A Twisted Ladder: Relating the Iron Superconductors and the High-Tc Cuprates

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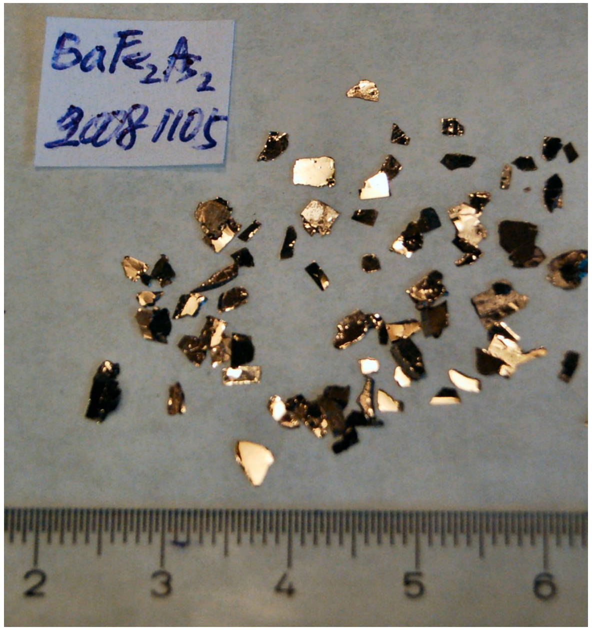
The cuprates and the pnictides

Two "High Tc" families

$YBa_2Cu_3O_{7-y}$,
Tc(max) ~ 90K

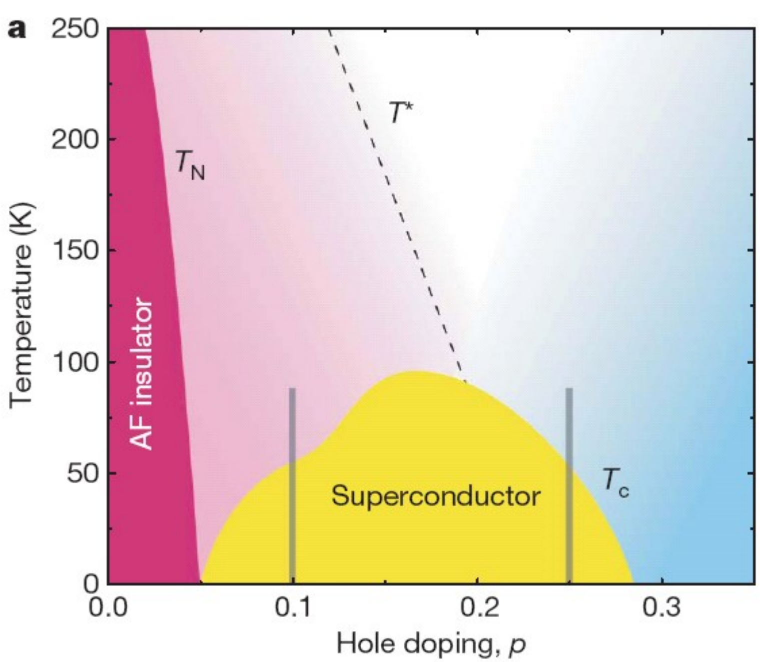
$Ba_{1-x}K_xFe_2As_2$
Tc(max)~40K



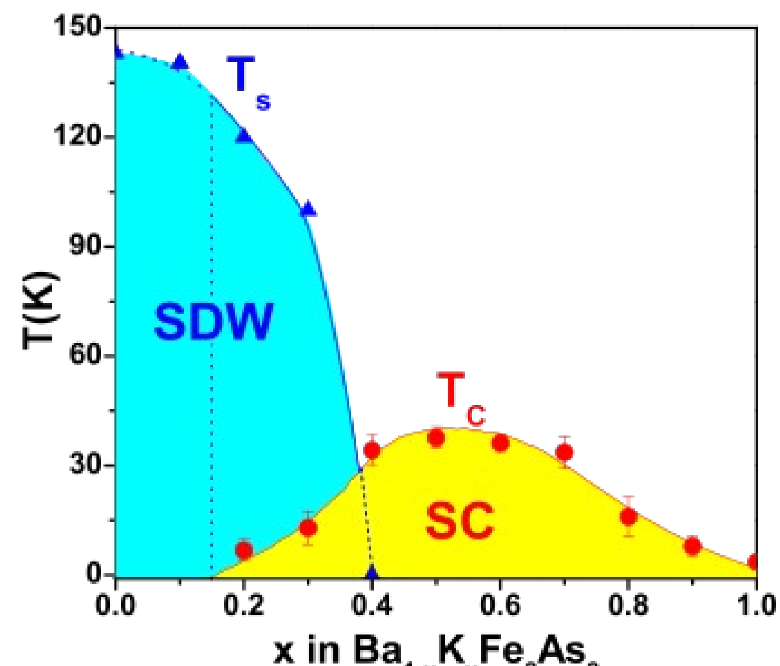
The cuprates and the pnictides

- Striking similarity of the "topology" of the phase diagram: proximity of SC and magnetically ordered states

Cuprates ($YBa_2Cu_3O_{7-y}$)



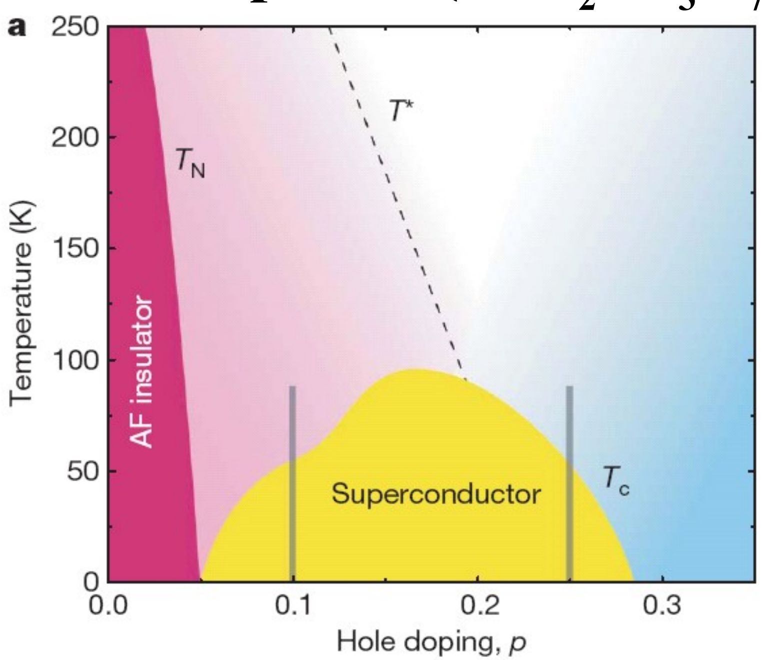
Iron pnictides ($Ba_{1-x}K_xFe_2As_2$)



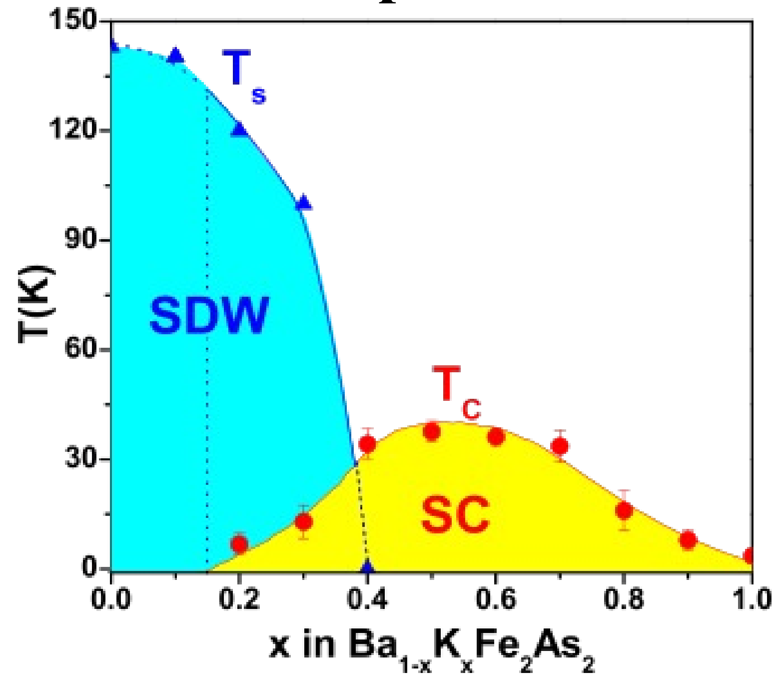
The Question

- One mechanism / Two mechanisms?
- Cuprates vs. Pnictides:
  "Similar"/"Different"?

Cuprates ($YBa_2Cu_3O_{7-y}$)



Iron pnictides



Experimentally: they are similar…

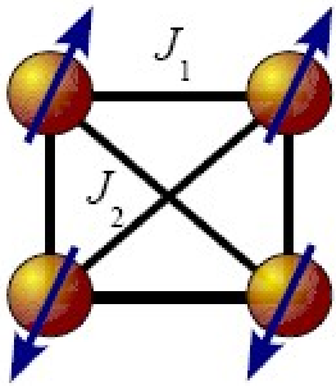
- Quasi-2D (Layered) materials
- Square lattice
- High resistivity in the normal state ("bad metal")
- Close-by magnetism
- "resonant peak" in $\chi''(q,\omega)$ at $q \approx Q_{mag},\ \omega \approx \Delta$

…But also different

- Single-band (cuprates) vs. multi-band (pnictides)
- Mott insulating vs. metallic parent compound
- d-wave vs. (possibly) s-wave order parameter

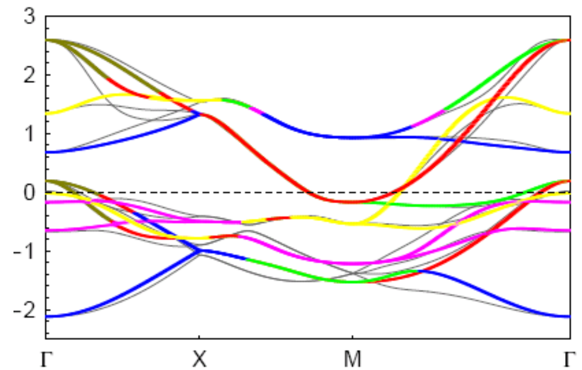
A related question: weak/strong coupling?

