Superconductivity in Iron Pnictides: From DFT to a functional RG Study

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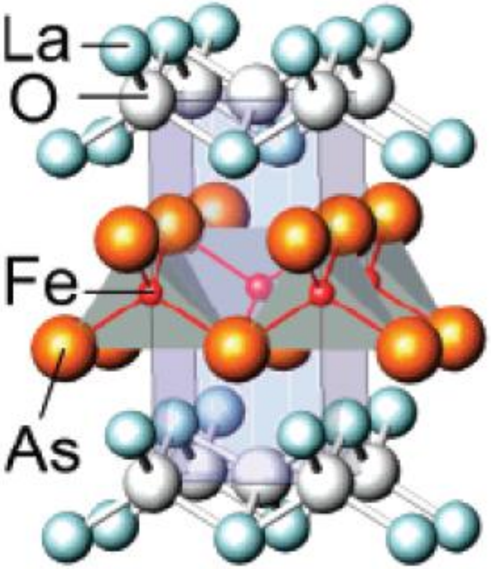
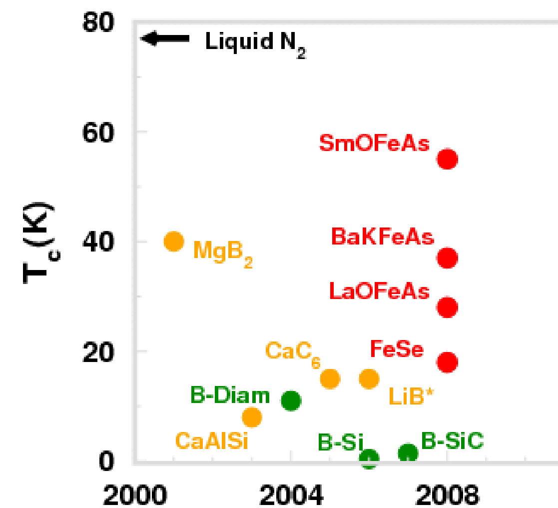


The Impact of Iron-based Superconductors :

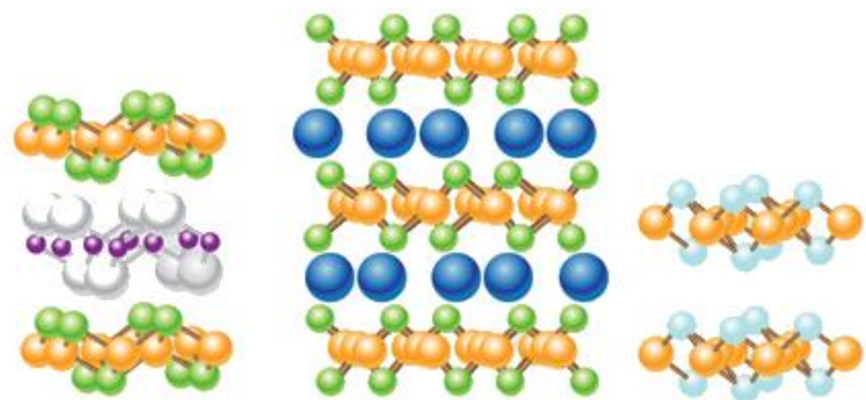
– Discovery of superconductivity in doped LaOFeAs by Kamihara *et al.* (Feb. 2008)

– Other iron-based SC followed shortly

– Possibility of higher-T_c in new iron-based compounds



Are iron pnictides new cuprates ?



R OFeAs
R: rare earth
iron arsenide 1111

A Fe_2As_2
A: alkaline earth
iron arsenide 122

FeSe, FeTe
(iron chalcogenides)

Overview

Introduction

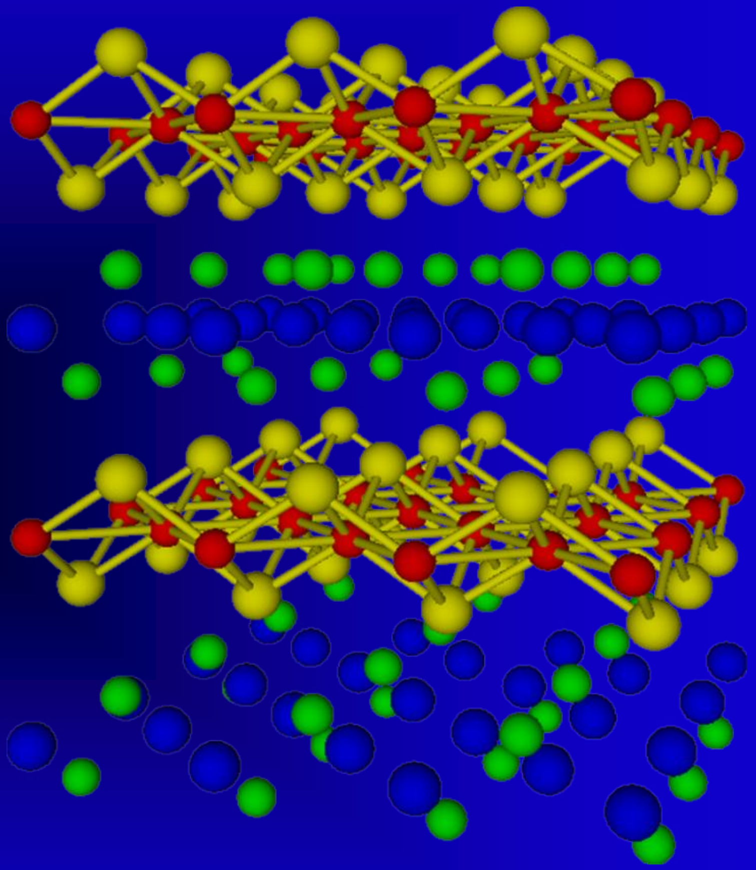
Band structure and Tight-binding approximations

Competing Orders at low Temperatures

Functional Renormalization Group (fRG)

Superconductivity in Pnictides (and Cuprates)

Conclusions



Central Question:

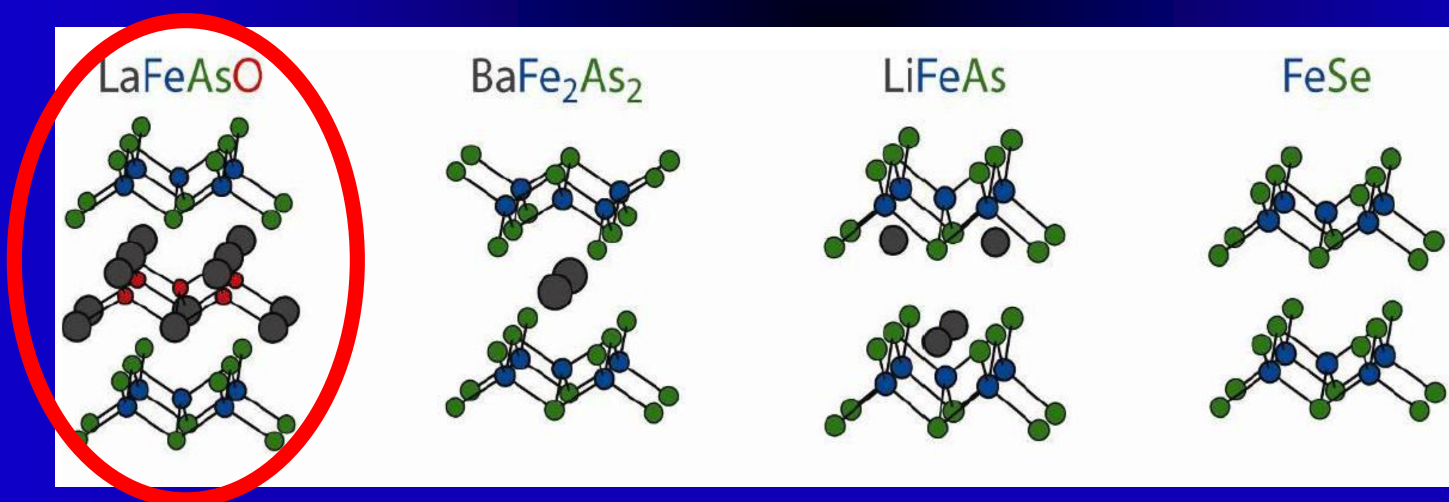
What is universal and what ist material-dependend?

New J. Phys. 11, 055058 (2009)

Introduction

Motivation

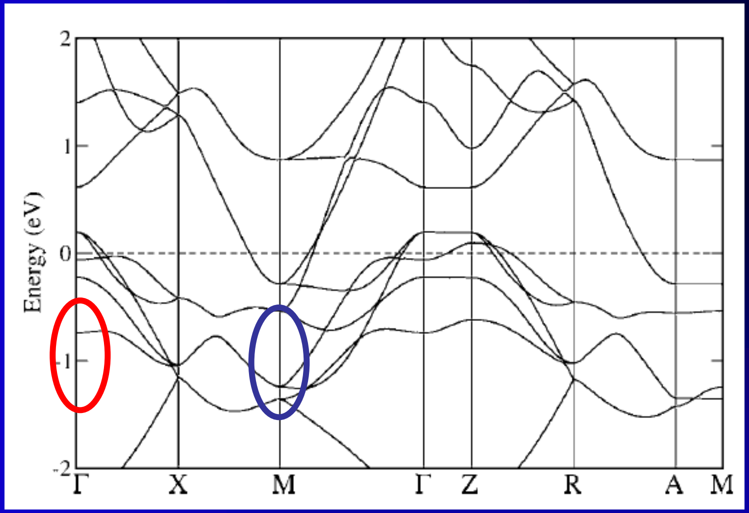
- Multiple disconnected Fermi surface sheets allow interesting superconducting states
- *s*-wave and *d*-wave are no longer synonyms for nodeless and nodal gaps
- New class of materials with similar electronic properties, but also remarkable differences



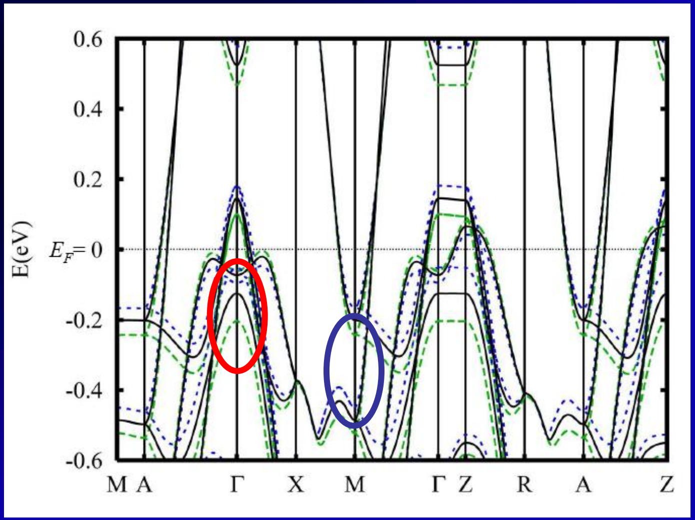
Bandstructure calculations

DFT bands

- DFT results for LaOFeP and LaOFeAs very similar
- Hole pocket around Γ and electron pocket around M



DFT of LaOFeP, Lebègue (2007)

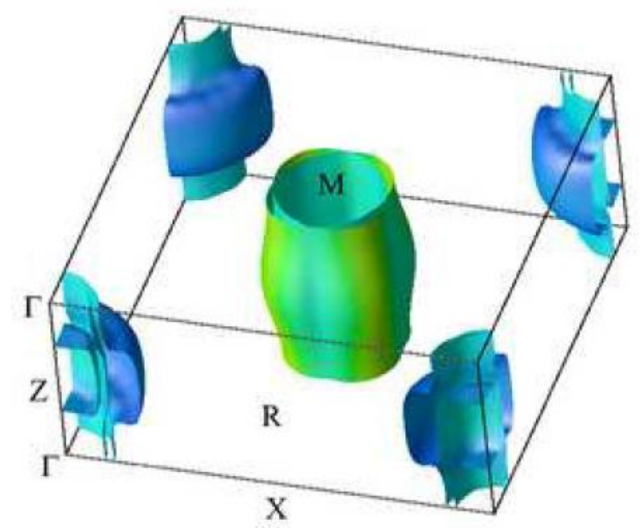


LaOFeAs, Singh and Du (2008)

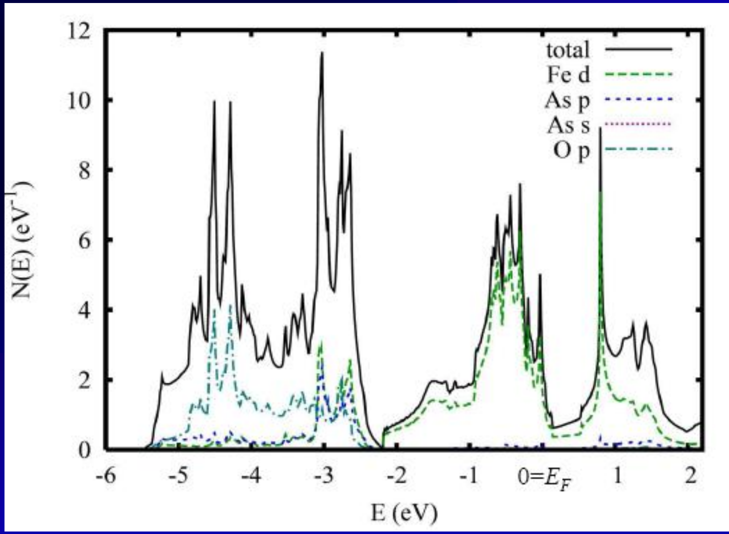
Bandstructure calculations

Fermi surface and DOS

- Fermi surface shows strongly 2D behavior
- DOS at the Fermi level: Fe 3d (and As 4p) orbitals



LDA FS, LaOFeAs, Singh and Du

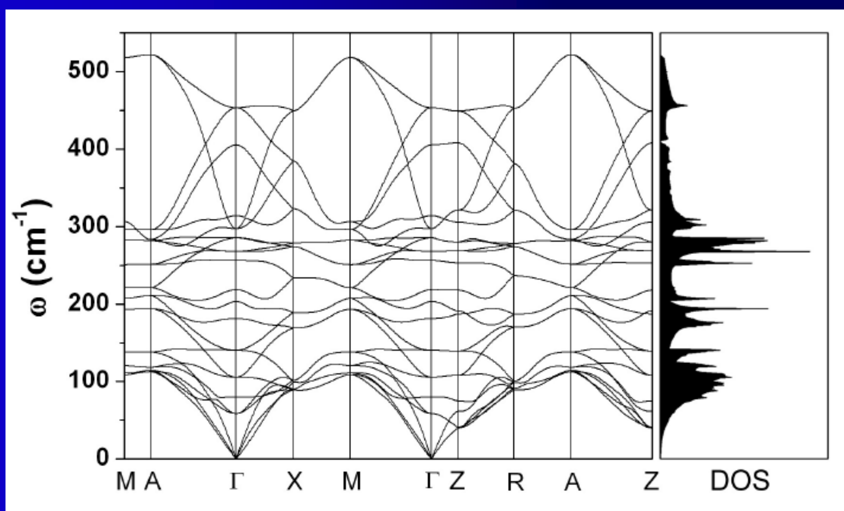


LDA DOS of LaOFeAs, Singh and Du

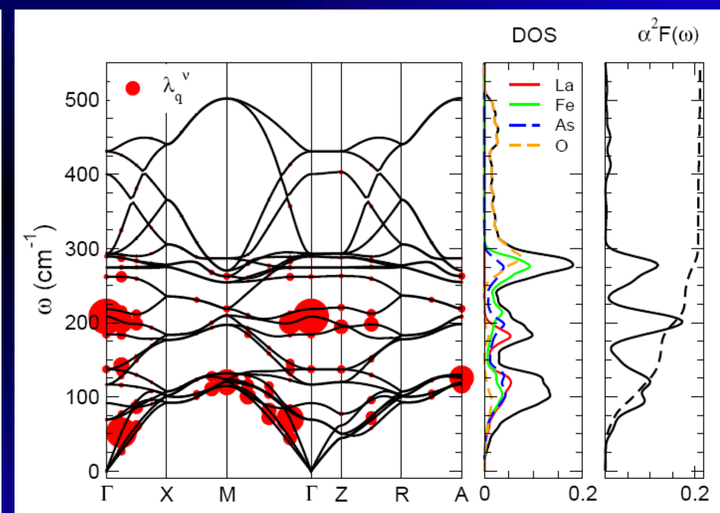
Bandstructure calculations

Electron-phonon coupling

• Only modest phonon densities in LaOFeAs, not sufficient for high T_c (λ=0.21)



Phonon dispersion and DOS, Singh and Du

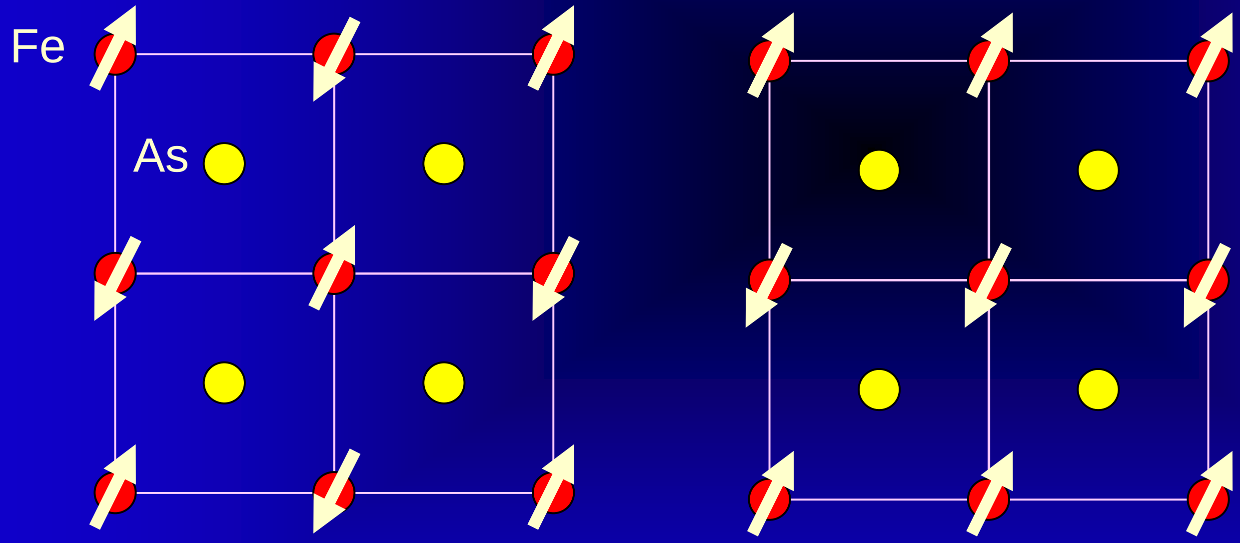


Electron-phonon properties, Boeri *et al.*

Bandstructure calculations

Parent compound is antiferromagnetic

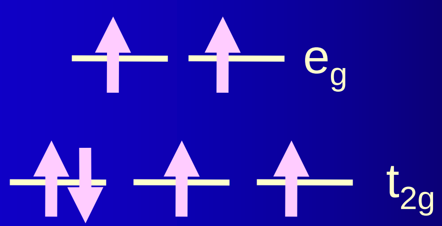
• For the parent compound: AF order is 40 meV lower in energy than pm state
Linear SDW state is 100 meV lower



