How to model holes doped into a cuprate layer

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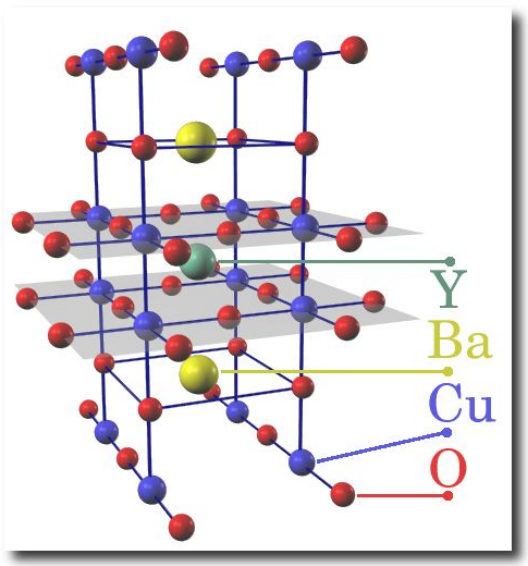
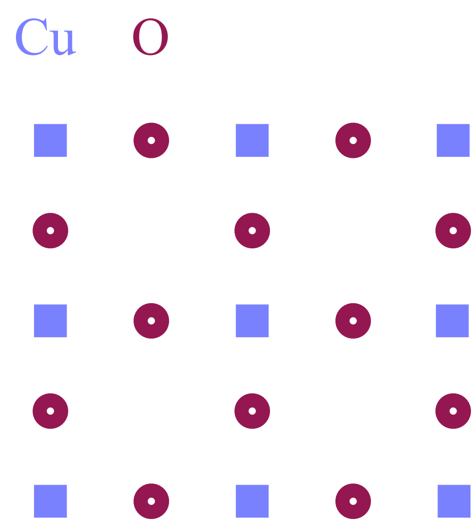
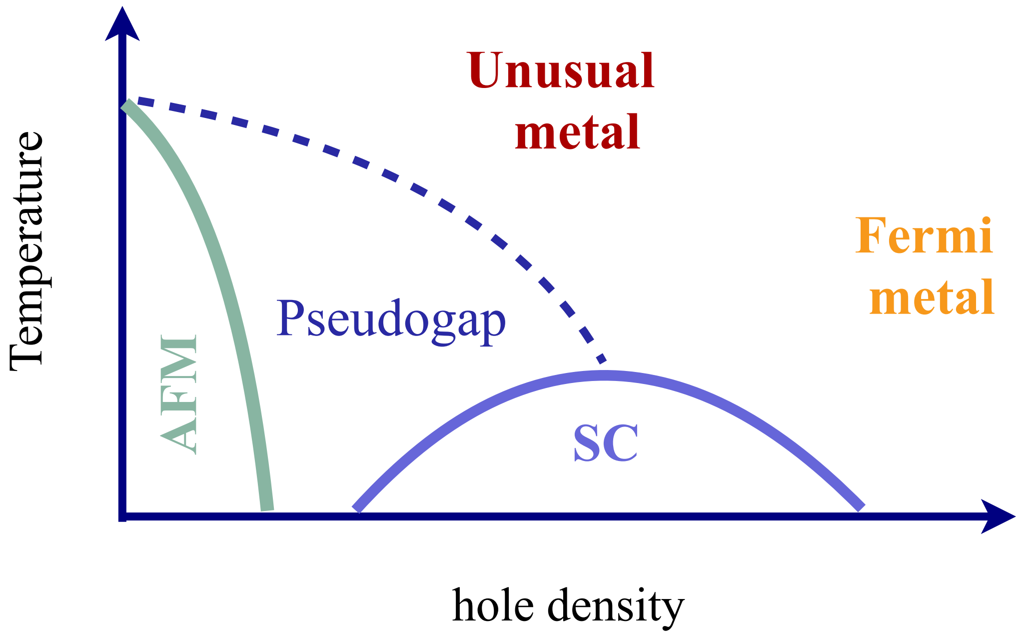
Why holes in a CuO_2 layer?

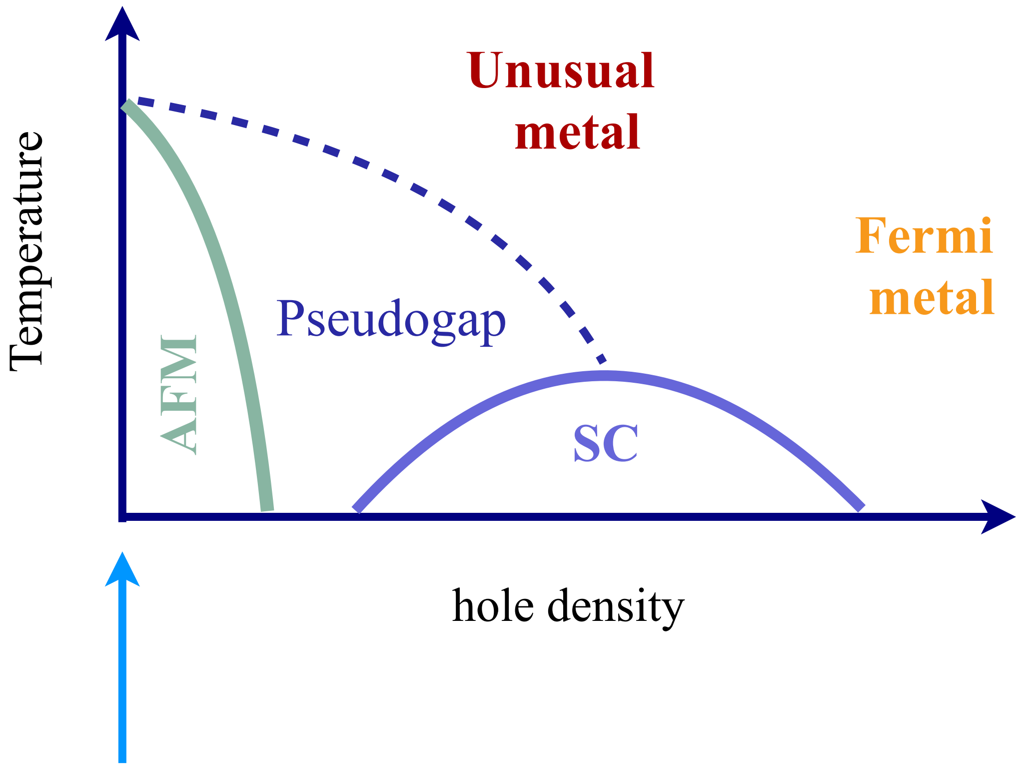
→ "cuprates" = family of high-temperature superconductors (high-Tc record)

→ layered compounds, common feature are CuO_2 layers believed to host superconductivity upon doping






Unusual
metal
Fermi
metal
Temperature
Pseudogap
AFM
SC
hole density



parent compound
= Mott insulator with AFM order

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→ ”cuprates” = family of high-temperature superconductors (high-Tc record)

→ layered compounds, common feature are CuO_2 layers believed to host superconductivity upon doping

→ origin of pairing still not resolved, although it is widely believed to have something to do with the AFM order

First step: understand what happens when one hole is added

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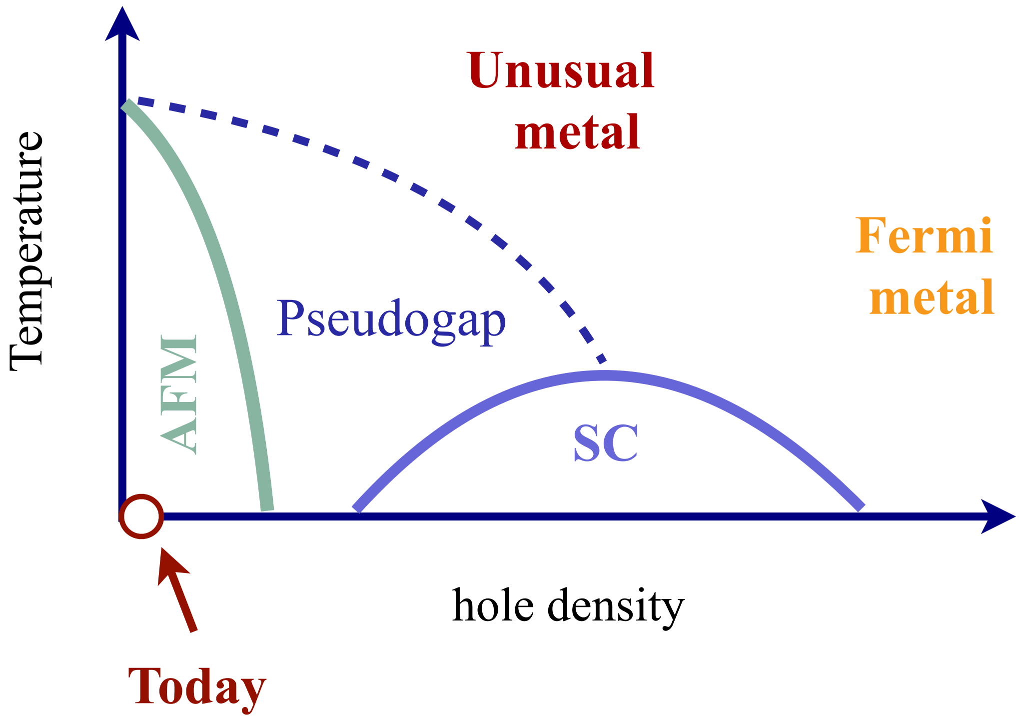
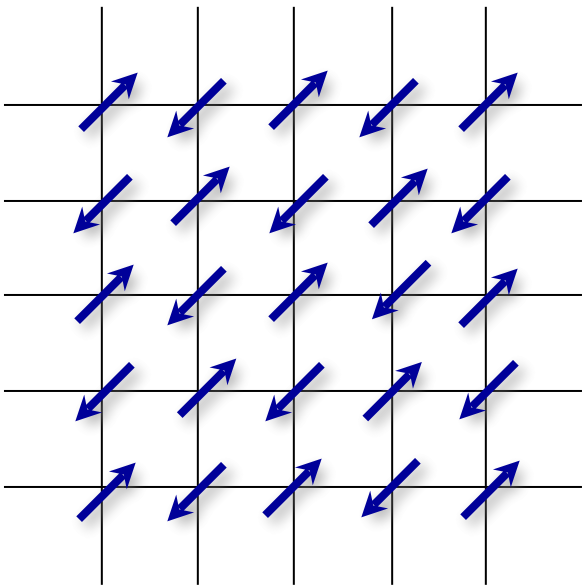


How to model this problem?

