Microscopic nematicity in iron superconductors

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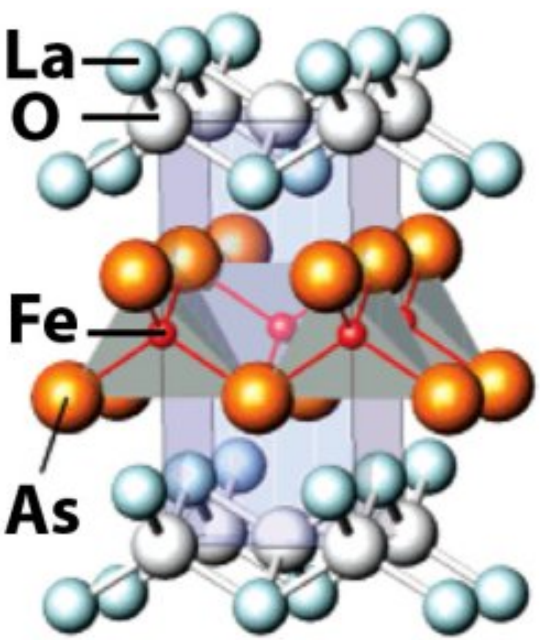
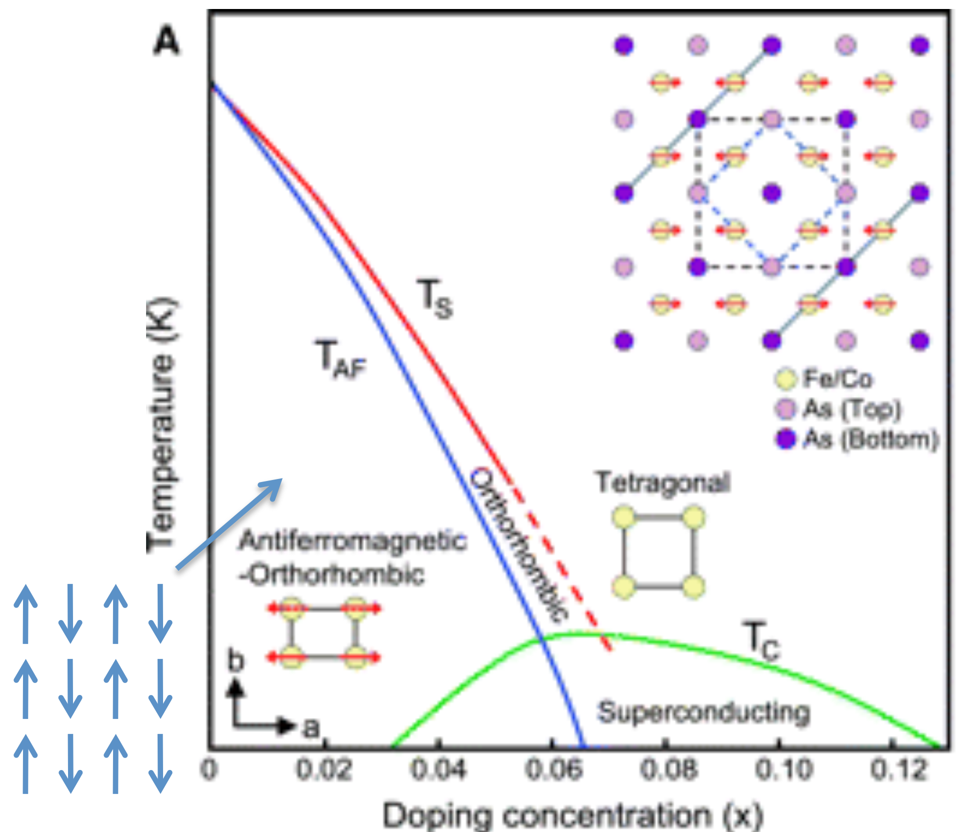
- Introduction: Iron superconductors and the nematic phase
- Theoretical proposal, spin nematic: effective action without information about the orbital degree of freedom. Multiorbital Hamiltonian (vortex)
- Our proposal: An effective action derived from a multiorbital Hamiltonian
  - Magnetic susceptibility
- Conclusions

Iron pnictides: Crystal structure and phase diagram



Kamihara'08



$(\pi,0)$ AF

High Tc SC on As-Fe layers

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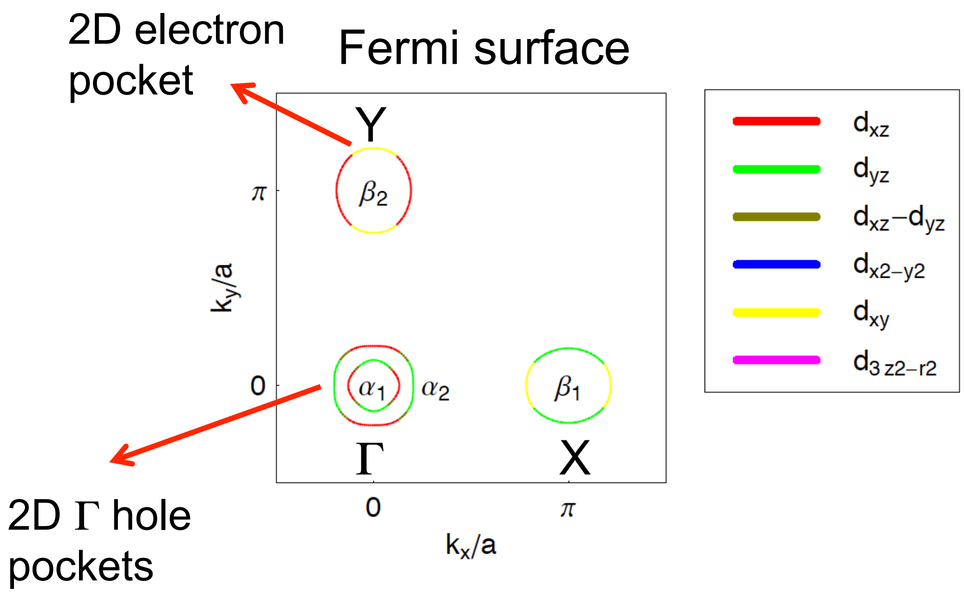
Multiorbital system

