Three-Orbital Spin-Fermion Model for CuO_2 Planes

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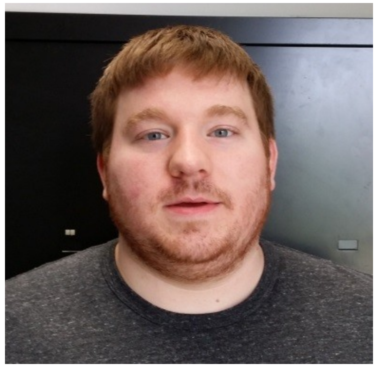
Collaborators



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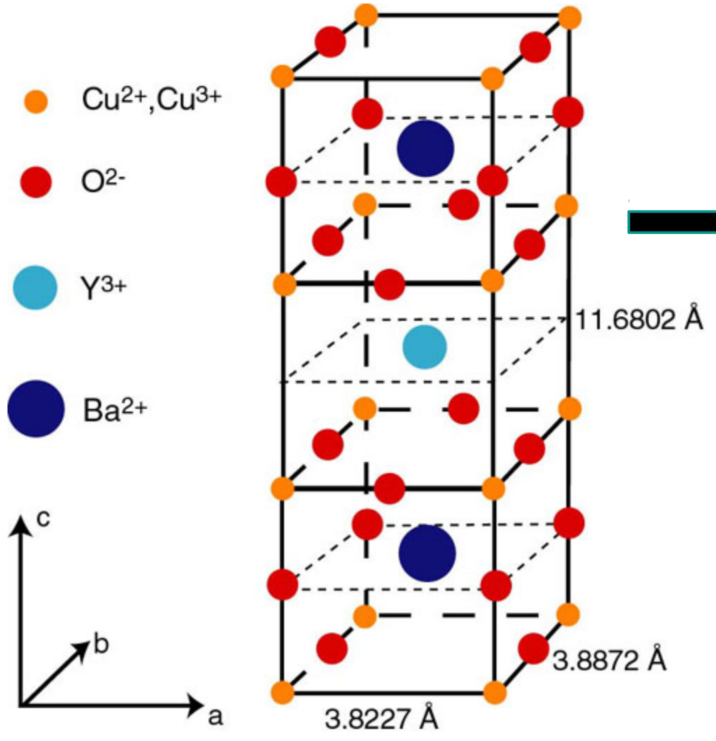
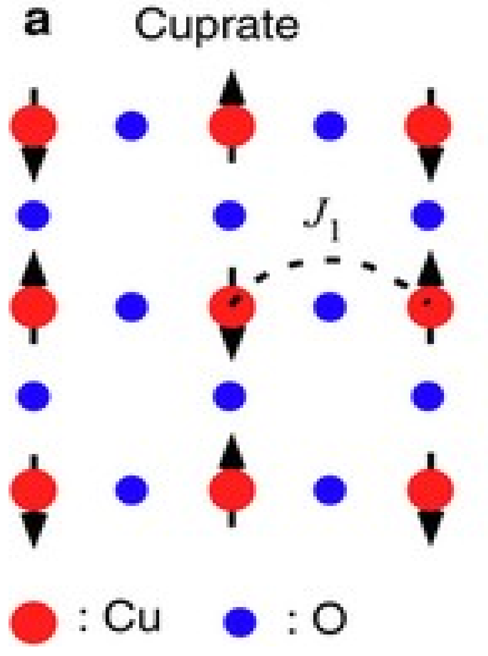
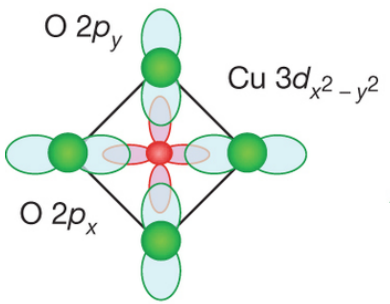
(Stuttgart)