→ parent compound: each Cu has one hole in $3d_{x2-y2}$ orbital, while O 2p are full

unpaired spin $\rightsquigarrow$ AFM order



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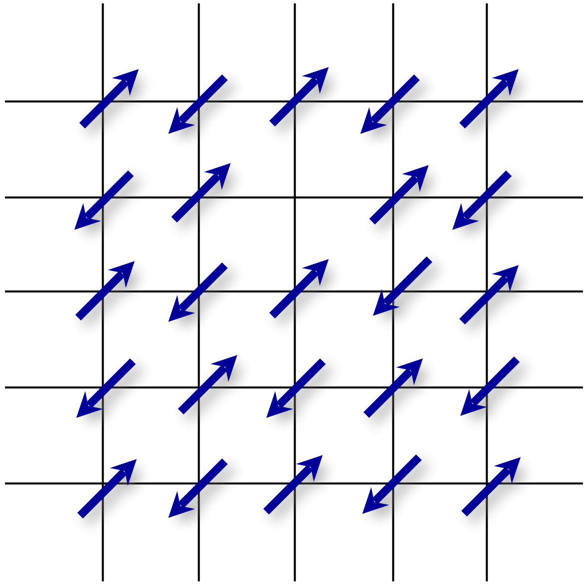

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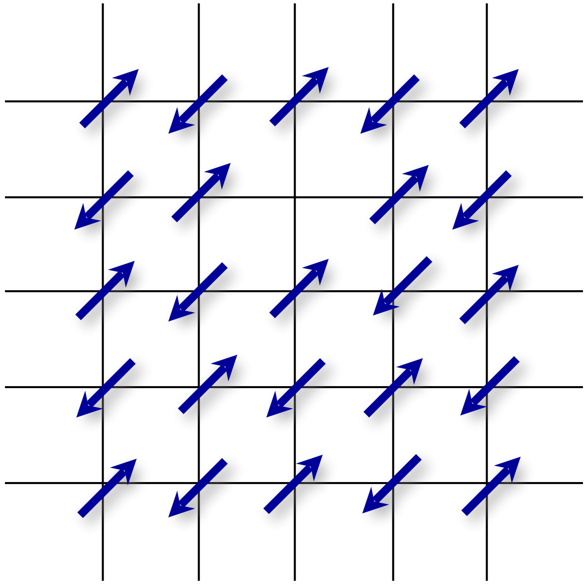

Use Hubbard or t-J model

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} \left(c^{\dagger}_{i,\sigma} c_{j\sigma} + h.c. \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

$$\xrightarrow{U \gg t} P \left[-t \sum_{\langle i,j \rangle} \left(c^{\dagger}_{i,\sigma} c_{j\sigma} + h.c. \right) \right] P + J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$

Hole in an AFM background: the t-J model results

→ could use ED or some flavour of MC, but not so good for gaining intuition

→ instead, use a variational method — not exact but we can understand the important phenomenology because we can identify the key aspects + we can study infinite layers + generalize to few holes **M. Berciu, PRL 107, 246403 (2011);**

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→ Challenge: the 2D AFM is a very complicated state because of the quantum spin fluctuations

$$\vec{S}_i \cdot \vec{S}_j = S_i^z S_j^z + \boxed{\frac{1}{2}\left[S_i^+ S_j^- + S_i^- S_j^+\right]}$$

$$\uparrow\downarrow \quad \leftrightarrow \quad \downarrow\uparrow$$

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→ Challenge: the 2D AFM is a very complicated state because of the quantum spin fluctuations

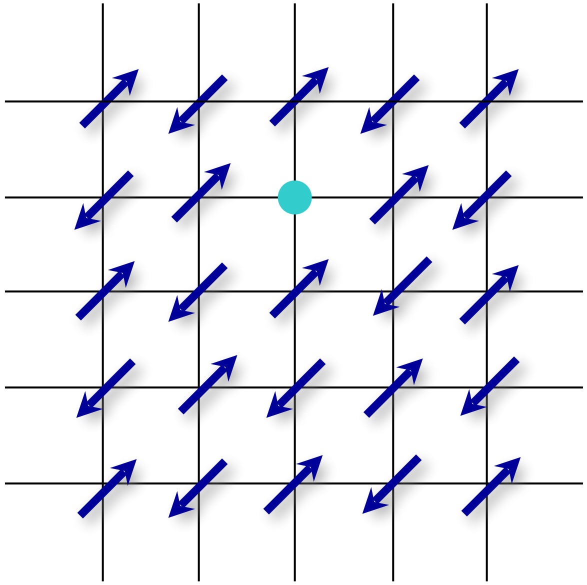
→ Two-step solution:

1. ignore background spin fluctuations, ie use a semi-classical Neel state

2. allow for "local" spin fluctuations only in the vicinity of the doped hole

Hole in the t-J_z model (spin fluctuations not allowed)

→ "Common wisdom": the hole is confined by the string of wrongly oriented spins (= magnons) generated through its motion



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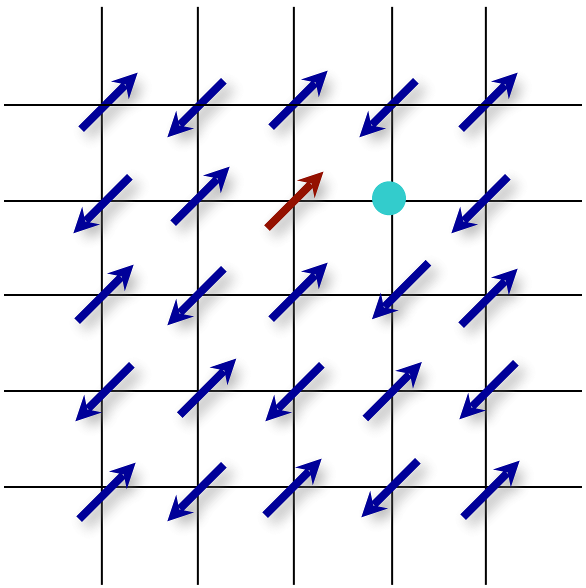

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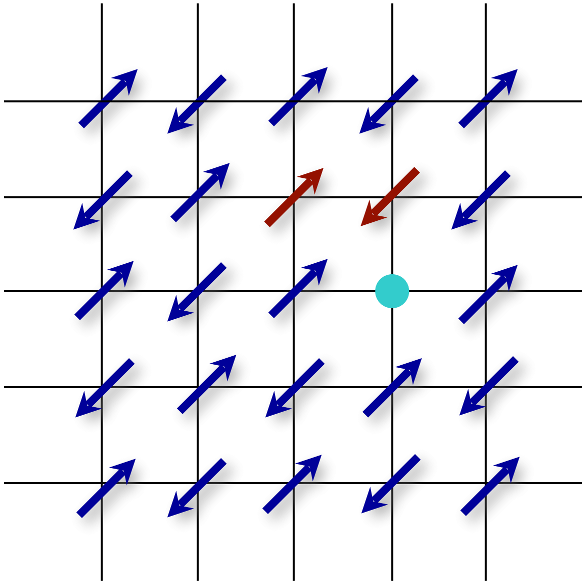

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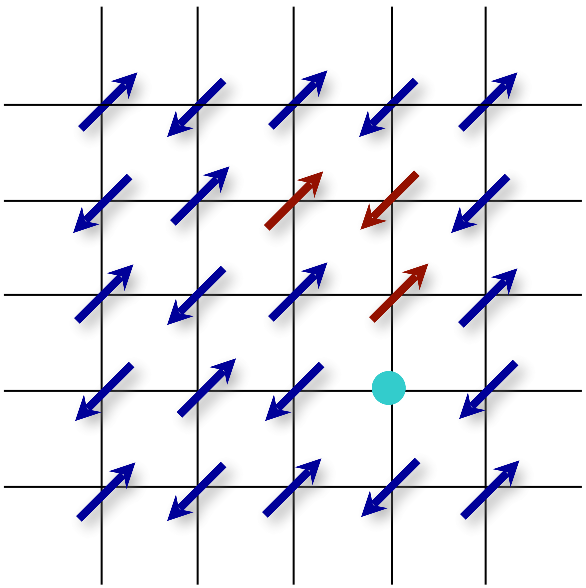

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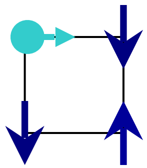

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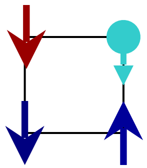

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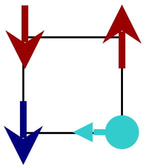

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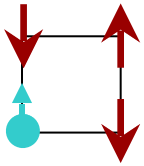

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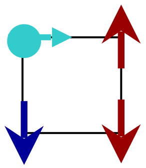

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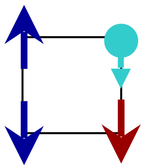

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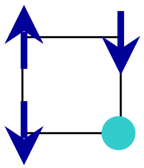

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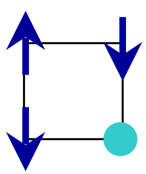


→ Effective 2nd nn hopping (and 3rd nn) are dynamically generated through these loops, so the hole can move anywhere on its sublattice

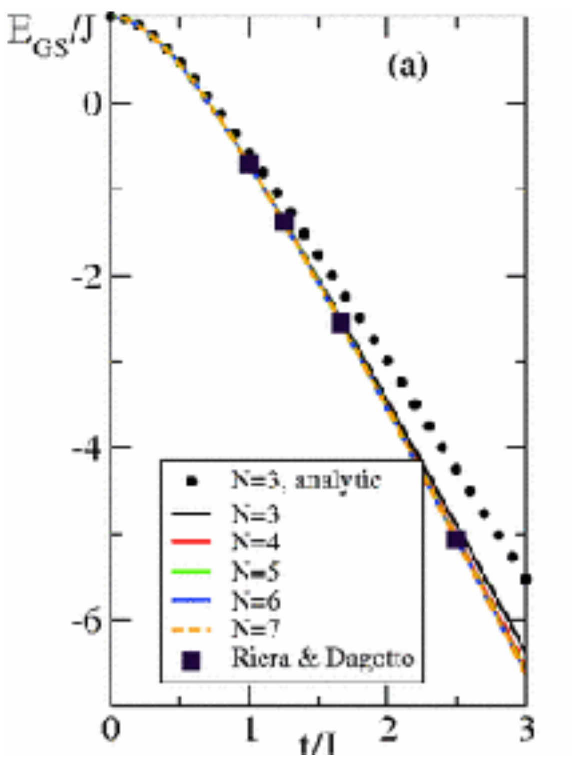
→ What is the resulting dispersion?