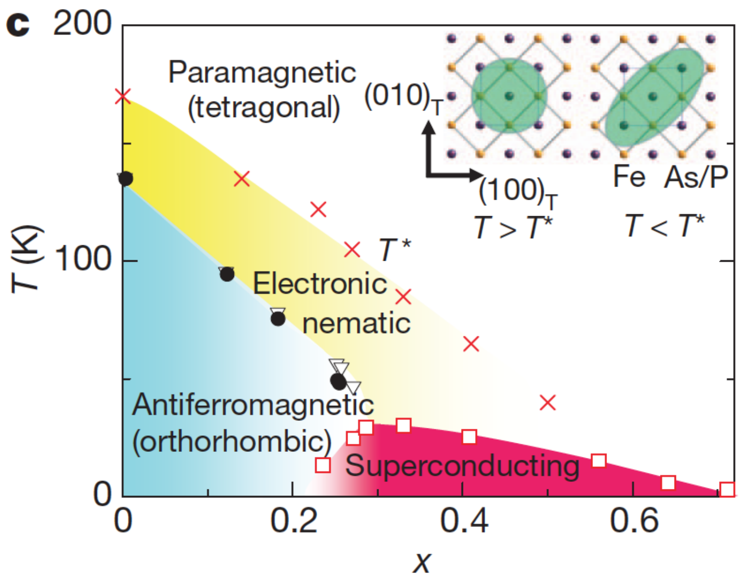
AB-initio calculations find that the 5 iron orbitals are the lower in energy-> Multiorbital physics in contrast to cuprates.
At the Fermi surface: dxz, dyz, dxy orbitals



Extended Brillouin zone,

Enigmatic nematic: ab anisotropy

The nematic phase is between the AF phase and the structural phase



Kasahara et al. Nature'12

Origin of nematicity:

- Lattice degrees of freedom?
- **Spin degrees of freedom?**
- **Orbital degrees of freedom?**

Symmetry dictates that the development of one of these orders immediately induces the other two: interrelation between spin, orbital and lattice d.o.f

'***chicken and egg problem***'

news & views

IRON-BASED SUPERCONDUCTORS

Enigmatic nematic

Iron pnictide superconductors often feature nematic, symmetry-breaking electronic states. These phenomena are now found to persist into the tetragonal phase of NaFeAs — a new piece of information that may help settle the fundamental origin of nematic electronic states.

J. C. Davis and P. J. Hirschfeld

nature physics REVIEW ARTICLE
PUBLISHED ONLINE: 31 JANUARY 2014 | DOI: 10.1038/NPHYS2877

What drives nematic order in iron-based superconductors?

R. M. Fernandes[1*], A. V. Chubukov[2*] and J. Schmalian[3*]

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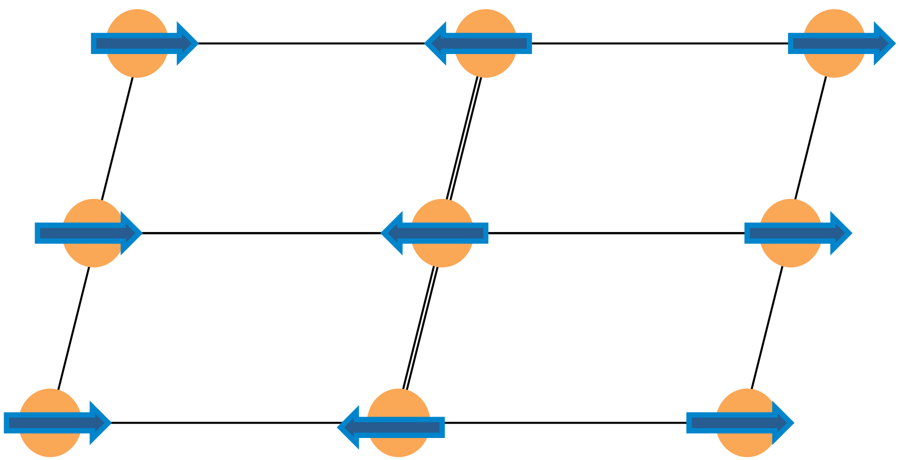
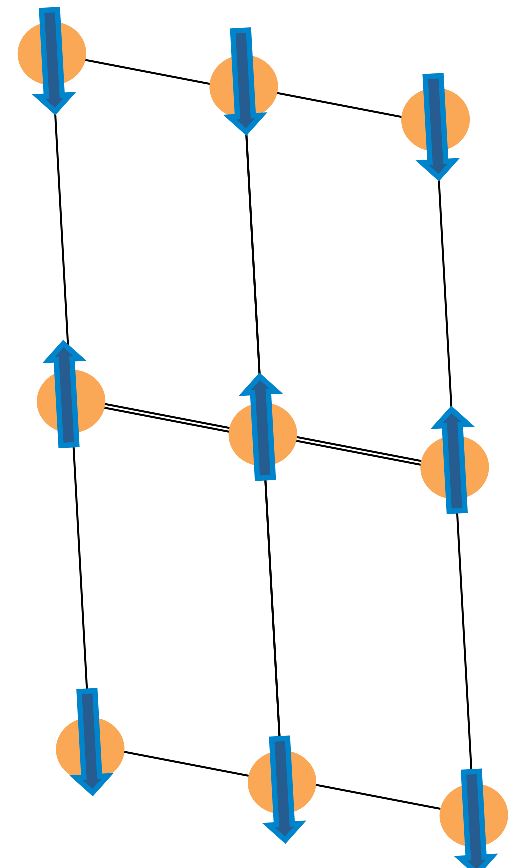
Theoretical approaches: Spin nematic

Spin-nematic: $(\pi,0)$ magnetism breaks 2 symmetries: O(3) and Z_2.

Z_2 is discrete symmetry -> is broken before O(3)



$(\pi,0)$ magnetism



$(0,\pi)$ magnetism

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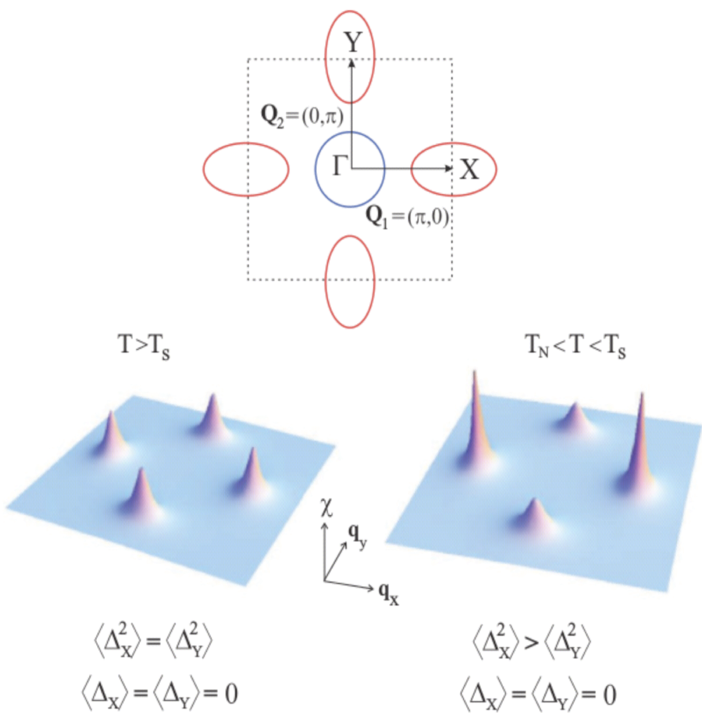
Spin nematic scenario