High T_c Cuprates

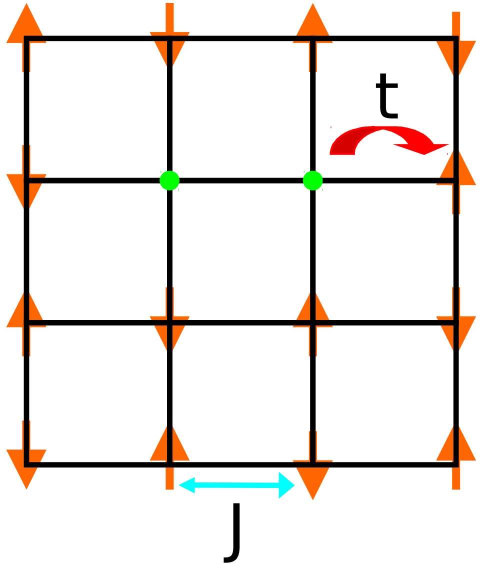


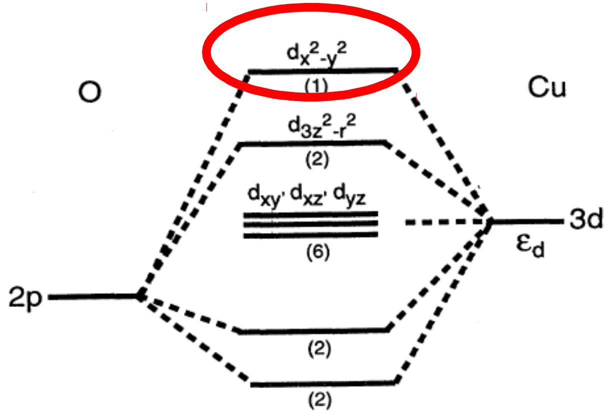




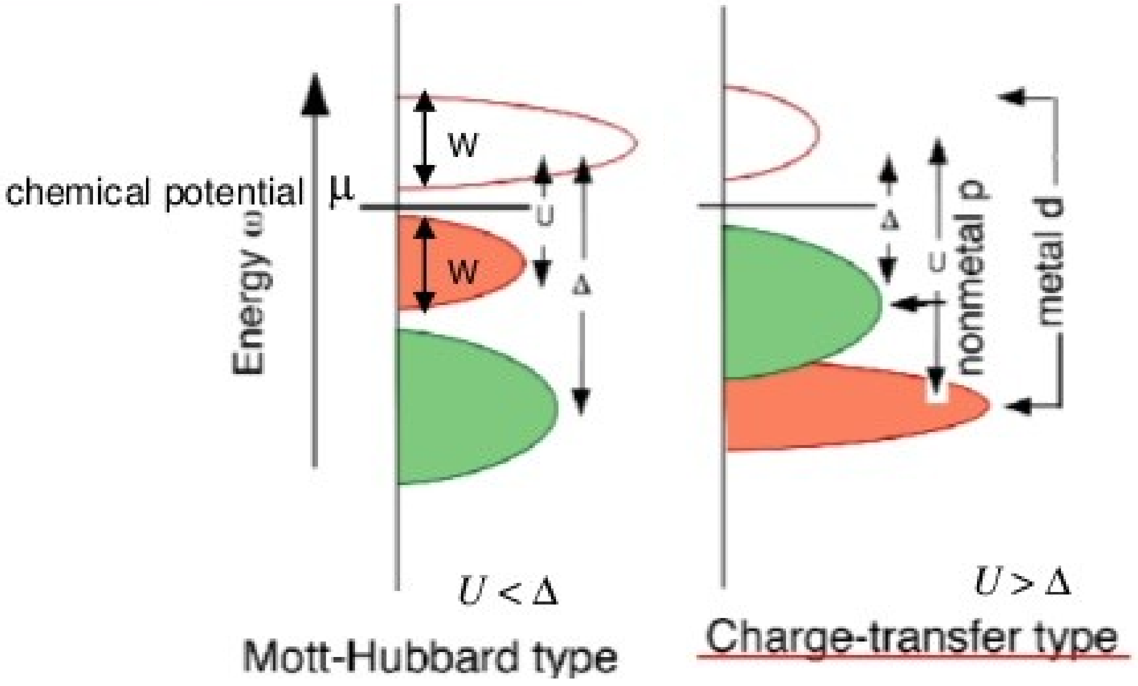
3-orbital model

1-orbital model





Mott versus Charge-Transfer Insulators



Single-Orbital models

Multi-Orbital models

Single-orbital models are often used:

- ARPES show one single band at the Fermi surface.
- Zhang-Rice singlet transforms the three-orbital model to a t-J model.

However, cuprates are charge-transfer insulators.

- Do oxygen p_σ orbitals play an important role?
- Is the Zhang-Rice picture correct?

We need a three-orbital model that can be studied numerically in large lattices and at all temperatures.