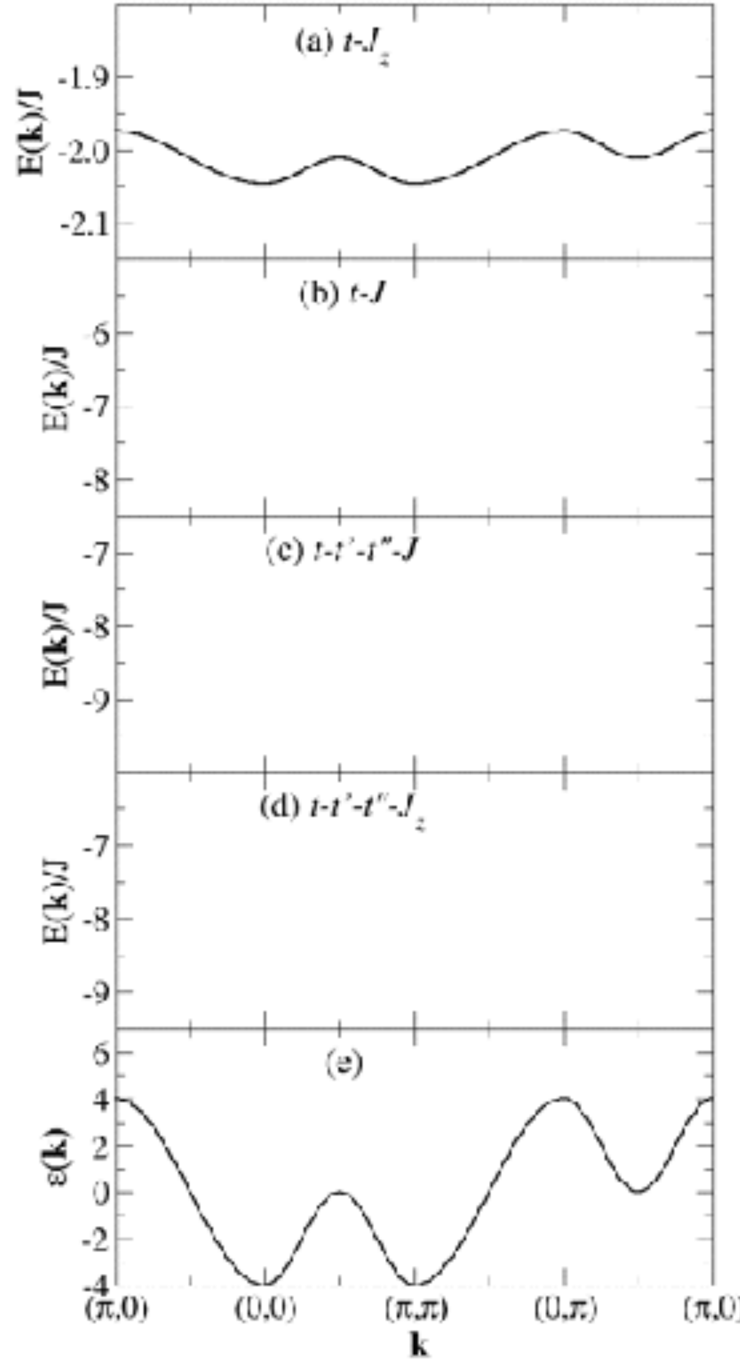
Hole in the t-J_z model

→ very heavy qp

M. Berciu and H. Fehske, PRB 84, 165104 (2011)

J. Riera and E. Dagotto, PRB 47, 15346(R) (1993)





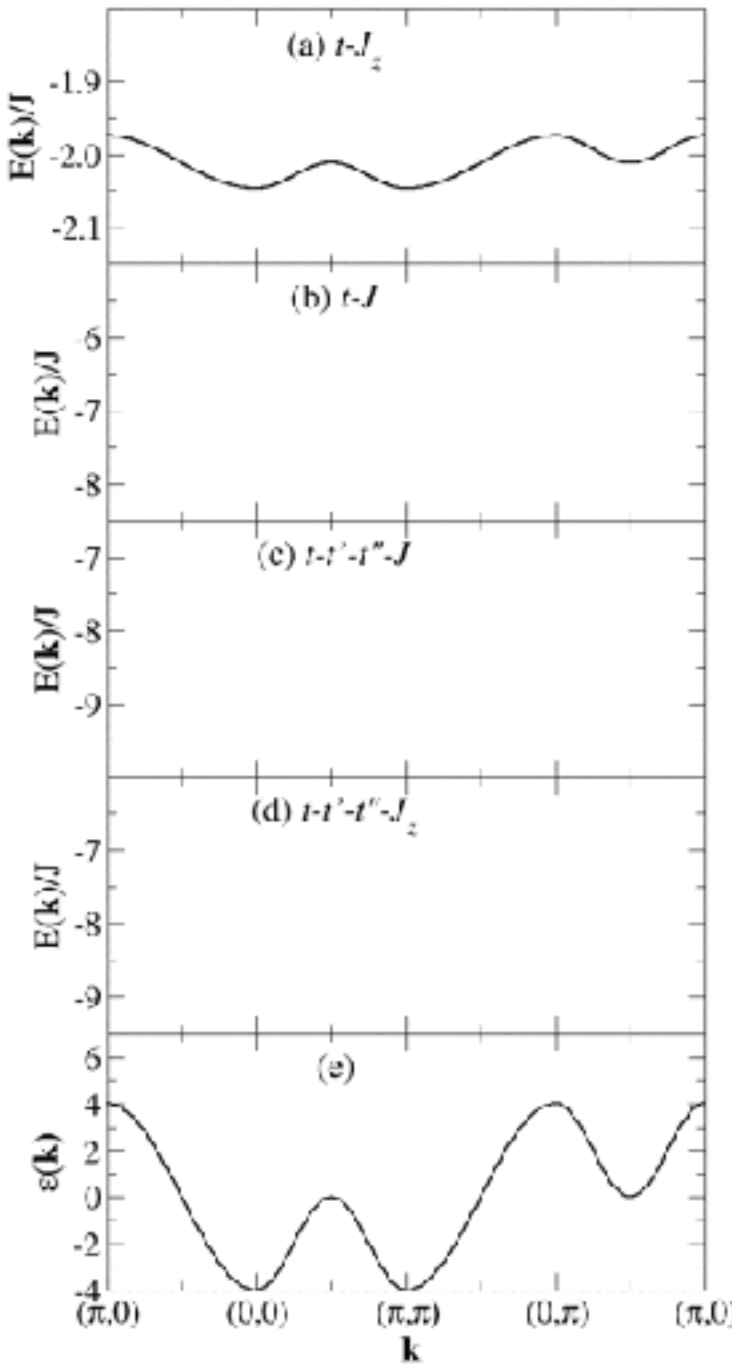
Hole in the t-J_z model

→ very heavy qp + wrong dispersion

→ In LR-AFM, qp dispersion MUST be

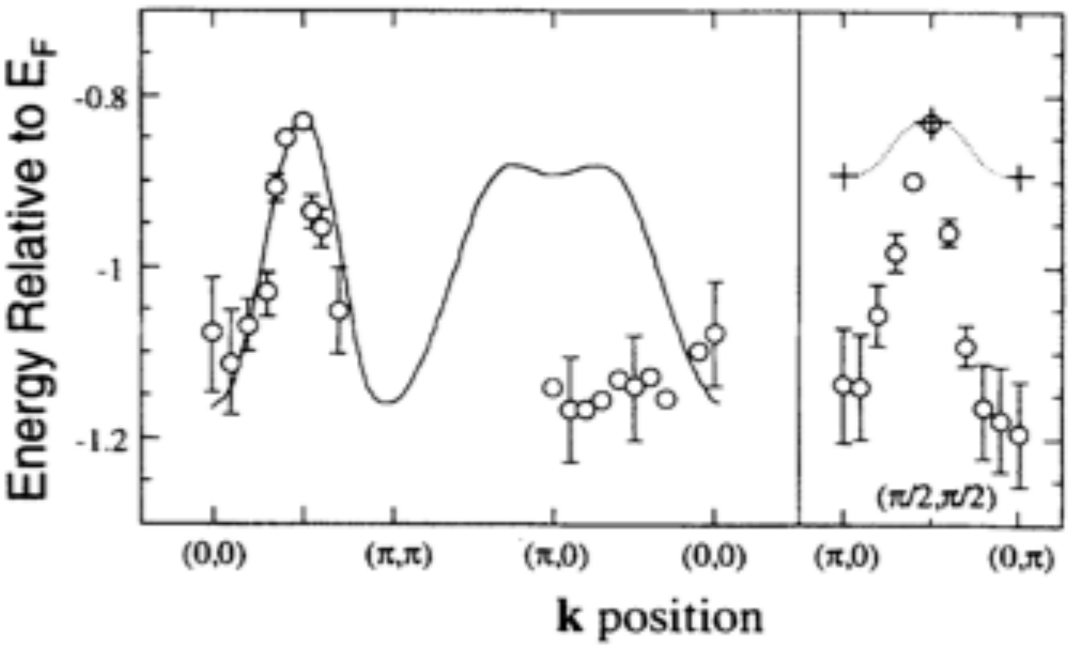
$$E_{qp}(\mathbf{k}) = 4t_2 \cos k_x \cos k_y$$
$$+2t_3[\cos(2k_x) + \cos(2k_y)]$$

→ For Trugman loops $|t_2| >> |t_3|$; then the curve has a saddle point at $(\pi/2,\pi/2)$



Can we measure the dispersion of one hole in parent compound?