Strong coupling: local moments



- Bad metal ($K_f l$~1)
- Magnetism is commensurate
- Large band renormalizations

Weak coupling:energy bands



From Graser et al. (2009)

- Metallic parent compound,
  small moments
- Rough agreement between ARPES and DFT
- Q_{AF} close to a nesting vector

What does theory have to say?

- Needed: a theoretical model that can interpolate between the different regimes
- Numerical simulations on small clusters/one dimensional systems
- Can make sense since the coherence lengths are quite short

Outline

Construction of 1D "Ladder" models for the Iron superconductors.

- **Review of the Hubbard ladder model for the cuprates.**

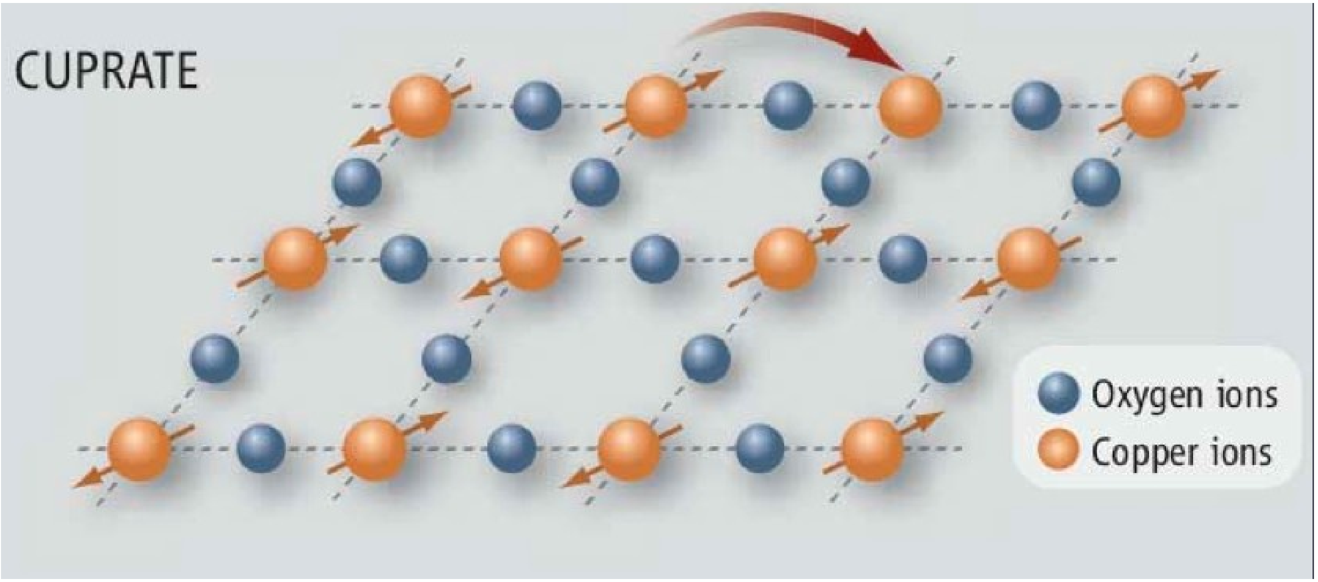
- **The pnictide one-orbital "twisted ladder"**

- **A hidden relation to the cuprates?**

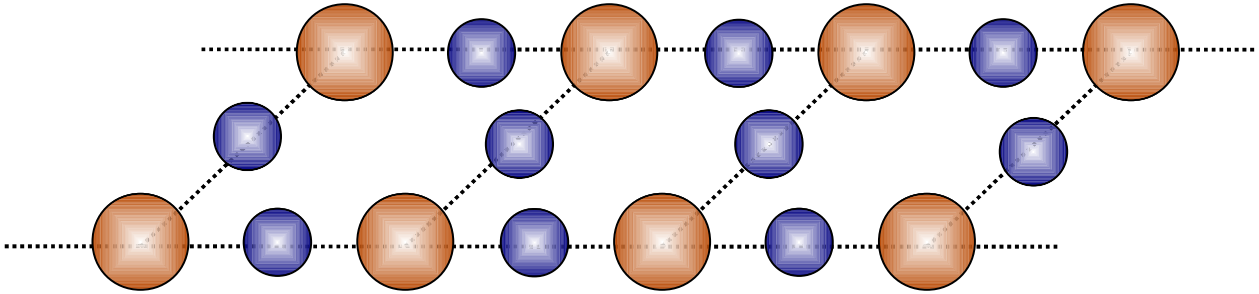
- **Beyond one orbital: preliminary results for the "diagonal ladder"**

The two-leg Hubbard model for the cuprates

Square CuO lattice:

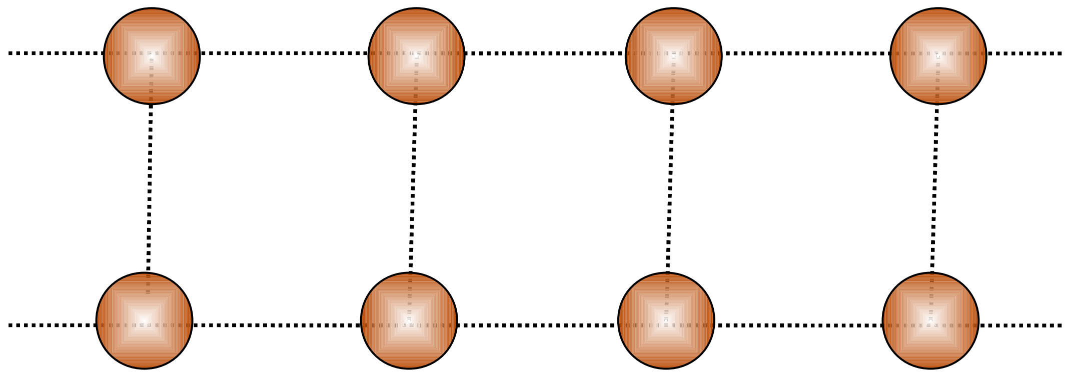


Cut out 2 chains:



The two-leg Hubbard model for the cuprates (2)

Reduce to effective 1-band model (Zhang,Rice):



With on-site interactions: the Hubbard model

$$H = -\sum_{\langle i,j \rangle, \sigma} t_{ij} (c^{\dagger}_{i,\sigma} c_{j,\sigma} + \mathrm{H.c.}) + \sum_{i} U_i n_{i,\uparrow} n_{i,\downarrow}$$

Properties of the 2-leg ladder

Dagotto, Riera, Scalapino, White, Rice,...

Undoped system:

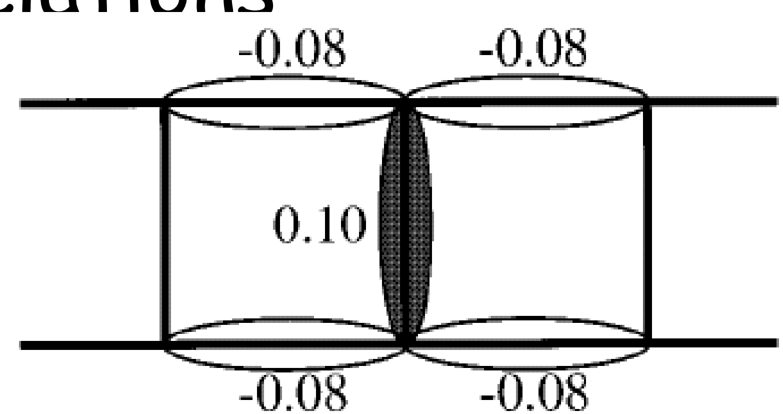
- Mott insulator for **any** U
- Finite spin gap, short range (π,π) spin correlations

Finite doping:

- Spin gap persists, d-wave like SC (and $4k_F$ CDW) power-law correlations

Pair structure:

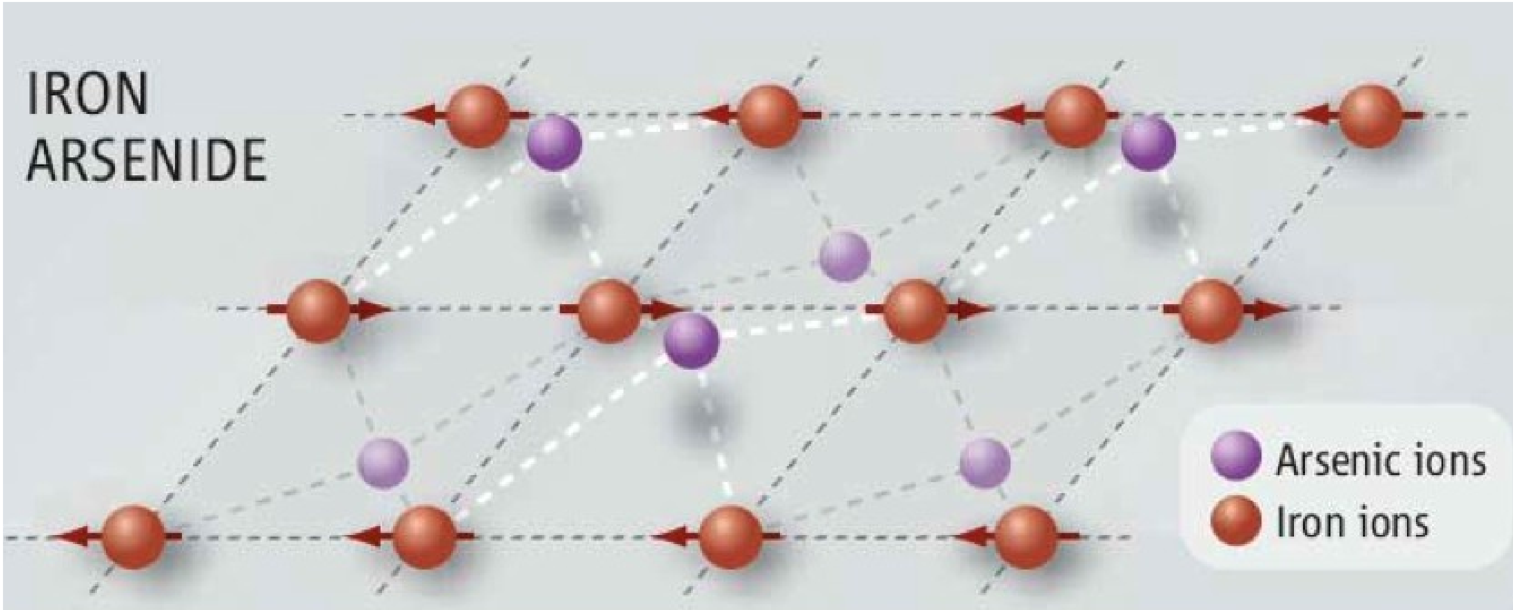
$$\Delta_{\mathbf{rr'}} = \langle N_2 | (c^\dagger_{\mathbf{r}\uparrow} c^\dagger_{\mathbf{r'}\downarrow} - c^\dagger_{\mathbf{r}\downarrow} c^\dagger_{\mathbf{r'}\uparrow}) | N_1 \rangle$$