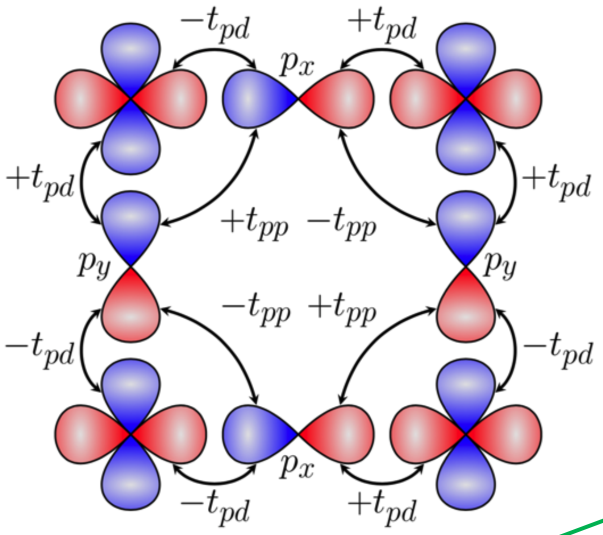
Spin-Fermion Model for the CuO_2 planes:

Three-band Hubbard model

$$H_{\mathrm{TB}} = \sum_{\mathbf{k},\alpha,\beta,\sigma} T^{\alpha,\beta}(\mathbf{k})\, \hat{c}^{\dagger}_{\mathbf{k},\alpha,\sigma} \hat{c}_{\mathbf{k},\beta,\sigma}$$

$$H_{\mathrm{int}} = U_d \sum_{\mathbf{i}} \hat{n}_{\mathbf{i},d,\uparrow} \hat{n}_{\mathbf{i},d,\downarrow}$$

$$\alpha = d, p_x, p_y$$



Spin-Fermion model

$$H_{\mathrm{SF}} = H_{\mathrm{TB}} + H_{\mathrm{d}} + H_{\mathrm{p}} + H_{\mathrm{Heis}}$$

$$H_{\mathrm{TB}} = \sum_{\mathbf{k},\alpha,\beta,\sigma} T^{\alpha,\beta}(\mathbf{k})\, \hat{c}^{\dagger}_{\mathbf{k},\alpha,\sigma} \hat{c}_{\mathbf{k},\beta,\sigma}$$

$$H_d = J_d \sum_i S_i \cdot s^d{}_i$$

Prevents double occupancy in d orbitals.

$$H_p = J_p \sum_{i,\mu} S_i \cdot s^p{}_{i+\mu/2}$$

Introduces frustration.

$$H_{\mathrm{Heis}} = J_{\mathrm{NN}} \sum_{\langle \mathbf{ij} \rangle} S_{\mathbf{i}} \cdot S_{\mathbf{j}}$$

Encourages AF order.

***S*$_i$ are phenomenological localized spins.**

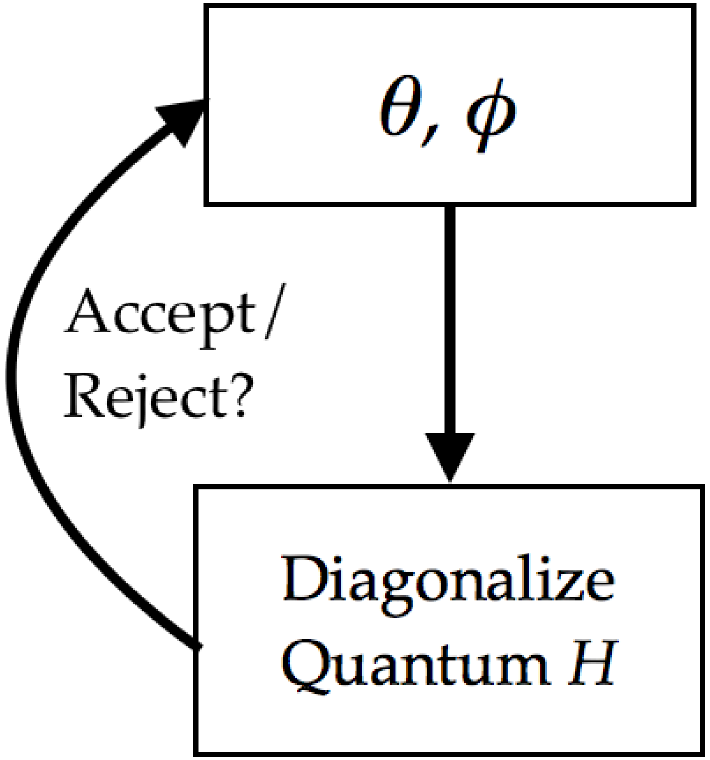
Simplification: classical localized spins can be studied with Monte Carlo

S. Liang et al., PRL **109**, 047001 (2012);
C. Buhler et al., PRL **84**, 2690 (2000);
E. Dagotto et al., PRB **58**, 6414 (1998).