→ YES, using ARPES **B.O. Wells et al, PRL 74, 964 (1995)**



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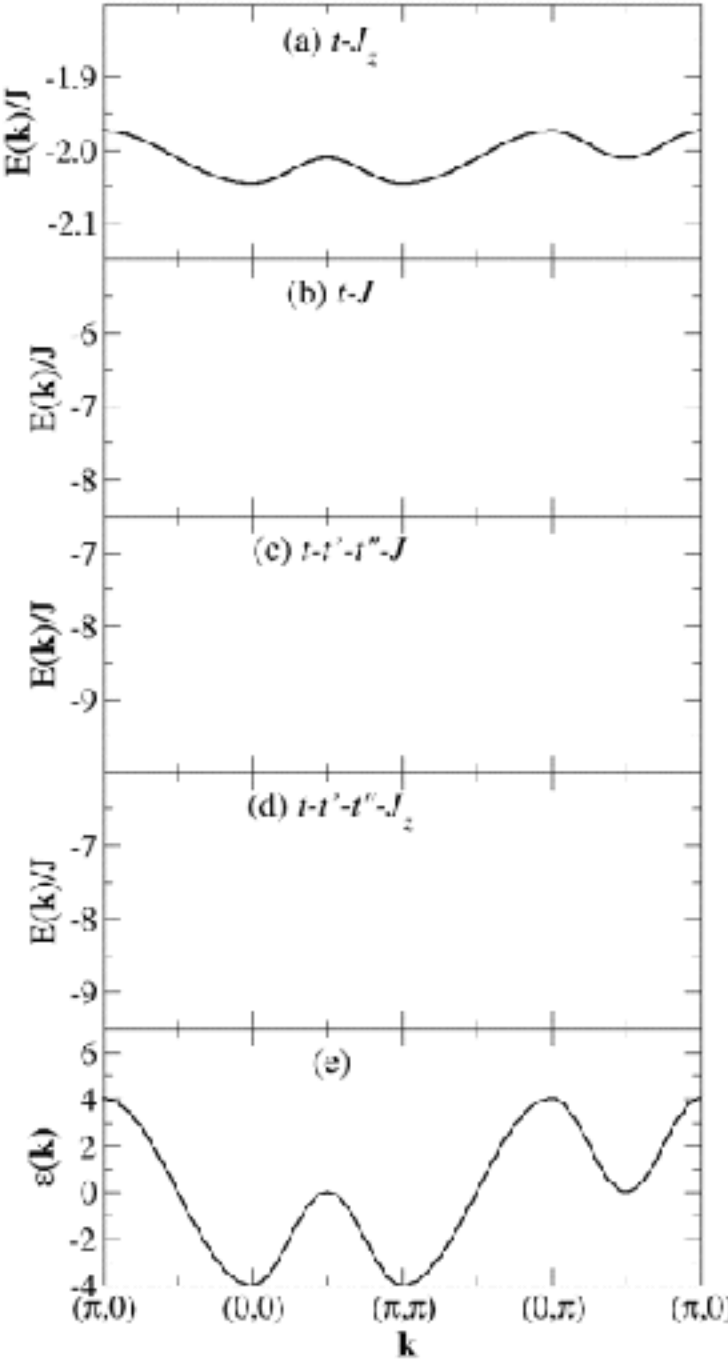
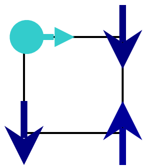


Hole in the t-J model (with local spin fluctuations)

→ Common wisdom: spin fluctuations can remove pairs of wrongly oriented spins so mass should be much lower …



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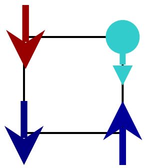

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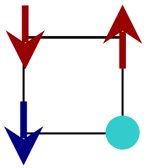

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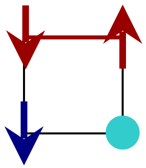

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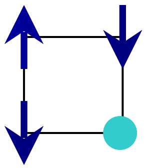
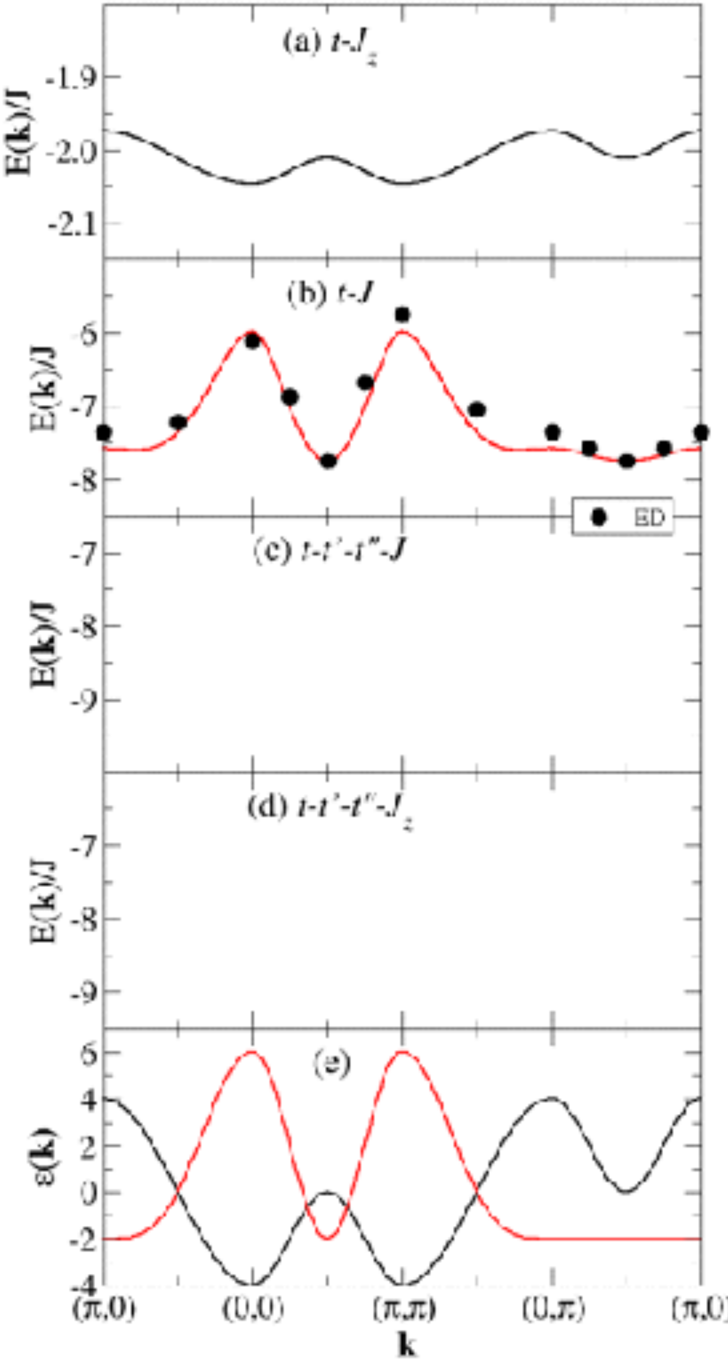


Hole in the t-J model

→ much lighter qp, but shape of dispersion is still wrong!

ED: PW Leung, RJ Gooding, PRB 52 R15711 (1995)



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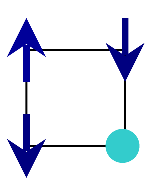

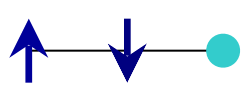

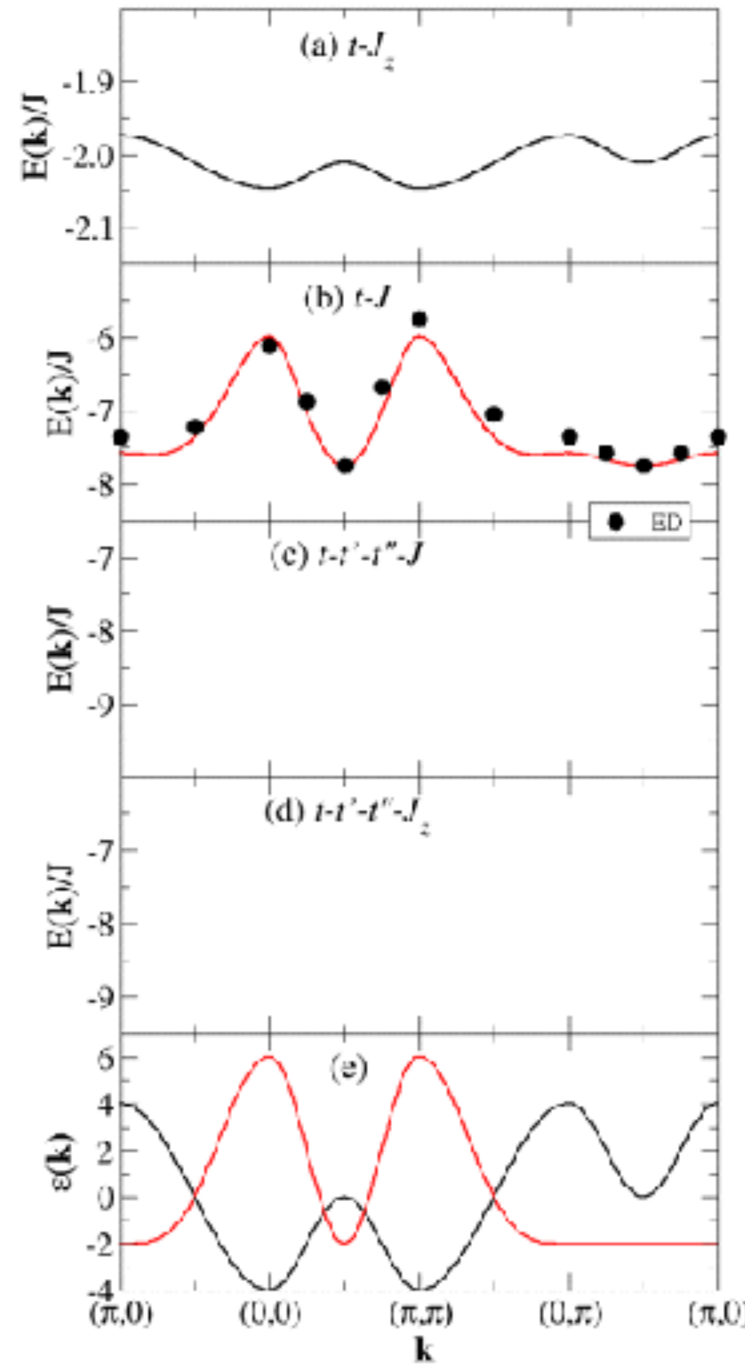

How to fix the wrong shape?