Weak coupling view: $\mathcal{H}_{\text{int}} = -\frac{1}{2} u_{\text{spin}} \sum_{i,\mathbf{q}} \mathbf{s}_{i,\mathbf{q}} \cdot \mathbf{s}_{i,-\mathbf{q}},$

$$S_{\text{eff}}\left[\boldsymbol{\Delta}_X, \boldsymbol{\Delta}_Y\right] = r_0 \left(\boldsymbol{\Delta}_X^2 + \boldsymbol{\Delta}_Y^2\right) + \frac{u}{2}\left(\boldsymbol{\Delta}_X^2 + \boldsymbol{\Delta}_Y^2\right)^2 - \frac{g}{2}\left(\boldsymbol{\Delta}_X^2 - \boldsymbol{\Delta}_Y^2\right)^2 + v\left(\boldsymbol{\Delta}_X \cdot \boldsymbol{\Delta}_Y\right)^2$$



Neel temperature $r_0 = \frac{2}{u_{\text{spin}}} + 2\int_k G_{\Gamma,k} G_{X,k},$

$$u = \frac{1}{2}\int_k G_{\Gamma,k}^2 (G_{X,k} + G_{Y,k})^2,$$

$$g = -\frac{1}{2}\int_k G_{\Gamma,k}^2 (G_{X,k} - G_{Y,k})^2,$$

Nematic coupling:
Strongly dependent on **ellipticity** of electron pockets.
Fine tunning?

Once the theoretical framework is stablized a lot of observables can be computed, Fernandes prb'12, …,
2 Nat. Phys'14, Nat. Mat.'14

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Iron superconductors: multiorbital physics

d Fe orbitals play the main role in the low energy physics

$$
\begin{aligned}
H &= \sum_{i,j,\gamma,\beta,\sigma} t_{i,j}^{\gamma,\beta} c_{i,\gamma,\sigma}^{\dagger} c_{j,\beta,\sigma} + h.c. + U \sum_{j,\gamma} n_{j,\gamma,\uparrow} n_{j,\gamma,\downarrow} \\
&+ (U' - \frac{J_H}{2}) \sum_{j,\gamma>\beta,\sigma,\tilde{\sigma}} n_{j,\gamma,\sigma} n_{j,\beta,\tilde{\sigma}} - 2J_H \sum_{j,\gamma>\beta} \vec{S}_{j,\gamma} \vec{S}_{j,\beta} \\
&+ J' \sum_{j,\gamma\neq\beta} c_{j,\gamma,\uparrow}^{\dagger} c_{j,\gamma,\downarrow}^{\dagger} c_{j,\beta,\downarrow} c_{j,\beta,\uparrow} + \sum_{j,\gamma,\sigma} \epsilon_{\gamma} n_{j,\gamma,\sigma} \,. \qquad (1)
\end{aligned}
$$

$U=U'+2J_H$

Difficult to calculate fluctuations in the PM phase

Hints from mean field

- **orbital ordering** appears in the magnetic phase*. Interplay between orbital and spin d.o.*f. (also in ab-initio calculations and other mean field, Daghofer, prb'09)
- ***Orbital ordering anticorrelated with experimental anisotropy.***
- Experimental anisotropy linked to the **magnetic reconstruction of the FS at low moment or close to the transition** (as in experiments).

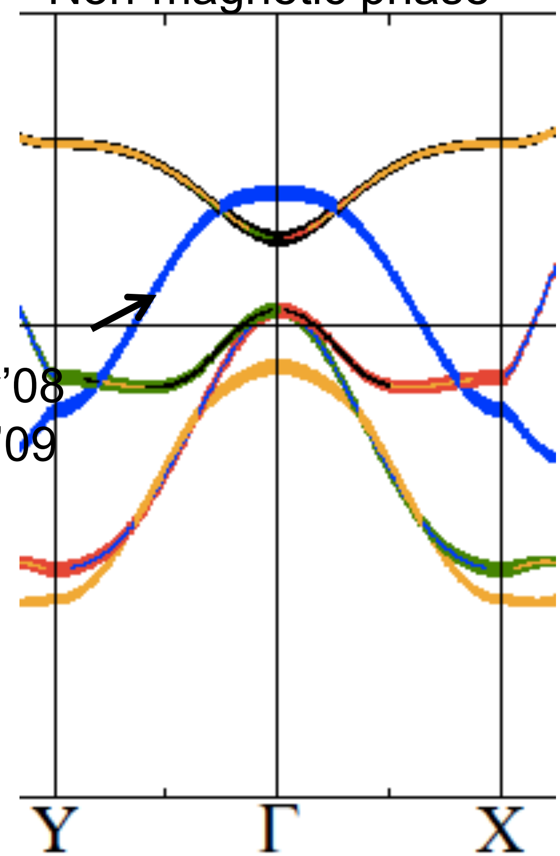
B.V., E. Bascones, M.J. Calderón, PRL'10

The quadratic band crossing point (QBCP) and magnetic reconstruction

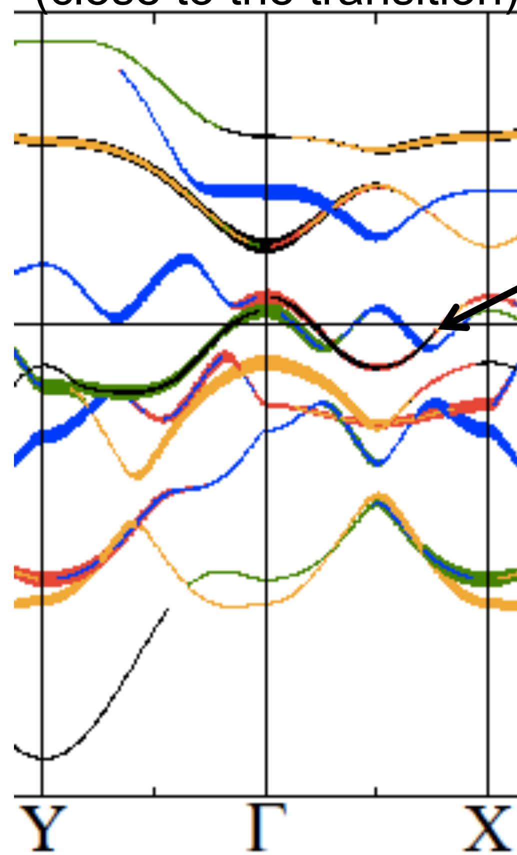
Red-yz orbital
Green-zx orbital

Γ pocket
QBCP
Vortex=2
Scalapino arXiv'08
DHL.et al. PRB'09

Non-magnetic phase



Magnetic phase at low moment
(close to the transition)



Two Dirac
Cones
1+1

QBCP are unstable under RG to nematic and topological phases, K. Sun et al. prl'09
(different context, pseudospin: 2 atoms per unit cell, bilayer graphene…)

A low energy theory should have this physics into account!

