Magnetic and pairing tendencies in quasi 1D multi-orbital models

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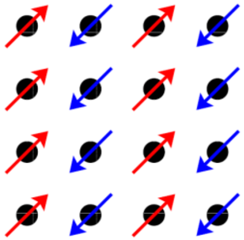
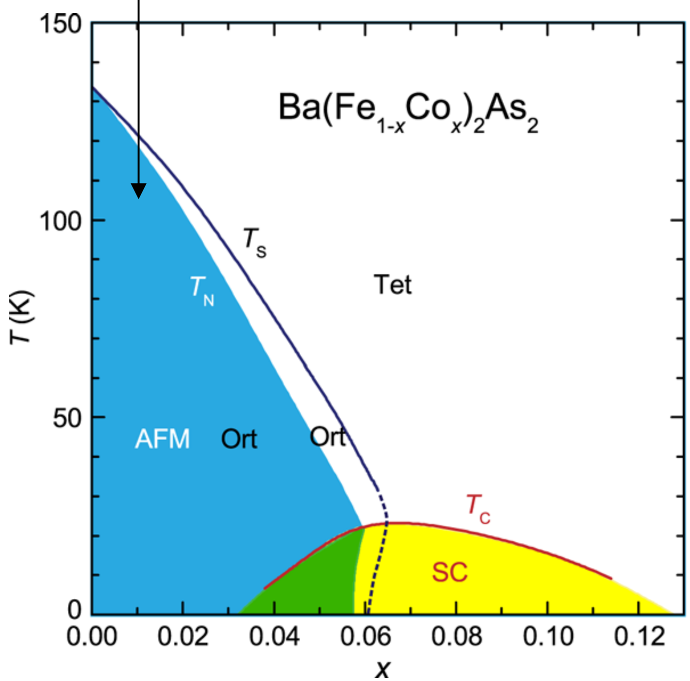
Overview of Fe-based High-T_c Scs



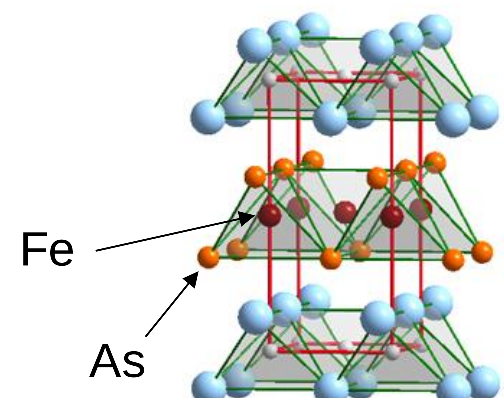


Similarities to cuprates

- Layered material.
- Superconducting order upon doping.
- Tetragonal to orthorhombic structural transition.

Differences to cuprates

- $(\pi, 0)$ magnetic ordering.
- Multiple d-orbitals are active.
- Bad-metal.



