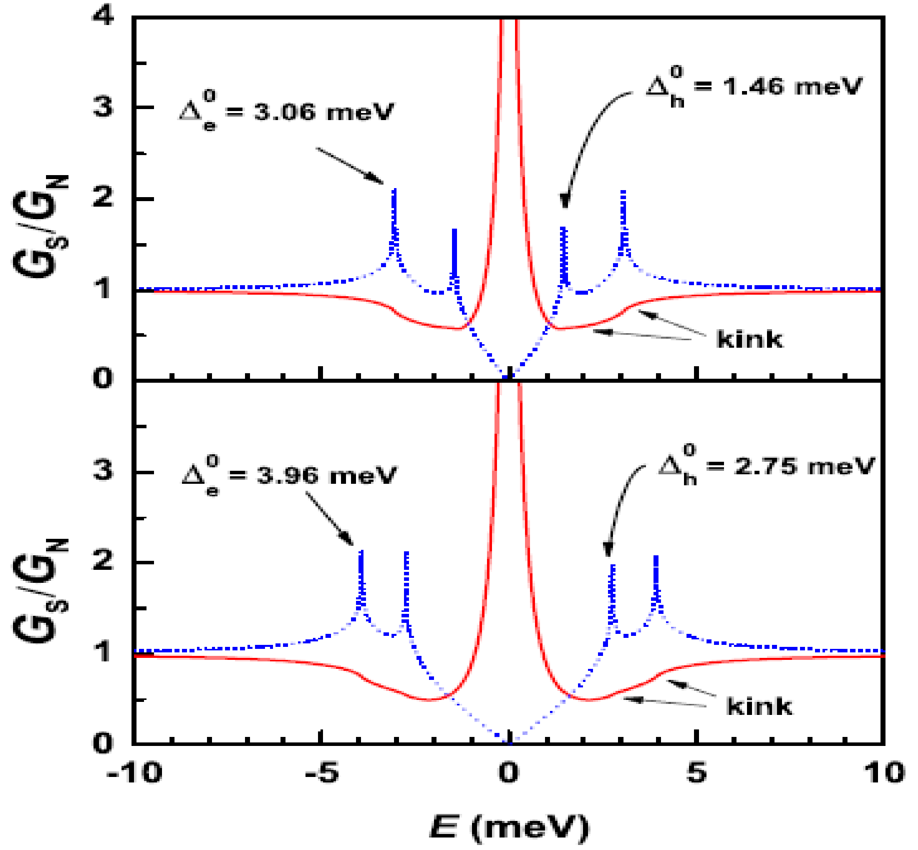
We choose the parameters as,

$$W_e=W_h=W,U_{eff}/W=0.3,J_{eh}/W=0.15,\varepsilon_0^{1,2}=0.05W$$

Phase Diagram



Zero-bias Coherent Peak



Nodal d-wave pairing
(two gaps behavior)

Useful Relations

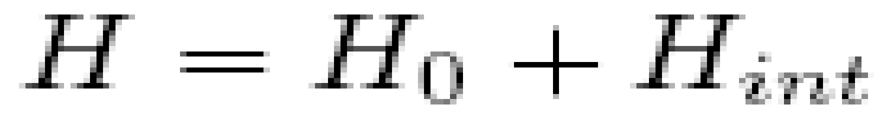
$$\frac{|-\ln(|\Delta_h^0|/T_c)+C_0-C_{T_c}|}{|-\ln(|\Delta_e^0|/T_c)+C_0-C_{T_c}|}\times|r_0r_c|=\frac{W_h}{W_e},$$

where $r_{0,c}=r(0),r(T_c)$ are respectively the above introduced gap ratio at zero and transition temperatures.