→ add longer range hopping …

Hole in the t-t'-t"-J model

→ interplay of spin fluctuations + longer range hopping — correct dispersion emerges

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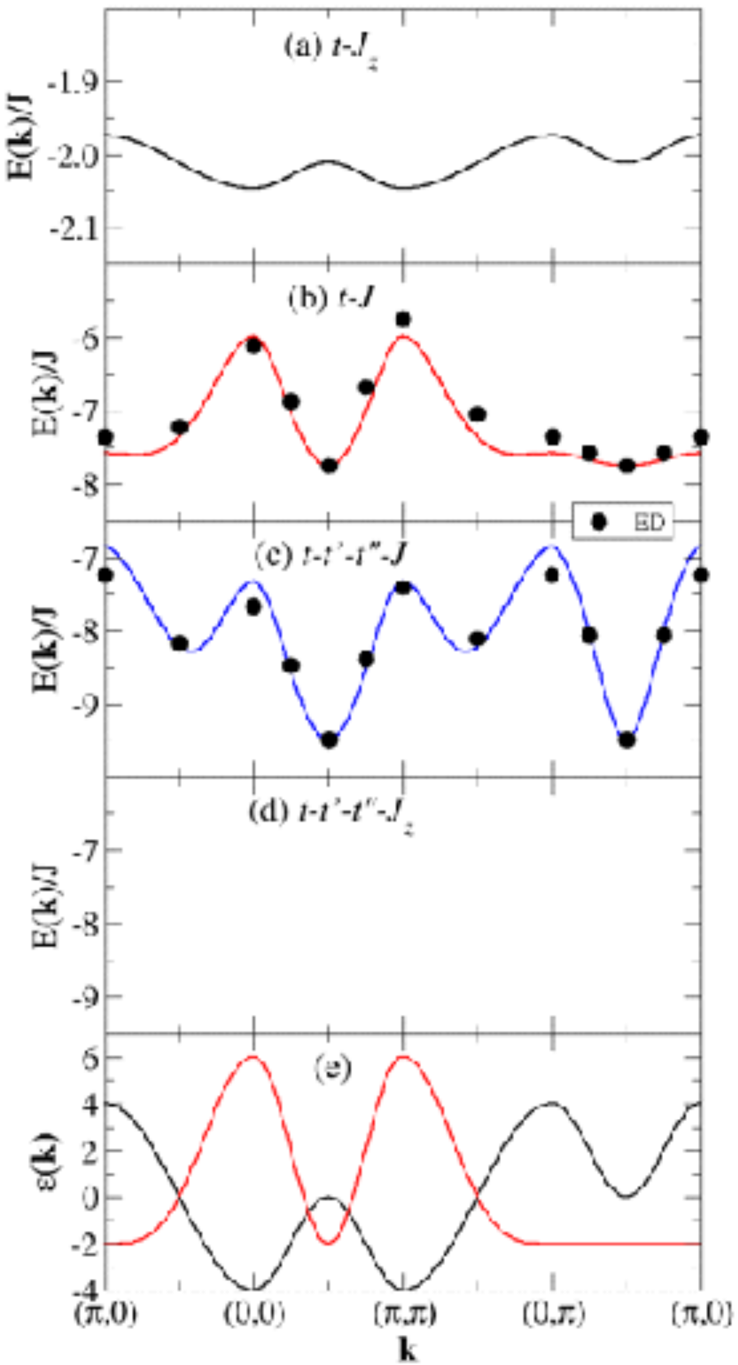

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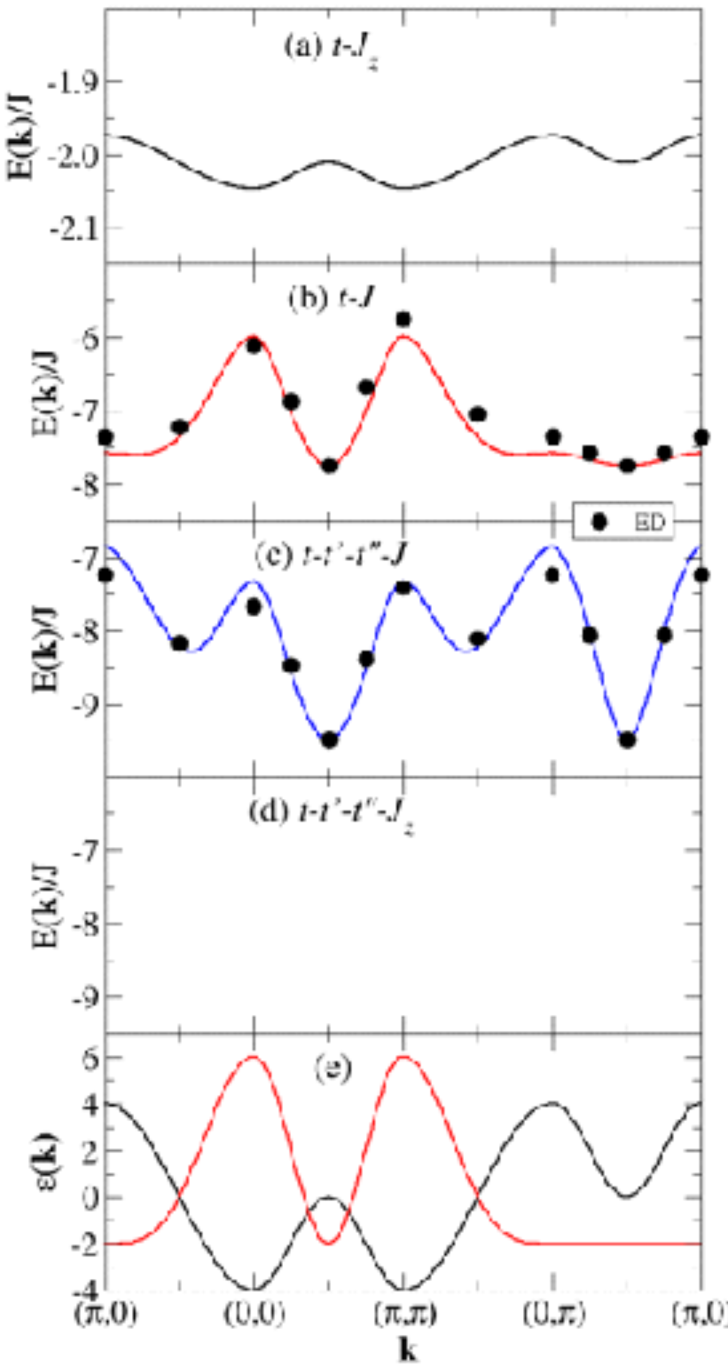
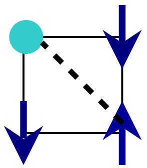
… but why?!



Hole in the t-t'-t''-J_z model (without spin fluctuations)

→ Longer range hopping should open additional options …

→ Hole can propagate freely, so t_2 = t', t_3= t''?



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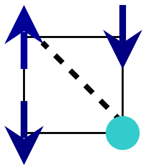

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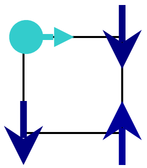

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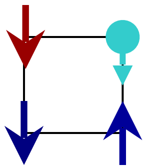

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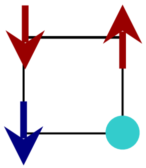

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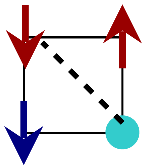

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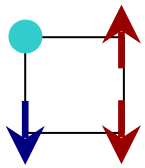

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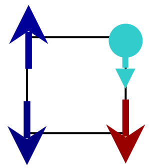
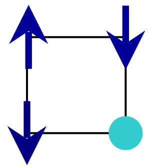


Hole in the t-t'-t"-J_z model (without spin fluctuations)

→ Longer range hopping should open additional options …

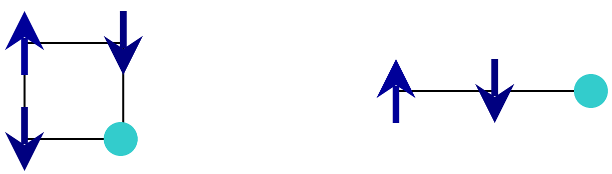
→ Such processes also contribute, so $t_2 = t' (1+ ….)$



Hole in the t-t'-t"-J_z model

→ The longer range hopping integrals get renormalized by similar amounts!

→ t_2/t_3 = t'/t" (= -1.5)



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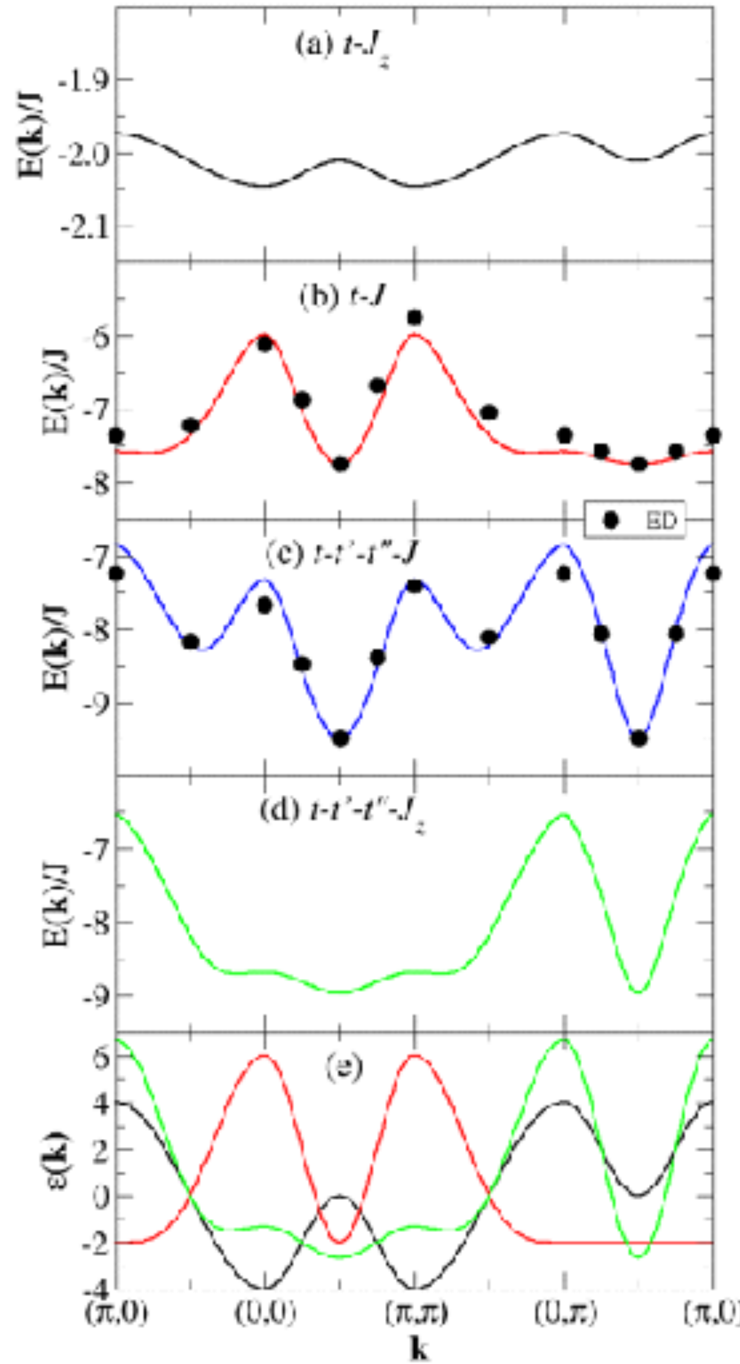


