The role of Hund’s coupling in the nematicity of iron superconductors:

E. Bascones
Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC)
Nematicity in FeSe

CeFeAsO$_{1-x}$F$_x$

Tetragonal symmetry is broken.
Orthorhombic distortion
Electronic properties strongly anisotropic

Zhao et al, Nat. Mat. 7, 953 (2008),
Sun et al, arXiv 1512.06951

E. Bascones  leni@icmm.csic.es
Nematicity in FeSe

CeFeAsO$_{1-x}$F$_x$

Zhao et al, Nat. Mat. 7, 953 (2008),

Spin degree of freedom
Ising-spin nematic?
Quadrupolar orders?

Orbital degree of freedom
Ferro-orbital onsite ordering $\Delta (n_{zx}-n_{yz})$?
d-wave nematic bond order $\Delta \Sigma_k (\cos k_x - \cos k_y) (n_{zx}(k)+n_{yz}(k))$?

Sun et al, arXiv 1512.06951
Correlations in iron superconductors: The role of multi-orbital physics

Experimentally electronic bands similar to those predicted by LDA but strongly renormalized (narrower bands with enhanced mass) are observed

Local correlations are important

LDA: Fe bands at the Fermi level.
Several orbitals involved

Minimum model: 5 orbitals
(6 electrons when undoped)

Multi-orbital character may play an important role in the correlations and instabilities

Hund’s coupling: key role in the correlations
The role of Hund’s coupling in the nematicity of iron superconductors

- Hamiltonian: 5 orbital Hubbard-Kanamori Hamiltonian (only local interactions included). Tight binding model from LDA for FeSe

- Interactions treated at single-site mean-field slave-spin.
  - Included: local correlations (quasiparticle weight-mass enhancement)
  - Not included: finite-range spin fluctuations

- Study of the response of the system to a nematic perturbation
  - Onsite order: Ferro-orbital ordering \( \Delta (n_{zx}-n_{yz}) \)?
  - Bond order: d-wave nematic \( \Delta \Sigma_k (\cos k_x - \cos k_y)(n_{zx}(k) + n_{yz}(k)) \) ?
  - Anisotropy in the hopping to 1st nn
The role of Hund’s coupling in the nematicity of iron superconductors

- Hamiltonian: 5 orbital Hubbard-Kanamori Hamiltonian (only local interactions included). Tight binding model obtained with LDA for FeSe.

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  - Not included: finite-range spin fluctuations

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  - Onsite order: Ferro-orbital ordering $\Delta (n_{zx}-n_{yz})$?
  - Bond order: d-wave nematic $\Delta \Sigma_k (\cos k_x - \cos k_y) (n_{zx}(k) + n_{yz}(k))$?
  - Anisotropy in the hopping to 1st nn
Outline

- Correlations in iron superconductors: the role of Hund’s coupling. Hund metals

- Nematicity:
  - Response of the system to an anisotropic perturbation: ferro-orbital ordering and correlations
  - Consequences in the band structure (ARPES)

- Summary
Thanks to my Collaborators

Nematicity and Correlations

Laura Fanfarillo
SISSA, Trieste
previously at ICMM-CSIC

Nematicity

Gianluca Giovanetti
SISSA, Trieste

Massimo Capone
SISSA, Trieste

Correlations

María José Calderón
ICMM-CSIC
Madrid

Belén Valenzuela
ICMM-CSIC
Madrid
Correlations in iron superconductors: The role of multi-orbital physics

\[ H = \sum_{i,j,\gamma,\beta,\sigma} t_{i,j}^{\gamma,\beta} c_{i,\gamma,\sigma}^\dagger c_{j,\beta,\sigma} + \text{h.c.} + U \sum_{j,\gamma} n_{j,\gamma,\uparrow} n_{j,\gamma,\downarrow} \]

Tight-binding (hopping)

\[ + \left( U' - \frac{J_H^2}{2} \right) \sum_{j,\gamma > \beta,\sigma,\tilde{\sigma}} n_{j,\gamma,\sigma} n_{j,\beta,\tilde{\sigma}} - 2J_H \sum_{j,\gamma > \beta} \vec{S}_{j,\gamma} \cdot \vec{S}_{j,\beta} \]

Inter-orbital repulsion

\[ + J' \sum_{j,\gamma \neq \beta} c_{j,\gamma,\uparrow}^\dagger c_{j,\gamma,\downarrow}^\dagger c_{j,\beta,\downarrow} c_{j,\beta,\uparrow} + \sum_{j,\gamma,\sigma} \epsilon_{\gamma} n_{j,\gamma,\sigma} . \]