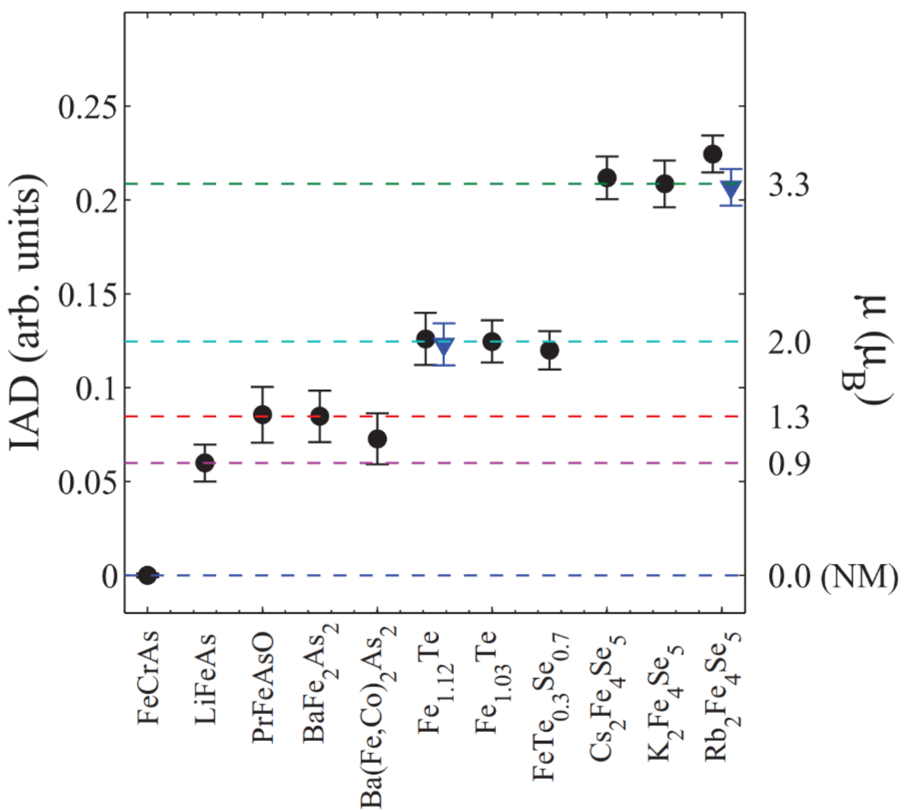
$d_{x^2-y^2}$

Copper: Cu^{+2} – 9 electrons in d-orbital

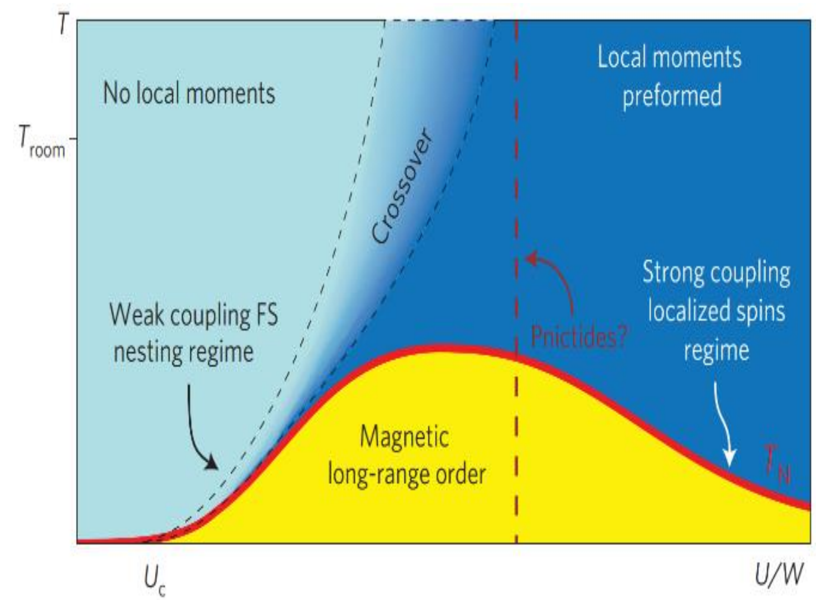
Iron: Fe^{+2} – 6 electrons in d-orbital $(d_{x^2-y^2}, d_{3z^2-r^2}, d_{xz}, d_{yz}, d_{xy})$

Correlation effects are not negligible

Local moments at room T



x-ray emission spectroscopy (room T)
H. Gretarsson et al., PRB **84**, 100509 (2011)