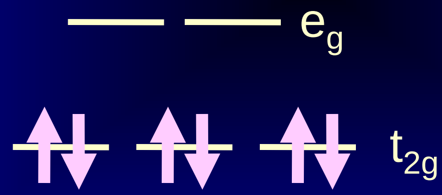
Bandstructure calculations

Possible explanation for small Fe moment

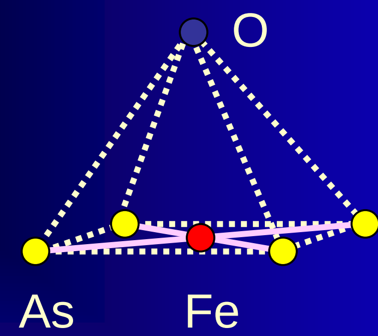
- La^{3+}, O^{2-}, As^{3-} → Fe^{2+} configuration
- *octa*hedral environment of Fe: splitting of t_{2g} and e_g orbitals



Hund's rule coupling dominates: S=2



Crystal field splitting dominates: S=0

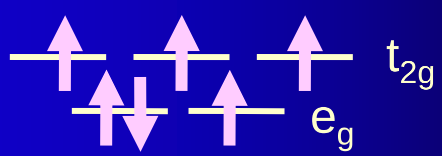


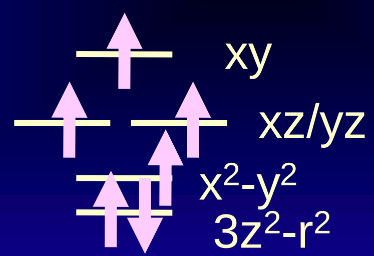
Bandstructure calculations

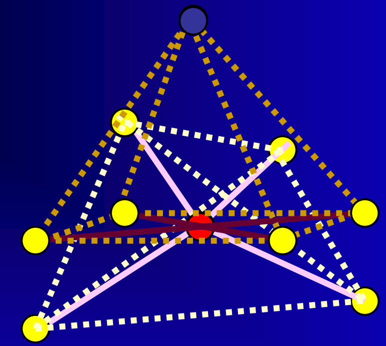
Possible explanation for small Fe moment

Cvetkovic and Tesanovic
Yildirim

- La^{3+}, O^{2-}, As^{3-} → Fe^{2+} configuration
- *tetra*hedral environment of Fe: splitting of t_{2g} and e_g inverted and reduced
- Band effects lead to further splitting of orbital states







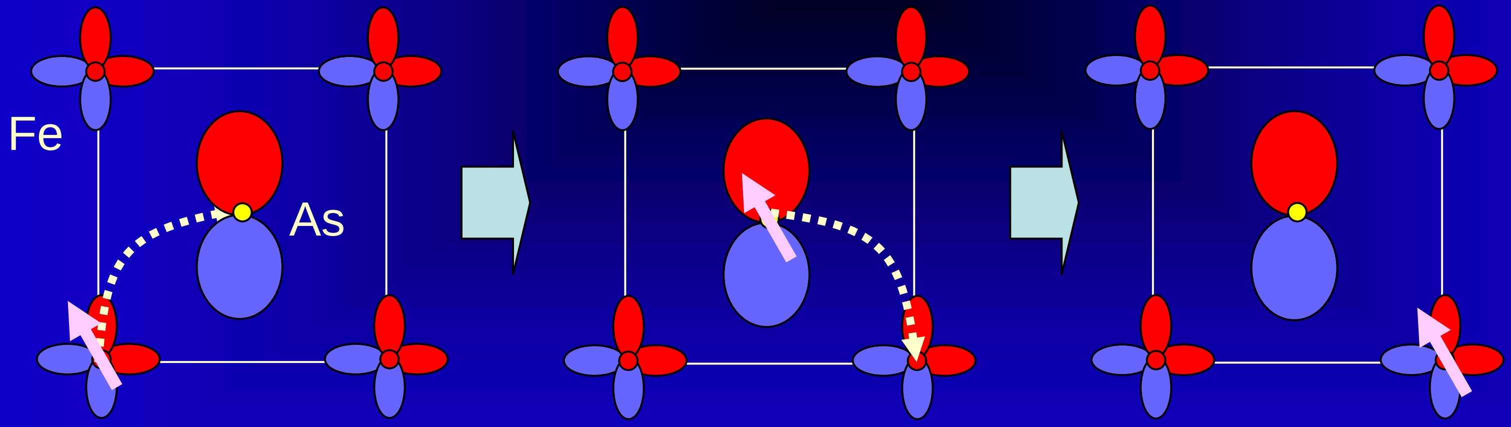
Large spin state: S=2

- Frustrated magnetism due to competing nn and nnn superexchange
  → small effective Fe moment

Tight-binding approximations

Basic considerations for simplification

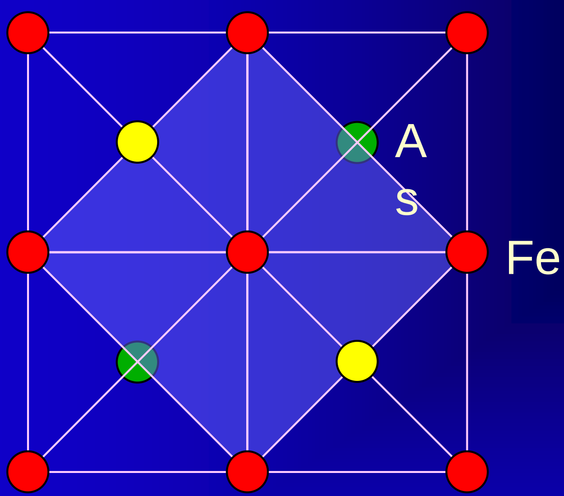
- Only the Fe (and As) bands are close to the Fermi level (16 important orbitals)
- LnO layers act as spacing layers, provide carriers by out-of-plane doping
- Description in an effective Fe-Fe model possible
- As *p* orbitals mediate hopping between Fe *d* orbitals and hybridize the Fe bands



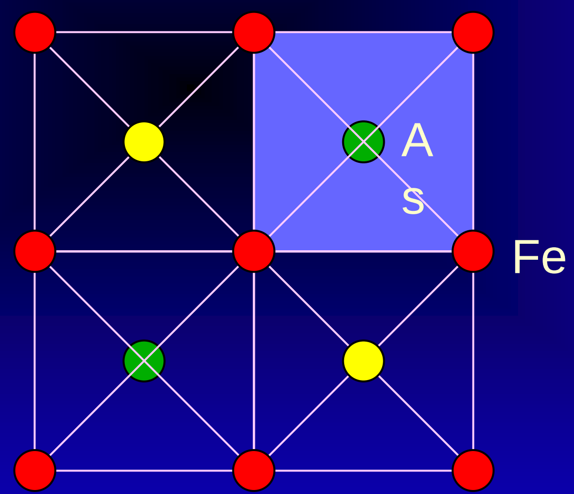
Tight-binding approximations

Basic considerations for simplification

- FeAs plane similar to CuO plane in cuprates, but As is out of plane
- 8 atoms per unit cell, although high degeneracy of As/La positions makes it convenient to work with reduced unit cell



real unit cell

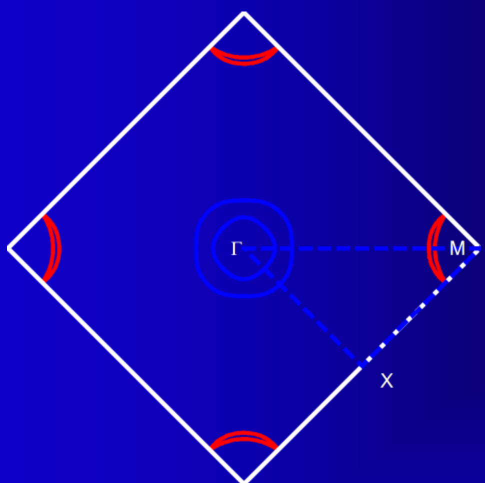


reduced effective unit cell

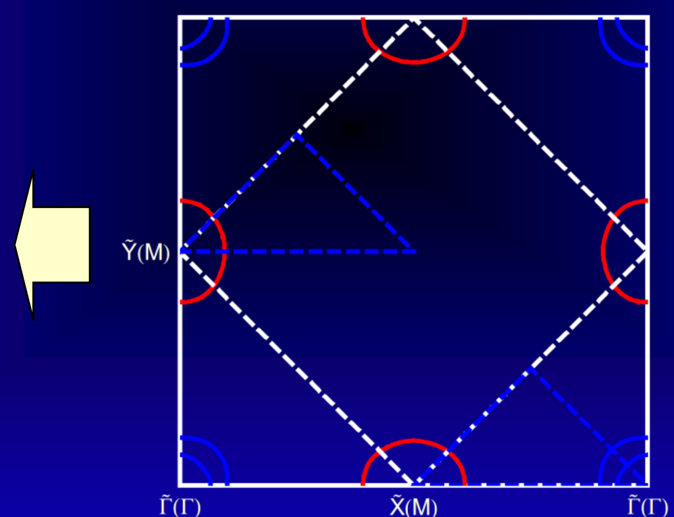
Tight-binding approximations

Basic considerations for simplification

- *Effective* Brillouin zone has to be „backfolded“ to give the *real* Brillouin zone



real Brillouin zone

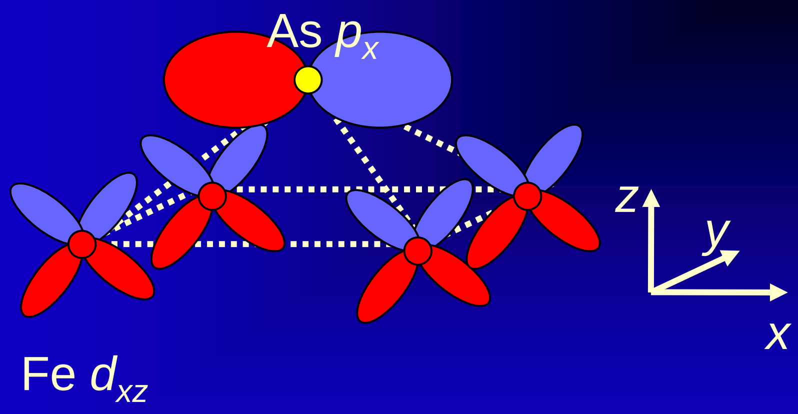


effective Brillouin zone

Tight-binding approximations

Two-orbital model

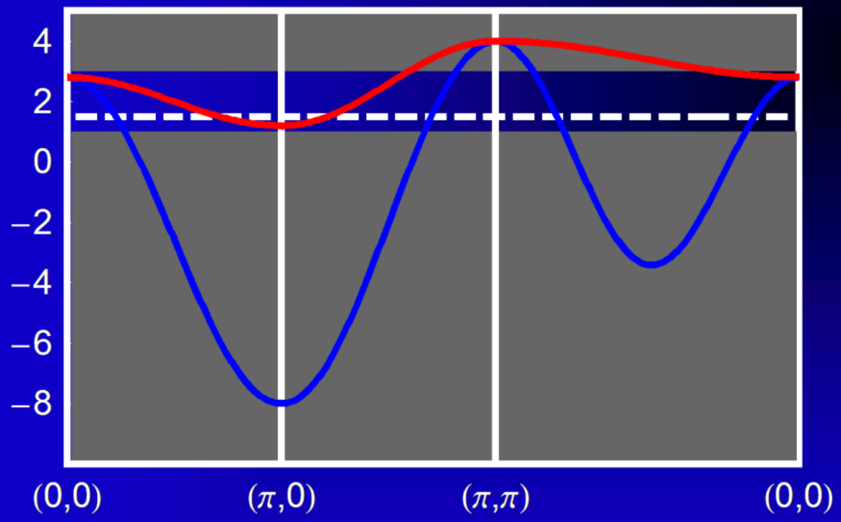
- Multiple bands crossing the Fermi level cannot be explained in an effective one band model, unlike the cuprates
- Simplest model: 2 band model
- Direction of the Fe d_{xz} and d_{yz} orbitals maximize overlap with As *p* orbitals

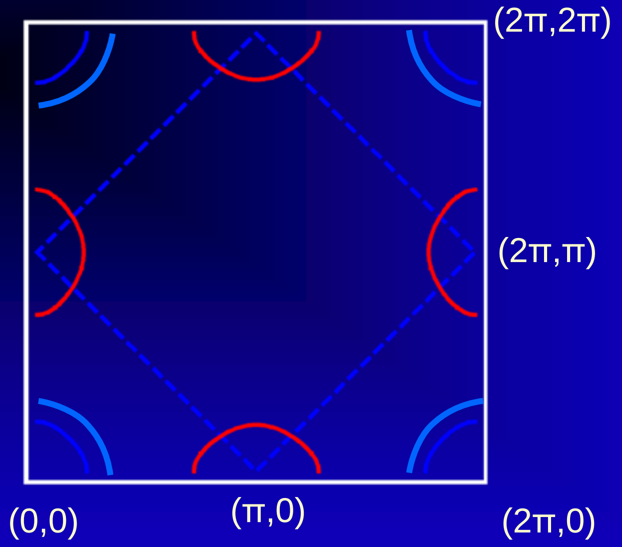


Tight-binding approximations

Two-orbital model

- Problem: Relative value of Fermi velocities by factor of 5 incorrect
- Problem: In the extended „effective“ BZ both hole pockets should be around (0,0) instead of the one around (π,π) → incorrect band character

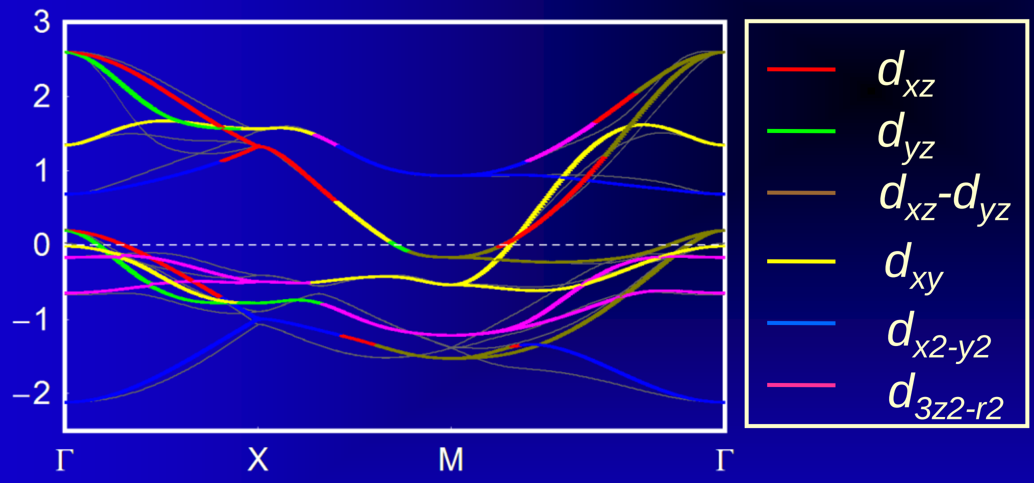


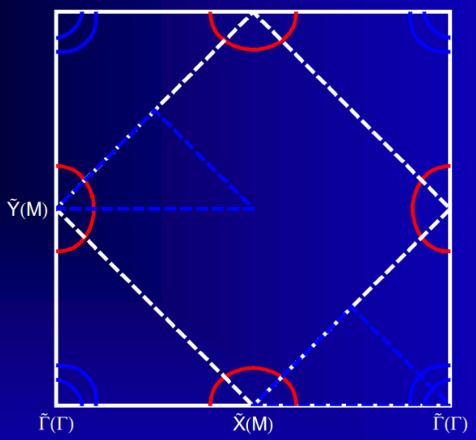


Tight-binding approximations

Five-orbital model

- Fourth orbital necessary to remove spurious FS around (π,π)
- Fifth band can improve approximation further, to allow the study of electron or hole doped compounds

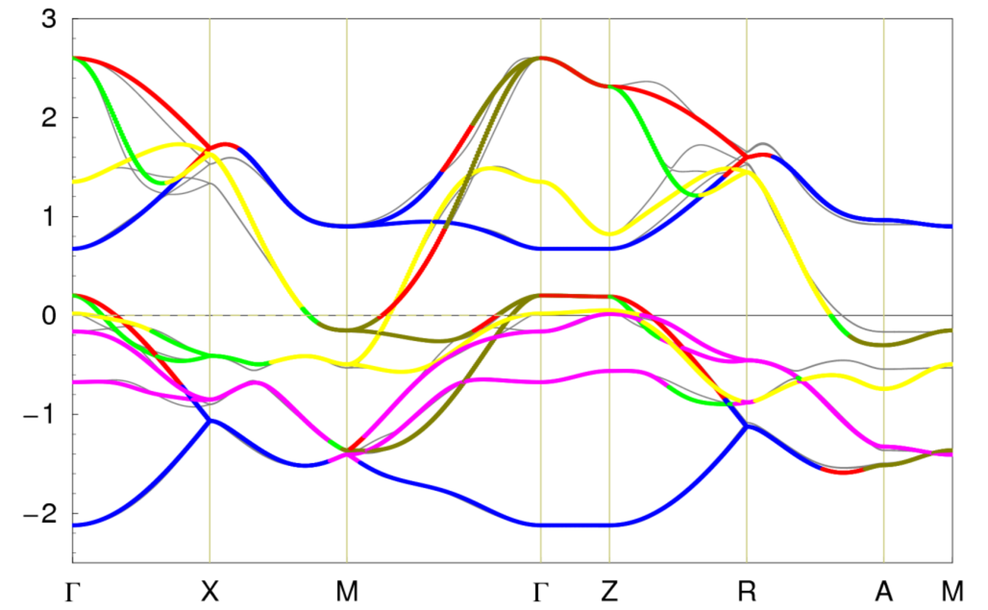




— DFT bandstructure by Cao *et al.*

Tight-binding approximations

Five-orbital model



Numerical re-fitting of the band structure keeps correct orbital weights and leads to very accurate results

— DFT bandstructure by Cao *et al.*

Superconducting ground state

The 5-orbital tight-binding Hamiltonian

$$H_0 = \sum_{k\sigma} \sum_{mn} \left(\xi_{mn}(k) + \epsilon_m \delta_{mn}\right) d^\dagger_{m\sigma}(k) d_{n\sigma}(k)$$

- fitted to approximate band structure by Cao *et al.*
- here $d^\dagger_{m\sigma}(k)$ creates particle with momentum *k*, spin σ in orbital *m*,
- ξ is kinetic energy, *ε* is onsite energy

Superconducting ground state

- General form of the interaction Hamiltonian (only intrasite)

$$H_{int} = U \sum_{is} n_{i,s\uparrow} n_{is\downarrow} + \frac{V}{2} \sum_{i,s,t\neq s} n_{is} n_{it} - \frac{J}{2} \sum_{i,s,t\neq s} \vec{S}_{is} \cdot \vec{S}_{it} + \frac{J'}{2} \sum_{i,s,t\neq s} \sum_{\sigma} c^{\dagger}_{is\sigma} c^{\dagger}_{is\bar{\sigma}} c_{it\bar{\sigma}} c_{it\sigma}$$

- here *U* is the *intra*orbital interaction, *V* is the *inter*orbital interaction, *J* is the energy associated with the Hund‘s rule coupling, and *J‘* is the pair hopping energy

- Derived from a single two-body term: *J‘*=*J*/2, *V*=*U*-3/4*J*-*J‘*

Why functional RG ?