Our work: derive a multiorbital effective action

Derive an effective action for the spin-nematic phase using the Hubbard-Stratonovich machinery from a multiorbital Hamiltonian. The Landau coefficients will depend on the U, J_H, the orbital content and the non trivial topology of the Γ pocket

The effective action

$$S_{eff} = \sum_{l=X,Y;\eta_1\eta_2} r_{\eta_1,\eta_2,l}\vec{\Delta}_{\eta_1 l}\cdot\vec{\Delta}_{\eta_2 l} + \\ + \frac{1}{16}\sum_{\eta_1\eta_2\eta_3\eta_4} u_{\eta_1\eta_2\eta_3\eta_4}\psi_{\eta_1\eta_2}\psi_{\eta_3\eta_4} + \\ - g_{\eta_1\eta_2\eta_3\eta_4}\phi_{\eta_1\eta_2}\phi_{\eta_3\eta_4} + 2v_{\eta_1\eta_2\eta_3\eta_4}\psi_{\eta_1\eta_2}\phi_{\eta_3\eta_4}. \quad (5)$$

$$\psi_{\eta_1\eta_2} = \frac{1}{2}\left(\vec{\Delta}_{\eta_1 X}\cdot\vec{\Delta}_{\eta_2 X} + \vec{\Delta}_{\eta_1 Y}\cdot\vec{\Delta}_{\eta_2 Y}\right),$$

$$\phi_{\eta_1\eta_2} = \frac{1}{2}\left(\vec{\Delta}_{\eta_1 X}\cdot\vec{\Delta}_{\eta_2 X} - \vec{\Delta}_{\eta_1 Y}\cdot\vec{\Delta}_{\eta_2 Y}\right),$$

Landau coefficients

$$r_{l\eta_1\eta_2} = U^{-1}_{\eta_1\eta_2} + \frac{1}{2}\sum_k G_\Gamma G_l \omega^{\eta_1}_{\Gamma l}\omega^{\eta_2}_{\Gamma l} \quad (8a)$$

$$U_{\eta_1\eta_2} = \frac{4}{3}U\delta_{\eta_1\eta_2} + 2J_H(1-\delta_{\eta_1\eta_2}),$$

$$\omega^{\eta}_{\Gamma l}(\mathbf{k},\mathbf{k}+\mathbf{q}) = a_{\Gamma\eta}(\mathbf{k})a_{l\eta}(\mathbf{k})$$

$$u_{\eta_1\eta_2\eta_3\eta_4} = \frac{1}{2}\sum_{kl} G^2_\Gamma\left(G_l\omega^{\eta_1}_{\Gamma l}\omega^{\eta_2}_{\Gamma l}\right)\left(G_X\omega^{\eta_3}_{\Gamma l}\omega^{\eta_4}_{\Gamma l}\right), \quad (8b)$$

$$g_{\eta_1\eta_2\eta_3\eta_4} = -\frac{1}{2}\sum_{kl,s=1(X),-1(Y)} G^2_\Gamma\left(sG_l\omega^{\eta_1}_{\Gamma l}\omega^{\eta_2}_{\Gamma l}\right)\left(sG_l\omega^{\eta_3}_{\Gamma l}\omega^{\eta_4}_{\Gamma l}\right), \quad (8c)$$

Nematic coupling:
Different from zero if ellipticity is zero.
It is not so sensitive to ellipticity

To be compared to:

$$S_{\text{eff}}[\boldsymbol{\Delta}_X,\boldsymbol{\Delta}_Y] = r_0\left(\boldsymbol{\Delta}_X^2+\boldsymbol{\Delta}_Y^2\right) + \frac{u}{2}\left(\boldsymbol{\Delta}_X^2+\boldsymbol{\Delta}_Y^2\right)^2 - \frac{g}{2}\left(\boldsymbol{\Delta}_X^2-\boldsymbol{\Delta}_Y^2\right)^2 + v\left(\boldsymbol{\Delta}_X\cdot\boldsymbol{\Delta}_Y\right)^2$$

$$r_0 = \frac{2}{u_{\text{spin}}} + 2\int_k G_{\Gamma,k}G_{X,k},$$

$$u = \frac{1}{2}\int_k G^2_{\Gamma,k}(G_{X,k}+G_{Y,k})^2,$$

$$g = -\frac{1}{2}\int_k G^2_{\Gamma,k}(G_{X,k}-G_{Y,k})^2,$$

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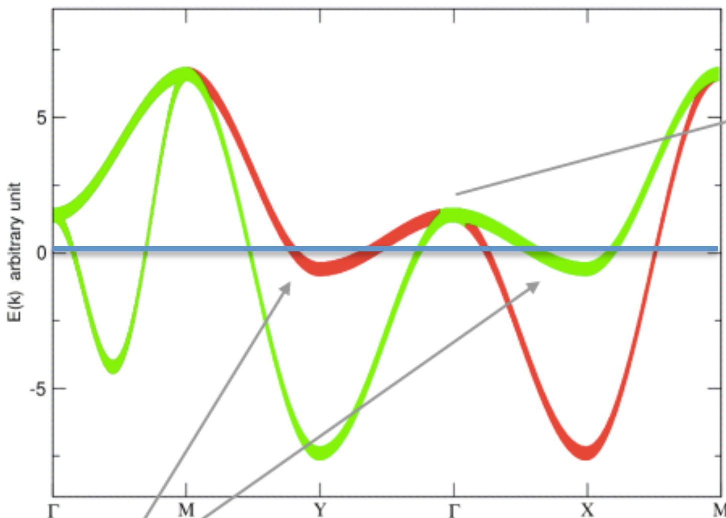
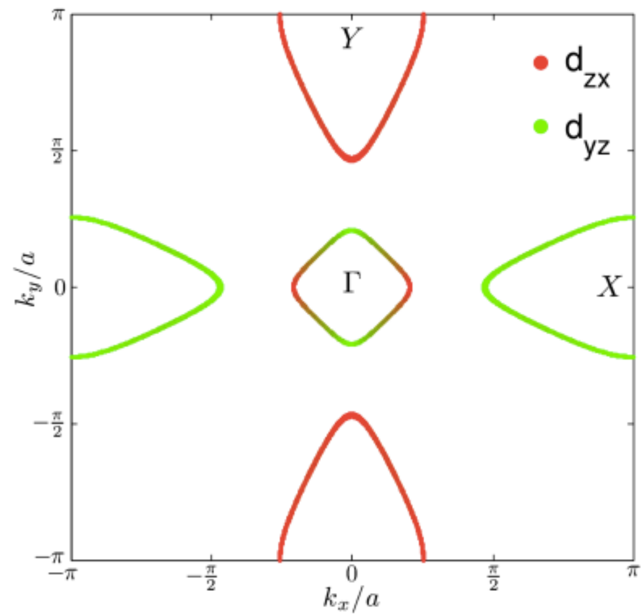
Analysis for the two orbital model



