Superconductivity and Spin Fluctuations in Iron Pnictides: FLEX Study

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Motivation

Understanding of mechanism of superconductivity in iron pnictides

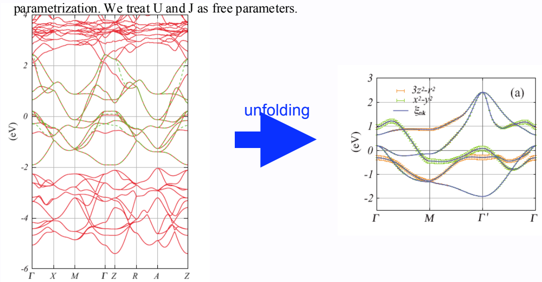
- 5-band Hubbard model
- Non-local correlations on bubble/ladder level - fluctuation exchange (FLEX)

Questions we address:

- Leading 2-particle instability (superconductivity vs magnetism)
- Doping and temperature dependent trends
- Normal state spin dynamics

5-band model for LaOFeAs

Starting from LDA bandstructure of undoped LaOFeAs for experimental lattice parameters we construct a 5-band model in unfolded Brillouin zone. We use on-site Coulomb interaction in Slater-Kanamori parametrization. We treat U and J as free parameters.



FLEX

Self-consistent weak-coupling perturbative method. Consists in replacing of the pp- and ph-irreducible vertices with their bare values and self-consistent solution of Bethe-Salpeter, Schwinger-Dyson and Dyson equations.

- 1-particle self-energy contains all bubble and ladder sums.
- Non-local reducible vertices are generated.
- Pairing vertices are generated.

Poor man's double counting - allows only minor modification of the non-interacting Fermi surface: $\delta\Sigma_{\ell m}(\boldsymbol{k},i\omega_n) = \Sigma_{\ell m}(\boldsymbol{k},i\omega_n) - \mathrm{Re}\,\Sigma^{R}_{\ell m}(\boldsymbol{k},0)$

Leading 2-particle instabilities:

1) Spin ordering

$$\hat{\chi}^s(q) = \hat{\chi}_0(q) + \hat{\chi}_0(q)\hat{U}^s\hat{\chi}^s(q) \quad \text{(Bethe-Salpeter eq.)}$$

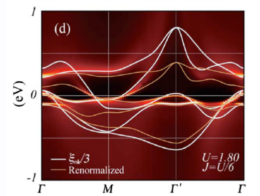
$$\chi^s(q) = \sum_{\ell m} \chi^s_{\ell\ell,mm}(q)$$

Magnetic instability: $\chi^s \approx 100$
Pairing intability: $\lambda = 1$

2) Superconductivity

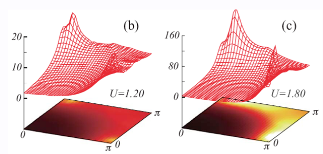
$$\Delta_{\ell m}(k) = -\lambda \sum_{k'} V^s_{\ell\ell'',m''m}(k-k')\mathcal{G}_{\ell''\ell'}(k')\mathcal{G}_{m''m'}(k')^*\Delta_{\ell' m'}(k') \quad \text{(Eliashberg eq.)}$$

Undoped system

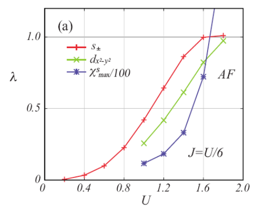


Renormalized FLEX band structure of LaOFeAs compared with uniformly rescaled LDA bands.

The static spin susceptibility for two values of the on-site repulsion at T=35 K. The peaks at $(\pi,0)$ are precursors of the stripe order.



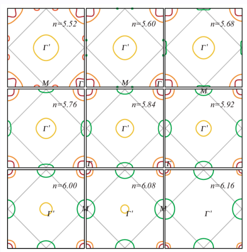
U-dependence of the Eliashberg eigenvalue λ and the spin susceptibility $\chi^s(\pi,0)$ at 35 K.



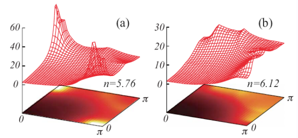
Dominant spin fluctuations due to scattering between the sheets around M and Γ' points. Survives down to electron fillings around n=5.7.

Effect of doping

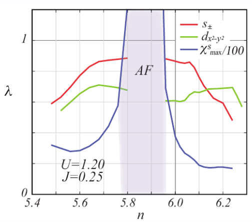
Evolution of the Fermi surface as a function of the d-band filling. Electron sheets are marked in green, hole sheets in red, orange and yellow.



The static spin susceptibility for hole and electron doping.

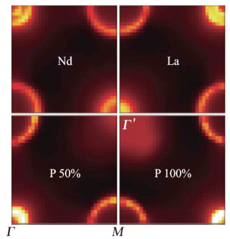


Doping dependence of the Eliashberg eigenvalue λ and the spin susceptibility $\chi^s(\pi,0)$ at 35 K.



Upon electron doping above 6.15 the Γ' sheet disappears and the low-energy spin fluctuations become dominated by scattering between different M sheets.

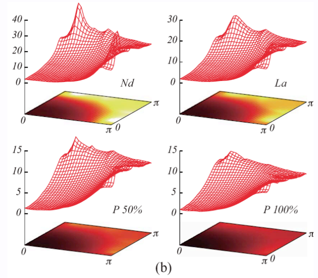
Pnictogen height



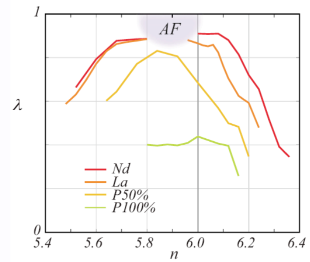
Evolution of the Fermi surface as a function of the pnictogen height. The main changes take place around Γ' point.

	Pnictogen hight (Å)	Internal coord. z
Nd	1.38	0.6580
La	1.32	0.6512
P 50%	1.23	0.6408
P 100%	1.14	0.6304

Evolution of the static spin susceptibility with the pnictogen height.



Doping dependence of the Eliashberg eigenvalue λ for the $s_\pm$ paring for several pnictogen heights.



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Summary

- FLEX is a weak coupling approach and thus provides a description qualitatively similar to non-selfconsistent RPA, i.e. description in terms of Fermi surface geometry. It takes into account variation of orbital character over the Fermi surface and T-, **k**- and orbital-dependent renormalization of quasiparticles.
- Both magnetic ordering and superconductivity are driven by Fermi surface nesting. A perfect nesting picks a single **q** and thus favors magnetic ordering, the superconducting pairing can make use of a whole (**q**,ω)-range of strong spin fluctuation modes and thus is favored by near nesting.
- The preferred pairing mode in the hole-doped region is $s_\pm$ with a small amplitude variation over FS sheets. In the electron-doped region the $s_\pm$ exhibits a large amplitude variation and eventually is replaced with $d_{x^2-y^2}$. The spin-dipole fluctuations account for 60-70% of the pairing while the rest comes from higher spin multipoles.