Iron-Pnictides:
a weakly correlated multi-band system

Local repulsion U in pnictides smaller than in cuprates:

- Underdoped state is itinerant antiferromagnet
- Constrained DFT gives smaller values for **U < bandwidth (W)**

  (Anisimov *et al.* , Z. X. Shen *et al.* : U ≈ 2eV, W≈ 5eV PRB 2008)

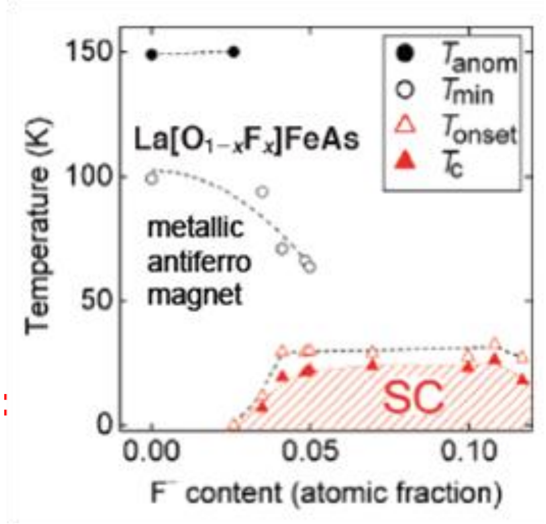
- Band structure matters (nesting!)

Pairing is most likely due to electron-electron interactions:

- Electron-phonon coupling strength too weak

  (coupling λ ≈ 0.2, Boeri *et al. PRL 2008* , Mazin *et al.* PRL *2008*)

All 5 iron orbitals contribute to electronic structure near FS

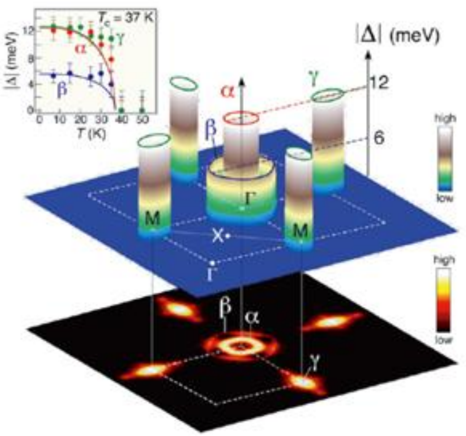


Kamihara *et al.* *(JACS 2008)*

functional RG should be ideal method !!

Facts and Open Issues

sc - gap

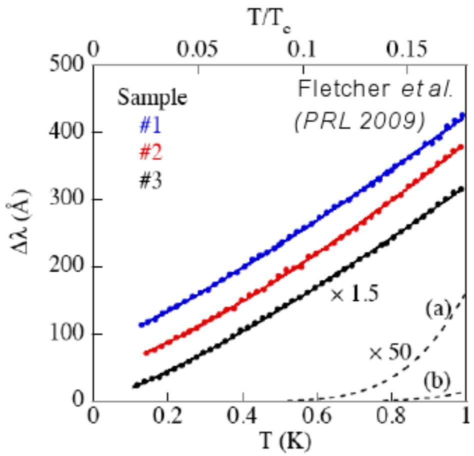


Ding *et al. (EPL 2008)*

Important question: gap symmetry ?

– ARPES and Andreev-reflection suggest:
nodeless sc-gap (Wray et al. PRB 08, Chen et al. Nature 09)

– penetration-depth results and NMR imply:
sc-gap with nodes (Fletcher et al. PRL 09; Grafe et al. PRL 08)



Answer from theory ?

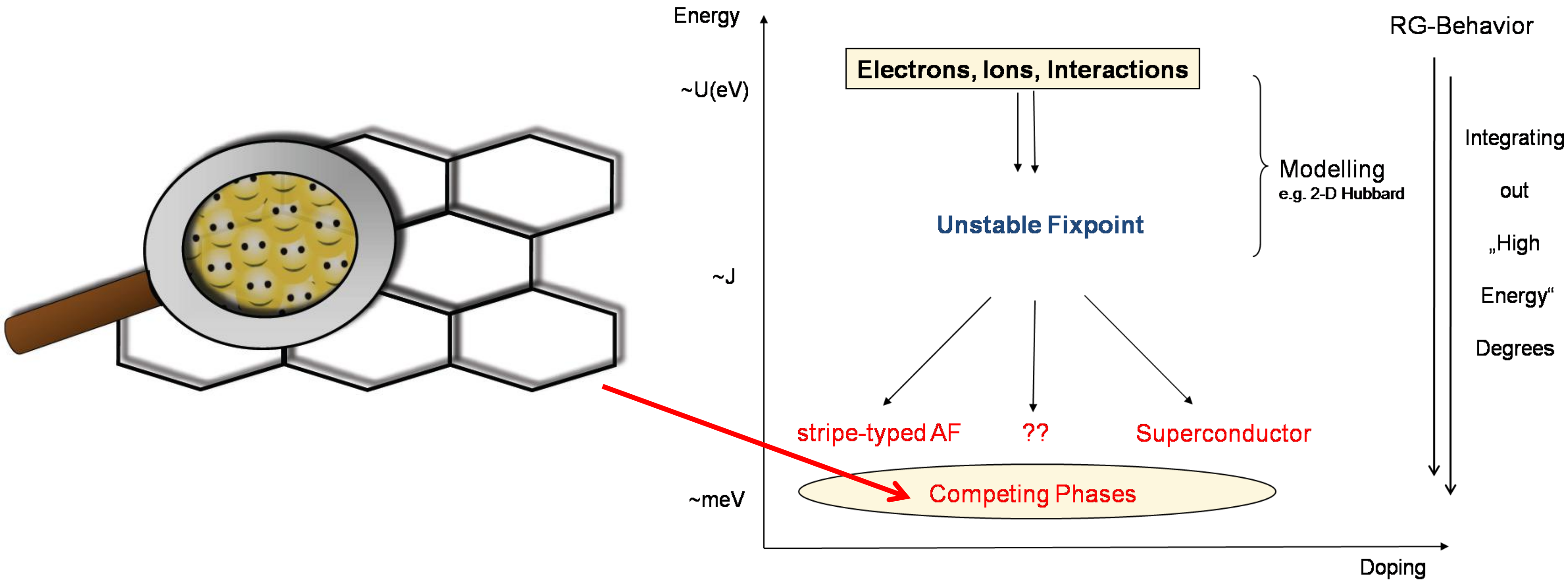
Not so easy: various possibilities …

Nodes or full gap depending on details ?

(F. Wang, D. H. Lee *et al.* PRL 2009; Maier, Scalapino *et al.* PRB 2009)

Pairing symmetry and mechanism not yet clear !

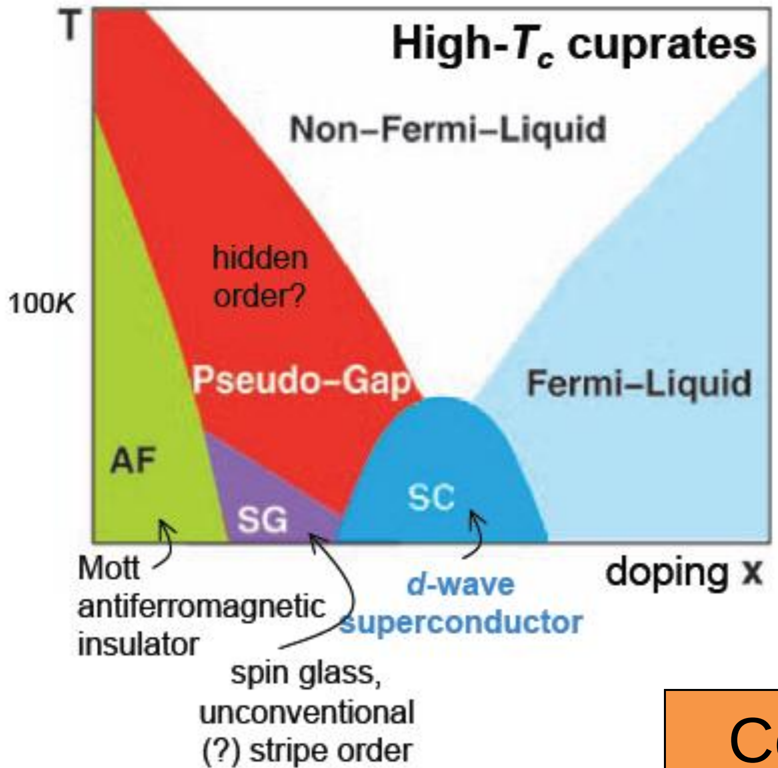
The functional RG method



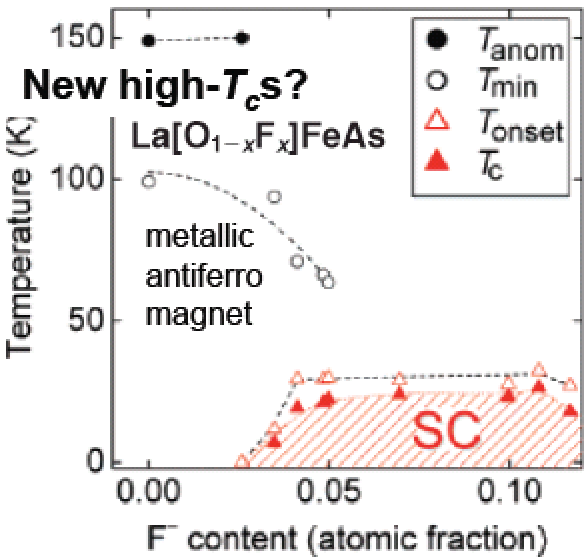
Exploring the World of
Interacting Fermions with the functional
Renormalization group

Correlated electrons

<u>Layered copper-oxides:</u>



<u>Layered iron-arsenides:</u>

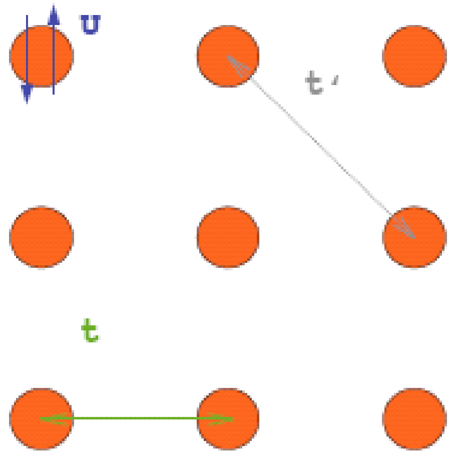


Correlated electrons exhibit large variety of many-body ground states

⟶ **Challenge for theory**

Standard model for strongly correlated fermions: Hubbard model

$$H = -t \sum_{\mathrm{nn},s} c^{\dagger}_{i,s} c_{j,s} - t' \sum_{\mathrm{nnn},s} c^{\dagger}_{i,s} c_{j,s} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

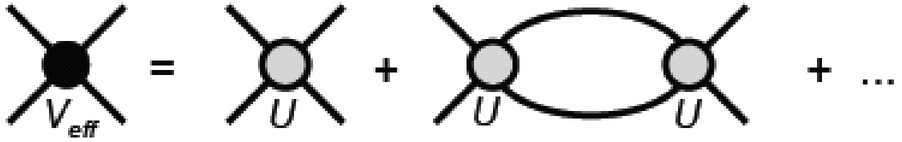


& variants:
multi-orbital,
lattice, …

Complexity from simplicity

$$H = -t \sum_{\mathrm{nn},s} c^\dagger_{i,s} c_{j,s} - t' \sum_{\mathrm{nnn},s} c^\dagger_{i,s} c_{j,s} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

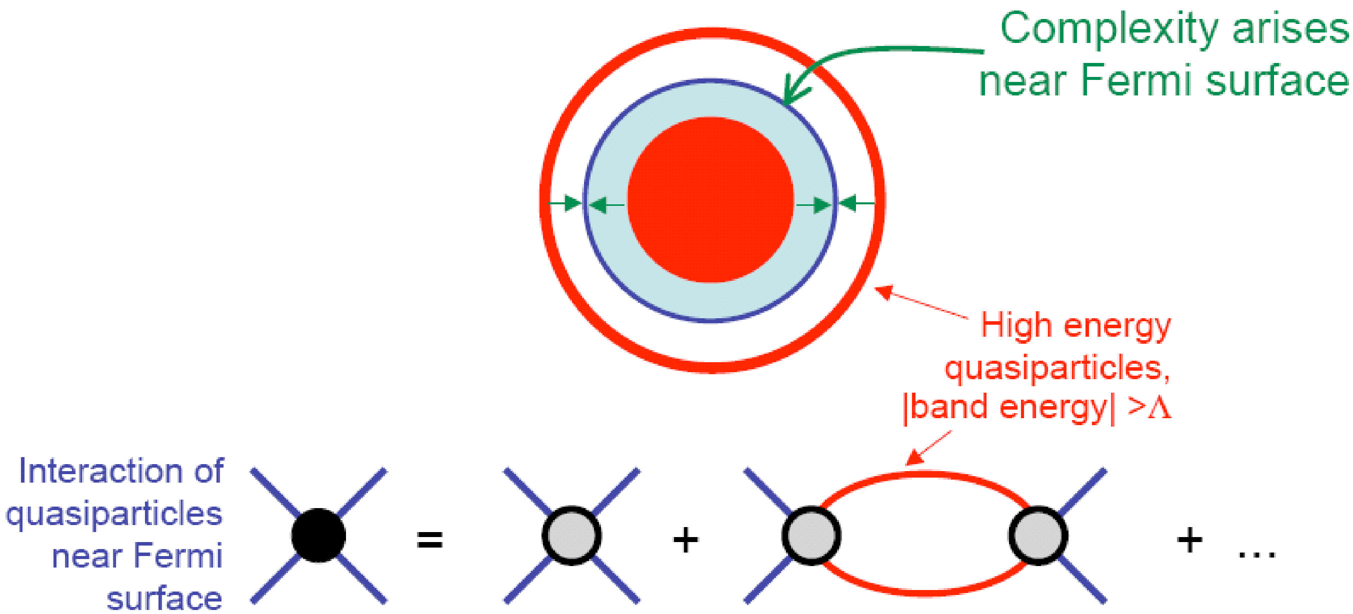
How can structure-less onsite/short-range interaction lead to diversity ?



→ **More is different ! It‘s a many-body problem !**

Dynamics of other particles (affected by band structure & tuning parameters) change effective interactions !

Renormalization group



Vary/decrease energy scale Λ:

→Take into account **(“integrate out”)** degrees of freedom **step by step**

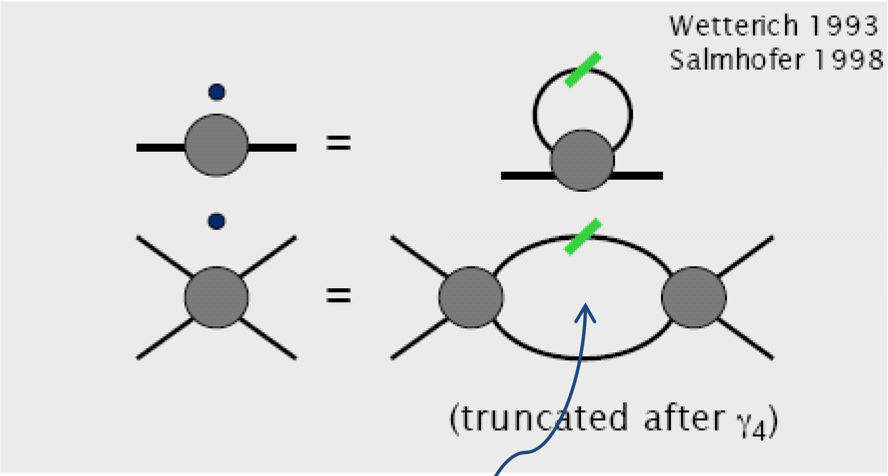
→ Approach low energy scales in controlled way

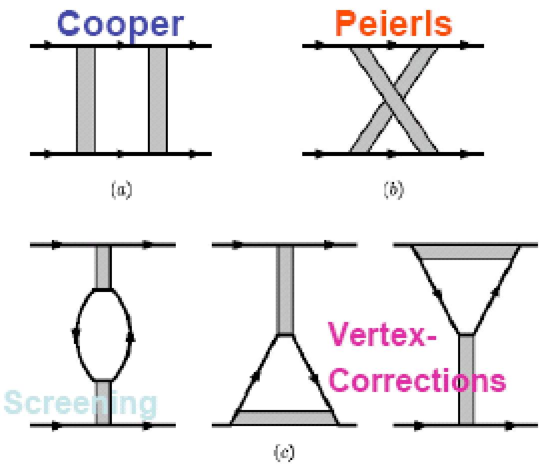
→ RG differential equation $d/d\Lambda\, V_{eff} = \ldots$

Infinite hierarchy of RG equations…but unbiased

– Exact flow equation for generating functional when Λ is changed → hierarchy of 1-loop equations for 1 PI vertices

– Needs truncation, 6pt vertex set to 0 → perturbative treatment

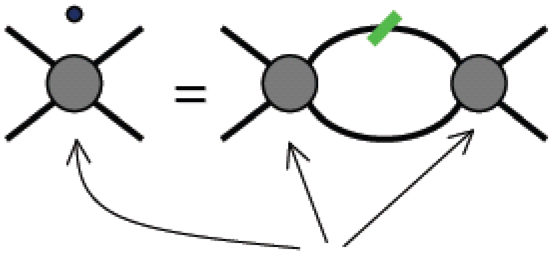




Includes all important fluctuations on equal footing !