Pair hopping

\[ U' = U - 2J_H \quad J' = J_H \]

Two interaction parameters: \( U \), \( J_H \)

Local Interactions

E. Bascones  leni@icmm.csic.es
Correlations in iron superconductors: The role of multi-orbital physics

Local density-density interactions only

\( H_{\text{int}} = U \sum_a n_{a\uparrow} n_{a\downarrow} + (U' - J_H) \sum_{a<b,\sigma} n_{a\sigma} n_{b\sigma} \)

\( + U' \sum n_{a\uparrow} n_{b\downarrow} \)

- two electrons in the same orbital
- two electrons in different orbitals with the same spin
- two electrons in different orbitals with different spin

Ising approximation:
Spin-flip part of Hund’s term & pair-hopping neglected

\( U' = U - 2J_H \)

Two interaction parameters: \( U, J_H \)
Correlations in iron superconductors: The role of multi-orbital physics

Correlations diagram corresponding to a 5 orbital Tight-binding model suitable for iron superconductors with n=6 electrons (undoped)

Correlated high-spin state but still itinerant (double exchange)

Fermi surface
Physics (nesting ...)

Technique:
Single site Slave-spin,
Local correlations

Local moment physics
(Heisenberg, exchange ...)

Yu & Si, PRB 86, 085104 (2012)
Similar diagram in (π,0) Hartree-Fock: EB et al, PRB 87, 174508 (2012)

Correlations in iron superconductors: The role of multi-orbital physics

high-spin state but still itinerant (double exchange)

Yu & Si, PRB 86, 085104 (2012)

Lanata et al, PRB 87, 045122 (2013)
Fanfarillo & EB, PRB 92, 075136 (2015)

Review: Bascones et al, Comptes Rendus Physique 17,36 (2016)
Correlations in iron superconductors: The role of multi-orbital physics

Technique: Single site Slave-spin, Local correlations

Yu & Si, PRB 86, 085104 (2012)

Review: E B et al, Comptes Redus Physique 17,36 (2016)
Hund metals: decoupling

two electrons in the same orbital

two electrons in different orbitals with the same spin

two electrons in different orbitals with different spin

As the atoms becomes spin polarized the effective interaction between the electrons in different orbitals decreases. It vanishes at $J_H = U/3$

$H_{int} = U \sum_a n_{a\uparrow} n_{a\downarrow} + (U' - J_H) \sum_{a < b, \sigma} n_{a\sigma} n_{b\sigma} + U' \sum_{a \neq b} n_{a\uparrow} n_{b\downarrow}$

$U' = U - 2J_H$

Fanfarillo & EB, PRB 92, 075136 (2015)
Correlations in iron superconductors: The role of multi-orbital physics

Strong correlations: Forbidden process
(increases # of **double occupied orbitals** & decreases spin polarization)

Metallicity: Allowed process
(no increase in # of **double occupied orbitals** & increases spin polarization)

Fanfarillo & EB, PRB 92, 075136 (2015)
Iron superconductors in the correlations diagram

Weakly correlated
Fermi surface physics

High-spin (double exchange like physics)
Strong correlations: mass enhancements
Orbital differentiation
Metal (partial itinerancy)

Strongly correlated
Hund metal

Metal moderate
correlations
Z>0.5
Low spin

Localized spin moments
(Heisenberg models ...)

E. Bascones  leni@icmm.csic.es
Iron superconductors in the correlations diagram

FeP compounds

Undoped FeAs compounds (more correlated when hole-doped)

From comparison with: ARPES, Quantum oscillations, specific heat, doping dependence, X-ray, neutron spectroscopy, optical Conductivity, spin susceptibility, Orbital selectivity, and predictions from DMFT+constrained LDA, ...

Review: E B et al, Comptes Redus Physique 17,36 (2016)

E. Bascones  leni@icmm.csic.es
Iron superconductors in the correlations diagram

FeSe

ARPES and Quantum oscillations experiments in FeSe are consistent with orbital dependent renormalization mass. Close to the Fermi surface

\[ m^*_{zx/yz} \approx 3 \quad m^*_{xy} \approx 5 \]

Inverse renormalization of the mass

Review: E B et al, Comptes Redus Physique 17,36 (2016)
Correlations in FeSe

Shrinking of the Fermi surface not due to local correlations

1-Fe unit cell
Hund’s coupling and ferro-orbital ordering

Response of the system to an onsite level splitting

$$n_{yz} - n_{zx} = \frac{d(n_{yz} - n_{zx})}{d(\delta \varepsilon_0)} \delta \varepsilon_0$$

$$\delta \varepsilon_0 = \varepsilon_{zx} - \varepsilon_{yz}$$

How does the response of the system depend on interactions?
Hund’s coupling and ferro-orbital ordering