Noack et. al. (1997)

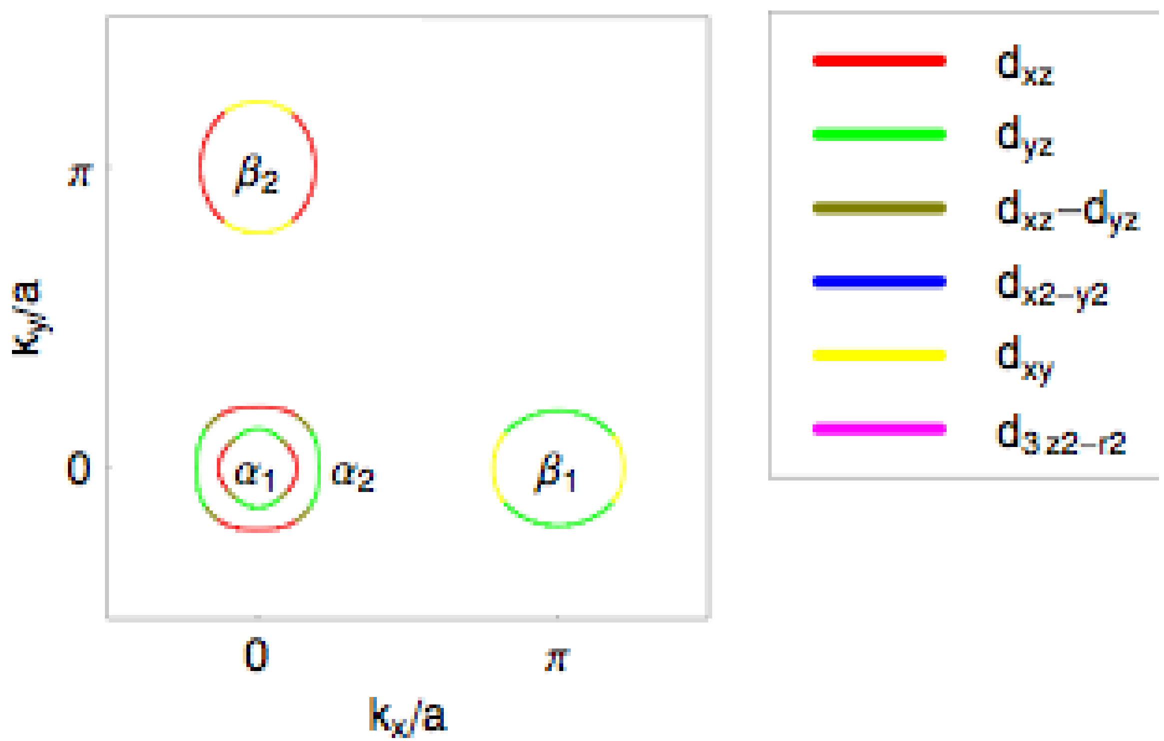
Can we play a similar game for the iron superconductors?

FeAs square lattice:



Can we play a similar game for the iron superconductors?

Tight binding fit to DFT
and orbital structure near the FS

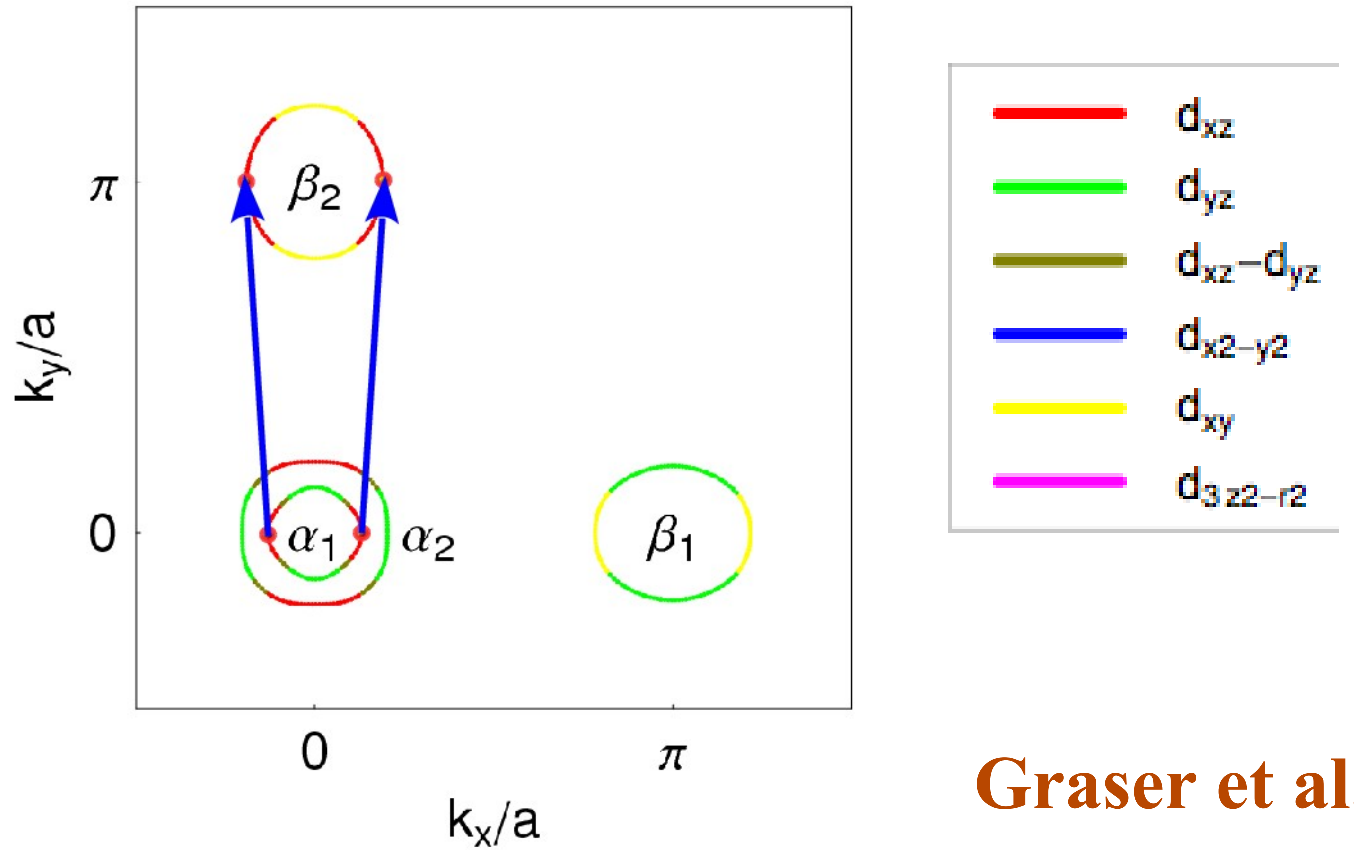


Graser et al. (2009), Cao et al. (2008)

Can we play a similar game for the iron superconductors?

Weak coupling analysis (Graser et al.):

Large contribution to pairing from intra-orbital pair scattering by $(0,\pi)$ or $(\pi,0)$ spin fluctuations

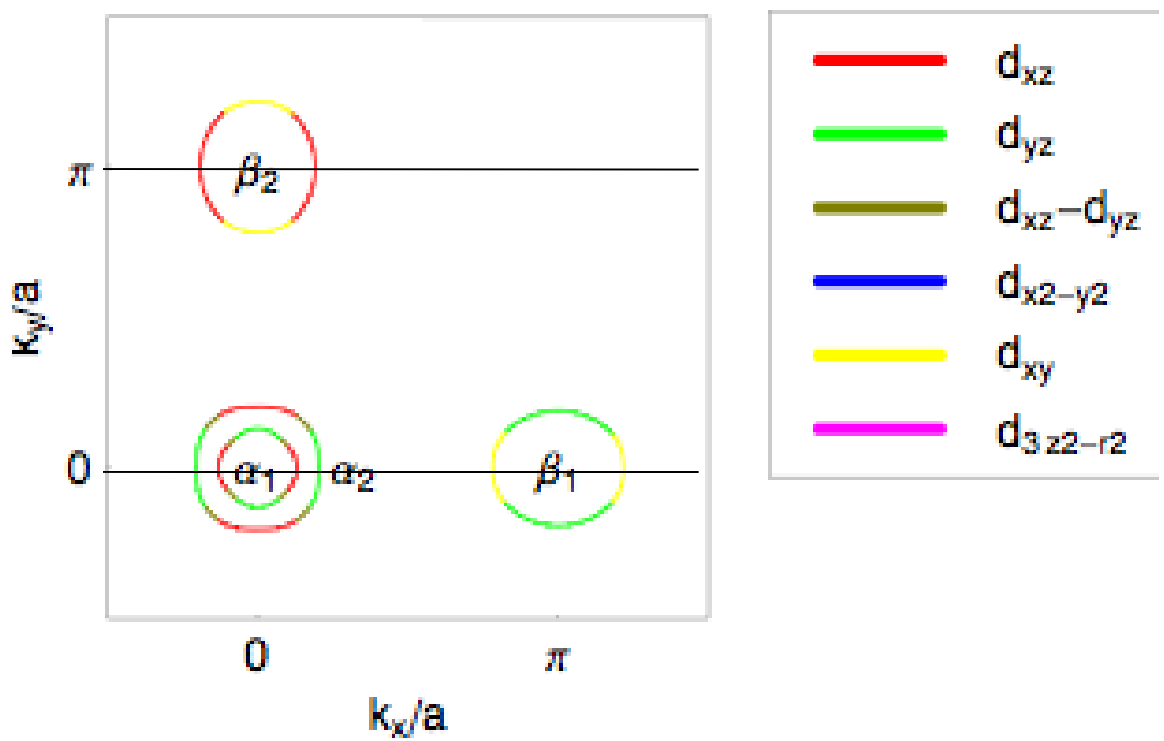


Graser et al. (2009)

Can we play a similar game for the iron superconductors?