Numerical Study of the Spin-Fermion Model:

Simplification: classical localized spins can be studied with Monte.

$$\mathbf{S_i} = \left(\sin\theta_i \cos\phi_i, \sin\theta_i \sin\phi_i, \cos\theta_i\right)$$



1K-5K warmups
3K-10K measurement steps

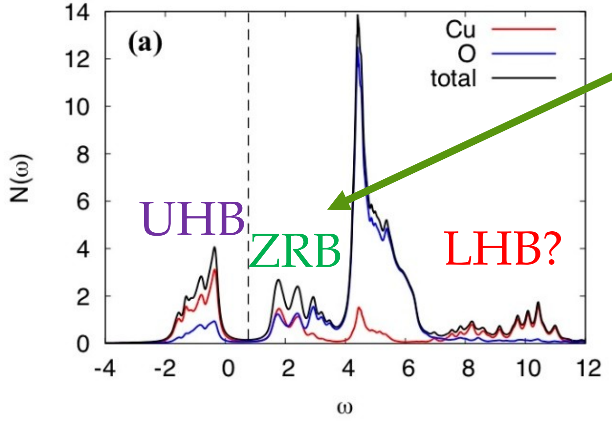
Green functions
and observables

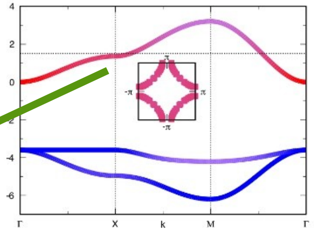
Metropolis
Algorithm

Results

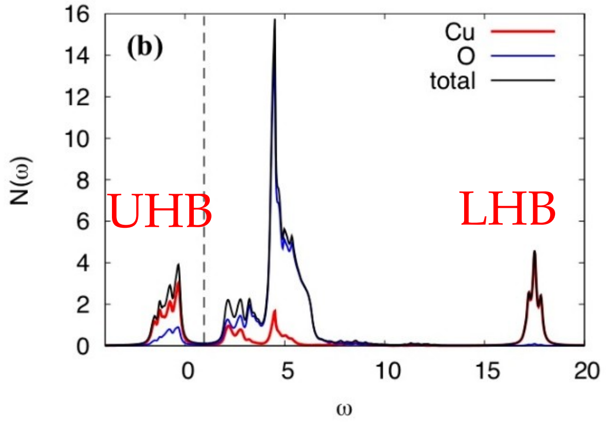
Three-band Hubbard model

Hole representation





$U_d/t=8$
Physical case
50/50 p-d in ZRB



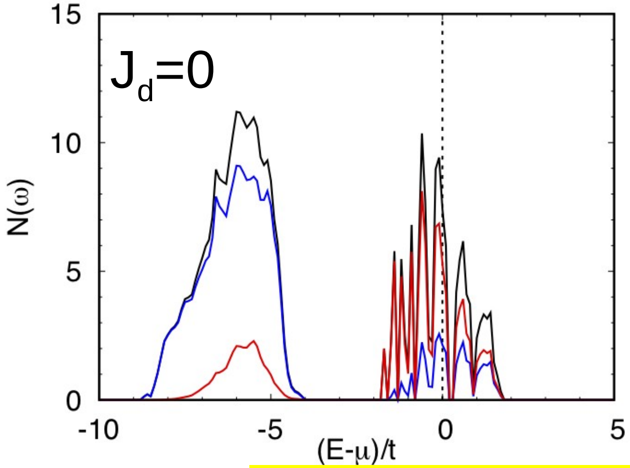
$U_d/t=16$

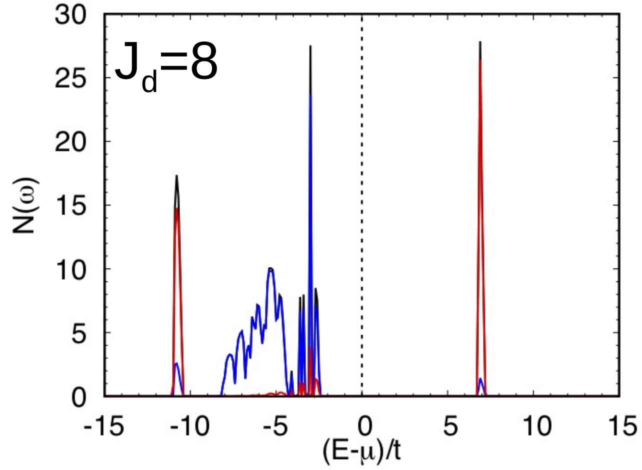
Variational Cluster Approach:
E. Arrigoni et al., NJP **11**, 055066 (2009).