Hole in the t-t'-t"-J model

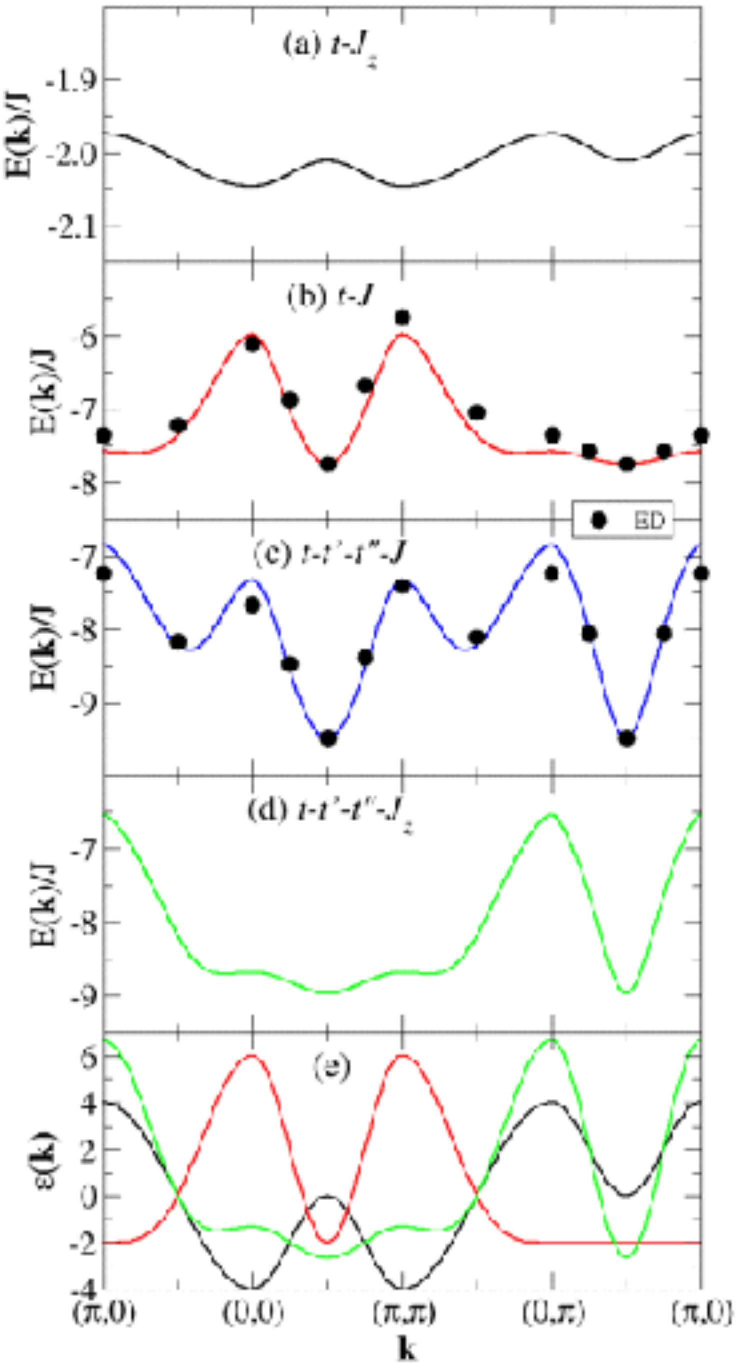
→ interplay of spin fluctuations + longer range hopping — correct dispersion emerges

→ isotropic dispersion around GS is an accident!

On $(0,0)$–(π,π) bandwidth set by J

On $(\pi,0)$–$(0,\pi)$ bandwidth set by t'

One needs to chose t'=J to get isotropy …



H. Ebrahimnejad, G. Sawatzky and M. Berciu, JPhys:CondMat 28, 105603 (2016)

Hole in the t-t’-t”-J model

→ dispersion agrees with that measured experimentally

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→ How to check?! Go back to the model …

What really happens when we dope the cuprate layer?

→ not Mott insulators, but instead a charge-transfer insulator!

→ doped holes go into the O band, not onto Cu orbitals

→ doped system described (minimally) by three-band Emery model
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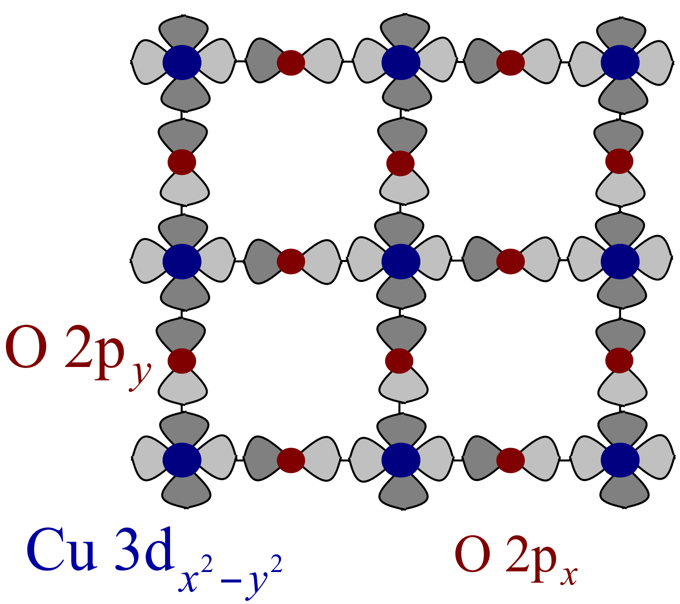

$$H = T_{pd} + T_{pp} + \Delta \sum_{i \in O} n_i + U_{dd} \sum_{i \in Cu} n_{i\uparrow} n_{i\downarrow} + U_{pp} \sum_{i \in O} n_{i\uparrow} n_{i\downarrow} + \ldots$$

t_{pd} = 1.3eV, t_{pp} = 0.65 eV, Δ_{pd}=3.6 eV, U_{pp} = 4 eV, U_{dd}= 8 eV

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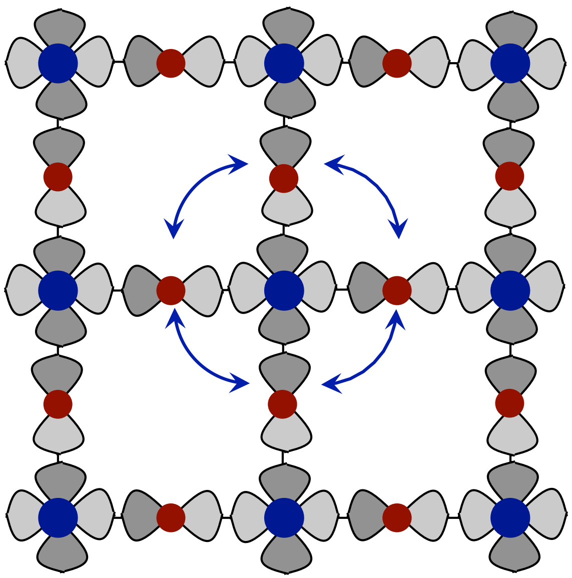
→ why should we expect to be able to continue to ignore the O and use a one-band model instead?

The Zhang-Rice singlet

→ **F. C. Zhang and T. M. Rice, Phys. Rev. B 37, 3759(R) (1988)**



$$P_{i\sigma}^{(S)} = \frac{1}{2}\sum_{l\in i}\left(-1\right)^{l} p_{l\sigma} \qquad (5)$$

(not orthogonal to each other!)

$$\phi_{i\sigma} = \frac{1}{\sqrt{N}}\sum_{k} e^{ikR_i} P_{k\sigma} \qquad (7)$$

$$P_{k\sigma} = \frac{1}{\sqrt{N}}\beta_k \sum_{i} e^{-ikR_i} P_{i\sigma}^{(S)} \qquad (8)$$

$$\beta_k = \frac{1}{\sqrt{1-\frac{1}{2}\left(\cos(k_x)+\cos(k_y)\right)}} \xrightarrow{k\to 0} \infty \qquad (9)$$

Zhang-Rice singlet:

$$\psi_{\mathrm{i}} = \frac{1}{\sqrt{2}}\left(\phi_{i\uparrow}d_{i\downarrow} - \phi_{i\downarrow}d_{i\uparrow}\right) \qquad (10)$$

The Zhang-Rice singlet (ZRS)

→ **F. C. Zhang and T. M. Rice, Phys. Rev. B 37, 3759(R) (1988)**

→ doped hole goes into x^2-y^2 linear combination of O orbitals and locks into a singlet with the hole on the central Cu (spins on Cu sites!)

→ Zhang and Rice argued that ZRS dynamics is described by the t-J model.

→ Can the ZRS = a composite object that combines both charge and spin degrees of freedom, properly describe the low-energy properties of the three-band Emery model?

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→ Can the ZRS = a composite object that combines both charge and spin degrees of freedom, properly describe the low-energy properties of the three-band Emery model?

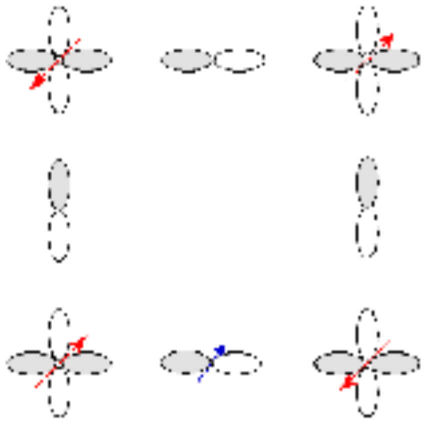
→ Direct comparison beyond our abilities to perform.