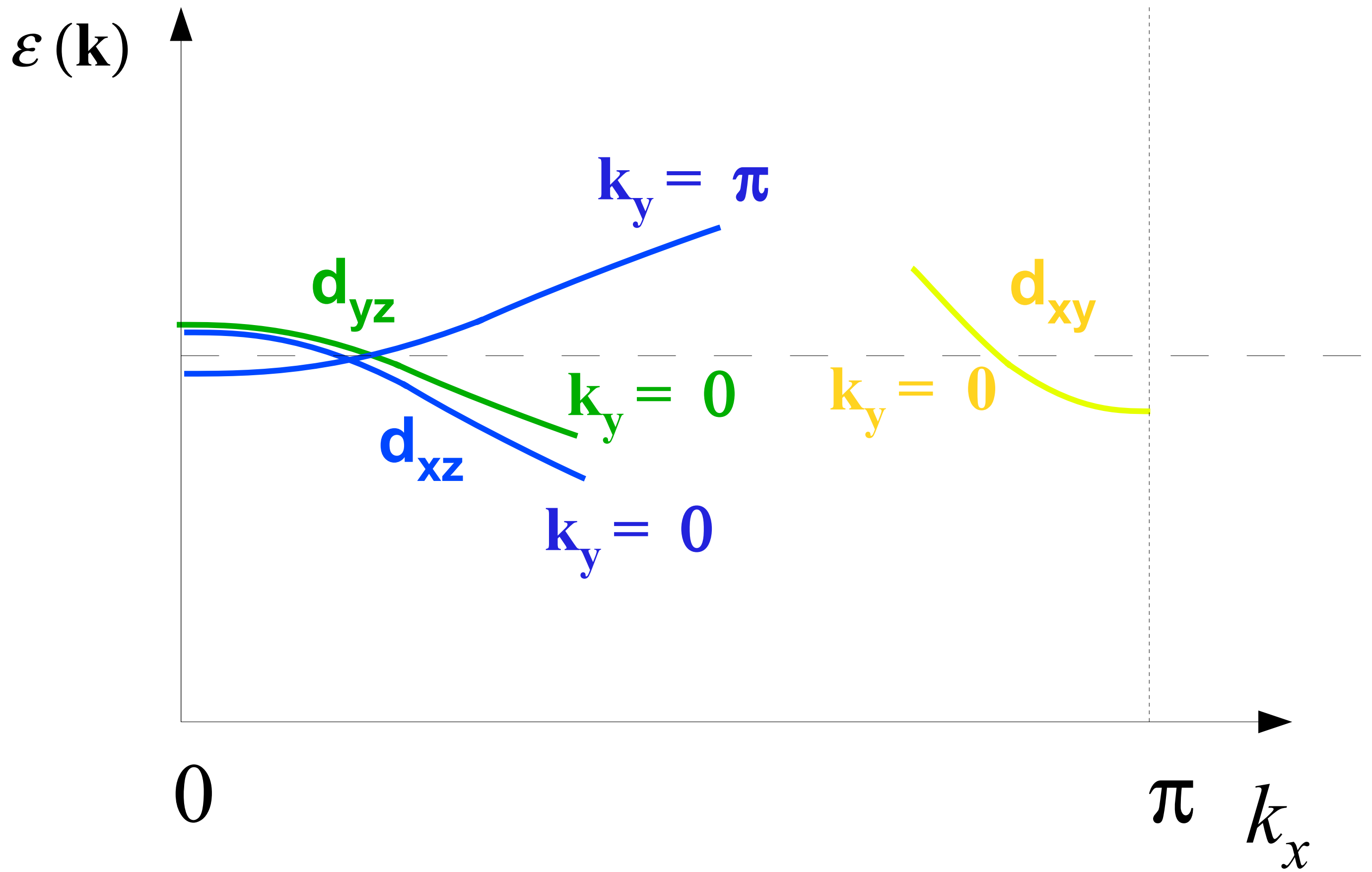
Two-leg ladder geometry:

Cut the Brillouin zone through $k_y = 0, \pi$



Band structure

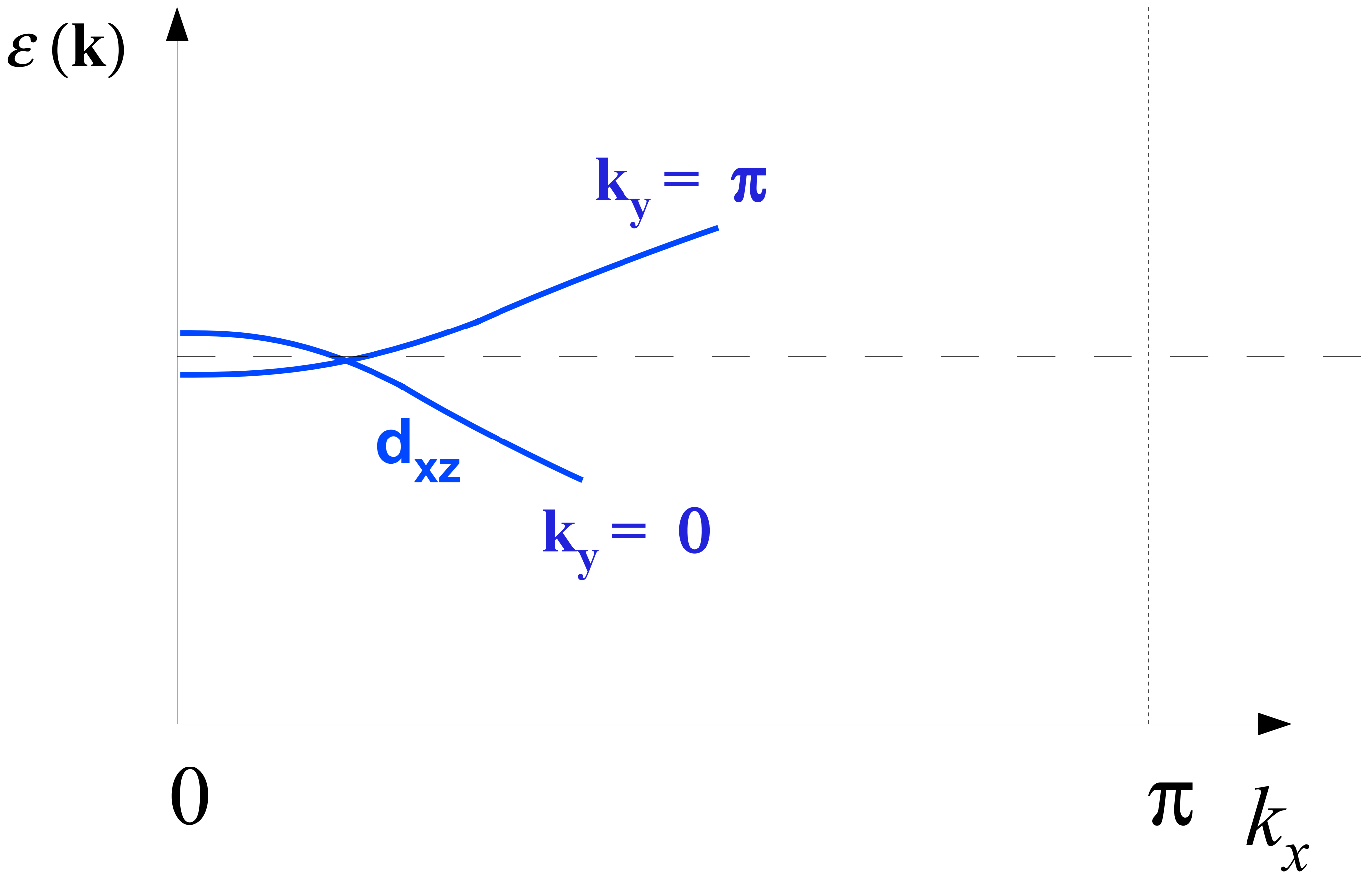
Ladder band structure near the Fermi level (schematic)



DFT calculation: Cao, Hisrchfeld, Cheng (2008)

Band structure

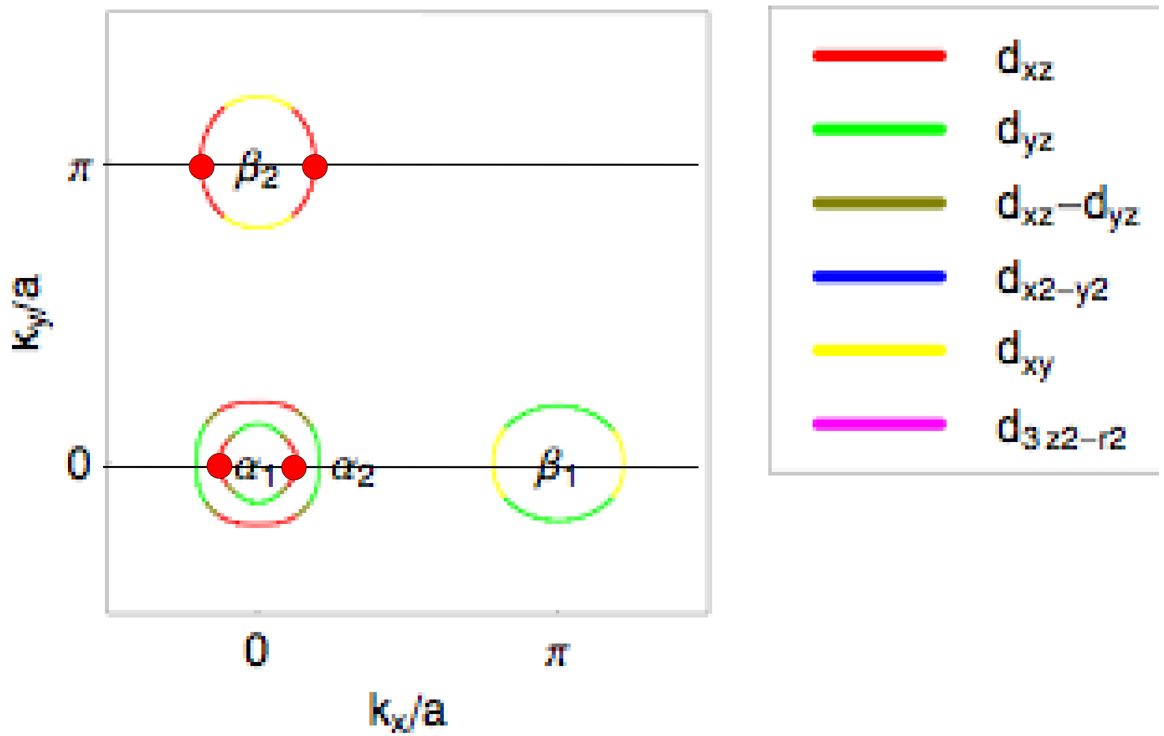
Keep only d_{xz}: (α_1 and β_2 pockets)



DFT calculation: Cao, Hisrchfeld, Cheng (2008)

Can we play a similar game for the iron superconductors?