Spin-Fermion model

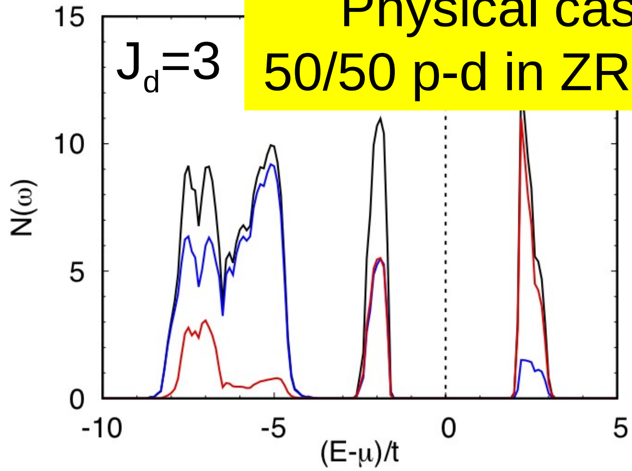
Electron representation

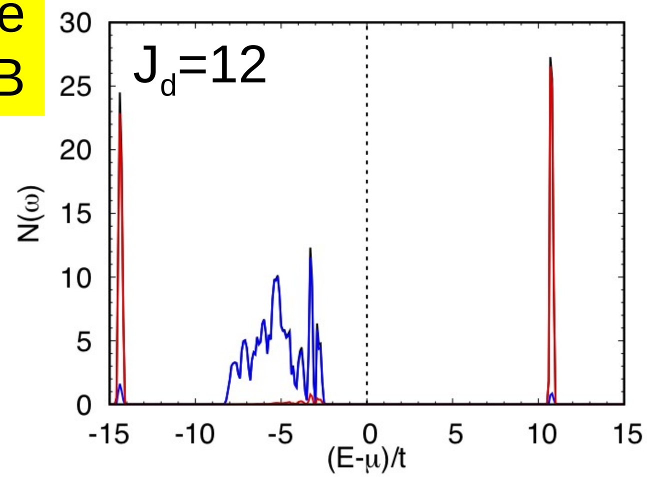
TB





Physical case
50/50 p-d in ZRB

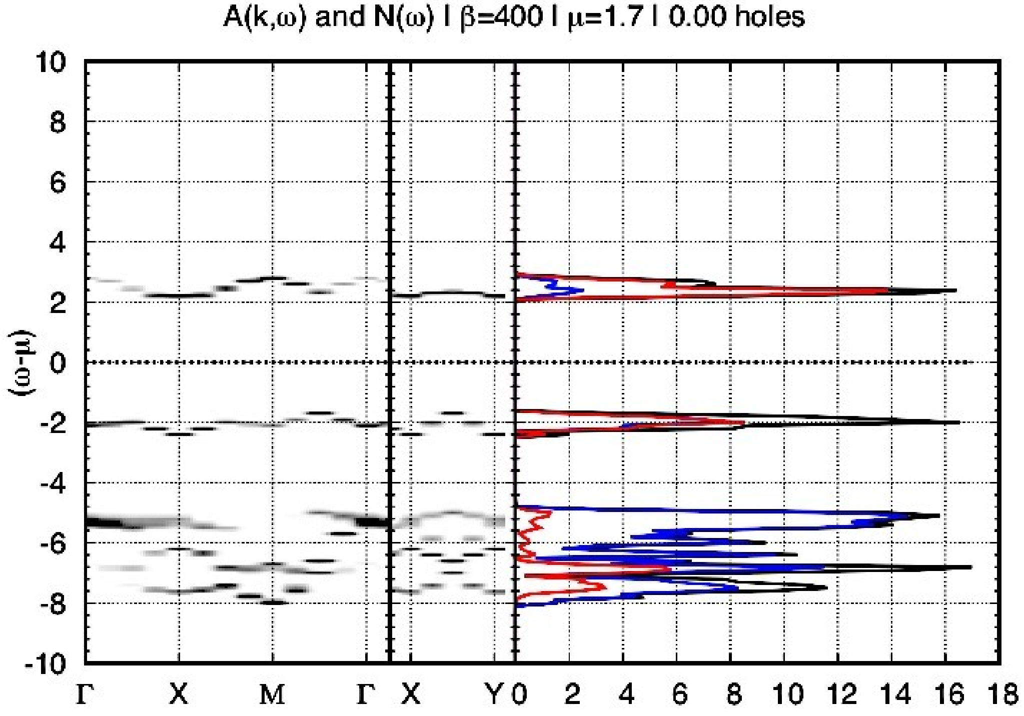




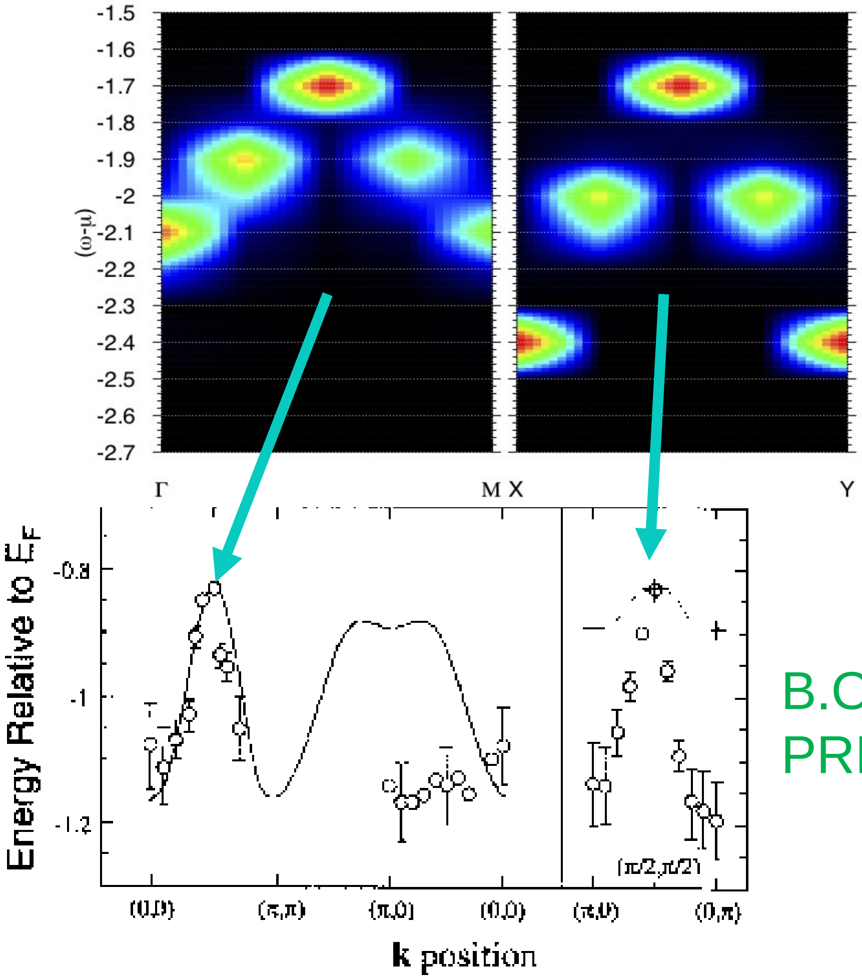
$J_p=1$, $J_{Heis}=0.1$, 8x8 lattice, $\beta=100$

Spectral Functions A(**k**,ω)

Undoped Case: 5 electrons per unit cell.



- The ZRB appears.
- Its dispersion is ~ 0.5-0.8 eV, close to experimental result.
- Dispersion symmetric about (π/2,π/2) not captured by t-J model.