Diversity enters here !

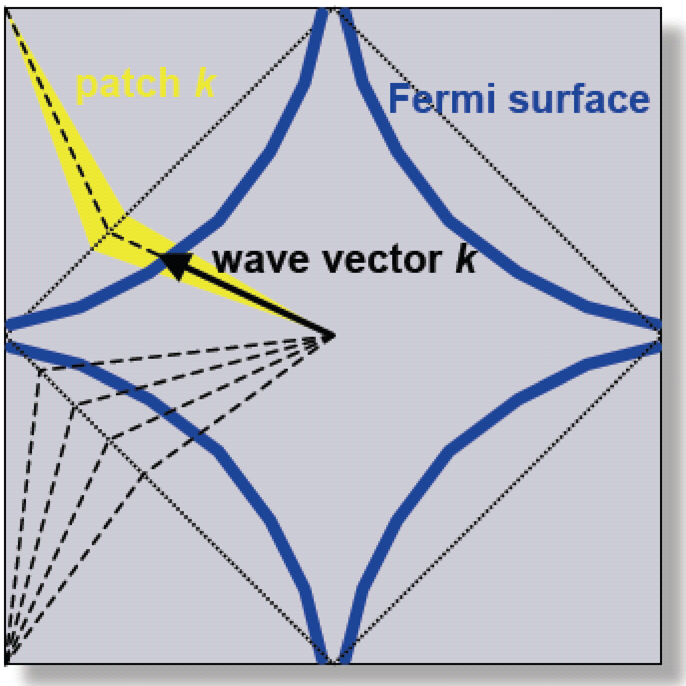
Implementation for two-dimensional systems



– **Coupling function** $\mathbf{V_\Lambda(k_1, k_2, k_3)}$ with two incoming wavevectors $\mathbf{k_1, k_2}$ and outcoming $\mathbf{k_3}$ $(k_4 = k_1 + k_2 - k_3)$

– Discretize: approximate $\mathbf{V_\Lambda(k_1, k_2, k_3)}$ as **constant** for $\mathbf{k_1, k_2}$ and $\mathbf{k_3}$ **in same patch**

– Frequency dependence can be taken into account

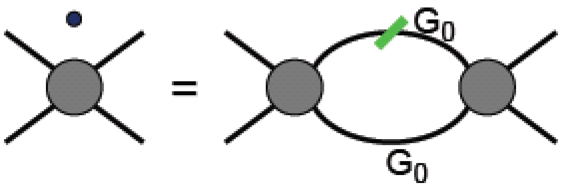


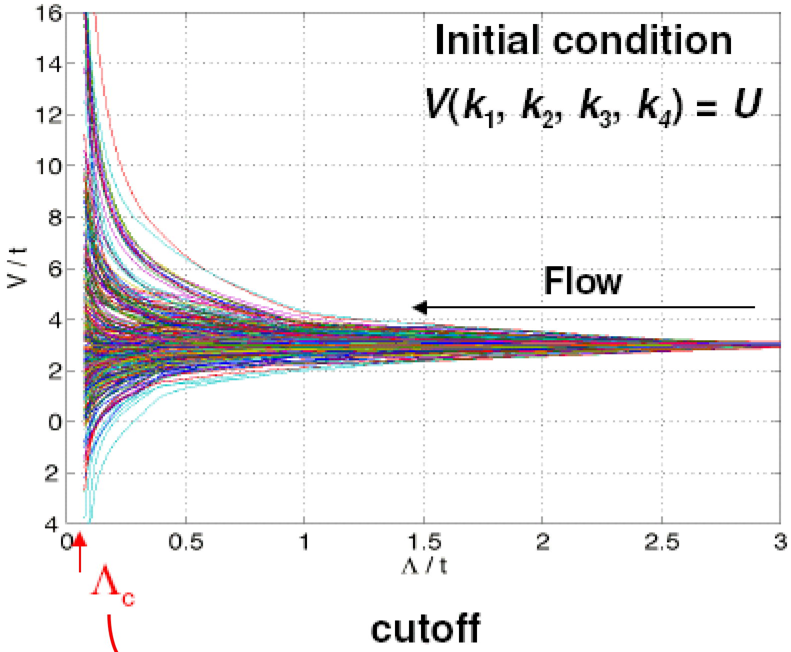
Zanchi and Schulz PRB 2000

Functional RG:
flow of coupling function derived from RG eqn of generating functional

Flow to strong coupling

<u>Flow without self-energy feedback:</u>
<u>Analysis of flow to strong coupling</u>

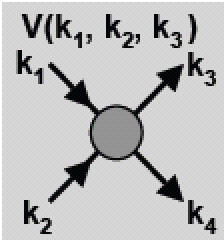




Upper bound for T_c

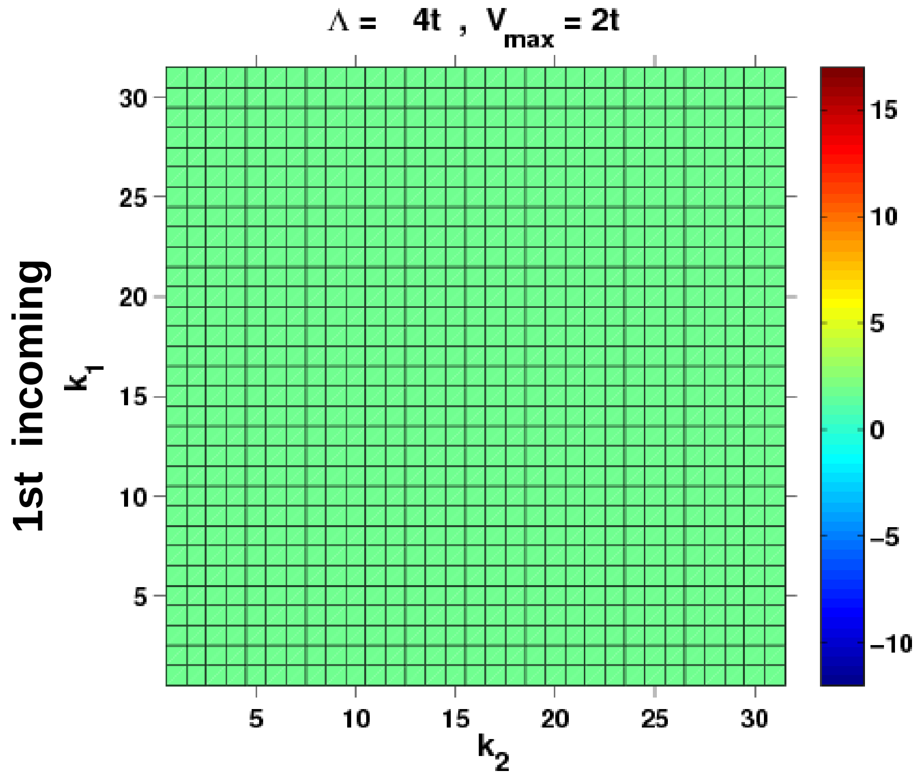
Leading low-energy correlations ?

Energy scales ?



1st outgoing k_3 fixed at point 1

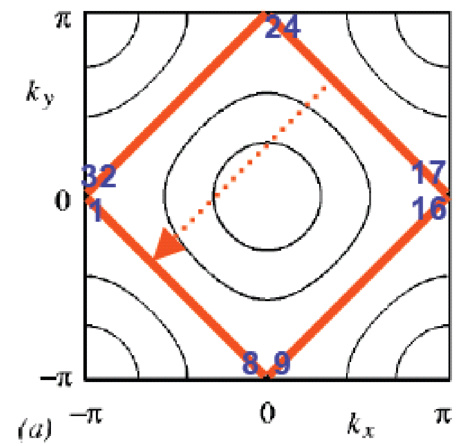
Spin-density wave:

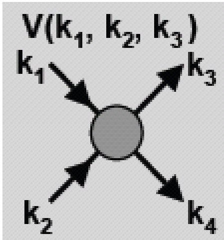


– Fully nested Fermi surface

– U = 2t, t‘ =0.0,

T = 0.001t





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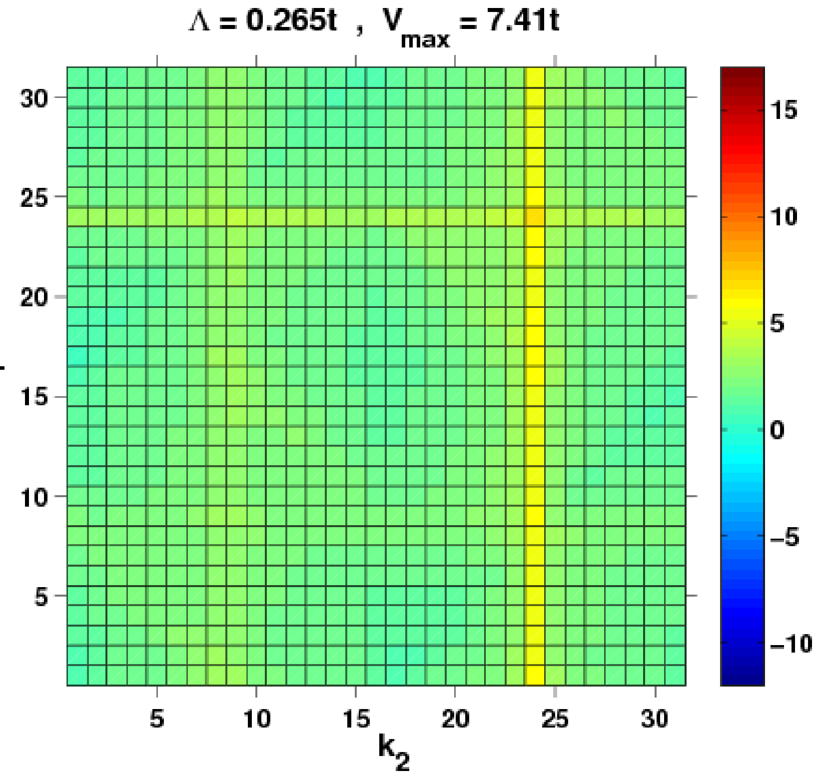
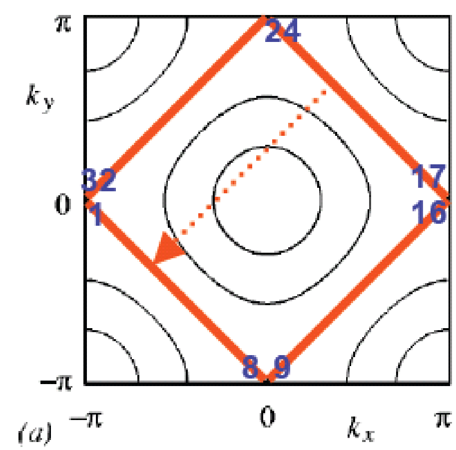


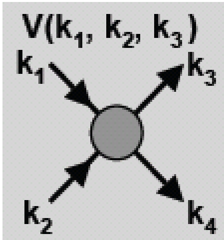
1st incoming

2nd incoming

- Fully nested Fermi surface
- U = 2t, t‘ =0.0, T = 0.001t



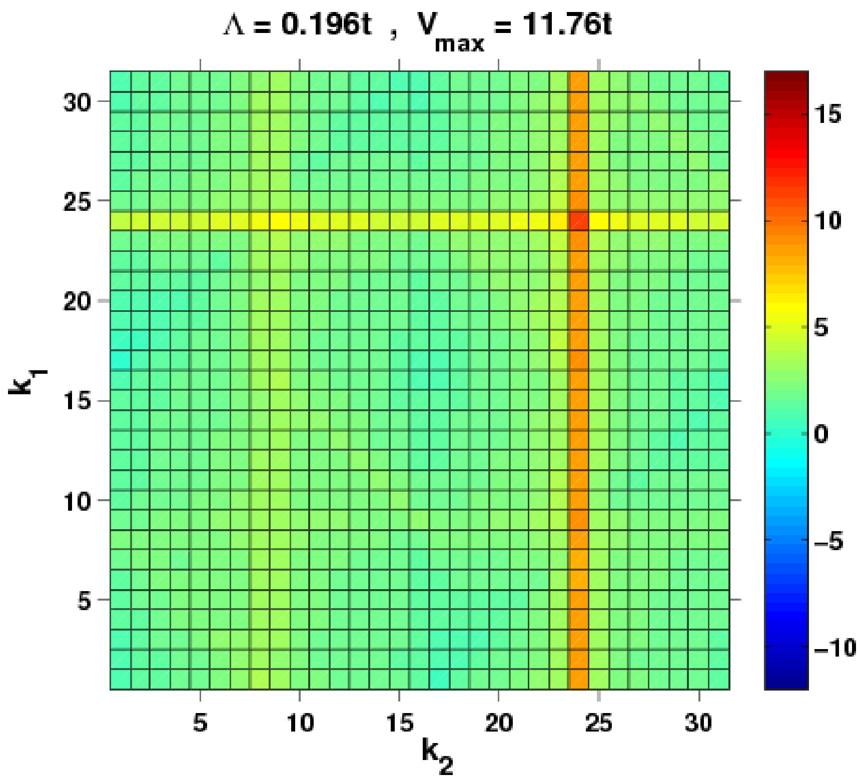
Emergent collective behavior in cuprates



1st outgoing k_3 fixed at point 1

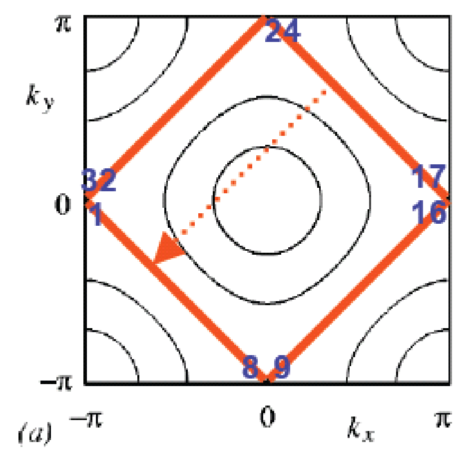
Spin-density wave:

1st incoming

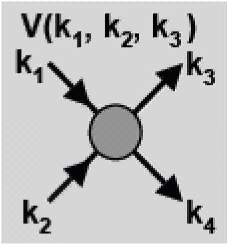


2nd incoming

- Fully nested Fermi surface
- U = 2t, t‘ =0.0, T = 0.001t

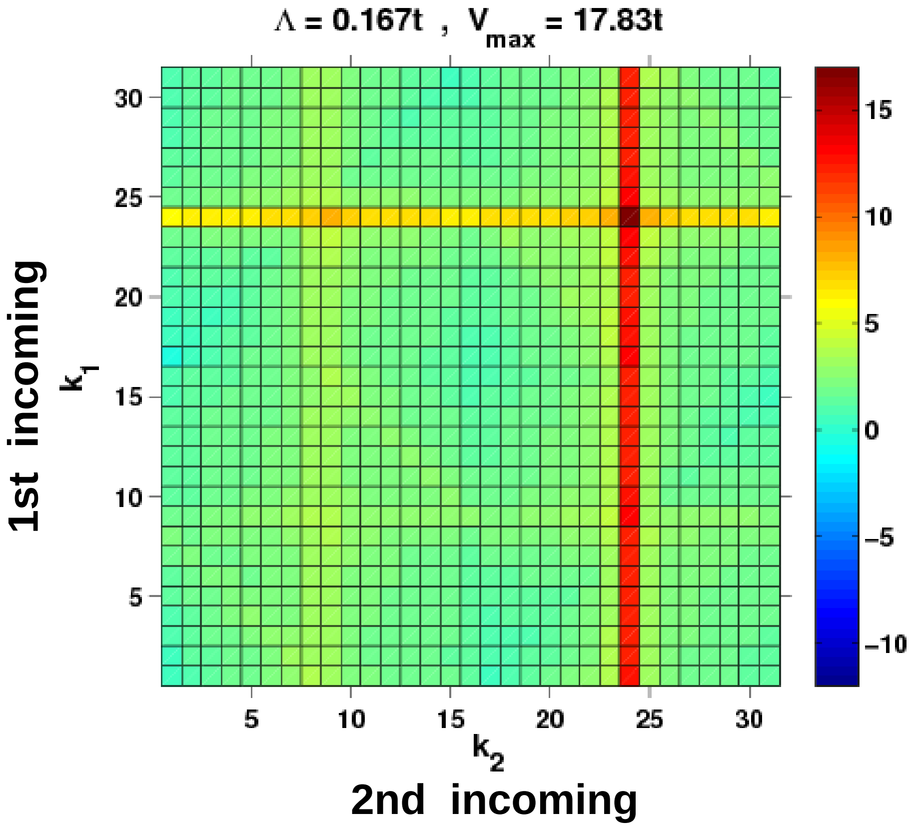


Emergent collective behavior in cuprates



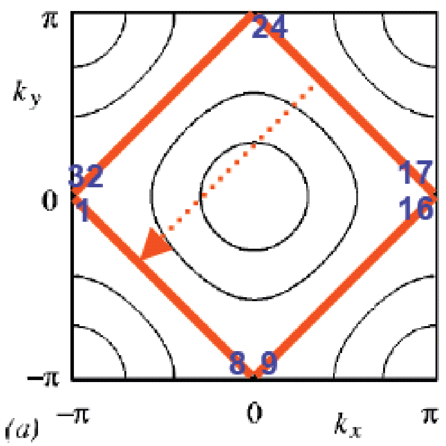
1st outgoing k_3 fixed at point 1

Spin-density wave:

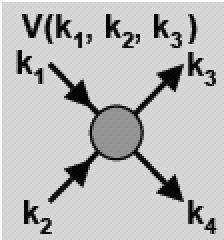


– Fully nested Fermi surface

– U = 2t, t‘ =0.0, T = 0.001t

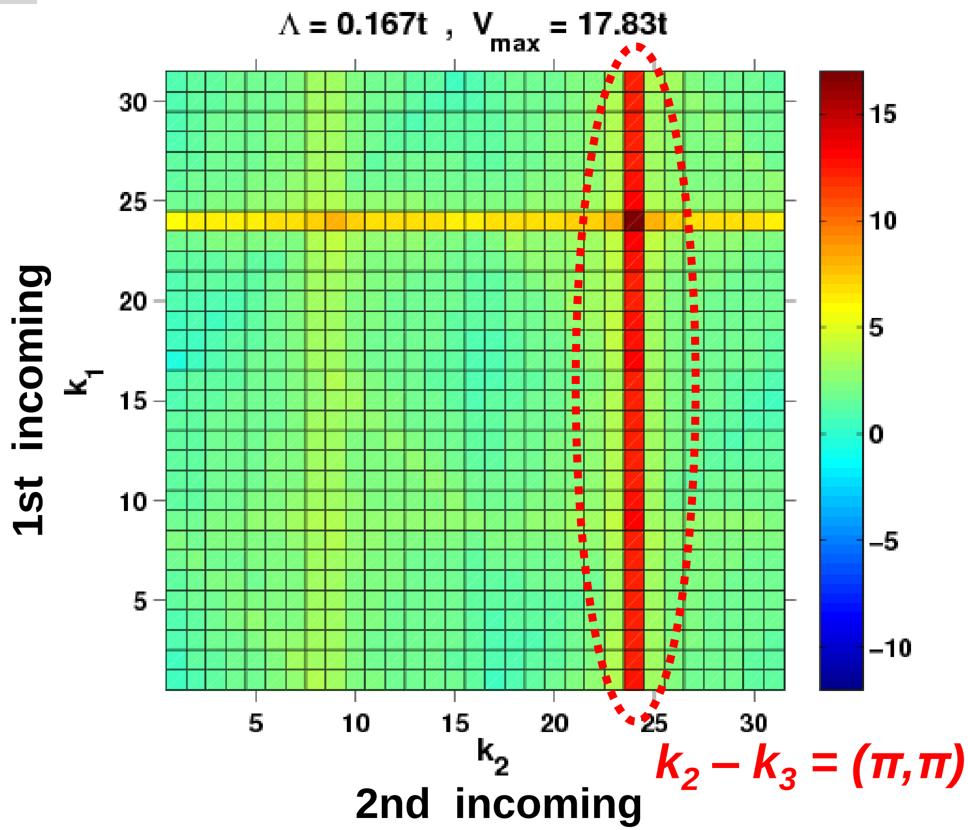


Emergent collective behavior in cuprates

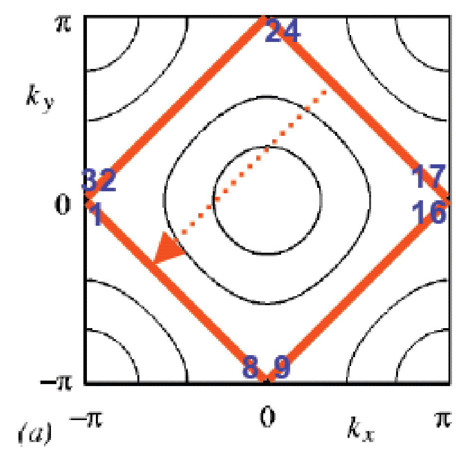


1st outgoing k_3 fixed at point 1

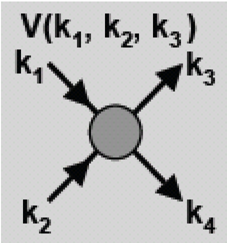
Spin-density wave:



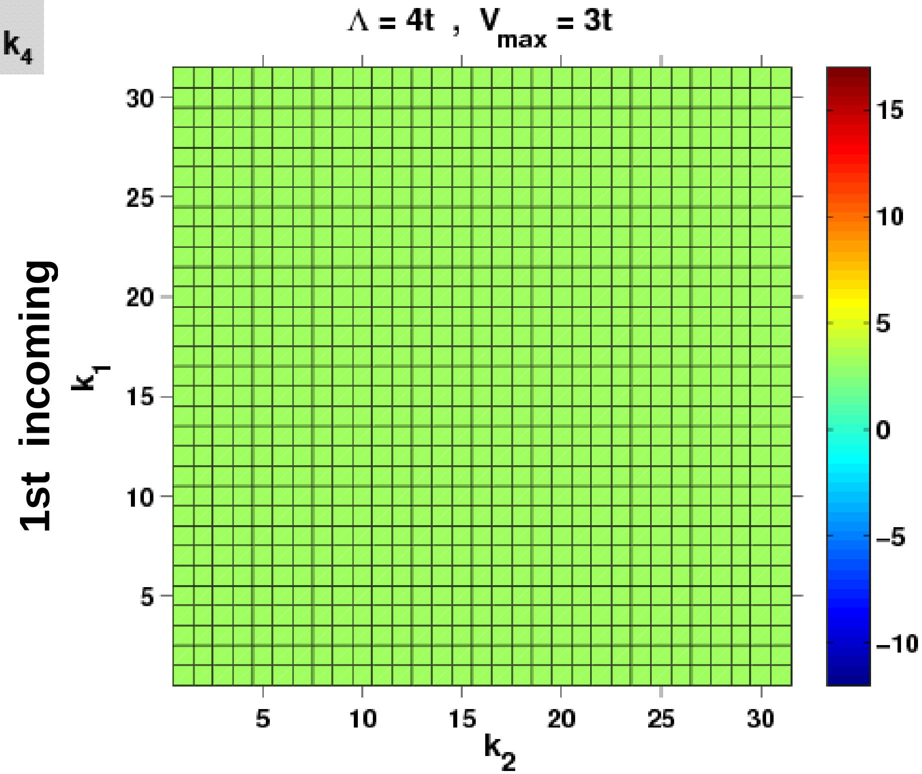
- Fully nested Fermi surface
- U = 2t, t‘ =0.0, T = 0.001t



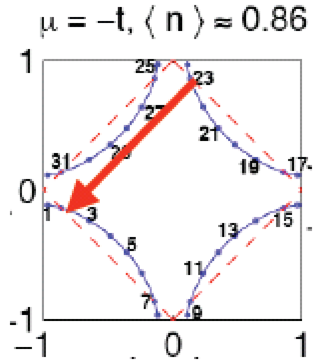
Interpretation: antiferromagnetic spin-density wave

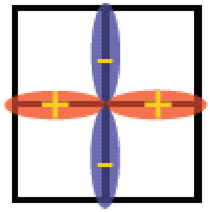


d-wave pairing on square lattice:

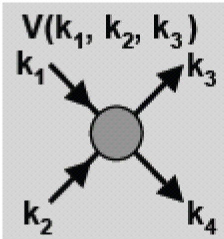


- imperfectly nested „high-T_c" Fermi surface
- U = 3t, t' = -0.3, T = 0.001t

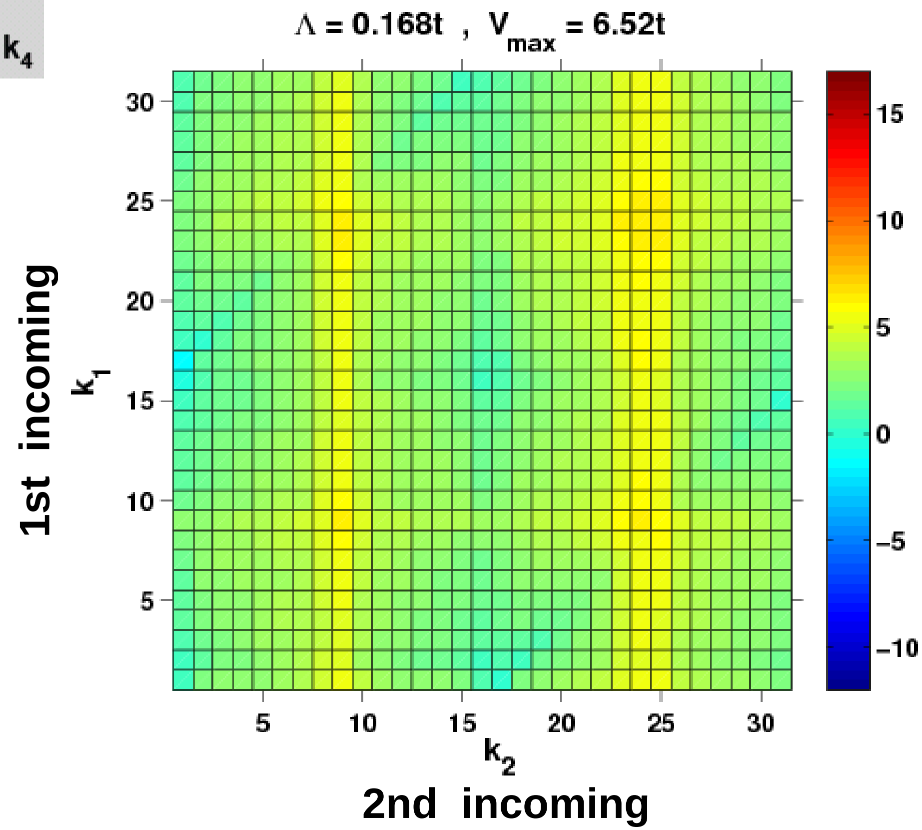




Emergent collective behavior in cuprates



d-wave pairing on square lattice:



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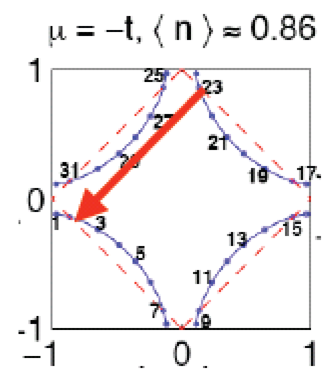
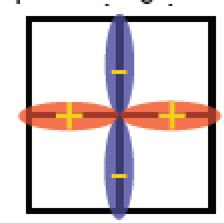
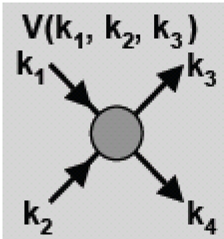
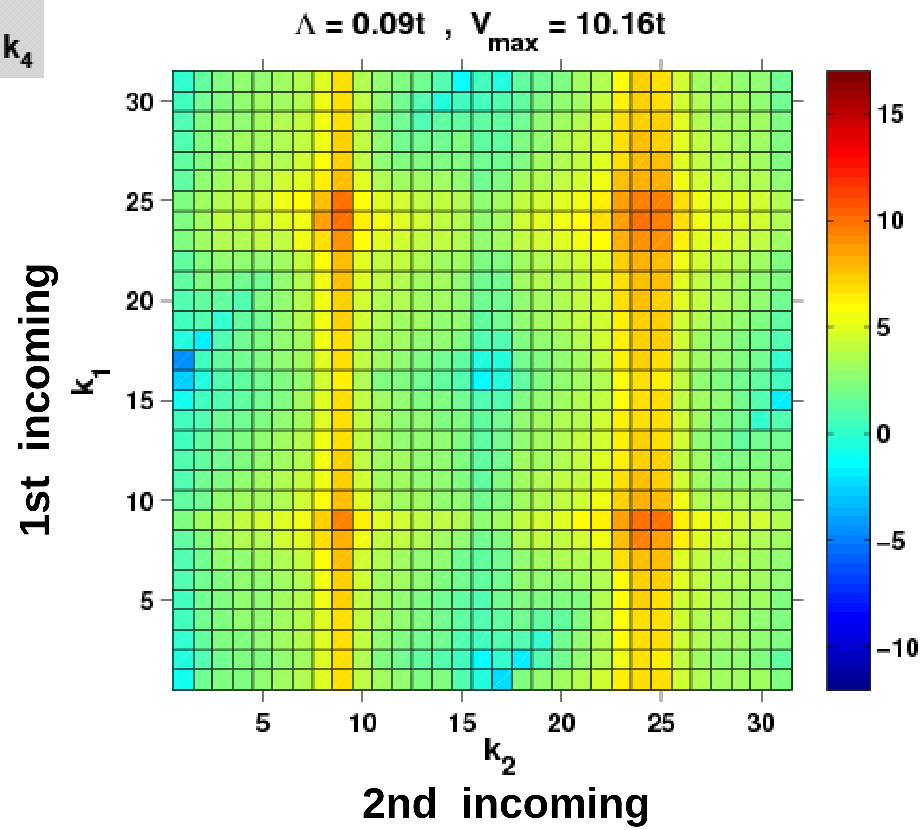




d-wave pairing on square lattice:





- imperfectly nested „high-T_c“ Fermi surface
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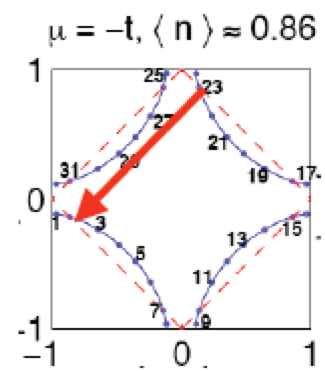
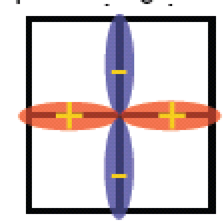
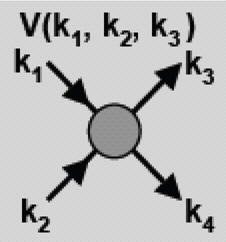
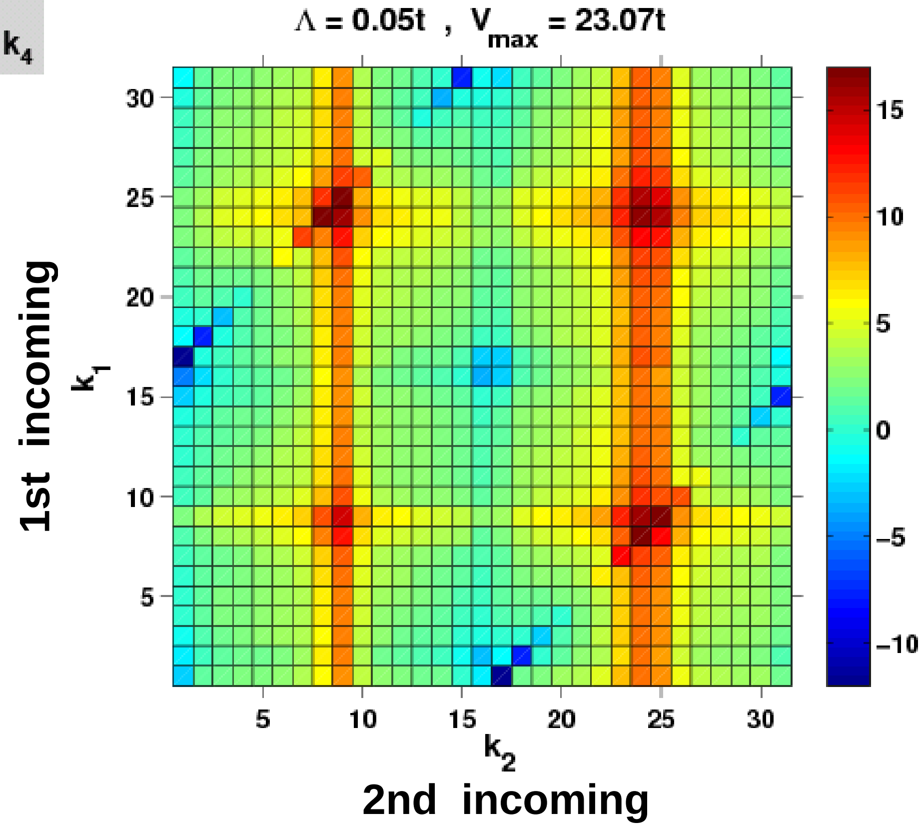


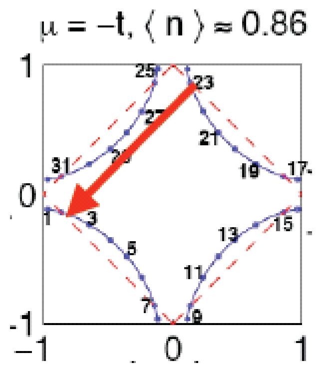


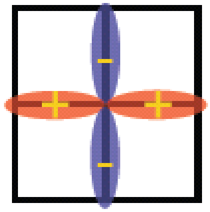


d-wave pairing on square lattice:

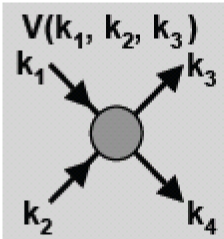


- imperfectly nested „high-T_c“ Fermi surface
- U = 3t, t‘ = -0.3, T = 0.001t

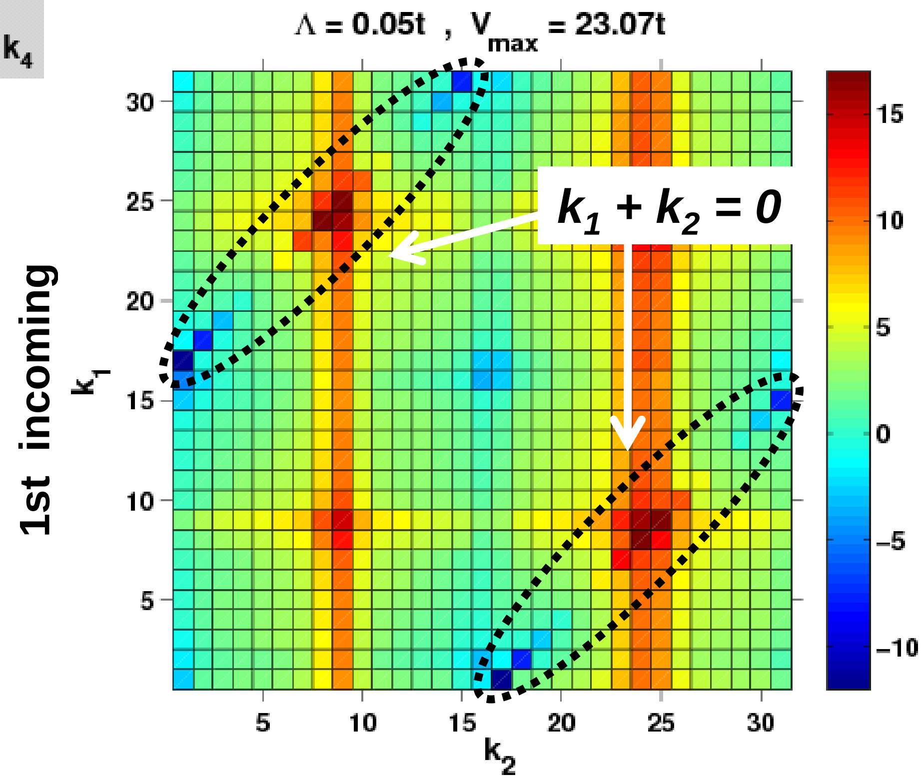




Emergent collective behavior in cuprates

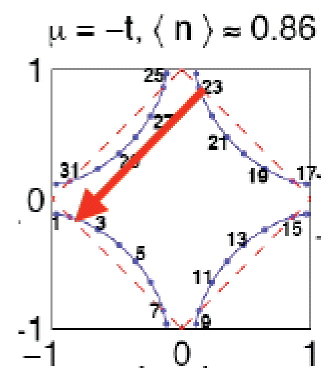


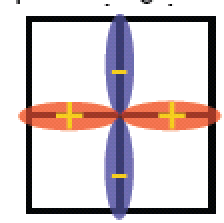
***d*-wave pairing on square lattice:**



– imperfectly nested „high-T_c" Fermi surface

– U = 3t, t' = -0.3, T = 0.001t





***d*–wave Cooper pairing instability**

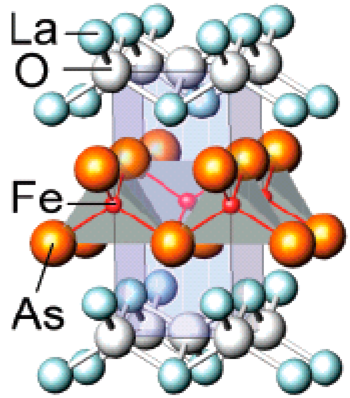
Iron-Pnictides:
a weakly correlated multi-band system

Local repulsion U in pnictides smaller than in cuprates:

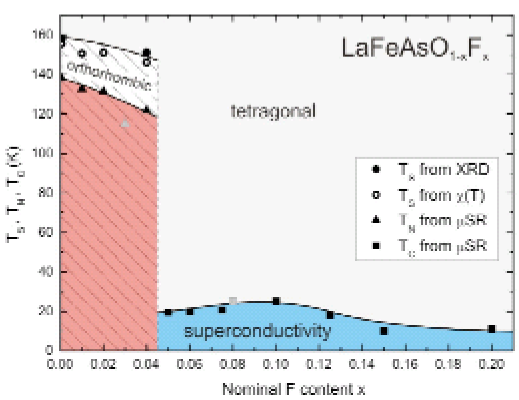
- Underdoped state is itinerant antiferromagnet
- Constrained DFT gives smaller values for **U < bandwidth**
- Band structure matters (nesting!)

All 5 iron orbitals contribute to electronic structure near FS

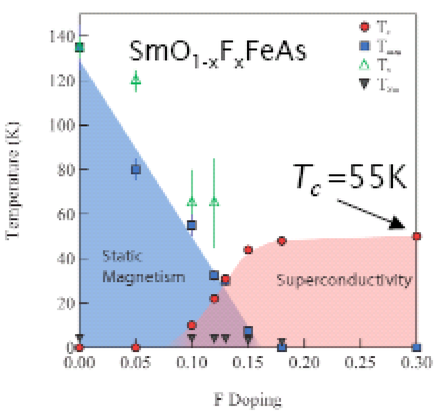
functional RG should be ideal method !!



Kamihara *et al.* *(JACS 2008)*



Luetkens *et al.* Nature 2008



Motivation

D.-H. Lee‘s group (PRL 2009)

- full five-orbital band structure, find extended s-pairing

A. Chubukov‘s group (PRB 2008)

- simplified, „two-circle model“ , find extended s-pairing

Great ! But is everything understood ? …not quite …

Our group:

- Interpolate between two treatments
- Use different band structures

Questions to be studied:

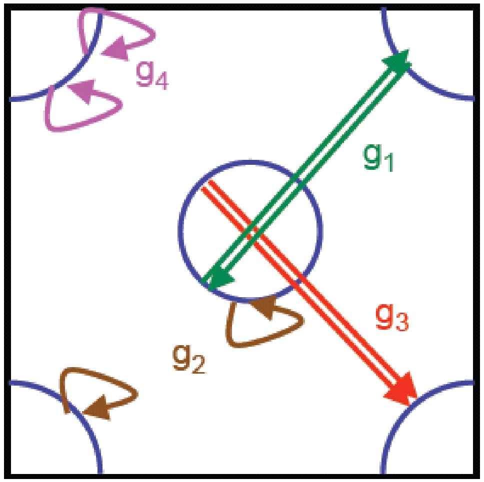
- Universal behavior ? What is material- or model-specific ?
- Parallels between cuprates and pnictide superconductivity ?

Iron pnictides and cuprates

Chubukov *et al.* (PRB 2008):

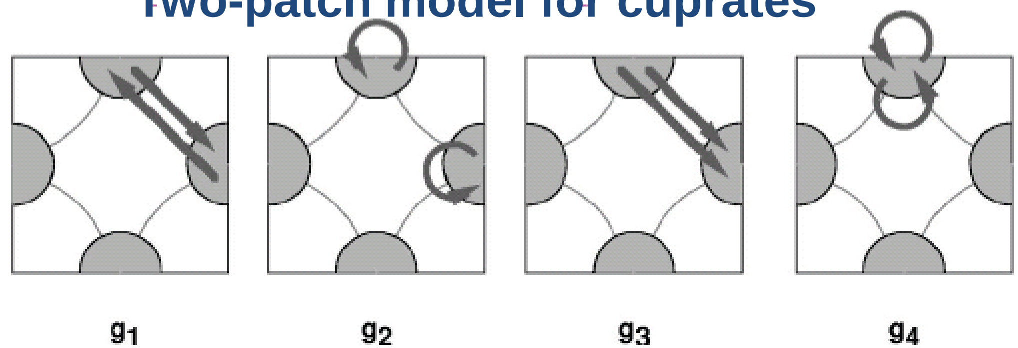
„g-ology“ for pnictides

couplings depend only on pocket



Furukawa, Salmhofer, Rice (PRL 1998):

Two-patch model for cuprates



For perfect nesting, one-loop equations are the same:

$$\begin{aligned}
\dot{g}_1 &= 2d_1 g_1 (g_2 - g_1), \\
\dot{g}_2 &= \dot{d}_1 (g_2^2 + g_3^2), \\
\dot{g}_3 &= -2\dot{d}_0\, g_3 g_4 + 2\dot{d}_1\, g_3 (2g_2 - g_1) \\
\dot{g}_4 &= -\dot{d}_0 (g_3^2 + g_4^2).
\end{aligned}$$

Flow to strong coupling: g_2, $g_3 \longrightarrow \infty$, $g_4 \longrightarrow -\infty$, g_1 diverges more weakly

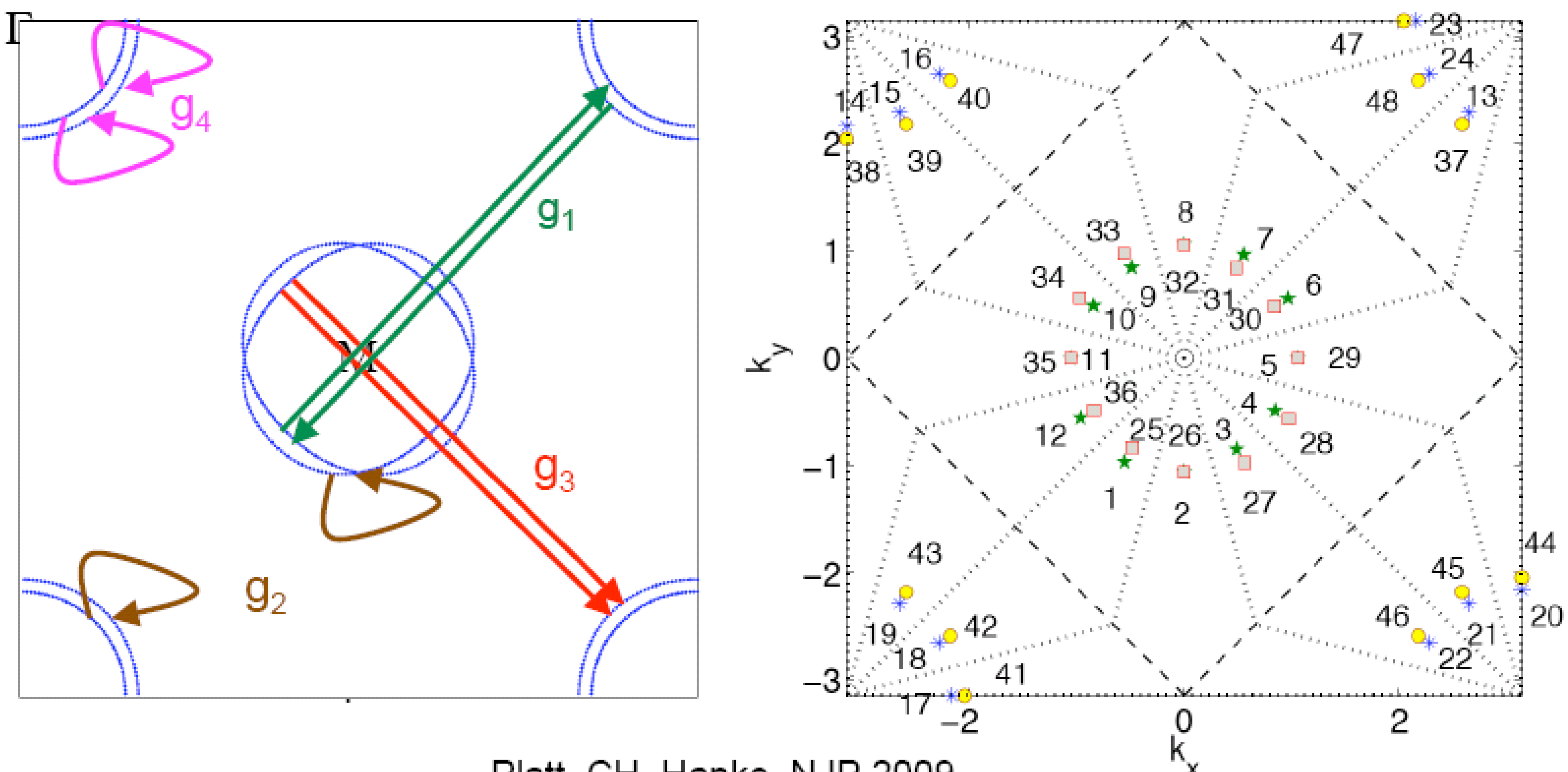
SDW: $g_2 + g_3$ **pairing:** $g_3 - g_4$ **uCDW:** $g_2 + g_3 - 2g_1$ **dPomeranchuk:** $2g_2 + g_1 - g_4$

Several channels diverge (SO(6)), driven by same („umklapp“) processes

Cannot have one winning channel alone !?

fRG for pnictides with g-ology inital cond's

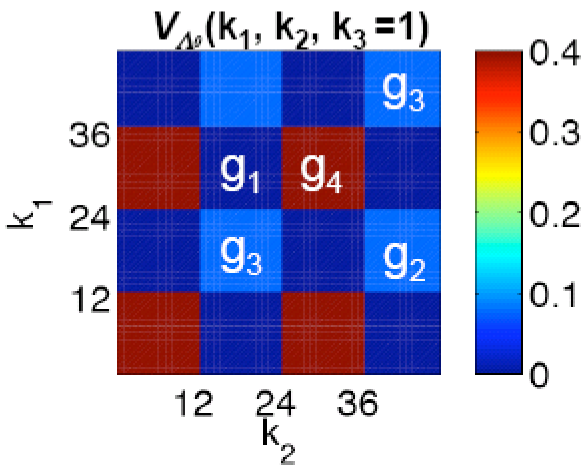
- 4-band dispersion (Korshunov & Eremin, EPL 08), bare couplings à la (Chubukov, Efremov, Eremin)
- Allow for *k*-dependence of effective interactions around Fermi surfaces
- All one-loop diagrams
- Study doping dependence

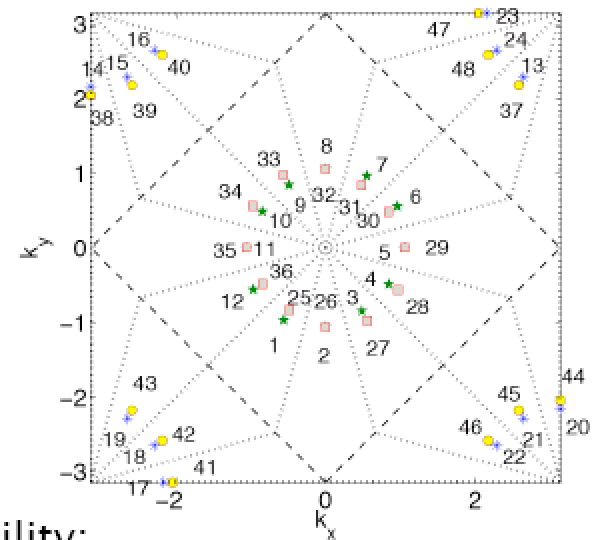


Platt, CH, Hanke, NJP 2009

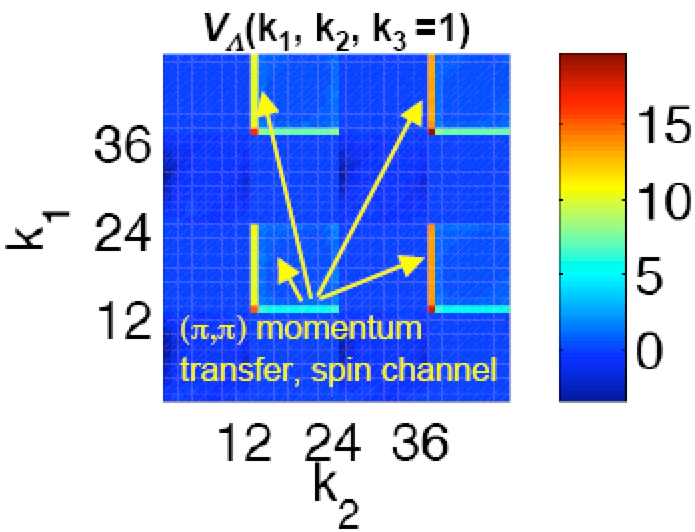
Undoped system: single-channel SDW instability

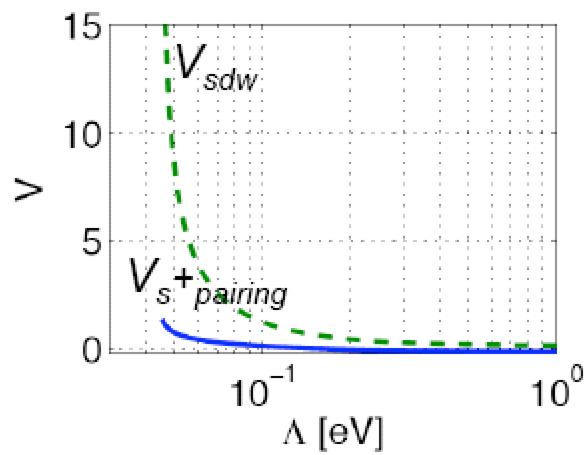
Initial (bare) interactions:





Final (effective) interactions near instability:

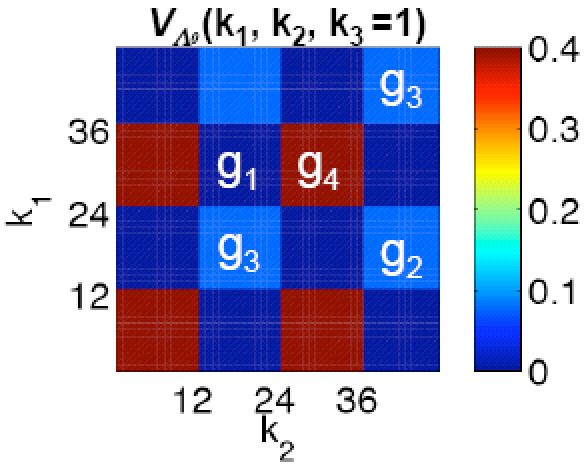


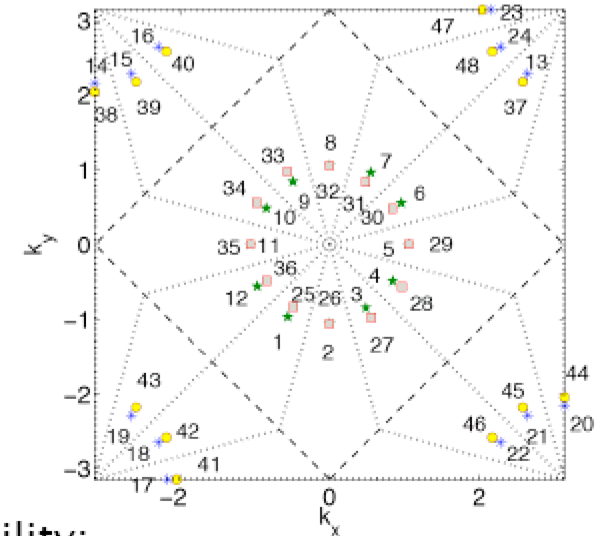


μ=0, half filling,
clearcut AF SDW instability

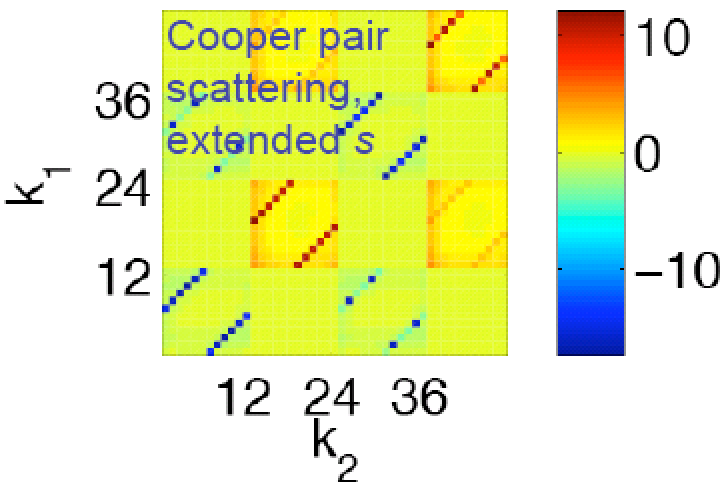
Doped case: single-channel pairing instability