→ What we can do is compare to an (intermediary) model where we have spins on the Cu sites, but doped hole is on O sublattice

(Simplified) three-band model

→ strongly-correlated limit of the Emery model, with spins at Cu sites and doped holes on the O →in between Emery model and one-band models

→ For a single doped hole the Hamiltonian is (for more holes, there are additional terms): **B. Lau, M. Berciu and G. A. Sawatzky, PRL 106, 036401 (2011)**



$$H = H_{J_{dd}} + T_{pp} + T_{swap} + H_{J_{pd}}$$

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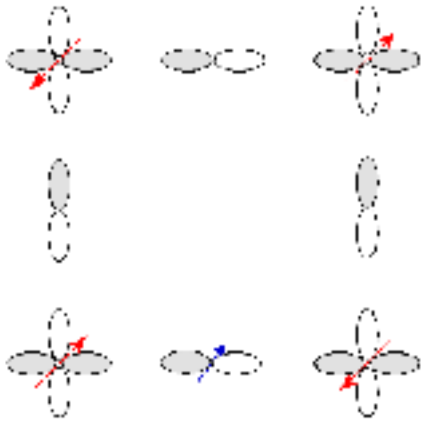

$$J_{dd} = \frac{4t_{pd}^4}{\Delta^2 U_{dd}} + \frac{8t_{pd}^4}{\Delta^2(2\Delta + U_{pp})}$$

J_{dd} ~ 125-150 meV = unit of energy from now on

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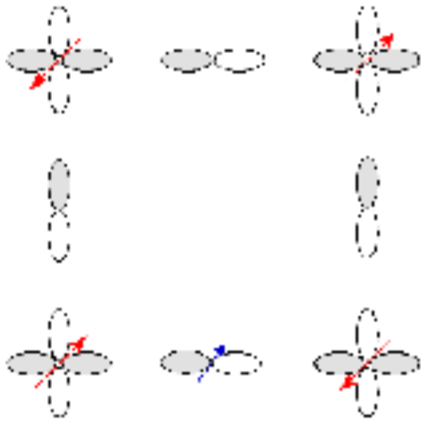

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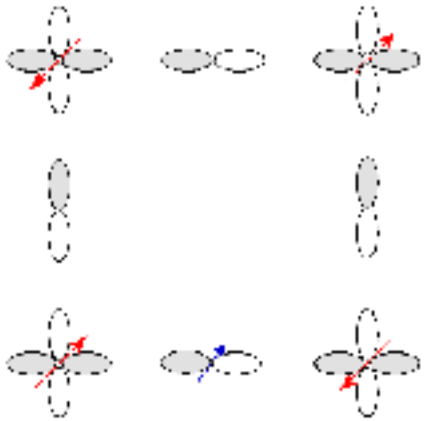

$t_{pp} = 4.1, \ \ t'_{pp} = 2.4$

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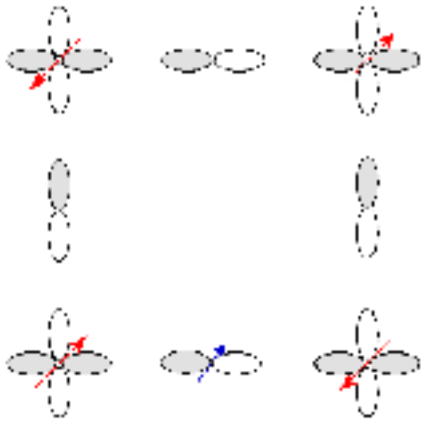

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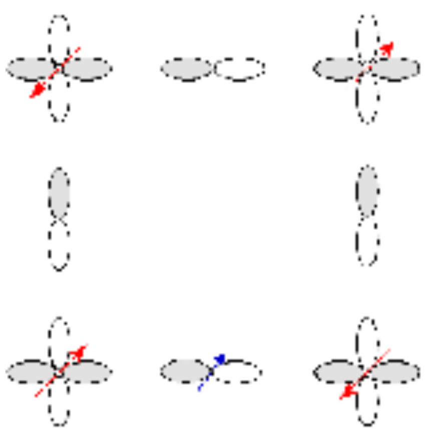

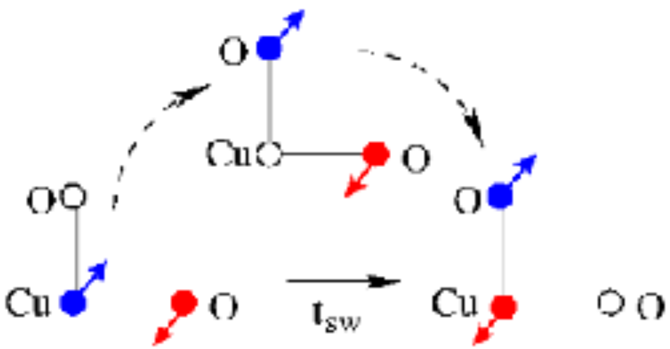

$$t_{sw} = t'_{sw} = \frac{t_{pd}^2}{\Delta} = 3.0$$

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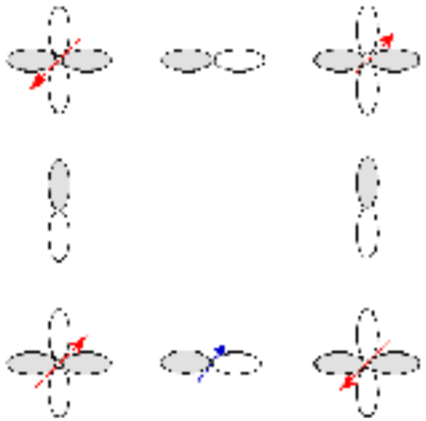

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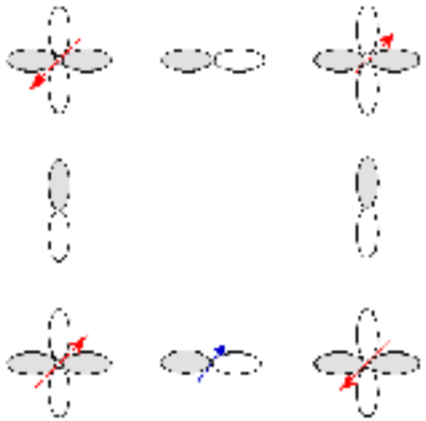

$$J_{pd} = \frac{2t_{pd}^2}{U_{pp} + \Delta} = 2.8$$

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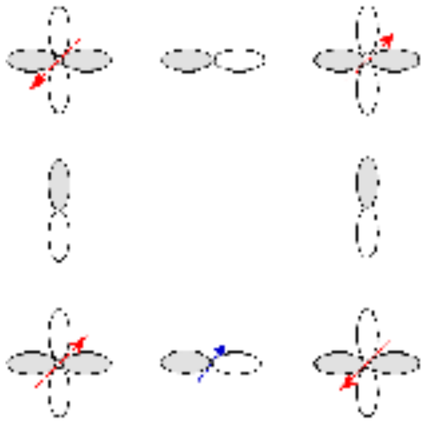


$$H = H_{J_{dd}} + T_{pp} + T_{swap} + H_{J_{pd}}$$

J_{dd} =1, t_{pp} = 4.1, t'_{pp} =2.4, t_{sw}=3.0, J_{pd}=2.8

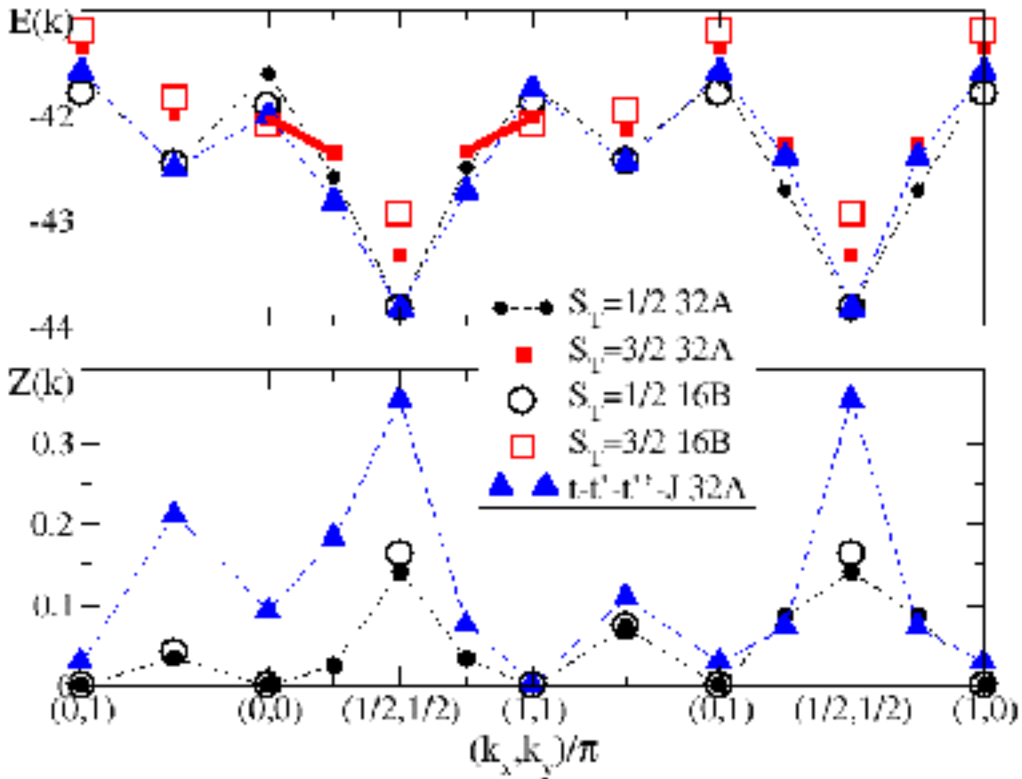
Hole in the (simplified) three-band model — ED results

→ exact diagonalization for 1 hole on clusters of 32 Cu + 64 O sites:

Bayo Lau, Mona Berciu and George A. Sawatzky, PRL 106, 036401 (2011)

Good agreement!

Problem solved, no?