At the Γ point: Both orbital components, Quadratic Band Crossing point (QBCP) (non trivial topology)



Y and X electron pockets has one orbital component

$$H = \sum_{\mathbf{k}\alpha\eta\eta'} c^{+}_{\eta\alpha}(\mathbf{k})\left(\tau_0^{\eta\eta'} h_0(\mathbf{k}) + \tau_1^{\eta\eta'} h_1(\mathbf{k}) + \tau_3^{\eta\eta'} h_3(\mathbf{k})\right) c_{\eta'\alpha}(\mathbf{k})$$

Pseudospin: orbital degree of freedom

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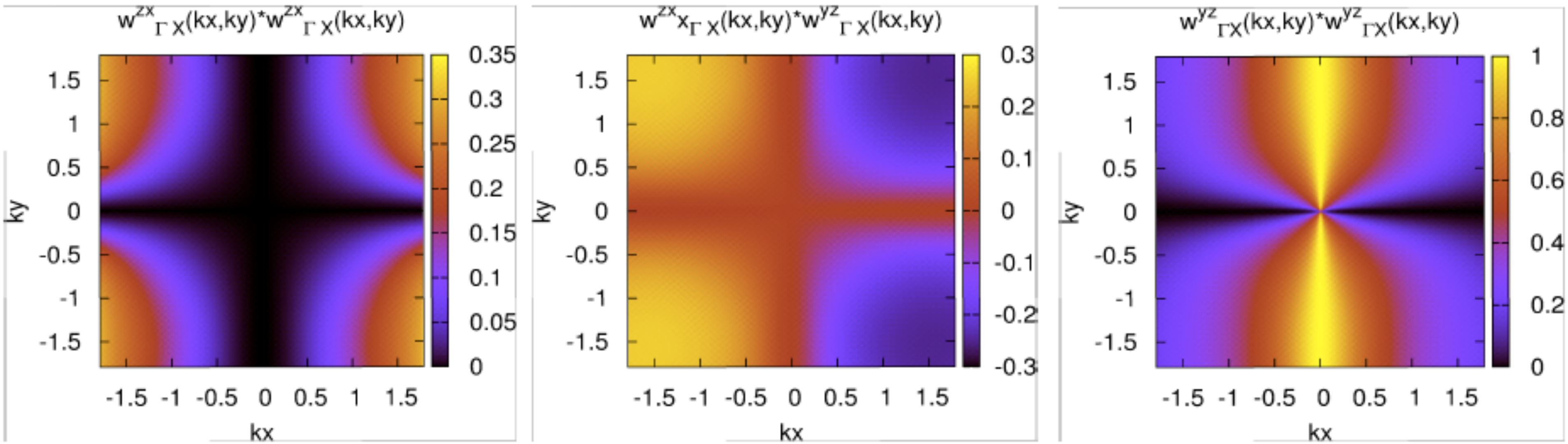
Spin susceptibility

$$\chi^{-1}(\mathbf{q},\Omega) = \sum_{\eta_1\eta_2} \hat{U}^{-1}_{\eta_1\eta_2} - \Pi^l_{\eta_1\eta_2}(\mathbf{q},\Omega) \qquad \Pi^l_{\eta_1\eta_2} = \sum_{i\omega,\mathbf{k}} G_\Gamma G_l \omega^{\eta_1}_{\Gamma l}\omega^{\eta_2}_{\Gamma l}$$

q=0 Q=(π,0)



There is a structure from the orbital degree of freedom in the BZ
yz more magnetic in agreement with mean field.
Along x every contribution is suppressed-> anisotropy?

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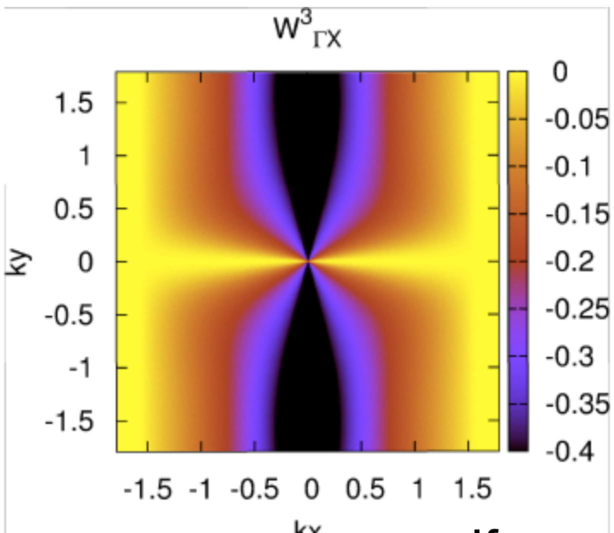
Spin susceptibility

$$\chi^{-1}(\mathbf{q},\Omega) = \sum_{\eta_1\eta_2} \hat{U}^{-1}_{\eta_1\eta_2} - \Pi^l_{\eta_1\eta_2}(\mathbf{q},\Omega) \qquad \Pi^l_{\eta_1\eta_2} = \sum_{i\omega,\mathbf{k}} G_\Gamma G_l \omega^{\eta_1}_{\Gamma l}\omega^{\eta_2}_{\Gamma l}$$

$$\chi^{-1} = [4/3U\tau_0 - 2J_H\tau_1]/det\hat{U} + \sum_{i\omega\mathbf{k}} G_\Gamma G_X [W^0_{\Gamma X}\tau_0 + W^1_{\Gamma X}\tau_1 + W^3_{\Gamma X}\tau_3]$$



Renormalizes U $\quad J_H$

Generation of orbital anisotropy in the spin channel

If we allow for charge degrees of freedom it will couple to the charge channel generating **orbital ordering.** Agrees with Mean field result but from the PM phase. **Spin-orbital are intertwined**

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Spin susceptibility, continuum limit and QBCP

$$\vec{H}_\Gamma(\mathbf{k}) = 2bk_xk_y\tau_0 + a(k_x^2 - k_y^2)\tau_z \to \vec{n}_\Gamma(k,\phi) = k^2(a\cos 2\phi, b\sin 2\phi)$$

$$r^l_{\eta_1\eta_2} = \int \frac{d^2\mathbf{k}}{(2\pi)^2} \frac{(1 - \vec{n}_l(\mathbf{k})\cdot\vec{n}_\Gamma(\mathbf{k}))\tau_0 + \vec{\tau}\cdot(\vec{n}_l(\mathbf{k}) - \vec{n}_\Gamma(\mathbf{k}))}{\Omega + E_P(\mathbf{k}) - E_\Gamma(\mathbf{k})} \equiv r^0_l\tau_0 + r^1_l\tau_1 + r^3_l\tau_3.$$