D. Liu et al., Nature Communications **3**, 931 (2012)
P. Dai et al., Nat. Phys. **8**, 709 (2012)

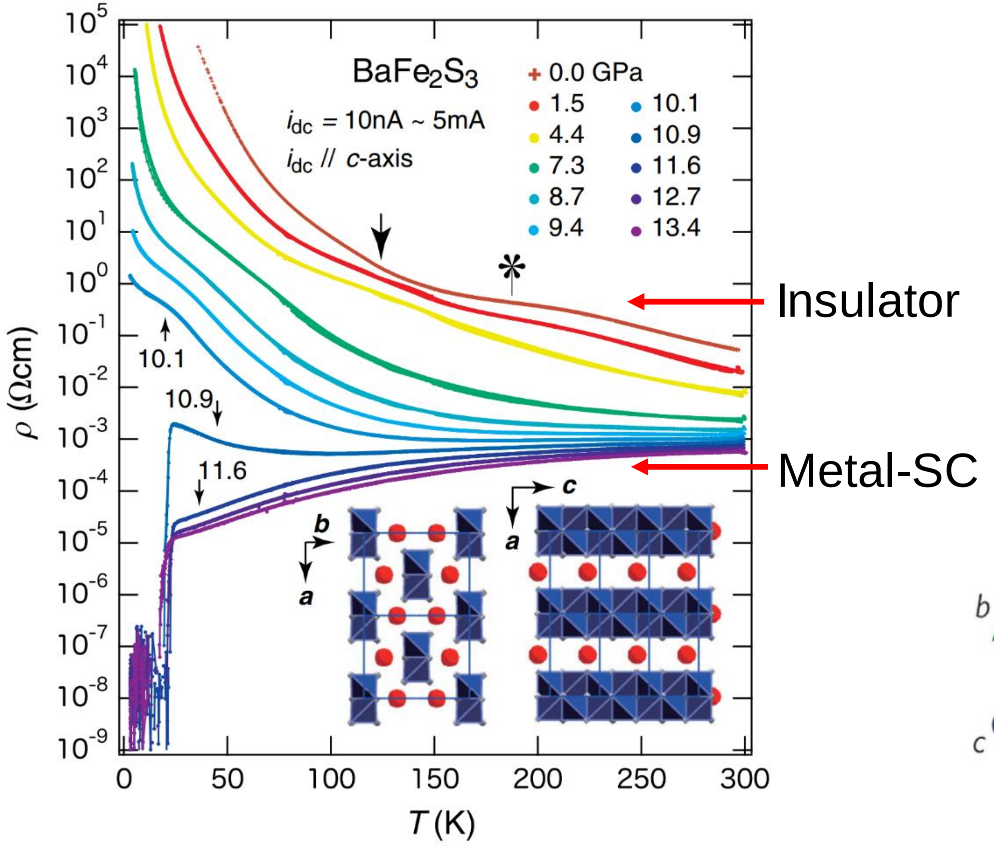
Interesting field is emerging

Iron ladders

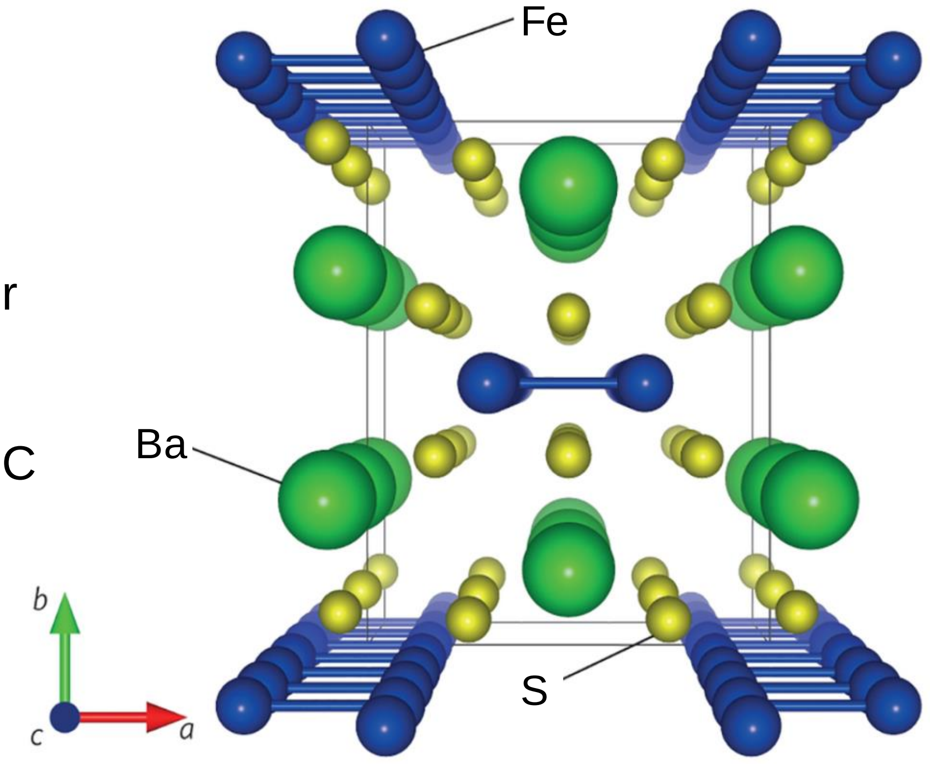
Why is this important?

First time that iron-based superconductivity is found in a non-layered geometry.

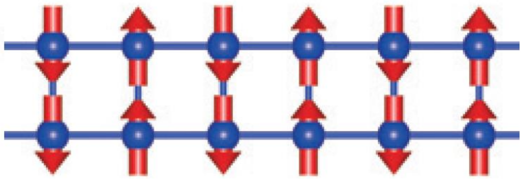
Iron-based ladders: 1D geometry
Superconductor at T_c = 24K (10 Gpa) reported



$BaFe_2S_3$



Spin moment (μ_B)
1.2 – 1.6



$(\pi, 0)$ order T_N ~ 120 K

H. Takagashi et al., Nature Materials **14**, 1008 (2015)
T. Yamauchi et al., Phys. Rev. Lett. **115**, 246402 (2015)

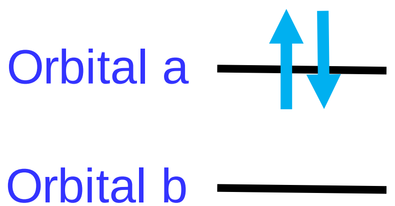
Model: Multiorbital Hubbard Model
Method: Density Matrix Renormalization Group (DMRG)