Response of the system to an onsite level splitting

\[ n_{\text{yz}} - n_{\text{zx}} = \frac{d(n_{\text{yz}} - n_{\text{zx}})}{d(\delta \varepsilon_0)} \delta \varepsilon_0 \]

\[ \delta \varepsilon_0 = \varepsilon_{\text{zx}} - \varepsilon_{\text{yz}} \]

Graph showing the response of the system to different values of \( J_H / U \):
- \( J_H / U = 0.05 \)
- \( J_H / U = 0.20 \)

FeSe

Strongly correlated Hund metal

Mott Insulator

Metal moderate correlations \( Z > 0.5 \)

\( U (\text{eV}) \):
- 0 to 15

\( J_H / U \):
- 0 to 0.25

Graph parameters:
- \( d(n_{\text{yz}} - n_{\text{zx}}) / d(\delta \varepsilon_0) \) in ev^{-1}
- U (eV):
- 1 to 4
Anisotropic Quasiparticle weight

Response of the system to an onsite level splitting

$$Z_{yz} - Z_{zx} = \frac{d(Z_{yz} - Z_{zx})}{d(\delta \varepsilon_0)} \delta \varepsilon_0$$

$\varepsilon_{zx}$ ↓ $\delta \varepsilon_0$

$\varepsilon_{yz}$

$\delta \varepsilon_0 = \varepsilon_{zx} - \varepsilon_{yz}$

Anisotropy in the correlation strength
Anisotropic Quasiparticle weight

Response of the system to an onsite level splitting

\[ Z_{yz} - Z_{zx} = \frac{d(Z_{yz} - Z_{zx})}{d(\delta \varepsilon_0)} \delta \varepsilon_0 \]

\[ \delta \varepsilon_0 = \varepsilon_{zx} - \varepsilon_{yz} \]

Anisotropic effective mass

Strongly enhanced response, but finite peak
Anisotropic Quasiparticle weight

Response of the system to an onsite level splitting

\[ Z_{yz} - Z_{zx} = \frac{d(Z_{yz} - Z_{zx})}{d(\delta \varepsilon_0)} \delta \varepsilon_0 \]

\[ \varepsilon_{zx} \quad \uparrow \quad \varepsilon_{yz} \quad \downarrow \delta \varepsilon_0 \]

\[ \delta \varepsilon_0 = \varepsilon_{zx} - \varepsilon_{yz} \]

Anisotropic effective mass

\[ \text{FeSe} \]

\[ J_H/U=0.20 \]

\[ J_H/U=0.05 \]

\[ \delta \varepsilon_0 \sim 75 \text{ meV} \]

\[ Z_{yz} - Z_{zx} \sim 0.025 \]

Similar effects for a d-wave nematic bond order

E. Bascones  leni@icmm.csic.es
Effect of the nematicity on the band structure

2-Fe unit cell

\[ zx: \text{green} \quad yz: \text{red} \]

In the tetragonal state (no nematicity):
Degeneracy of zx and yz bands at symmetry points
Effect of the nematicity on the band structure

2-Fe unit cell

In the nematic state finite splitting appears between zx and yz bands at the symmetry points.

The splitting gives information on the kind of nematic order

Naive splitting used to interpret ARPES experiments

Onsite order: $\delta \varepsilon_0 (n_{zx} - n_{yz})$

Splitting at $M_1 \sim \delta \varepsilon_0$

Splitting at $\Gamma \sim \delta \varepsilon_0$

Bond d-wave order:

$\Delta \Sigma_k (\cos kx - \cos ky) (n_{zx} + n_{yz})$

Splitting at $M_1 \sim 4\Delta$

Splitting at $\Gamma \sim 0$
Effect of the nematicity on the band structure

2-Fe unit cell

*zx: green yz:red*

In the nematic state finite splitting appears between zx and yz bands at the symmetry points. The splitting gives information on the kind of nematic order.