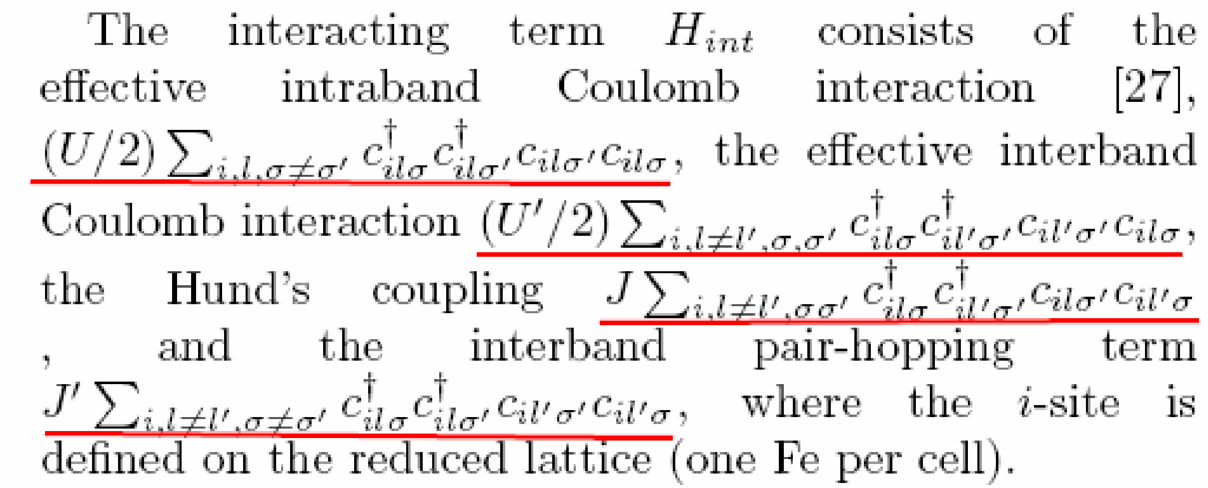
$$\frac{\ln|r_0|}{[1+(W_h/W_e)|r_0r_c|^{-1}](|r_c|-|r_0|)}=\frac{|J_{eh}|/W_h}{\tilde{J}_{eh}^2-\tilde{J}_{ee}\tilde{J}_{hh}}.$$