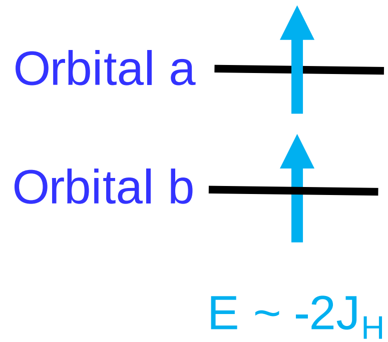
$$H_k = \sum_{\substack{i\sigma \\ \gamma\gamma'\alpha}} t^{\vec{\alpha}}_{\gamma\gamma'} (c^\dagger_{i\sigma\gamma} c_{i+\vec{\alpha}\sigma\gamma'} + \text{H.c.}) + \sum_{i\gamma\sigma} \Delta_\gamma n_{i\gamma\sigma}$$

$$U \sum_{i\gamma} n_{i\gamma\uparrow} n_{i\gamma\downarrow} + (U' - \frac{J_H}{2}) \sum_{\substack{i \\ \gamma < \gamma'}} n_{i\gamma} n_{i\gamma'} - 2J_H \sum_{\substack{i \\ \gamma < \gamma'}} \mathbf{S}_{i\gamma} \cdot \mathbf{S}_{i\gamma'}$$

Orbital repulsion

Hund's Coupling = Spins must Be aligned on site





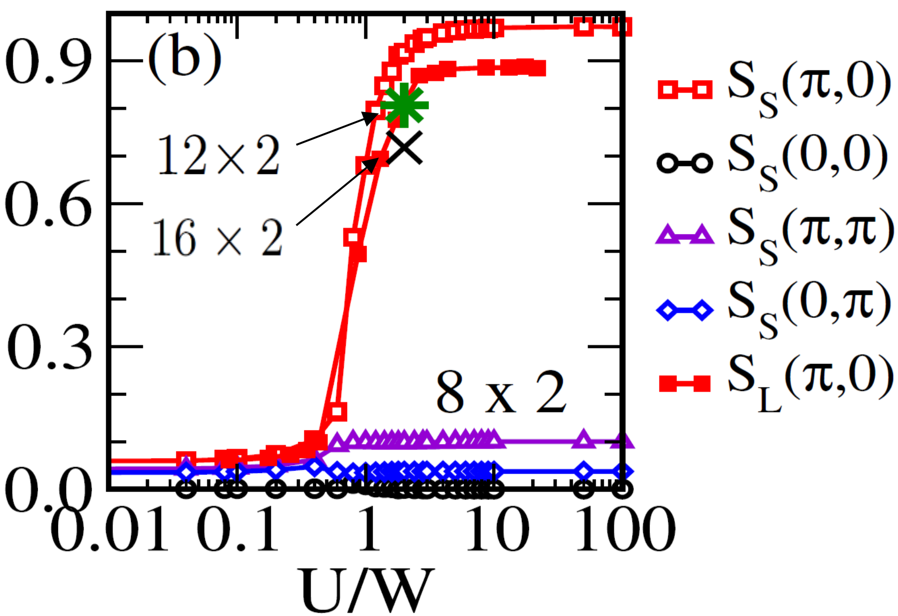
$$U' = U - 2J_H$$

Number operator: $n_{i\sigma\gamma} = c^\dagger_{i\sigma\gamma} c_{i\sigma\gamma}$

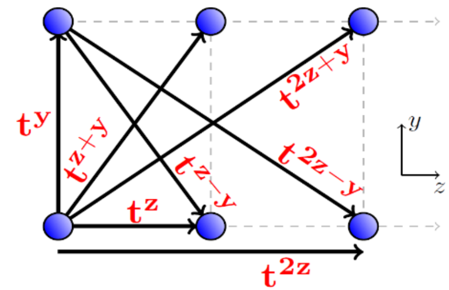
Spin operator: $\mathbf{S}_{i\gamma} = \sum_{\sigma\sigma'} c^\dagger_{i\sigma\gamma} \sigma_{\sigma\sigma'} c_{i\sigma'\gamma}$