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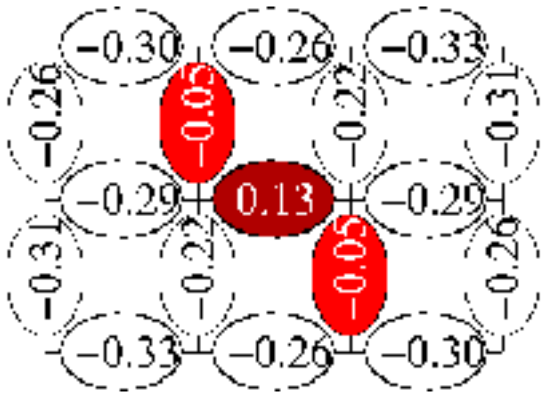
Problem: FM correlations near hole

and other facts hard (for us) to explain



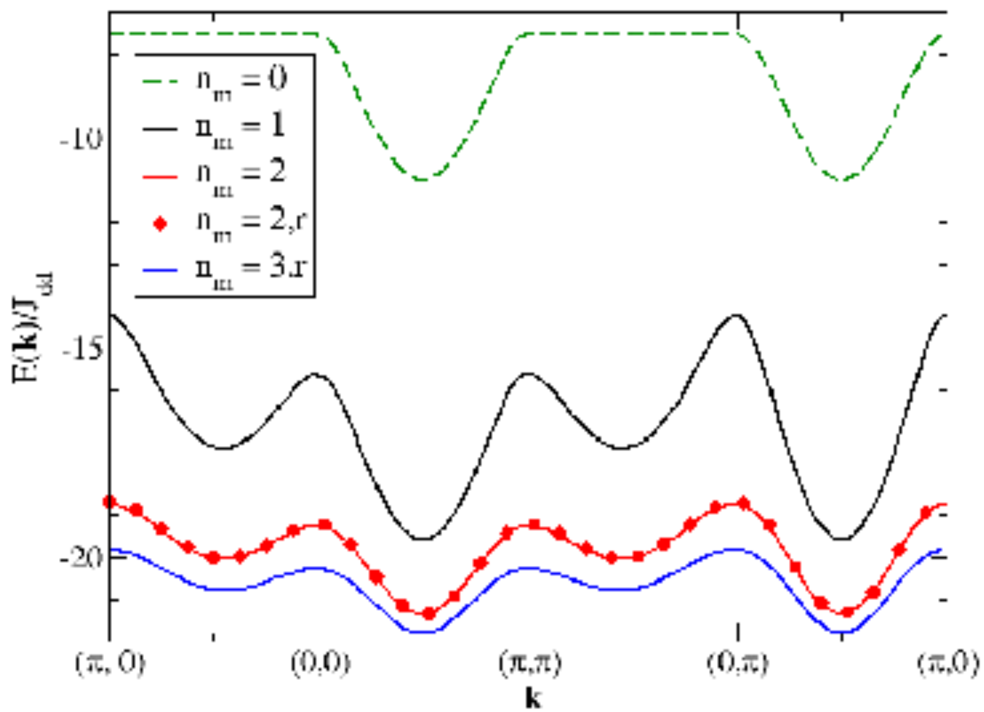
Bonus: a variational approach might work!

Hole in the (simplified) three-band model

→ Step 1: ignore spin fluctuations (Neel background)

→ Qp dispersion has the deep isotropic minima around (π/2, π/2) appear even for n_m=0!

→ For n_m=3, good quantitative agreement with Bayo's ED



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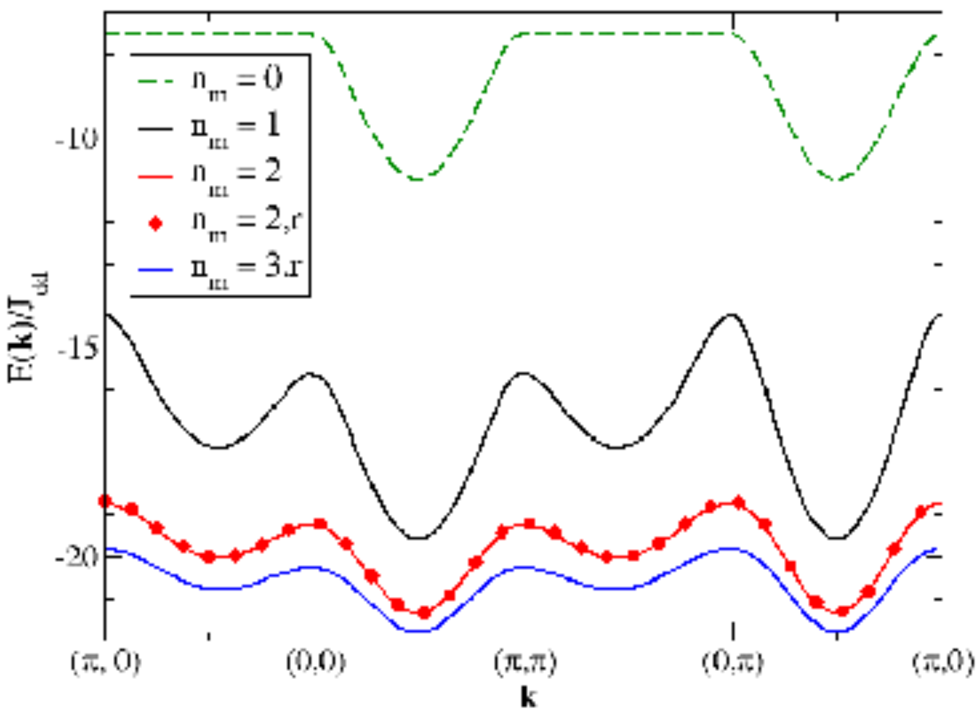
→ **WHAT?!**



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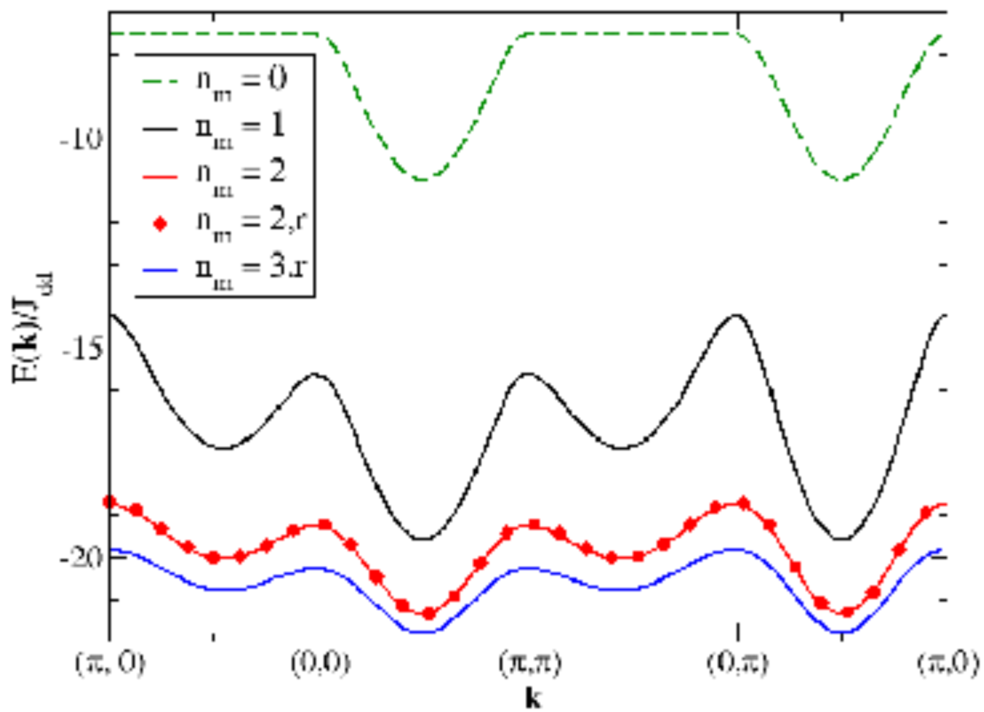


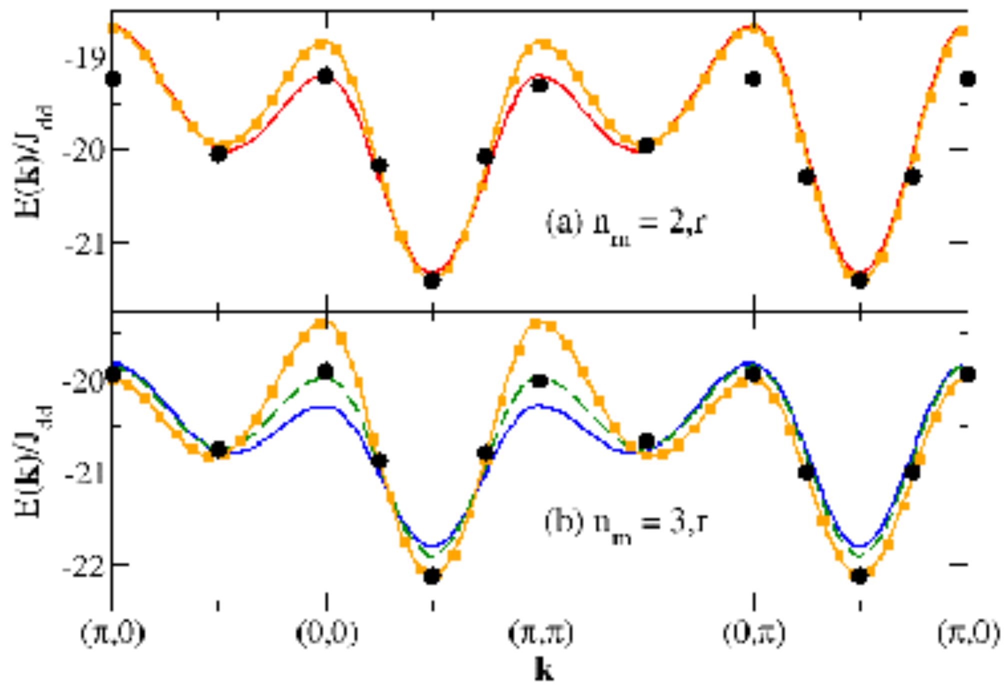
→ Spin fluctuations have no influence on qp dispersion in this model!

H. Ebrahimnejad, G. Sawatzky and M. Berciu, Nature Physics 10, 951 (2014)

Hole in the (simplified) three-band model

→ Step 2: add local spin fluctuations

→ Basically no effect



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What is the physical reason for this qualitative difference?

→ In the three-band model, the hole can move freely on the O sublattice without changing the spin configuration. The magnons in the qp cloud are created and absorbed by the hole through T_{swap} and J_{pd} processes. This is done on a faster time-scale than $1/J_{dd}$ of spin fluctuations, so they have no time to act and to influence the dynamics of the hole.

→ One-band models have very different physics (although same dispersion!)

- → Longer range t', t" hopping needed to mimic the role of Tpp
- → But these are taken to be comparable with J, not much larger than it → spin fluctuations are fast enough to significantly affect the structure of the qp cloud and therefore the qp dynamics.

Conclusions

→ we find that the (simplified) three-band model describes very different physics than the one-band t-J/Hubbard models

→ we believe that this is because the one-band models are way too simplified (many terms are ignored)

→ this needs to be tested further …

→ **warning**: different models can give a similar prediction for a given quantity for very different reasons …