II. FLEX Results

- Microscopic Model Hamiltonian

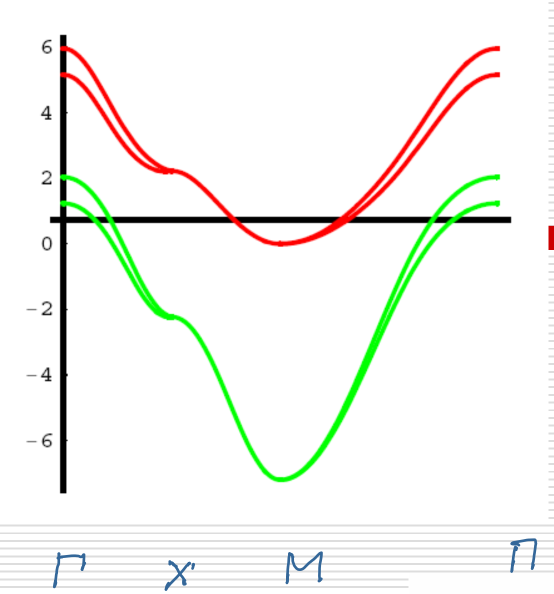


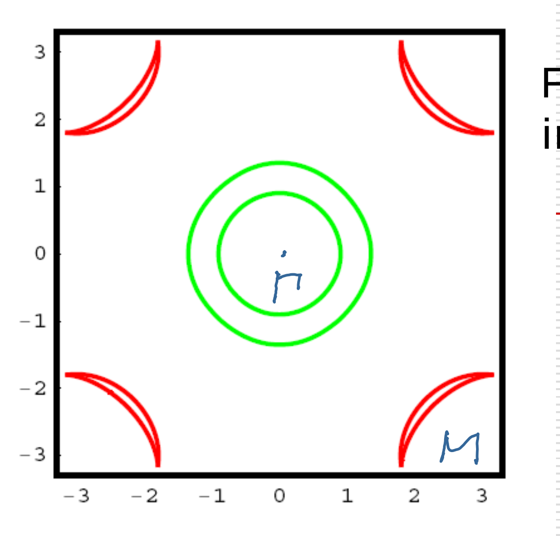
$$H = H_0 + H_{int}$$



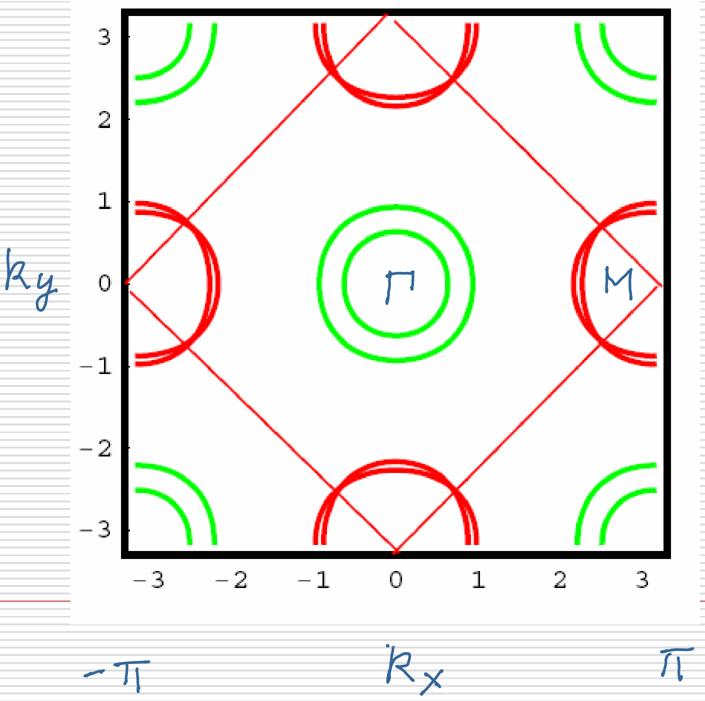
The interacting term H_{int} consists of the effective intraband Coulomb interaction [27], $(U/2)\sum_{i,l,\sigma\neq\sigma'} c^{\dagger}_{il\sigma} c^{\dagger}_{il\sigma'} c_{il\sigma'} c_{il\sigma}$, the effective interband Coulomb interaction $(U'/2)\sum_{i,l\neq l',\sigma,\sigma'} c^{\dagger}_{il\sigma} c^{\dagger}_{il'\sigma'} c_{il'\sigma'} c_{il\sigma}$, the Hund's coupling $J\sum_{i,l\neq l',\sigma\sigma'} c^{\dagger}_{il\sigma} c^{\dagger}_{il'\sigma'} c_{il\sigma'} c_{il'\sigma}$, and the interband pair-hopping term $J'\sum_{i,l\neq l',\sigma\neq\sigma'} c^{\dagger}_{il\sigma} c^{\dagger}_{il\sigma'} c_{il'\sigma'} c_{il'\sigma}$, where the i-site is defined on the reduced lattice (one Fe per cell).