Two-orbital Hubbard model - $BaFe_2S_3$ ladders
Half filling – 2e/site

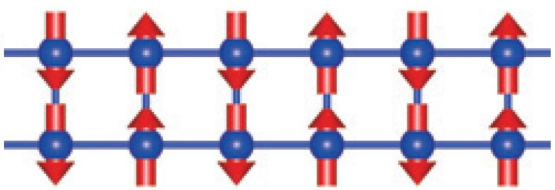
$$\frac{J_H}{U} = 0.25$$



2 orbitals/site



ab initio
W~2eV



$S(\pi, 0)$ magnetic ground state

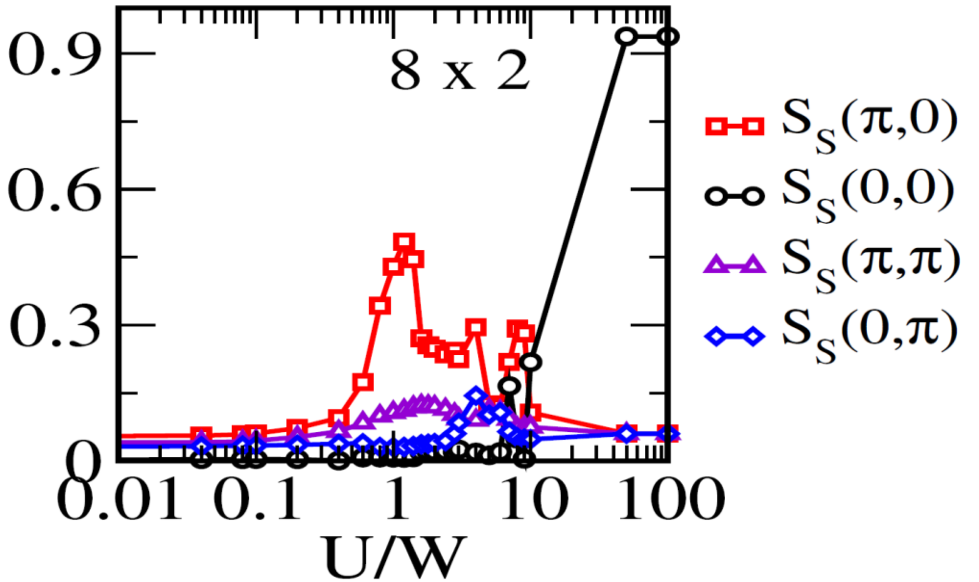
Explained by J_1-J_2 spin model

$$\frac{J_2}{J_1} \propto \frac{t_{z+y}^2}{t_z^2} \geq 0.5$$

$$S(k_z, k_y) = \frac{1}{N^2} \sum_{i,j} e^{-i\vec{k}\cdot\vec{r}_{ij}} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$$