Naive splitting used to interpret ARPES experiments

\[ \delta \varepsilon_0 = \varepsilon_{zx} - \varepsilon_{yz} = 75 \text{ meV} \]

U=0.2 eV
Weak interactions

Onsite order: \[ \delta \varepsilon_0 (n_{zx} - n_{yz}) \]
Splitting at \( M_1 \sim \delta \varepsilon_0 \)
Splitting at \( \Gamma \sim \delta \varepsilon_0 \)

Bond d-wave order:
\[ \Delta \Sigma_k (\cos kx - \cos ky)(n_{zx} + n_{yz}) \]
Splitting at \( M_1 \sim 4 \Delta \)
Splitting at \( \Gamma \sim 0 \)

Experiment still controversial
Effect of Onsite orbital ordering on the band structure

\[ \delta \varepsilon_0(n_{zx}-n_{yz}) \]

\[ J_{H}/U=0.20 \]

\[ \delta \varepsilon^{*}/\delta \varepsilon_0 \]

\[ Z_{zx/yz} \]

\[ U(eV) \]

Shift at the symmetry points

\[ \delta \varepsilon_{zx}(k) \sim \delta \varepsilon^{*}_{0,zx} + \delta Z_{zx}(2t^y_{zx,zx} \cos ky + 4t'_{zx,zx} \cos kx \cos ky) \]

\[ \delta \varepsilon_{yz}(k) \sim \delta \varepsilon^{*}_{0,yz} + \delta Z_{yz}(2t^x_{yz,yz} \cos kx + 4t'_{yz,yz} \cos kx \cos ky) \]

\[ t^y_{zx,zx} = t^x_{yz,yz} \sim -0.32 \text{ eV} \]

\[ t'_{zx,zx} = t'_{yz,yz} \sim 0.23 \text{ eV} \]

K dependence in 1-Fe unit cell

Tight binding parameters

E. Bascones  leni@icmm.csic.es
Effect of Ferro-orbital ordering on the band structure

Splitting at $M_1 \sim \delta \varepsilon^*_0 + \delta Z(2t^y_{zx,zx} + 4t'_{zx,zx})$

Splitting at $\Gamma \sim \delta \varepsilon^*_0 - \delta Z(2t^y_{zx,zx} + 4t'_{zx,zx})$

0.29 eV

J_H/U=0.20

Splittings at symmetry points between zx/yz orbitals are modified with respect to naive expectations

Accidental sign reversal
Effect of Ferro-orbital ordering on the band structure

Splitting at $M_1 \sim \delta \varepsilon_0^* + \delta Z (2t^y_{zx,zx} + 4t'_{zx,zx})$

Splitting at $\Gamma \sim \delta \varepsilon_0^* - \delta Z (2t^y_{zx,zx} + 4t'_{zx,zx})$

$0.29 \text{ eV}$

FeSe

2-Fe unit cell

$zx$: green  $yz$: red

$U = 3.4 \text{ eV}$  $J_H/U = 0.20$  $\delta \varepsilon_0 = 75 \text{ meV}$
Different splittings at $\Gamma$, $\Gamma^{up}$, $M_1$, $M_2$

\[ M_1 \sim \delta \varepsilon_0^* + \delta Z(2t^y_{zx,zx} + 4t'_{zx,zx}) \]
\[ \Gamma \sim \delta \varepsilon_0^* - \delta Z(2t^y_{zx,zx} + 4t'_{zx,zx}) \]
\[ \sim 0.29 \text{ eV} \]

\[ M_2 \sim \delta \varepsilon_0^* + \delta Z(-2t^y_{zx,zx} + 4t'_{zx,zx}) \]
\[ \Gamma^{up} \sim \delta \varepsilon_0^* - \delta Z(-2t^y_{zx,zx} + 4t'_{zx,zx}) \]
\[ \sim 1.56 \text{ eV} \]
Different splittings at $\Gamma$, $\Gamma^{up}$, $M_1$, $M_2$

\[ M_1 \sim \delta \varepsilon_0^* + \delta Z (2t_{zx,zx}^y + 4t'_{zx,zx}) \]
\[ \Gamma \sim \delta \varepsilon_0^* - \delta Z (2t_{zx,zx}^y + 4t'_{zx,zx}) \]
\[ M_2 \sim \delta \varepsilon_0^* + \delta Z (-2t_{zx,zx}^y + 4t'_{zx,zx}) \]
\[ \Gamma^{up} \sim \delta \varepsilon_0^* - \delta Z (-2t_{zx,zx}^y + 4t'_{zx,zx}) \]

$\sim 0.29$ eV

$\sim 1.56$ eV
Role of Hund’s coupling in the nematicity of iron superconductors

- Strong suppression of ferro-orbital ordering due to Hund’s coupling, operative for interactions suitable for FeSe.

- Anisotropic quasiparticle weight in presence of other sources of anisotropy (ferro-orbital ordering, hopping anisotropy, d-wave nematic, strain ....).

  Enhanced response at the crossover to the Hund metal (FeSe).

- Impact on the band structure: Splittings between zx/yz at symmetry points different from naive expectations. Important for the interpretation of ARPES experiments.

- Further information from the splittings at M₂ and Γ^up (optical conductivity).