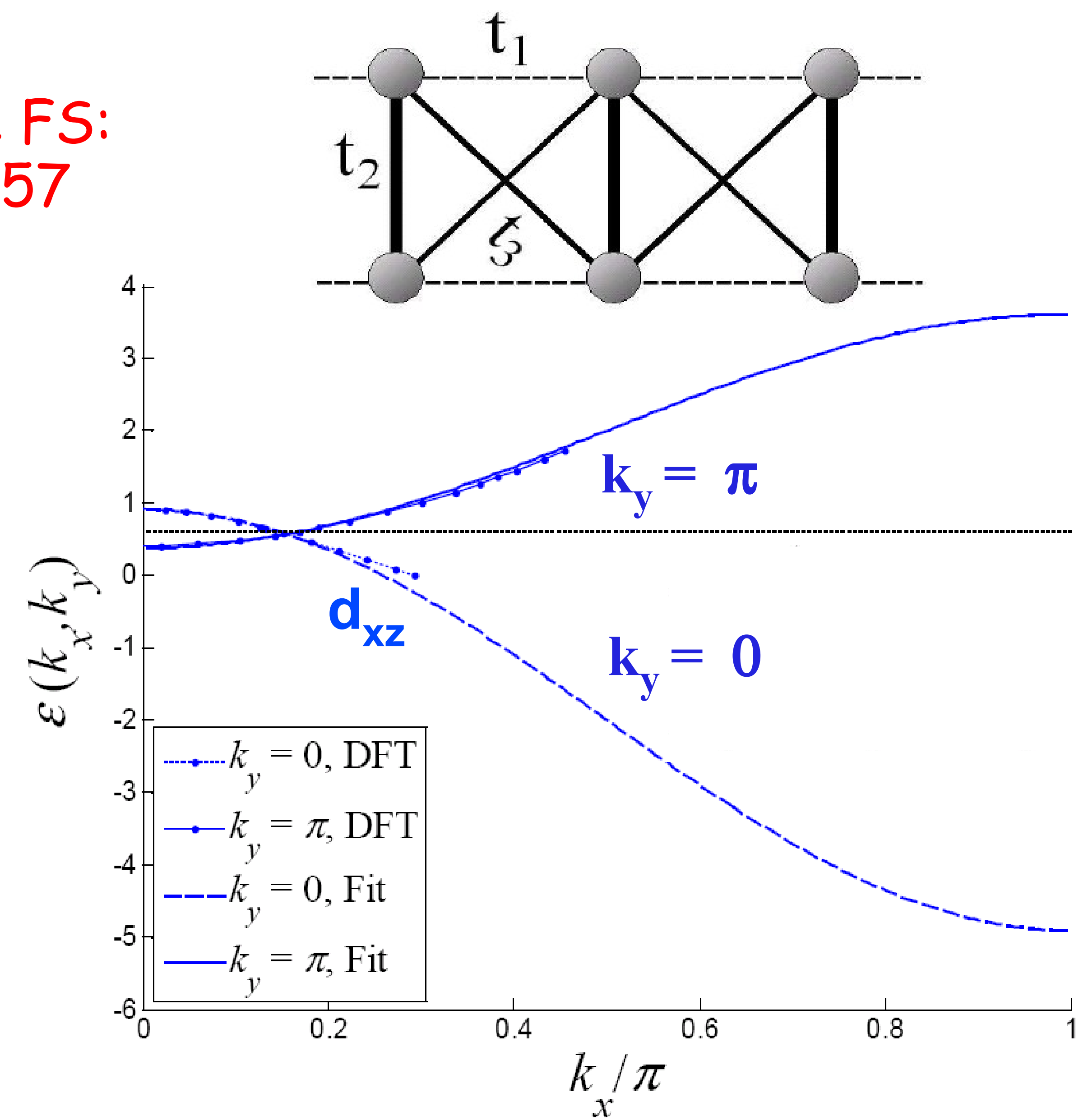
Four Fermi points with d_{xz} character



Ladder band structure

Fit to LDA near the FS:
t_1=–0.32, t_2=1, t_3=–0.57

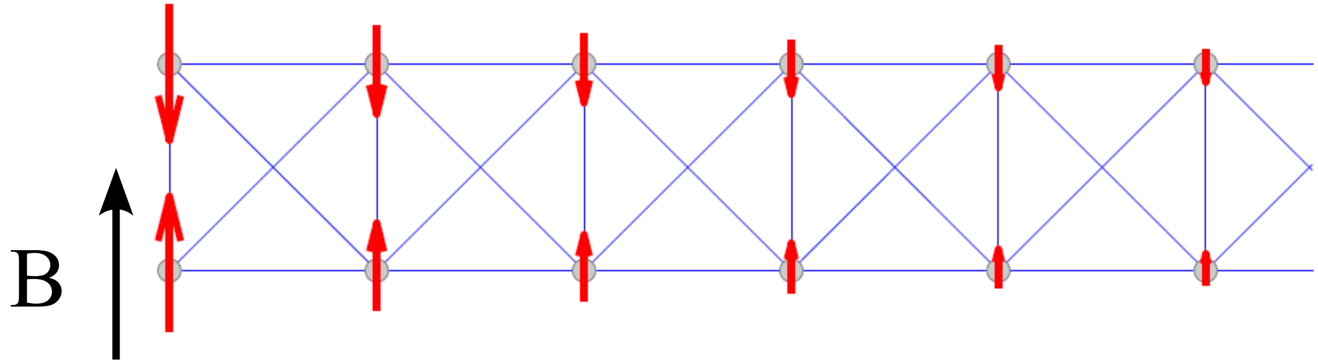
"Intermediate Coupling": U = 3



DFT calculations: Cao, Hisrchfeld, Cheng (2008)

Properties of the Fe ladder

DMRG results for the Undoped system: (n=1 per site)



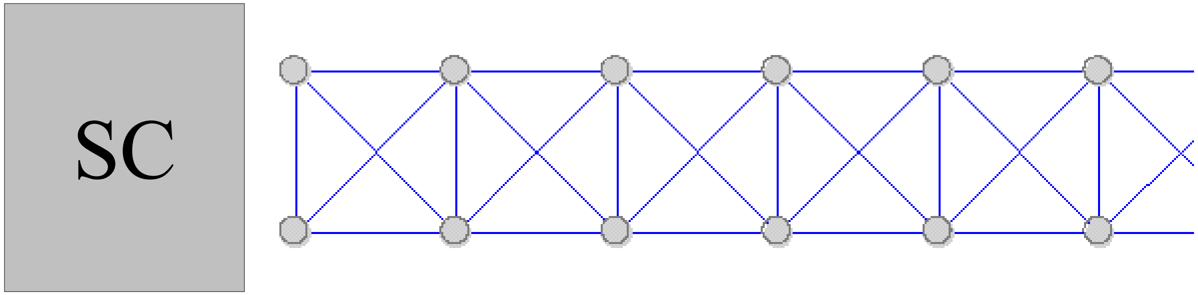
Short-range "stripe-like" magnetic correlations at $(0,\pi)$

Insulator for any non-zero U at n=1

Berg, Kivelson, Scalapino, New J. Phys. (2009)

Properties of the Fe ladder (2)

Hole doped system (n=0.9375 per site)
proximity-coupled to a bulk superconductor

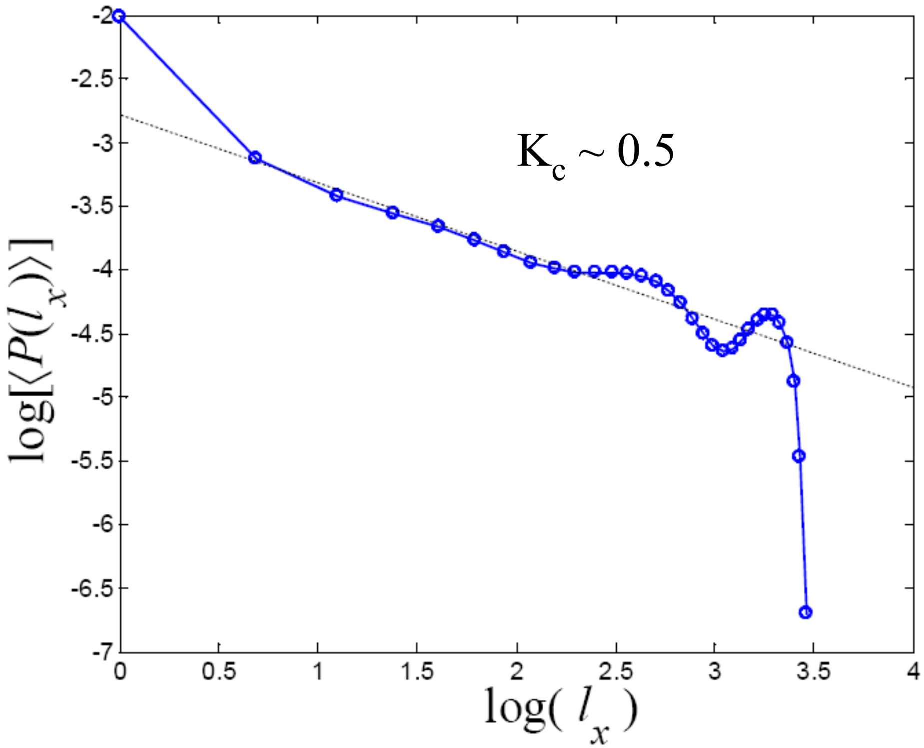


$$H_1 = \Delta_1 \left(P_1^\dagger + \text{h.c.} \right), \quad P_1^\dagger = \left(d_{1,1\uparrow}^\dagger d_{1,2\downarrow}^\dagger - d_{1,1\downarrow}^\dagger d_{1,2\uparrow}^\dagger \right)$$