N. D. Patel et al., Phys. Rev. B **94**, 075119 (2016)

2-Hole Doping - $BaFe_2S_3$ ladders



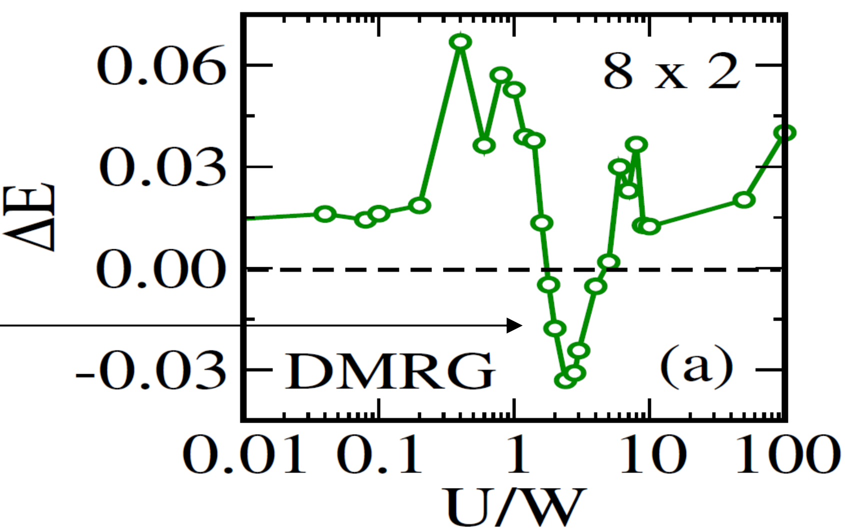
Suppressed $(\pi, 0)$
Magnetic order

two correlated holes

$$\Delta E = [E_{N-2} - E_N] \\ -2[E_{N-1} - E_N]$$

two independent holes

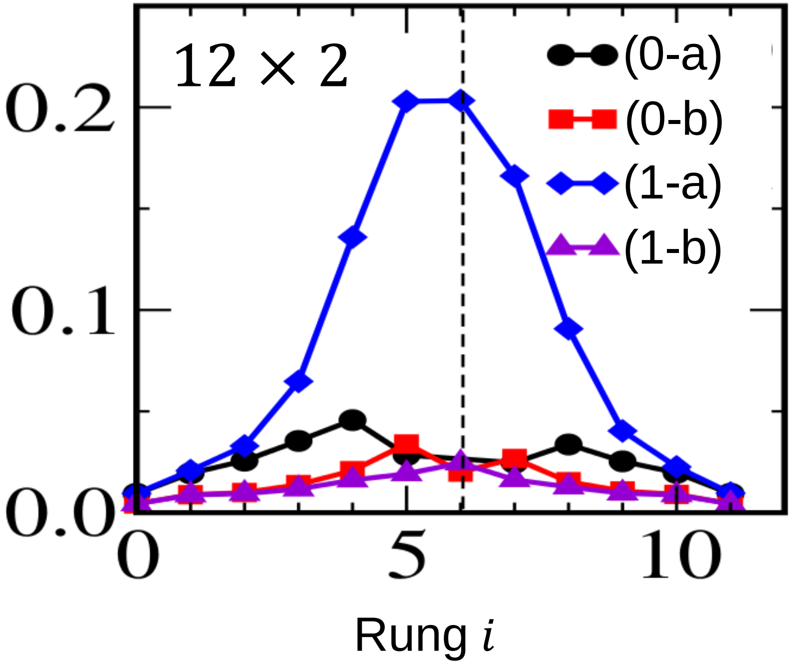
Bound state?



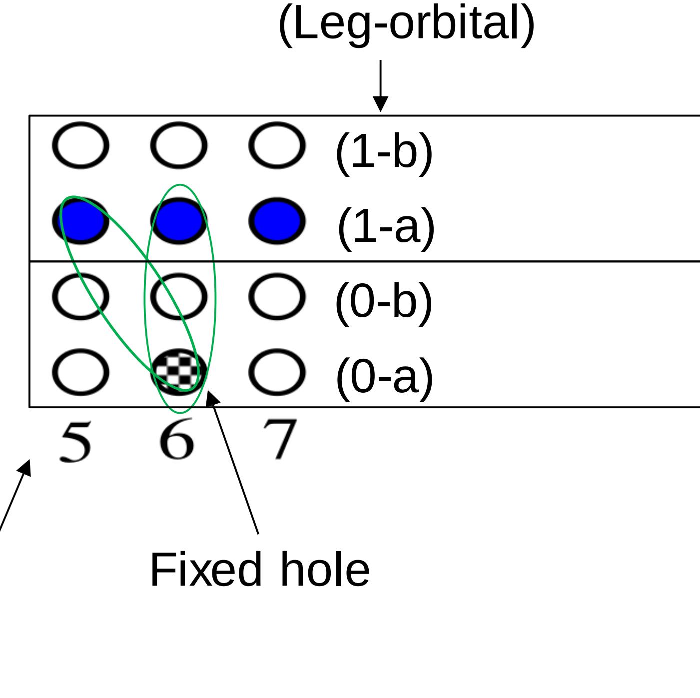
N. D. Patel et al., Phys. Rev. B **94**, 075119 (2016)

Pair Structure in - $BaFe_2S_3$ ladders

Probability of finding a hole at the i^{th} rung, given that one hole is located at 6^{th} rung – leg 0 – orbital a.



Two-orbital 2-leg ladder ~ One-orbital 4-leg ladder



<u>Rung and Diagonal Pairs</u>

Orbital Selective pairs?

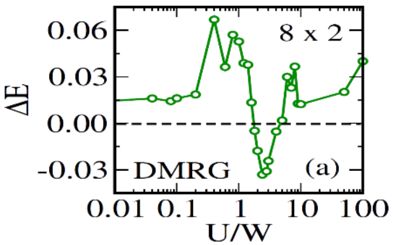
N. D. Patel et al., Phys. Rev. B **94**, 075119 (2016)

P. O. Sprau et al., "Discovery of Orbital-Selective Cooper pairing in FeSe" Science **357**, 75 (2017)

Multi-orbital ladders are numerical expensive to study.

How can I simplify my model to focus only on the pairing mechanism?