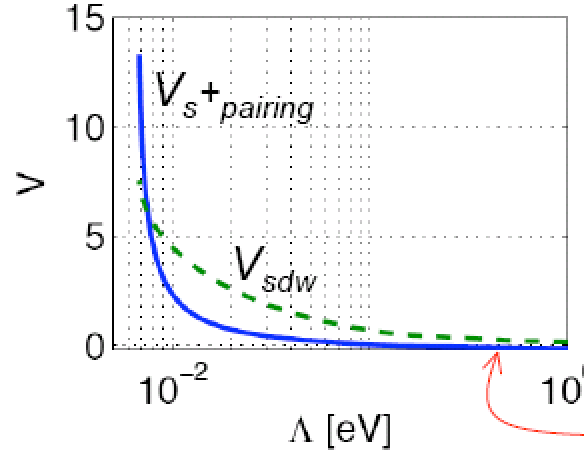
Initial (bare) interactions:





Final (effective) interactions near instability:





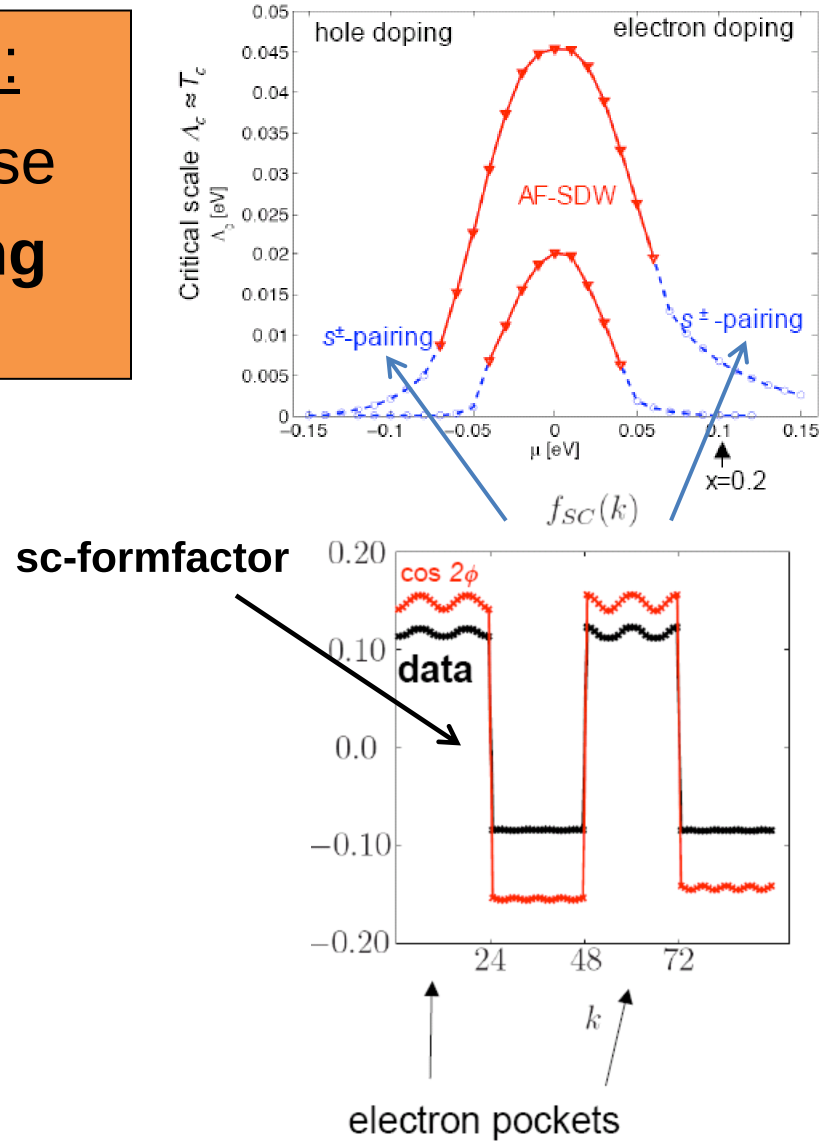
nonzero doping: extended **s-wave pairing instability**

initially repulsive

fRG with „g-ology initial conditions“

<u>fRG confirms basic picture:</u>

- **AF-SDW** for undoped case
- **Extended s-wave pairing** for both e- and h-doping



<u>Model dependence 1:</u>

Multichannel instability removed when *k*-space diversification of couplings is allowed

<u>Model dependence 2:</u>

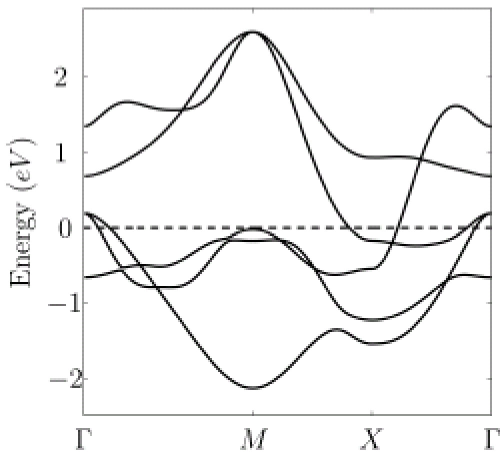
Very isotropic extended s-wave gap

How good are these approximations ?

$\longrightarrow$ Use more realistic band structure + interactions defined in orbital picture !

more realistic model for the iron-pnictides

tight binding fit to LDA results



Graser, Maier, Scalapino, Hirschfeld , NJP 2009

Free Hamiltonian for 5-Fe orbitals:

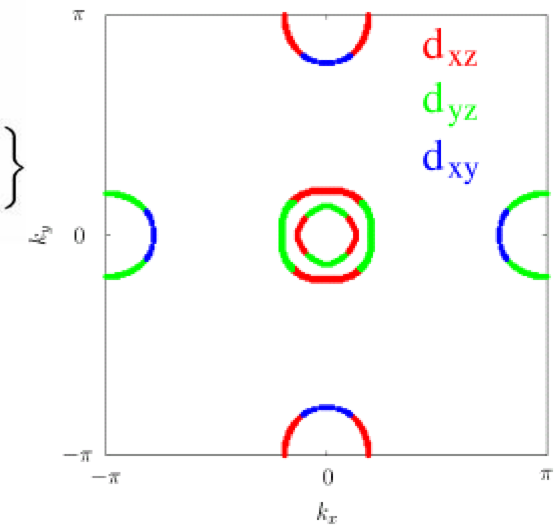
$$H_0 = \sum_{s=\uparrow,\downarrow} \sum_{\vec{k}} \sum_{a=1}^{5} \sum_{b=1}^{5} c^\dagger_{a\vec{k}s} K_{ab}(\vec{k}) c_{b\vec{k}s}$$

$$a, b \in \{d_{xz}, d_{yz}, d_{xy}, d_{x^2-y^2}, d_{3z^2-r^2}\}$$

Onsite interaction (U_1 = 4eV, U_2=2eV , J_H = J_{pair}=0.7eV):

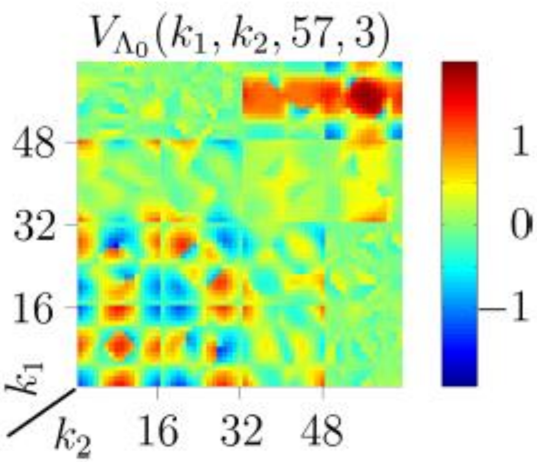
$$H_{\text{int}} = \sum_i \Big\{ U_1 \sum_a n_{i,a,\uparrow} n_{i,a,\downarrow} + U_2 \sum_{a<b} n_{i,a} n_{i,b} + J_H \Big[\sum_{a<b,s,s'} c^\dagger_{ias} c^\dagger_{ibs'} c_{ias'} c_{ibs} + (c^\dagger_{ias} c^\dagger_{ias'} c_{ibs'} c_{ibs} + \text{h.c.}) \Big] \Big\}$$

main orbital weights at FS



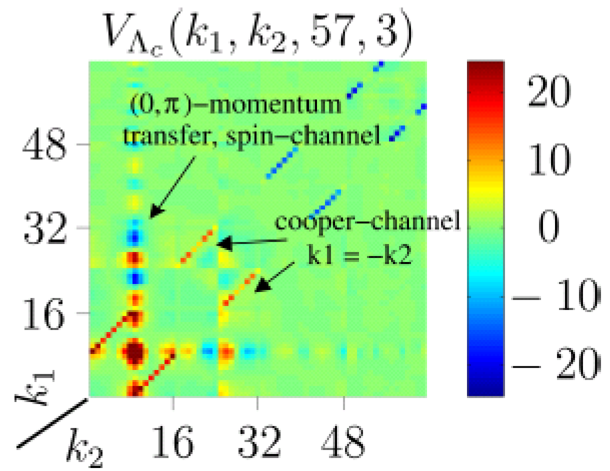
Starting the flow (5 orbital model)

Initial coupling at scale Λ_0 = 4 *eV* (bandwidth)

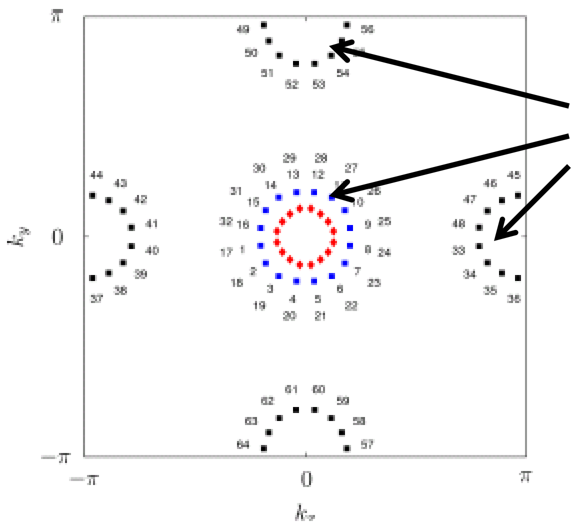


flow of coupling function

Effective coupling at scale Λ_c = 0.01 *eV*



SDW- and SC-ordering tendencies emerge at low energy scales !



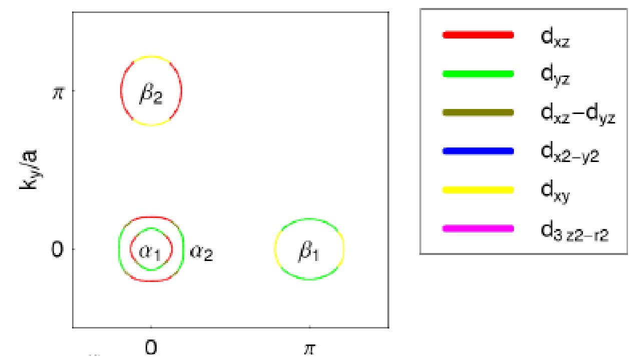
k_i - positions at FS (1 – 64) pts

Comparing different models for the iron pnictides….

How robust are these findings from fRG ?

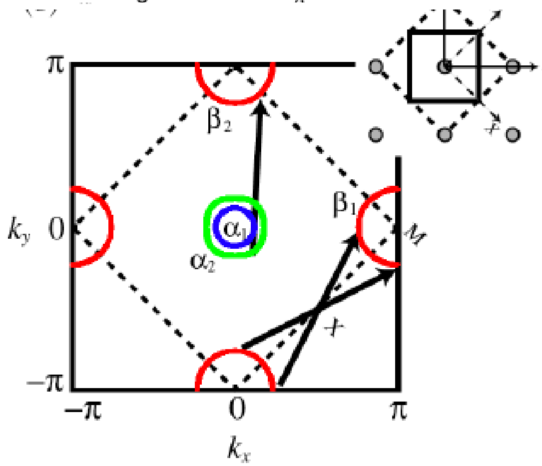
<u>Band structure 1:</u>

Graser, Maier, Hirschfeld, Scalapino NJP 2009: 5-orbital tight-binding fit to DFT by Cao, Hirschfeld, et al. (PRB 2008)



<u>Band structure 2:</u>

Kuroki et al. PRL 2009:
Minimal model with 5 maximally localized Wannier *d*-orbitals



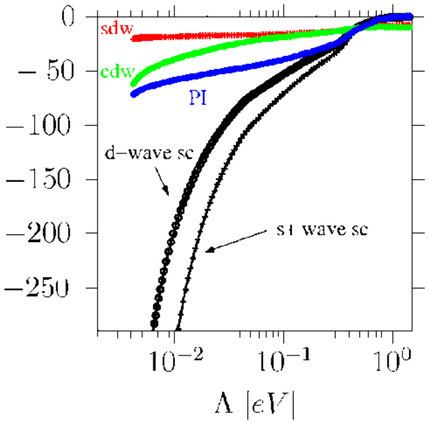
Model dependence I

10 % electron doping :
(same bare interaction in both models)

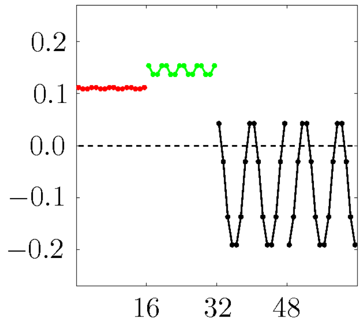
5-orbital model:

Graser, Maier, Hirschfeld, Scalapino NJP (2009)

flow of various channels:



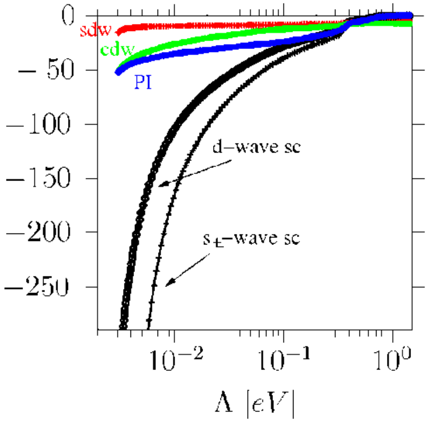
s± -formfactor:



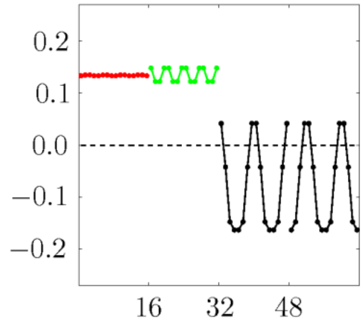
5-orbital model:

Kuroki et al. PRL (2008)

flow of various channels:



s± -formfactor:



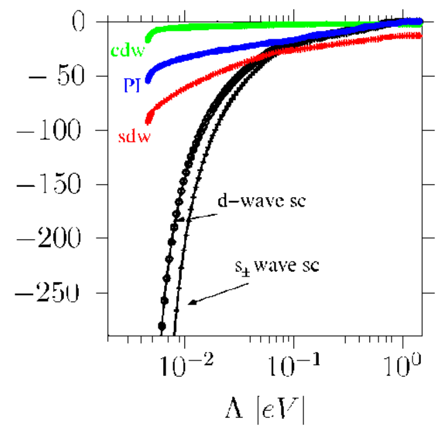
Both models show similar results at electron doping !

Model dependence II

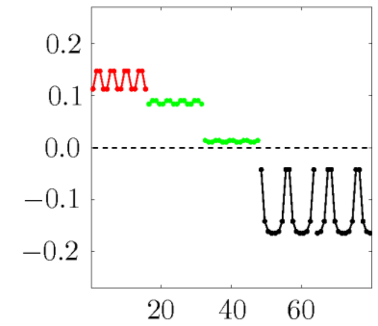
10 % hole doping:

5-orbital model:

Graser, Maier, Hirschfeld, Scalapino NJP (2009)

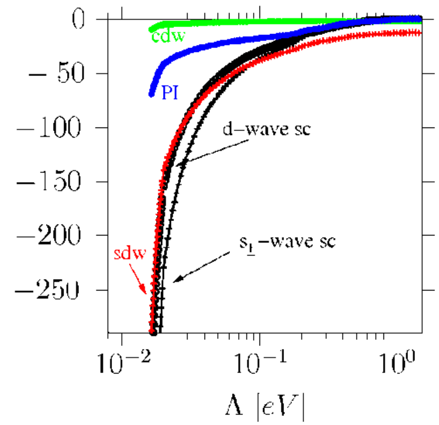


s± -formfactor:

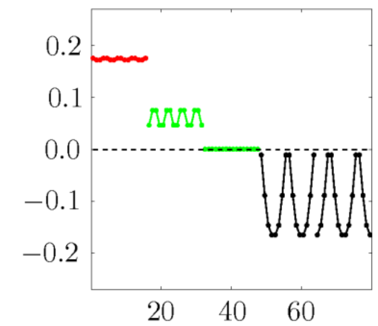


5-orbital model:

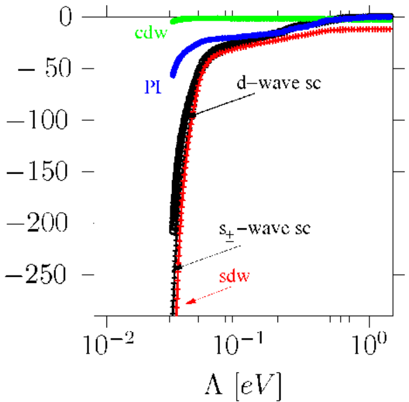
Kuroki et al. PRL (2008)



s± -formfactor:

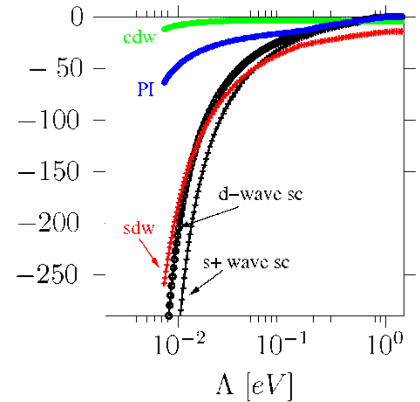


Undoped case:



model à la Kuroki :

- **sdw wins**
- **critical scale is higher despite same (bare) interaction**



model à la Graser :

- **no leading sdw-instability**

Model dependence III

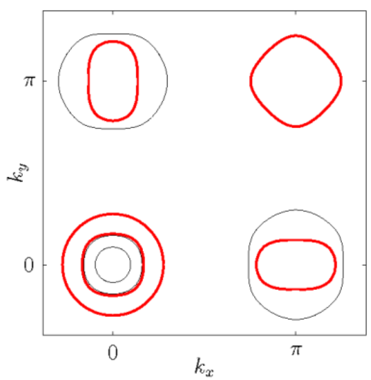
Both 5-orbital models (á la Kuroki & Graser) show:

- **nodeless s±** and nearby d-wave pairing **in electron doped regime**
- **s± pairing with nodes in hole doped case**

whereas:

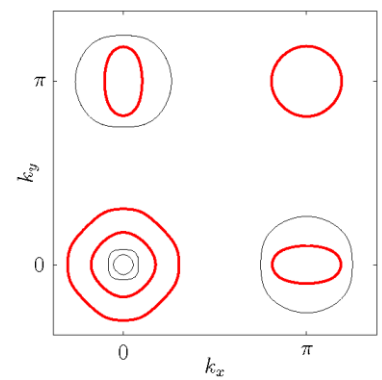
- **Kuroki's model** shows a **more pronounced propensity to sdw-order**
  (due to better nested FS in undoped and hole doped regime)
- no leading sdw-order in the undoped Graser model (for one special set of interaction pars.)