Two-band structure in the reduced (original) BZ





Fermi pockets in the BZ



Fermi pockets in the extended BZ

Spin susceptibility

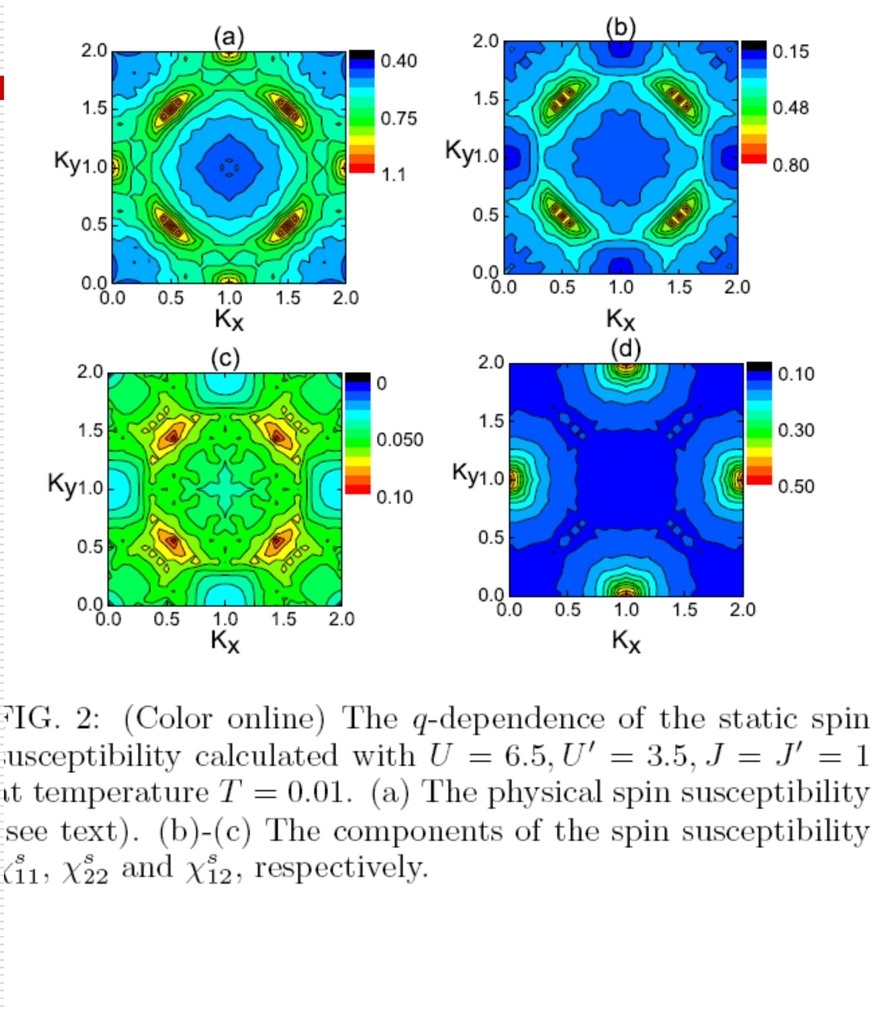


FIG. 2: (Color online) The q-dependence of the static spin susceptibility calculated with $U = 6.5, U' = 3.5, J = J' = 1$ at temperature $T = 0.01$. (a) The physical spin susceptibility (see text). (b)-(c) The components of the spin susceptibility χ^s_{11}, χ^s_{22} and χ^s_{12}, respectively.

Superconducting pairing

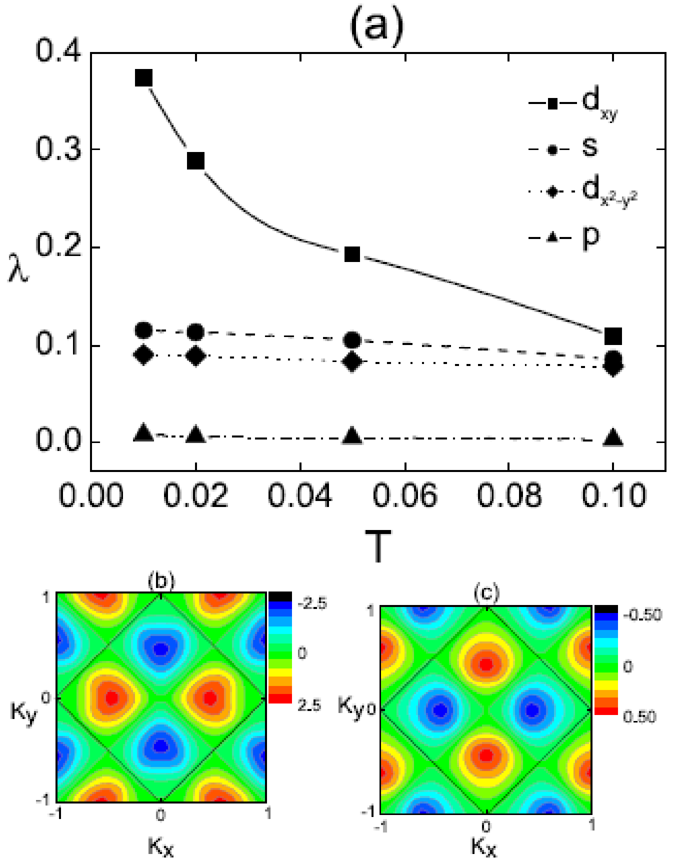


FIG. 3: (Color online) (a) Temperature dependence of the maximum eigenvalues for $U = 6.5, U' = 3.5, J = J' = 1.0$. (c) and (d): Momentum dependence of the gap functions $\Delta_{11,22}(k)$ corresponding to the largest eigenvalue at temperature $T = 0.01$.

Outlook

1. Origin of Fe-As Superconductivity: electron-electron interaction? If yes, intraband or interband SF fluctuations? Or both? Or doped Mott physics?
2. Pairing symmetry: s-, d-, or p- wave ? To be determined by experiments on single crystals(?)
3. Profound understandings on the above two key points may provide some clue to resolve a long standing issue of copper oxide SC mechanism.
4. Even higher Tc above 77K?
5. Novel phenomena and physics?
6. Applications?

Superconductors *redux*

Yet another surprise has been uncovered in the complex oxides.

Thank you!