$\hat{n}(k,\phi)$

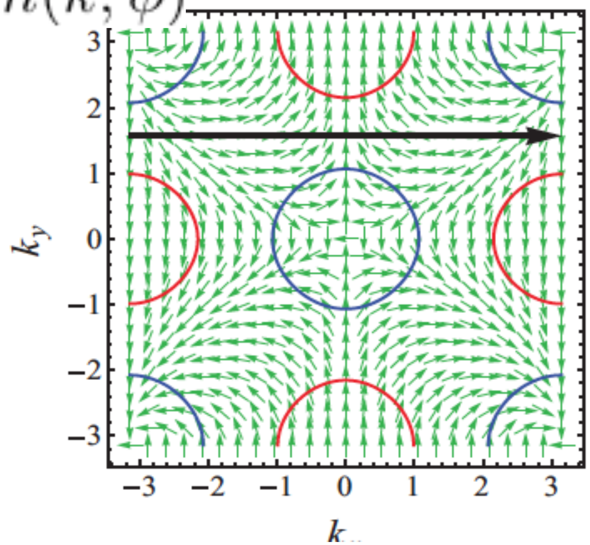

Fig from Lau, prb'13

Again:

- Orbital anisotropy generated dynamically
- *Anisotropy between k_x and k_y from the Q=(π, 0) nesting between the Γ pocket with vortex=2 and the X pocket: **topology of the Γ pocket behind anisotropy?***

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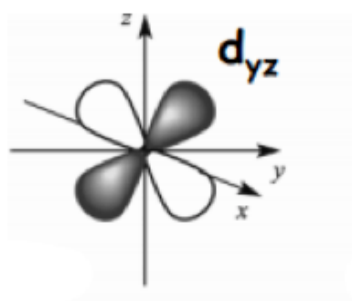
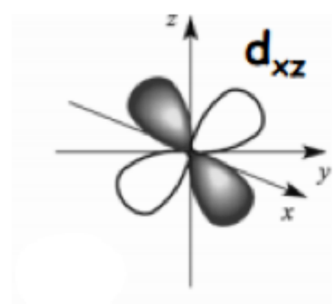
Conclusions

-We have built an effective action for Iron superconductors to study the spin-nematic phase. The Landau parameters depend on U, J_H, orbital content and topology of the FS. Nematic order parameter not so sensitive to ellipticity

Magnetic susceptibility for the 2-orbital model
-Orbital anisotropy is generated dynamically in the spin channel. It can generate orbital ordering in the charge channel. Interplay between spin-charge channels revealed from the paramagnetic phase.
-Anisotropy weight factors: No weight along x-> Has nematicity a topological aspect? This would explain why nematicity decreases with magnetic moment.

Under 90º xz transforms in yz





But under 90º yz transforms in -xz

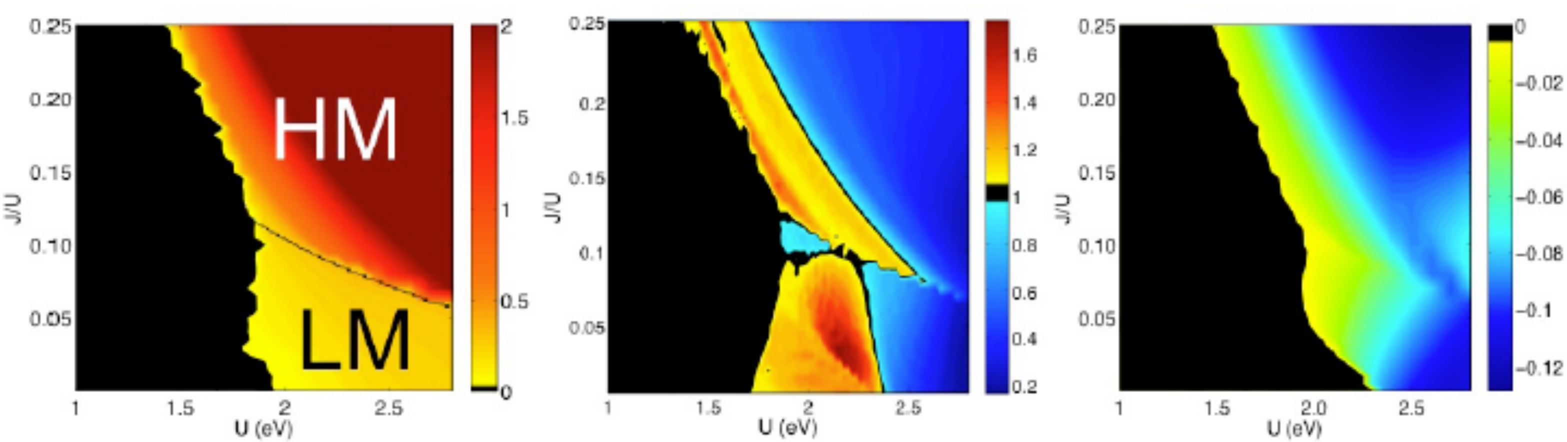
Future:
-With this action we or others can calculate the desired response function

Thank you!

Some hints from mean field in the magnetic state: orbital order

Mean field analysis and ab-initio calculations: orbital ordering appears in the magnetic phase but not alone.

Magnetism | Drude anisotropy: D_x/D_y | Orbital ordering

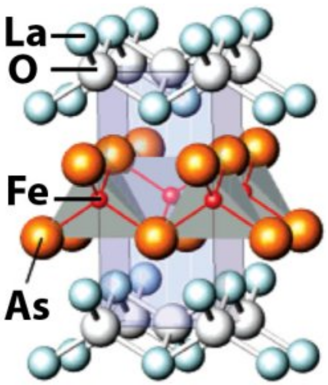


Orbital ordering ***anticorrelated with the experimental Drude anisotropy.***
Orbital order not behind anisotropy at the MFL in the magnetic phase
Experimental anisotropy found for ***weak magnetic moment*** as in experiments

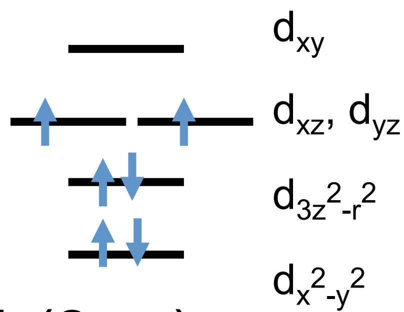
B. V., E. Bascones, M.J. Calderón, PRL 105, 207202 (2010)