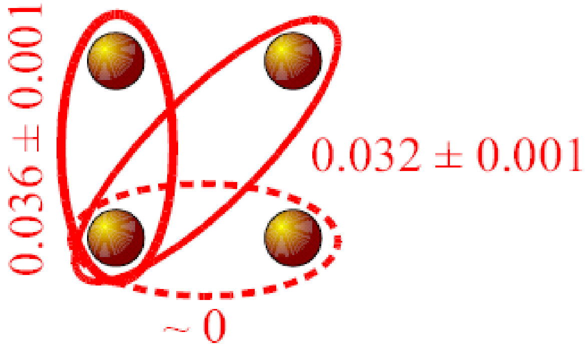
Berg, Kivelson, Scalapino, New J. Phys. (2009)

Properties of the Fe ladder (3)

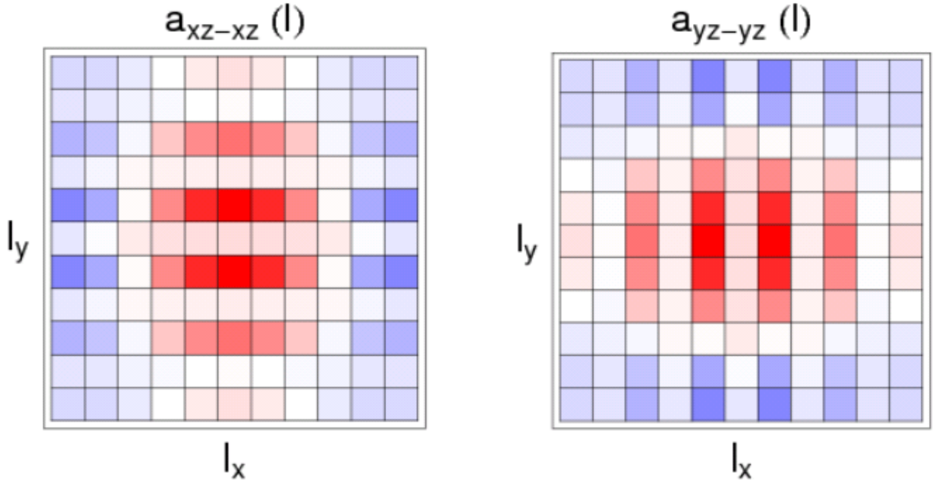
Induced rung SC order parameter for 32x2 system:



Pair structure near the middle of the system:



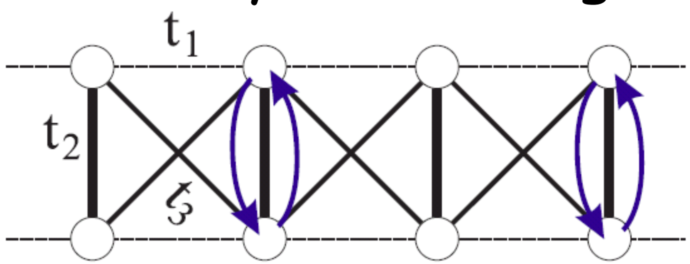
Compare to the RPA result for 5-band, 2D model (Graser et. al.) for an s± gap



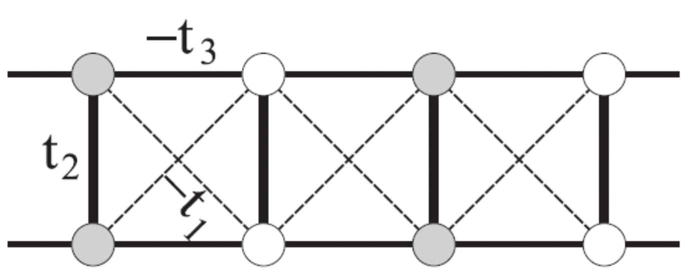
Relation to the Hubbard ladder

Under a simple "twist", the Fe ladder becomes the usual Hubbard ladder used to model the cuprates.

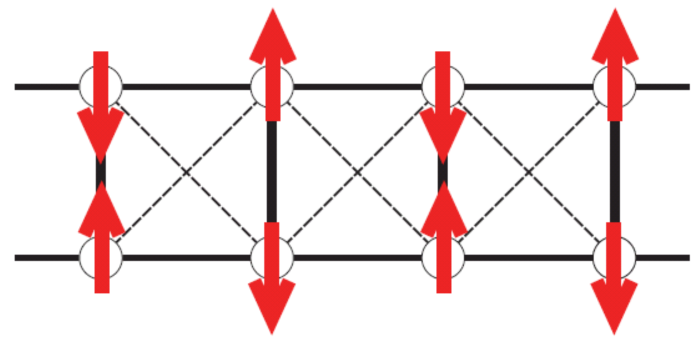
Interchange sites on every other rung



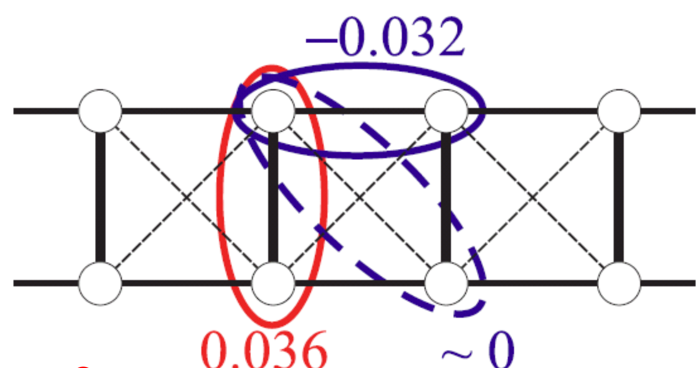
Change sign of orbitals of shaded sites $c_i \to -c_i$



Short range (π,π) magnetic correlations



Power-law $d_{x^2-y^2}$ like SC correlations



Hubbard ladder in the regime $t_2 \approx 2t_1, t_3 > 0$:

nearly optimal for pairing! (Noack et al.,1997)

Beyond one orbital?

The “Twister Ladder” model suggests a relation between the pairing mechanisms of the pnictides and the cuprates.

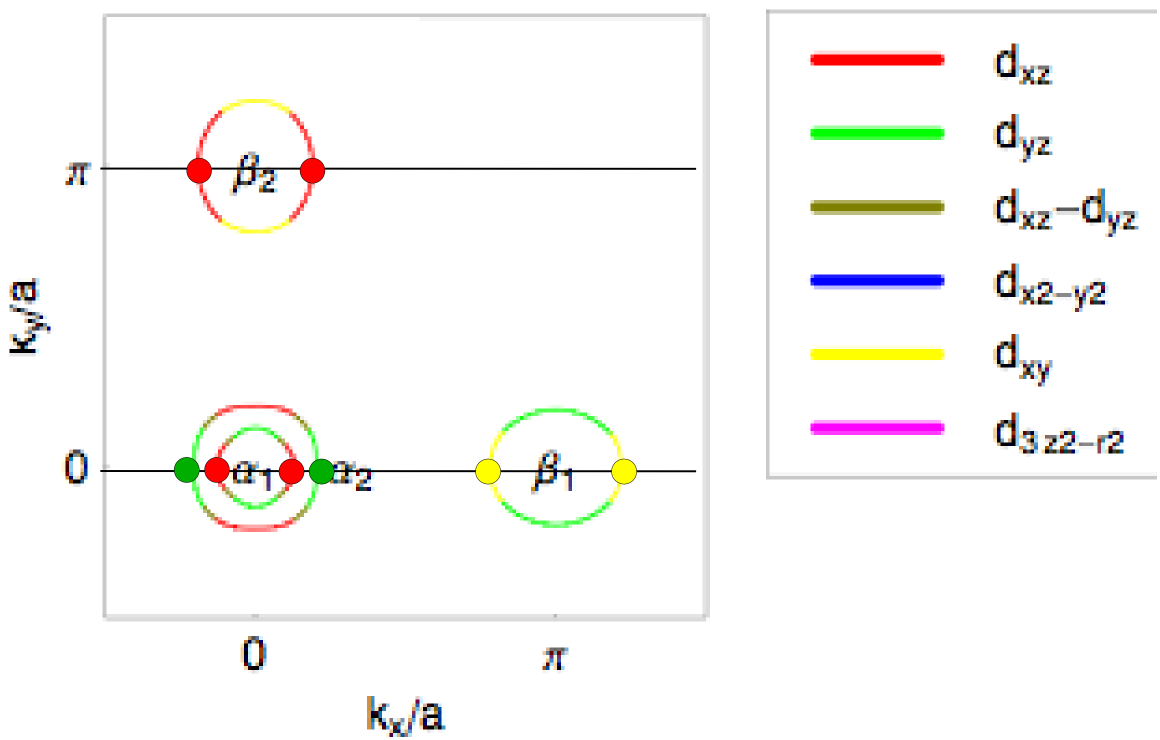
However, there are questions that it cannot address:

- d-wave vs. s-wave
- Nematic transition, orbital ordering

How to go beyond one orbital?

Beyond one orbital?