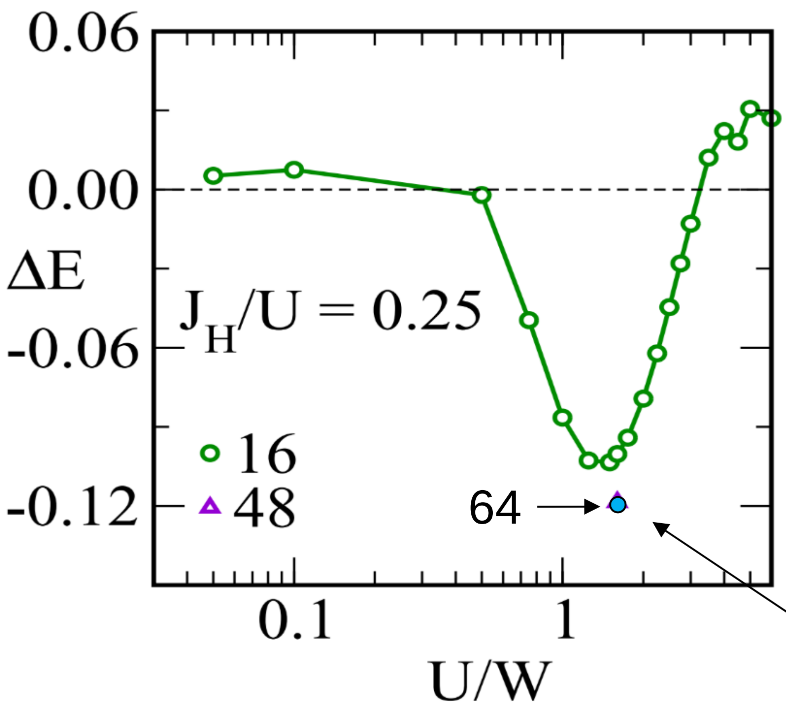
Multi-orbital chains



BaFe$_2$S$_3$ Ladder

two-orbital model on a chain

Only intra-orbital hopping (xz,yz)
no crystal field



two correlated holes

$$\Delta E = [E_{N-2} - E_N] \\ -2[E_{N-1} - E_N]$$

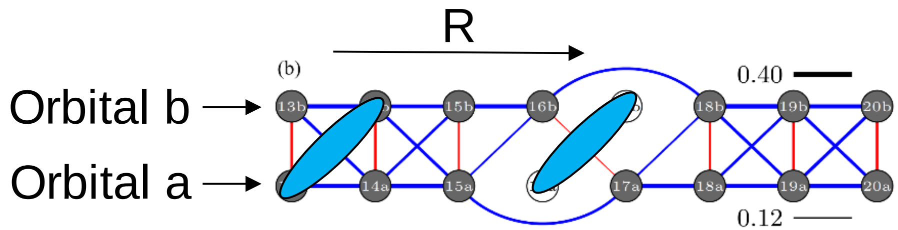
two independent holes

Bound pairs remain
in bulk limit.

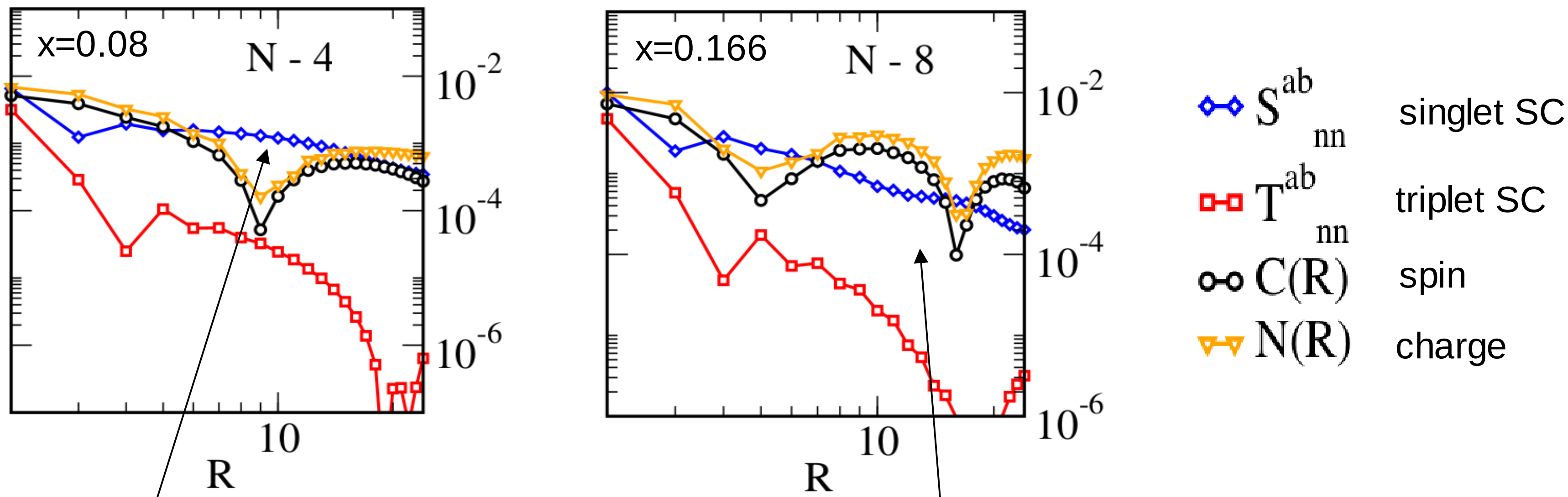
N. D. Patel et al., Phys. Rev. B **96**, 024520 (2017)