Multiorbital system

Pnictides: 6 electrons in 5 Fe orbitals in a tetrahedral environment:



Kamihara'08

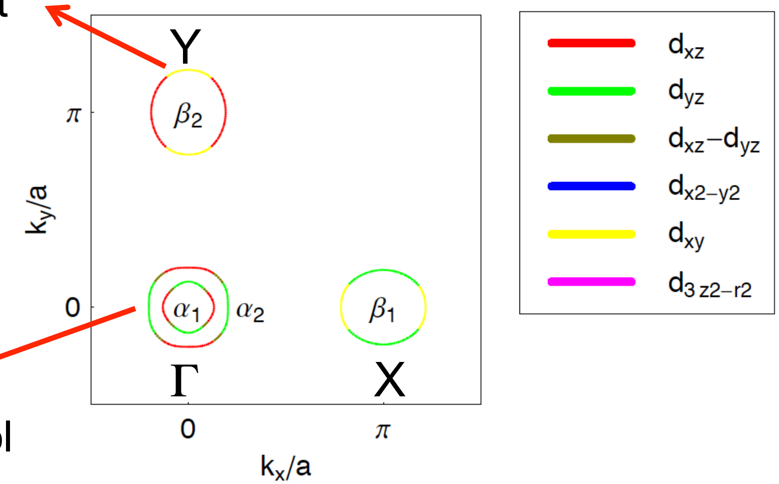


S=1 ($2m_B$)

Crystal field ~200 meV

2D electron pocket

Fermi surface



AB-initio calculations find that the 5 iron orbitals are the lower in energy-> Multiorbital physics in contrast to cuprates. At the Fermi surface: dxz, dyz, dxy orbitals

2D Γ hol pockets

Extended Brillouin zone,

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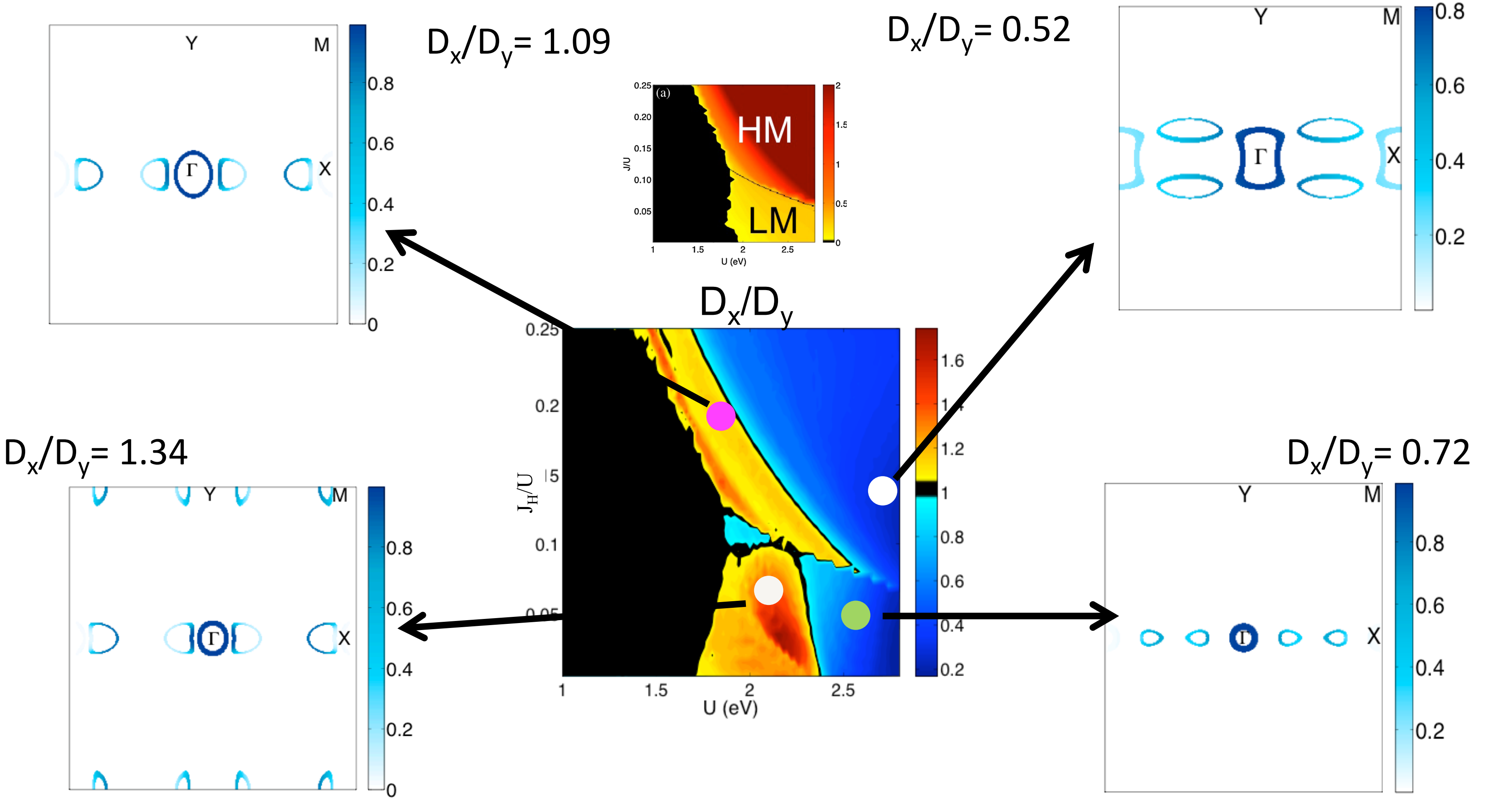
Magnetic reconstruction as origin of the conductivity anisotropy



Orbital ordering do not explain the experimental anisotropy
Anisotropy linked to magnetic reconstruction of the FS at low moment or close to the transition (as in experiments).