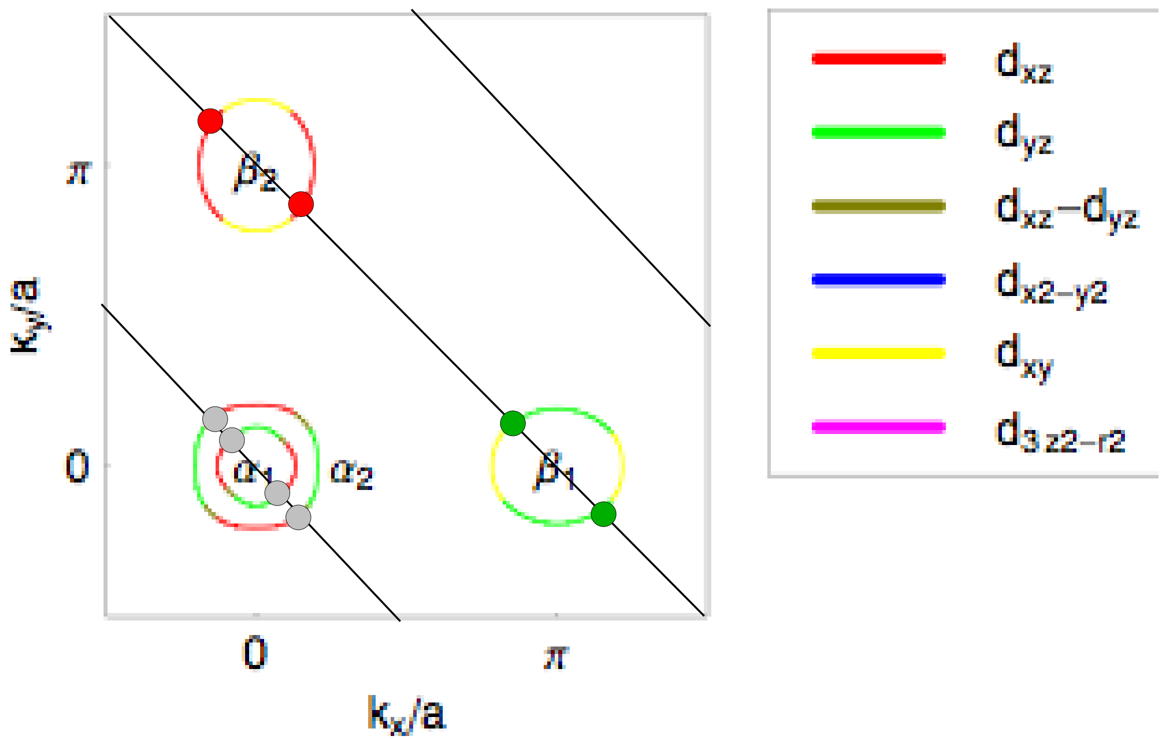
Natual extension: keep all the 2-leg ladder Fermi points (requires d_{xy}, d_{yz} orbitals)



Beyond one orbital?

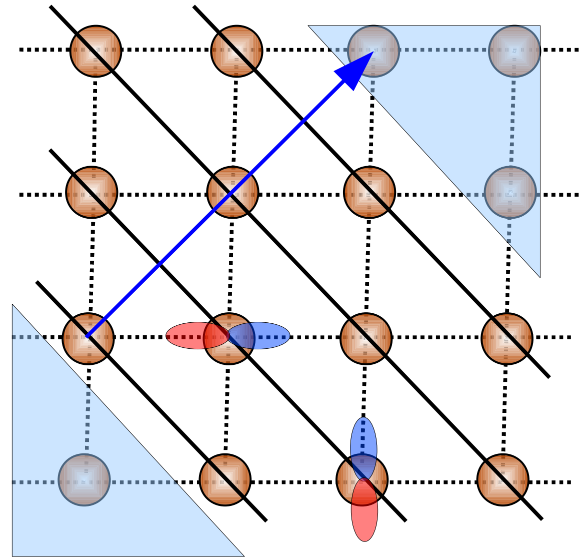
Altenatively, choose a diagonally oriented ladder

Treats the d_{xz} and d_{yz} orbitals symmetrically!



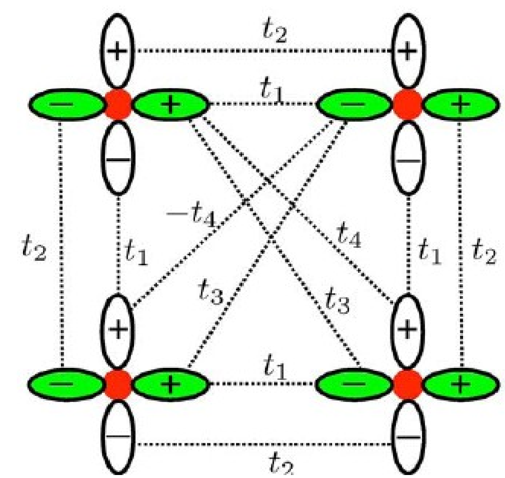
The Diagonal Ladder

Extended along (1,-1), periodic with period (2a,2a)



Keep d_{xz}, d_{yz} orbitals per site

Two band model: Raghu et. al. (2008)

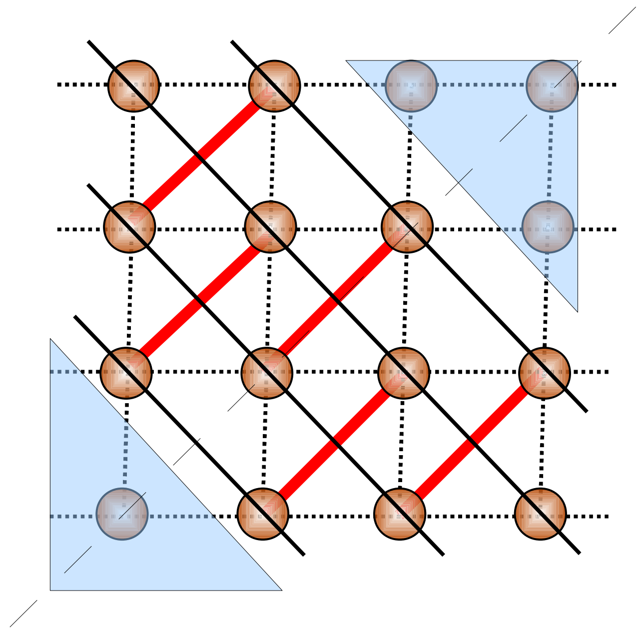


On-site Interactions:

$$H_{\text{int}} = \sum_{\mathbf{r}} \sum_{\alpha=xz,yz} \Big[U n_{\alpha\uparrow\mathbf{r}} n_{\alpha\downarrow\mathbf{r}} + V n_{x\mathbf{r}} n_{y\mathbf{r}} - J \mathbf{S}_{x\mathbf{r}} \cdot \mathbf{S}_{y\mathbf{r}} + J' \left(d^\dagger_{x\uparrow\mathbf{r}} d^\dagger_{x\downarrow\mathbf{r}} d_{y\downarrow\mathbf{r}} d_{y\uparrow\mathbf{r}} + H.c. \right) \Big]$$

The Diagonal Ladder

Essentially, a 2-leg, 2-orbital model



Properties of the 2-orbital diagonal ladder:

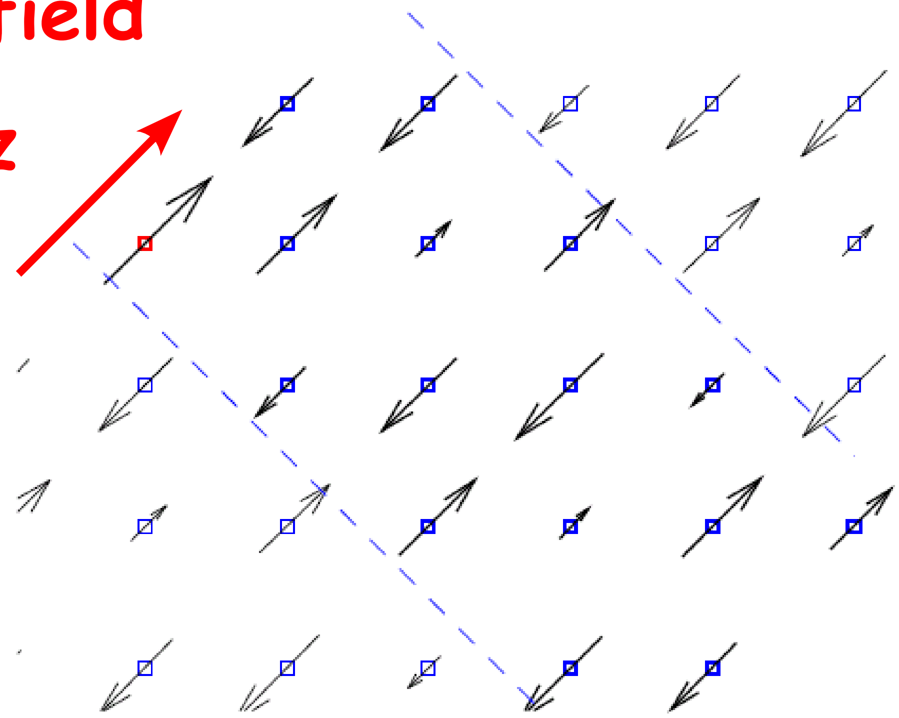
- Can be metallic at zero doping
  (Finite U_c for Mott insulaor)
- Reflection symmetry about the (1,1) direction:
  - Possible to have a nematic phase
  - Can distinguish d and s-wave pairing

Preliminary results

$U = 4, V = 3, J = U–V, J' = J/2$

Magnetic correlations in the undoped system (2 el. per site, 8x2)