Pair-Pair correlations & real-space decay

two-orbital chain



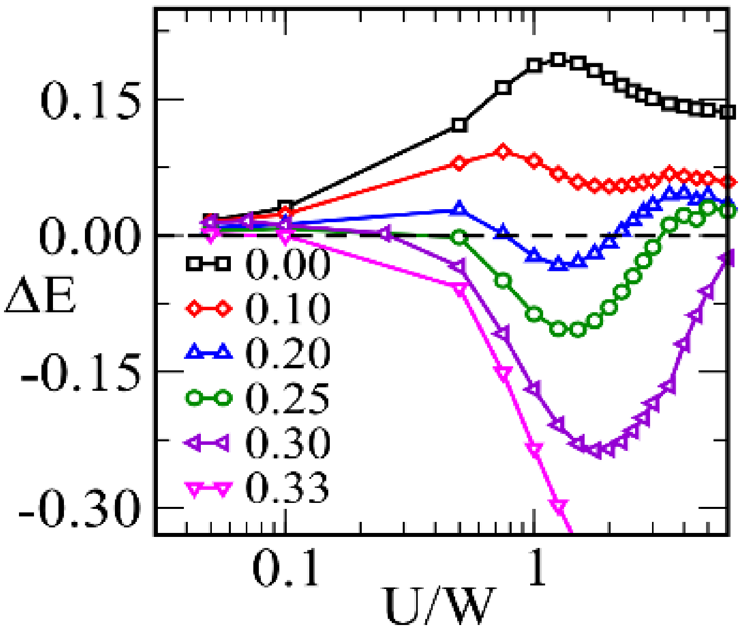
$$\mathcal{O}^{\gamma\gamma'}_{nn,\pm}(R) = \frac{1}{2N_R}\sum_i \langle \Delta^{\gamma\gamma'\,\dagger}_{nn,\pm}(i)\,\Delta^{\gamma\gamma'}_{nn,\pm}(i+R)\rangle$$

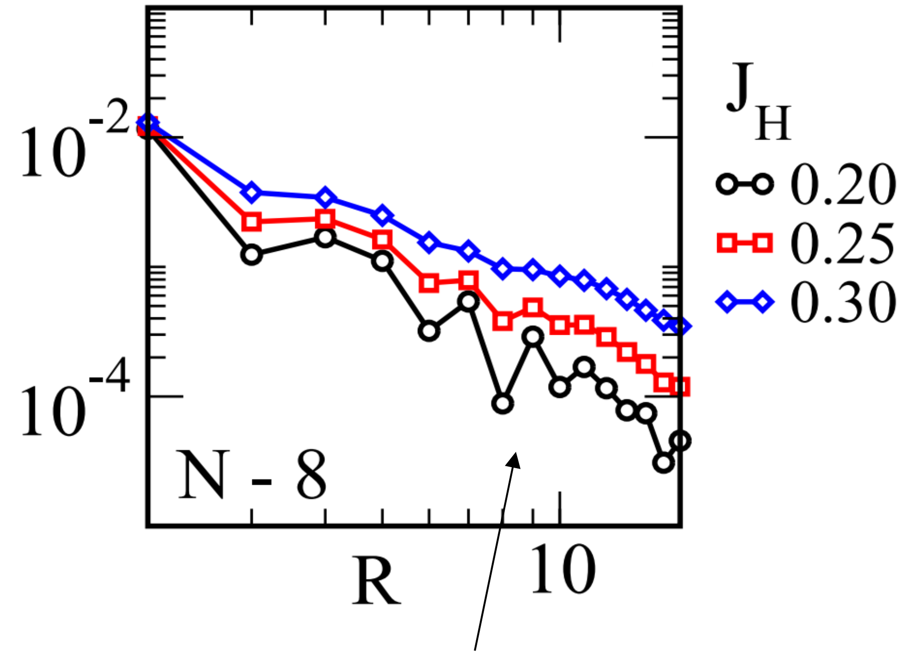


Pair-Pair correlations decay slower than the spin/charge density wave.

Competition SC, magnetism, and charge intertwined orders.

Work in progress:
What is responsible for singlet pairs?



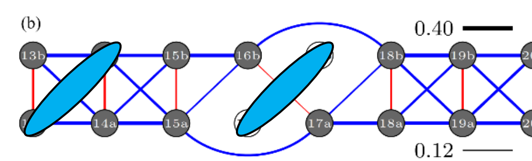


Upper limit of Hund coupling

$$U' \geq J_H$$

$$\frac{J_H}{U} \leq \frac{1}{3}$$

Hund coupling plays a crucial role in pairing



Summary

- Iron-based ladders become superconducting at high pressure, and they can be studied theoretically with accuracy.

Our main results are the following

- Binding of holes found even through the Hamiltonian is purely repulsive!
- In $BaFe_2S_3$ ladders, rung and diagonal hole-pair configurations are dominant.
- Pairing upon hole doping is also found in the two-orbital chains. Origin?