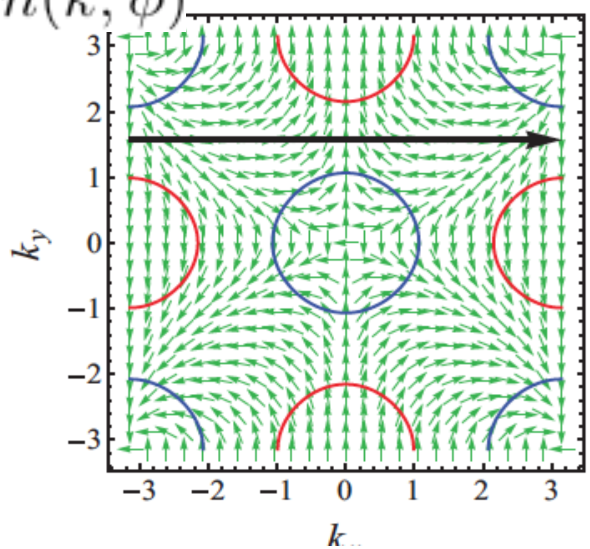
B. V., E. Bascones, M.J. Calderón, PRL 105, 207202 (2010)

Spin susceptibility, continuum limit and QBCP

$$\vec{H}_\Gamma(\mathbf{k}) = 2bk_xk_y\tau_0 + a(k_x^2 - k_y^2)\tau_z \to \vec{n}_\Gamma(k,\phi) = k^2(a\cos 2\phi, b\sin 2\phi)$$

$$r^l_{\eta_1\eta_2} = \int \frac{d^2\mathbf{k}}{(2\pi)^2} \frac{(1 - \vec{n}_l(\mathbf{k})\cdot\vec{n}_\Gamma(\mathbf{k}))\tau_0 + \vec{\tau}\cdot(\vec{n}_l(\mathbf{k}) - \vec{n}_\Gamma(\mathbf{k}))}{\Omega + E_P(\mathbf{k}) - E_\Gamma(\mathbf{k})} \equiv r_l^0\tau_0 + r_l^1\tau_1 + r_l^3\tau_3.$$

$\hat{n}(k,\phi)$



Again:

-Renormalization of U,J_H

-Generation of orbital anisotropy

-Anisotropy between k_x and k_y from the Q=(π,0) nesting between the Γ pocket with vortex=2 and the X pocket: ***topology of the Γ pocket behind anisotropy?***

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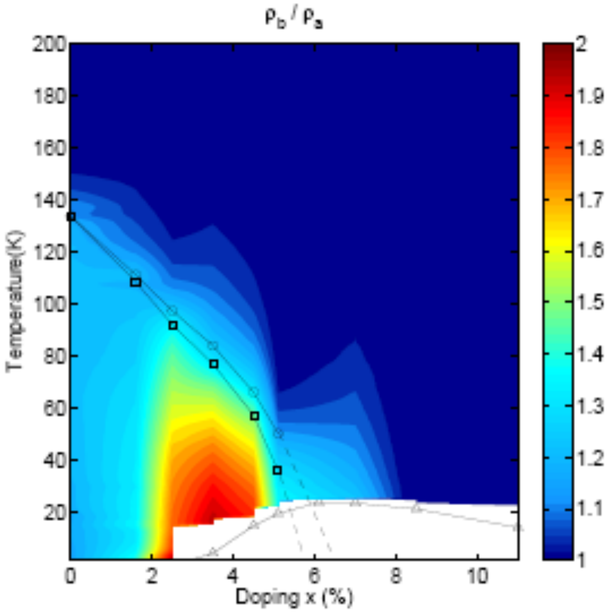
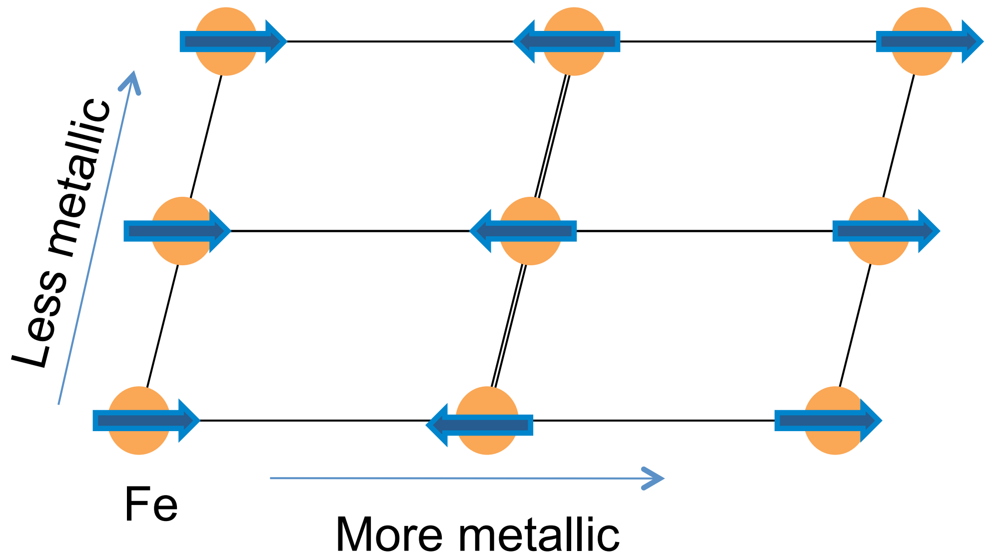
The nematic phase

Resistivity anisotropy in the phase diagram





Chu et al. Science'10

-Anisotropy measured experimentally in charge, spin an orbital channels
-Cuprates also present a nematic phase

From the microscopic model to the effective action

$$c^\dagger_{\mathbf{k}\mu\sigma} = \sum_n a^*_{\mu n}(\mathbf{k}) d^\dagger_{\mathbf{k}n\sigma} \longrightarrow c^\dagger_{\mu\sigma}(\mathbf{k}_j) = \sum_n a^*_{\mu n}(\mathbf{k}_j) d^\dagger_{n\sigma}(\mathbf{k}_j)$$

$$H_{int} = -\frac{1}{2}\sum_{\mathbf{q}}\sum_{\eta\eta'} U_{\eta\eta'}\mathbf{S}_\eta(\mathbf{q})\mathbf{S}_{\eta'}(-\mathbf{q}); \quad U_{\eta\eta'} = \frac{4}{3}U\delta_{\eta\eta'} + 2J_H(1-\delta_{\eta\eta'})$$

The effective coupling for the spin channel depends on U, J_H

$$\mathbf{S}_\eta(\mathbf{q}) = \sum_{\mathbf{k}}\sum_{l=X,Y} \omega^\eta_{\Gamma l}(\mathbf{k},\mathbf{k}+\mathbf{q})\mathbf{S}_{\Gamma l}(\mathbf{k},\mathbf{k}+\mathbf{q});$$

$$\mathbf{S}_{\Gamma l}(\mathbf{k},\mathbf{k}+\mathbf{q}) = \frac{1}{2}\sum_{\alpha\beta} d^\dagger_{\Gamma\mathbf{k}\alpha}\sigma_{\alpha\beta}d_{l\mathbf{k}+\mathbf{q}\beta}; \quad \omega^\eta_{\Gamma l}(\mathbf{k},\mathbf{k}+\mathbf{q}) = a_{\Gamma\eta}(\mathbf{k})a^*_{l\eta}(\mathbf{k}+\mathbf{q});$$

We retain all the information about the orbital structure