Three-Orbital Spin-Fermion Model for CuO$_2$ Planes

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High $T_c$ Cuprates

3-orbital model

1-orbital model
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 $p_\sigma$ 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**

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

\[ H_{\text{int}} = U_d \sum_{i} \hat{n}_{i,d,\uparrow} \hat{n}_{i,d,\downarrow} \]

\[ \alpha = d, p_x, p_y \]

Simplification: classical localized spins can be studied with Monte Carlo

**Spin-Fermion model**

\[ H_{\text{SF}} = H_{\text{TB}} + H_d + H_p + H_{\text{Heis}} \]

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

Prevents double occupancy in d orbitals.

Introduces frustration.

Encourages AF order.

S$_i$ are phenomenological localized spins.

S. Liang et al., PRL **109**, 047001 (2012);
C. Buhler et al., PRL **84**, 2690 (2000);
Numerical Study of the Spin-Fermion Model:

Simplification: classical localized spins can be studied with Monte.

\[ S_i = (\sin \theta_i \cos \phi_i, \sin \theta_i \sin \phi_i, \cos \theta_i) \]

1K-5K warmups
3K-10K measurement steps
Green functions and observables

\( \theta, \phi \)

Accept/Reject?

Diagonalize Quantum \( H \)

Metropolis Algorithm
Three-band Hubbard model

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

Results

Hole representation

U\textsubscript{d}/t=8
Physical case
50/50 p-d in ZRB

U\textsubscript{d}/t=16

Spin-Fermion model

Electron representation

J\textsubscript{d}=0

J\textsubscript{d}=8

Physical case
50/50 p-d in ZRB

J\textsubscript{p}=1, J\textsubscript{Heis}=0.1, 8x8 lattice, β=100
Spectral Functions $A(\mathbf{k},\omega)$

Undoped Case: 5 electrons per unit cell.

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

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

Points: experimental results
Solid line: t-J model
Doped Case: 16 holes in 8x8 cluster.

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

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

Undoped Case: 5 electrons per unit cell.

- Tendency towards AF long-range order.
- $T_N \sim 300-500 \text{K}$.
- 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 $A(k,\omega)$.
• The symmetry about $(\pi/2,\pi/2)$ in $A(k,\omega)$, 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.