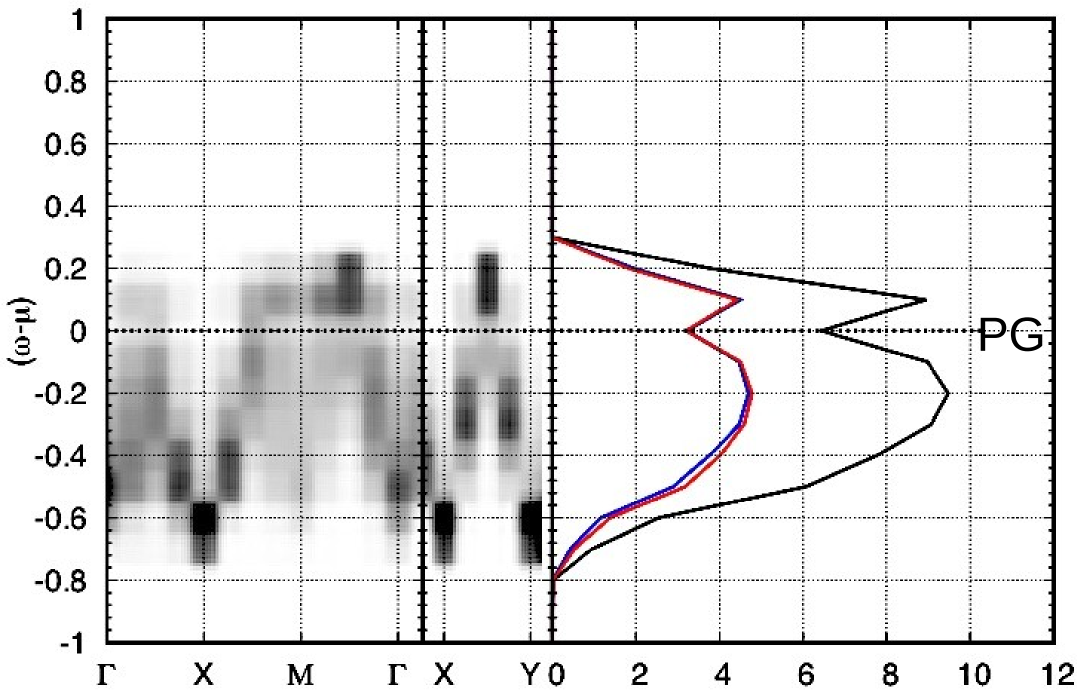


B.O.Wells et al., PRL **74**, 964 (1995)

Points: experimental results
Solid line: t-J model

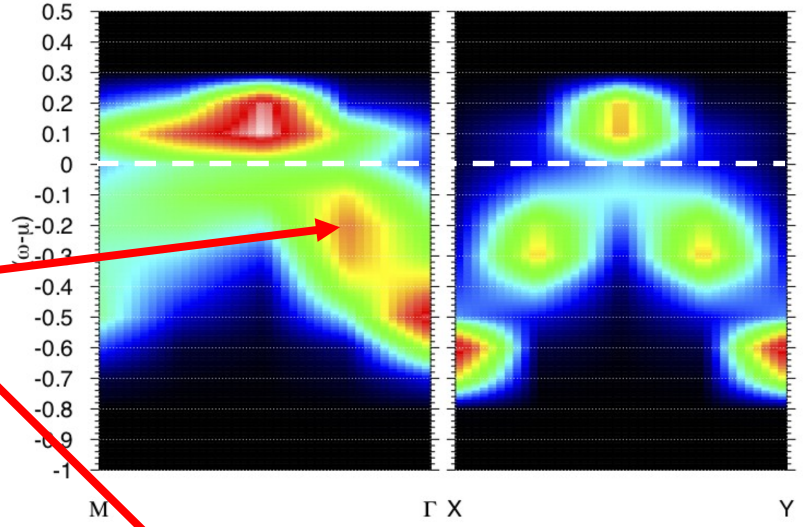
Spectral Functions A(**k**,ω)

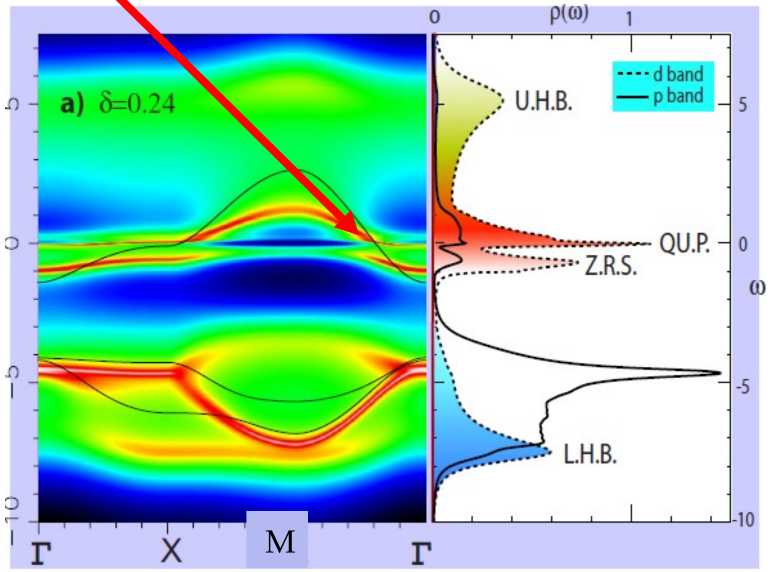
Doped Case: 16 holes in 8x8 cluster.