Magnetic field on the dxz orbital

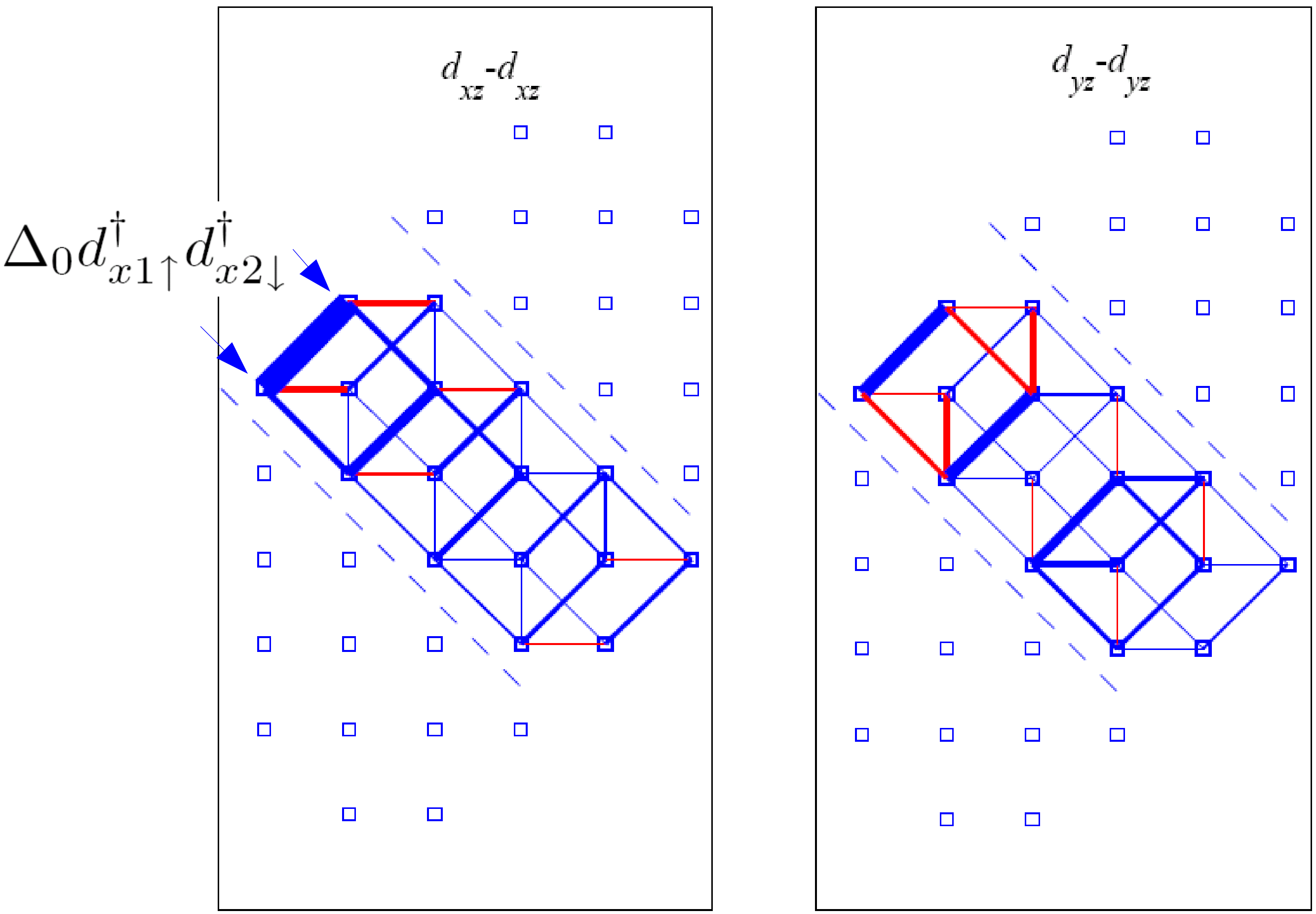


Preliminary results

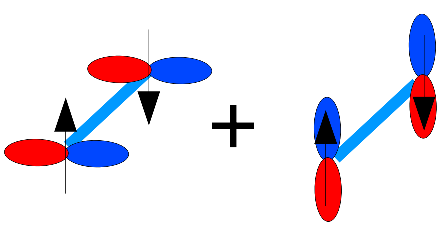
U = 4, V = 3, J = U–V, J' = J/2

Pairing correlations in a 8x2 system doped by 2 electrons: Proximity coupling to the last d_{xz} rung

Induced SC order parameter:



This calculation indicates s-wave!

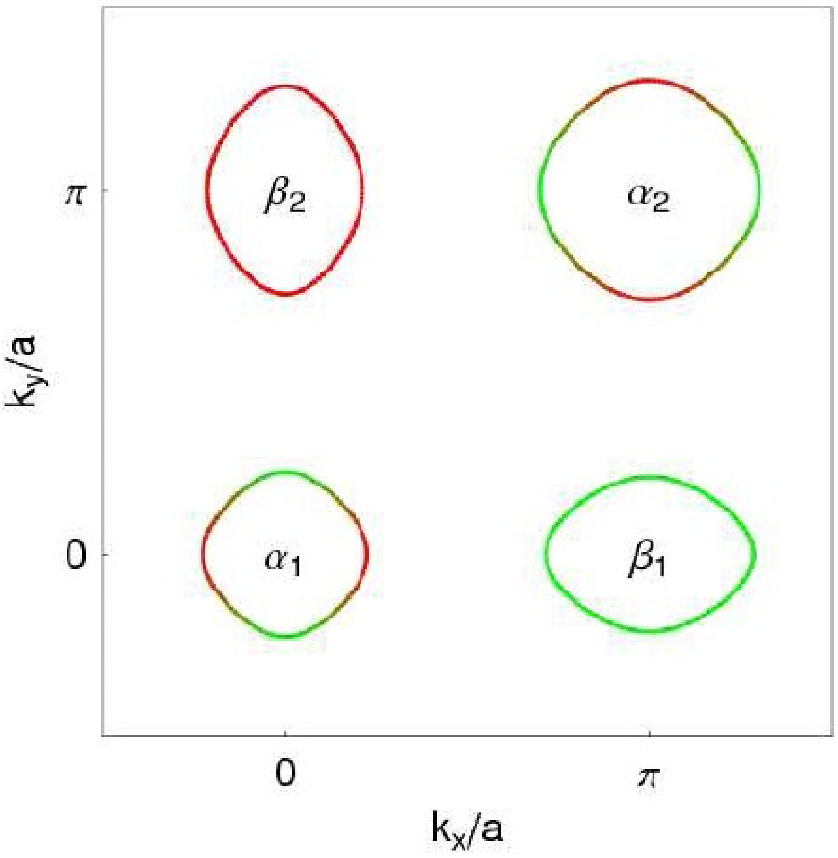


Conclusions

- A 2-leg ladder model of the Fe superconductors was used to understand some of their magnetic and superconducting correlations.
- The model turns out to be just a "twisted" version of the 2-leg Hubbard model often used to describe the Cuprates, suggesting that the mechanism of superconductivity is closely related to that of the cuprates.
- To answer more detailed questions, a diagonal two-orbital ladder model is proposed. This model can elucidate the pairing symmetry and the existence of other correlations (e.g. nematic order).

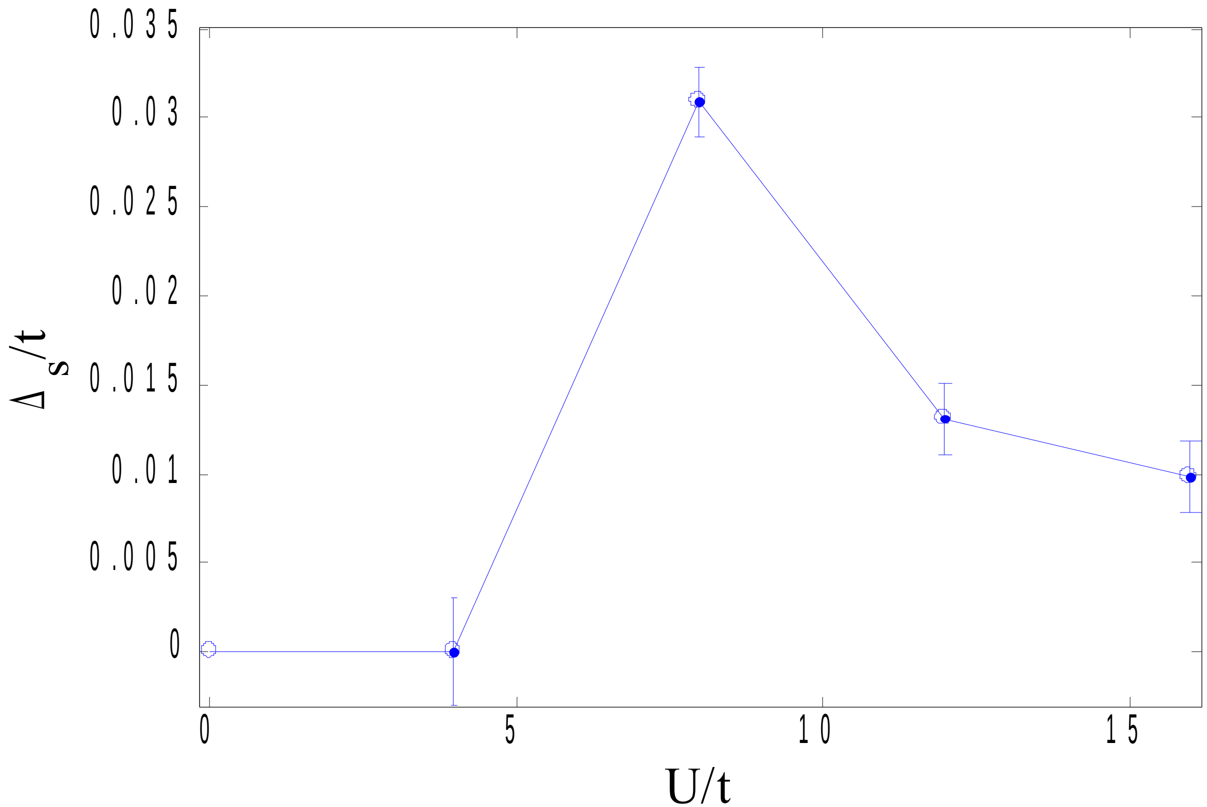
  Studies of the diagonal ladder (DMRG and weak coupling RG) are under way.

2-orbital model band structure



Properties of the 2-leg ladder

Spin gap vs. U/t:



Max. for U/t ≈ 8: **intermediate coupling!**

Outline

phase diagram, high value of the normal-state resistivity, magnetic resonance in the SC state) and differences (metallic/Mott insulating normal state, single/multi-orbital system, full gap/d-wave)

- The questions: two superconducting mechanisms or one? Weak or strong coupling? (1-2)
- SC from repulsive interactions:general features
- 1D: the 2-leg ladder Hubbard model for the cuprates
- Models for the pnictides: strong/weak coupling
- Graser, Maier, Hisrchfeld, Scalapino: band structure,importance of intra-orbital alpha-beta pocket scattering
- Fit to band structure. 2-leg model
- Results: spin correlations, spin gap, pairing correlations
- Relation to the Hubbard ladder
- The next step: treat two orbitals symmetrically. The diagonal ladder
- Preliminary results for the diagonal ladder
- Summary

A related question: weak/strong coupling?

- Possible answer: cuprates - "strong", pnictides - "weak". (insulating vs. metallic when undoped)
- ...But there are indications that both are "intermediately coupled".
- Optical conductivity data from M. Qazilbash, D. Basov et al (Nature Phys. 2009):