FS for Kuroki model (x=0.1 , x = -0.1)



different doping evolutions of FS

FS for Graser model (x=0.1 , x = -0.1)



What is universal ?

2 patch model for the pnictides
(Chubukov *et al.*)

↓

4-Band model with pocketwise interaction (g_1,….,g_4)

↓

Realistic 5-orbital model with full orbital interaction
(Kuroki *et al.*, Graser *et al.*)

} dominant pairing is **s± - wave**

} **sc gap-anisotropy** on electron pockets (even nodes)

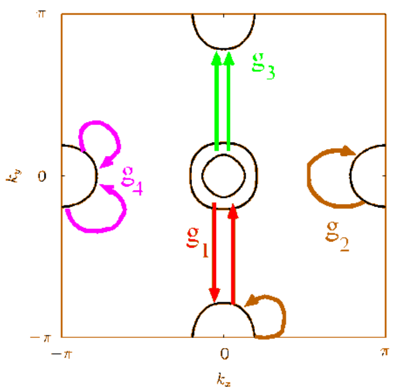
fRG suggests that in both cuprates and pnictide SC is driven by SDW-scattering

sc-gap anisotropy and existence of nodes depends on details (system parameters, doping,..)

Importance of orbital weights

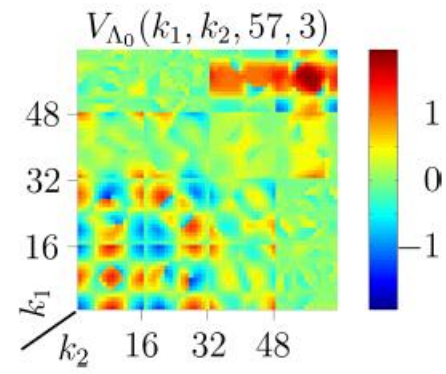
Without / with orbital structure in the initial interaction:

only 4 relevant scatterings:

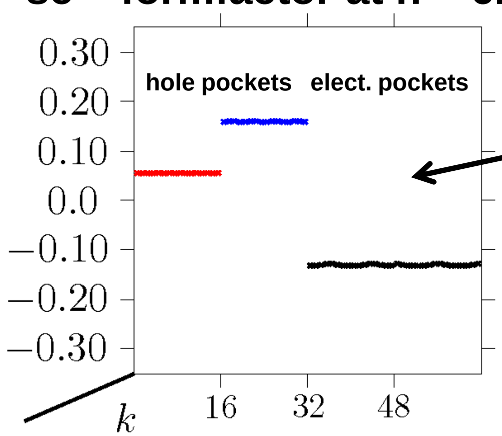


pronounced k-structure due to orbital weight

full orbital (initial) interaction:



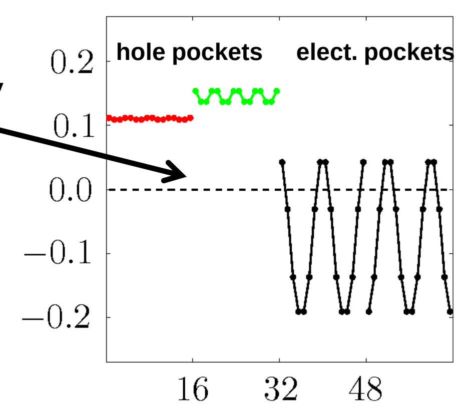
sc – formfactor at n = 6.10:



No gap fine-structure

sc – formfactor at n = 6.10:

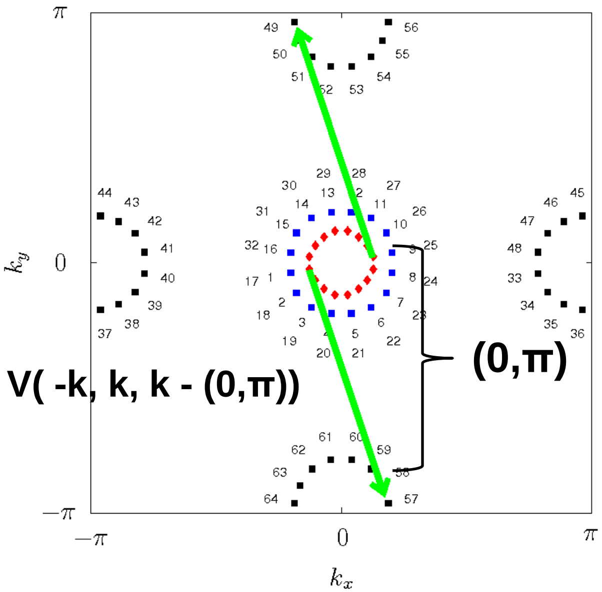
Gap-anisotropy



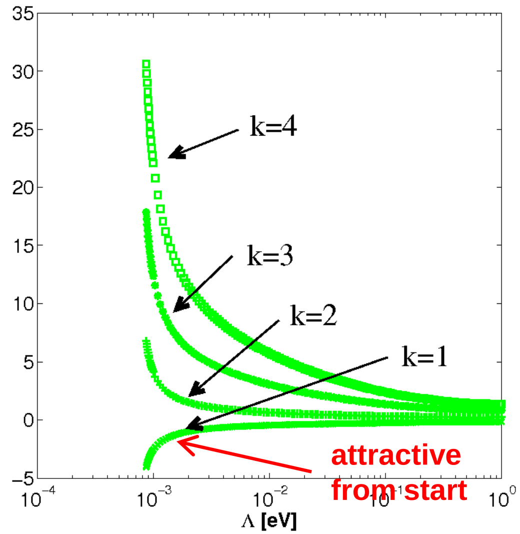
gap anisotropy is due to orbital – weights !!

Origin of nodes in sc-order parameter

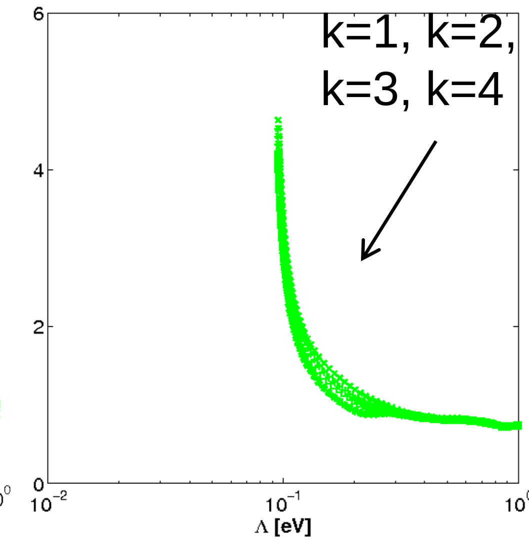
Dual SDW & SC scattering



V(-k, k, k - (0,π)) with orbital-weights:



V(-k, k, k - (0,π)) without orbital weights:



Certain (dual) sdw & sc channels diverge with negative sign

all (dual) sdw & sc channels remain repulsive

due to orbital weights: the sc-gap not necessarily favors $\langle\Delta_k\rangle\langle\Delta^\dagger_{k+(0,\pi)}\rangle < 0$ for all k !!

Conclusion

– Most dominant pairing instability at weak coupling is **extended s-wave (nodes/nodeless at electron/hole doping)**

– **Orbital weights are essential for gap anisotropy and nodes**

– Nearby (subleading) d-wave symmetry might cause **(s+id)-pairing**

Challenges for RG- (and other) theories:

– Analyze **renormalization effects in band structure** (orbital weights in bands may change !)

– **Include As-p orbitals** (p-d interaction)

– Study unconventional **electron (magnon) – phonon coupling**
large Fe-isotope effect (Liu et al. Nature 2009)
anomalous phonon dispersion in $CaFe_2As_2$ (Jülich, Karlsruhe 2009)

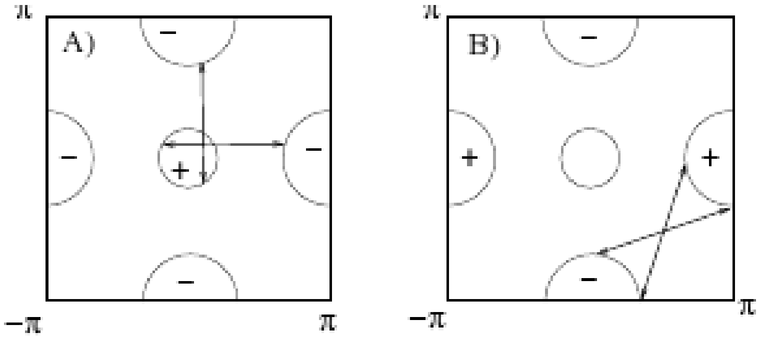
Platt, Honerkamp, Hanke, NJP 2009
Thomale, Platt, Hu, Honerkamp, Bernevig, arXiv: 0906
Thomale et al. to be published
Platt et al. to be published

Thank you for listening

Possibility of a time-reversal symmetry breaking (s+id) pairing:

Striking a compromise between different order parameters

(0,π) , (π,0)   (π, π/2) , (π/2, π)



In collaboration with S.C. Zhang (Stanford)

Possibility of (s+id) - pairing

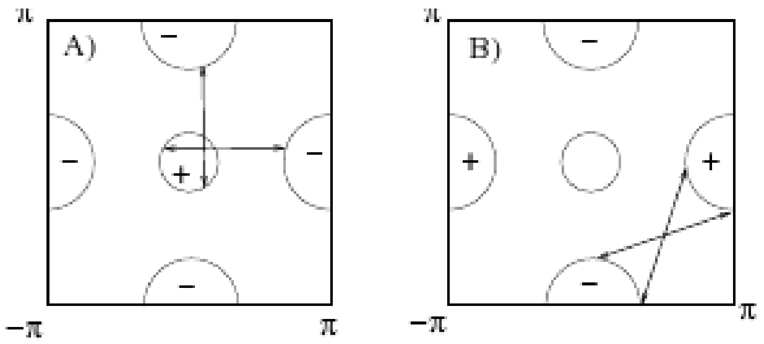
- Different nestings cause **frustration of the pairing order-parameter**:
  (in a spin-fluctuation based pairing)

- Competition of these two pairings **can lead to a mixed (s+id) state** after s-pairing occured

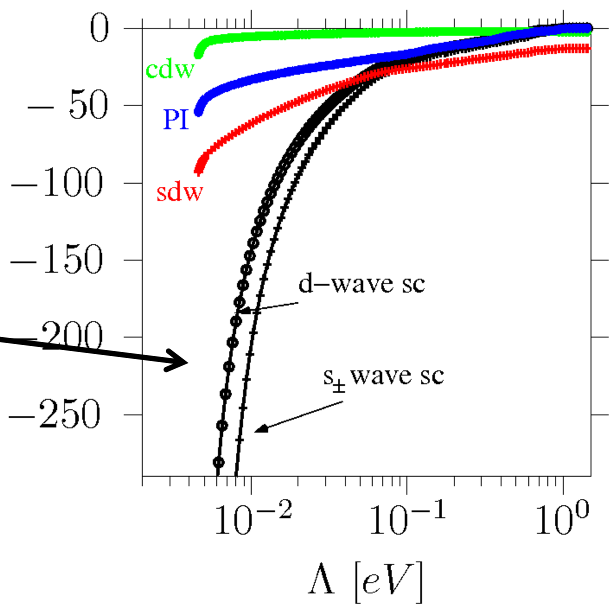
- B1g Raman mode can reveal if this mixed - state is favored or not

- Our fRG results show a **close competition between s- and d-wave pairing**

(0,π) , (π,0) (π, π/2) , (π/2, π)



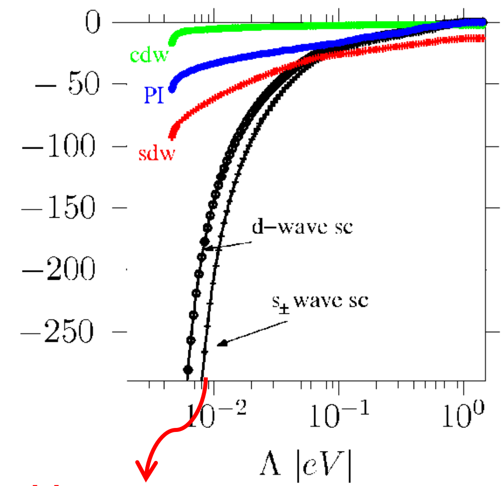
W. C. Lee, S. C. Zhang, C. Wu, PRL (2009)



Possibility of (s+id) - pairing

Solve gap equation after decoupling in the pairing channel at a scale Λ = 0.01 eV:

$$\Delta_k = -\sum_{k'} V_\Lambda(k,-k,k',-k') \frac{\Delta_{k'}}{2E_{k'}} \tanh\left(\frac{E_{k'}}{2T}\right)$$

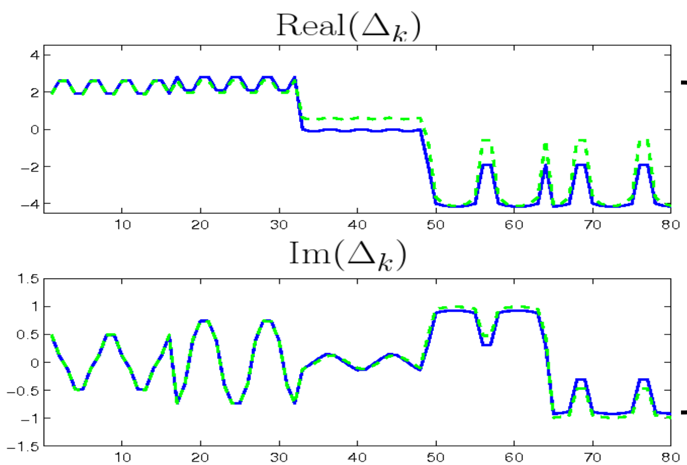


extract pairing vertex

(s+id)-pairing as selfconsistent solution:

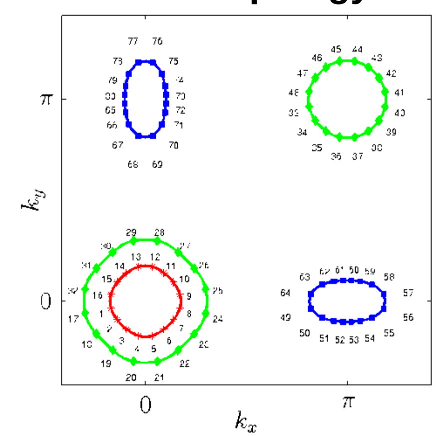
s - wave

d - wave



equal magnitude

FS topology



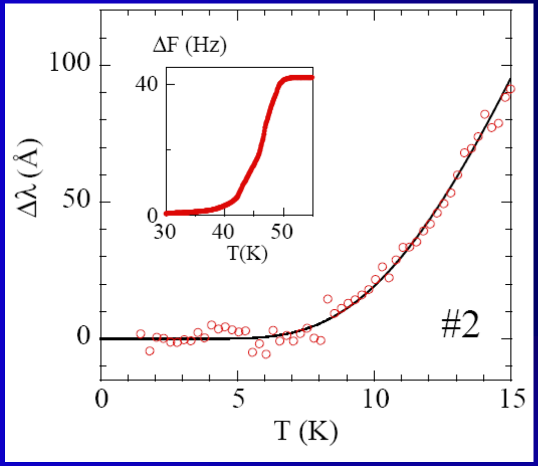
(s+id)-pairing is contained in the fRG result

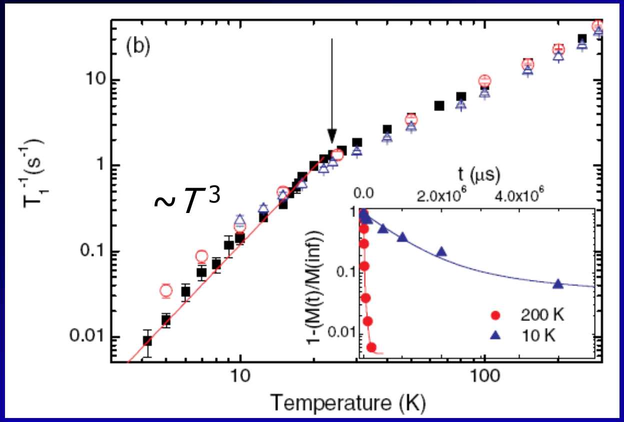
⟶ check free energy dependence

Introduction

Experimental facts

- Experiments not conclusive about the symmetry of the ground state
- Possibility: Different ground states in different materials?





L. Malone *et al*.:, Penetration depth shows exponential behaviour

H.-J. Grafe *et al*.: NMR relaxation rate shows powerlaw behaviour