- Pseudogap (PG) at chemical potential.
- Dispersion is ~ 1 eV, close to experiments.
- “Waterfall” feature along Γ-M.
- FS features along X-Y.

Waterfall

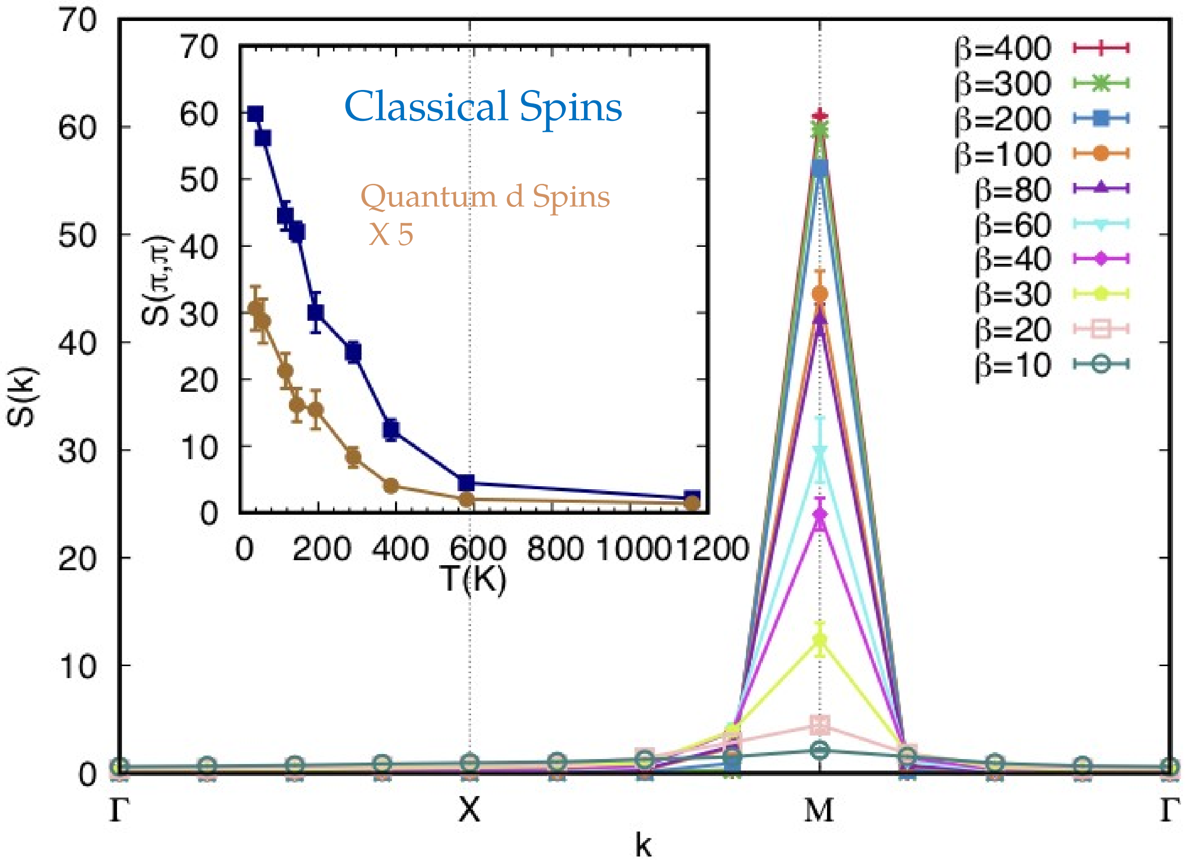




C. Weber et al., PRB **78**, 134519 (2008). DMFT

Magnetic Structure

Undoped Case: 5 electrons per unit cell.



- Tendency towards AF long-range order.
- T_N~300-500K.
- Quantum Cu spins follow classical spins.

Conclusions

A three-orbital spin-fermion model for the CuO_2 planes was presented.

- It captures the charge-transfer nature of cuprates.
- AFM state stabilizes in the undoped limit around 300 K.
- Zhang-Rice singlet band observed in $A(\mathbf{k},\omega)$.
- The symmetry about $(\pi/2,\pi/2)$ in $A(\mathbf{k},\omega)$, reproduced only with long range hoppings in single-orbital models, develops spontaneously.

Next steps: study charge-spin structures such as stripes, Zhang-Rice singlets, high spin polarons, intertwined orders, etc.

- The studied cluster sizes cannot be accessed with DMRG, Lanczos nor Quantum Monte Carlo.
  - 64x64 clusters possible with traveling cluster approximation.