SPATIAL CORRELATIONS AND THE INSULATING PHASE OF THE HIGH-TC CUPRATES:

insights from a configuration interaction based solver for dynamical mean-field theory

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• Method and model
  • Configuration interaction (CI) as an impurity solver
  • Three-band copper oxide model

• Results and discussion
  • Convergence with respect to the number of bath orbitals
  • Spectral gap and phase diagram
  • Optical conductivity and experimental relevance

• Summary
EXACT DIAGONALIZATION (ED) AS AN IMPURITY SOLVER

• No sign problem
• No significant increase of the computational cost for nondiagonal hybridization function
• Direct access to real frequencies: No analytic continuation

• Limited system size: $N_c+N_b \sim 15$
  • Dimension of the Hilbert space: $4^N$ for $N=N_c+N_b$
DO WE NEED ALL THE $4^N$ SDS?

• Example: half-filled Hubbard model, large $U$
DO WE NEED ALL THE $4^N$ SDS?

- Discard less important states

- Many body states can be represented in a truncated Hilbert space
CONFIGURATION INTERACTION (CI) AS AN IMPURITY SOLVER

\[ |\Psi\rangle \approx c_0|\Phi\rangle + \sum_{i,a} c_i^a |\Phi_i^a\rangle + \sum_{i,j,ab} c_{ij}^{ab} |\Phi_{ij}^{ab}\rangle + \cdots \]

: Ground state in the (intelligently) truncated Hilbert space

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- Bath orbitals are easier to add
  - \( N_c=4, N_b \sim 20 \) in 32-core machine. cf) \( N_c+N_b \sim 15 \) in ED
- Systematic improvement of accuracy is possible
  - Full CI = Exact diagonalization
- Multi-reference CI
EXAMPLE: 1D HUBBARD MODEL

\( N_c = 4 \)

\( N_c = 8 \)

\( N_c \): # of correlated orbitals, \( U/t = 6 \)

Larger \( N_c \): More continuous, closer to Bethe ansatz (gray lines)

The CI solver can solve the system beyond the ED limit!
THREE-BAND COPPER-OXIDE MODEL

Dynamic cluster approximation

\[ G^R(i\omega_n) = \sum_{\mathbf{k} \in K} \frac{1}{(i\omega_n + \mu)1 - H_0(\mathbf{k}) - \Sigma_\mathbf{K}(i\omega_n)} \]

- Oxygen \( p \)-band is included but only Cu ions are interacting, \( t_{pd} \sim 1.6 \text{eV} \)
- \( n_d^+n_p = 5 \) (one hole per unit cell): parent material of high-\( T_c \) cuprates
- Four site DMFT: Role of spatial correlations is studied
- Broad range of parameters is considered
• Converging behavior beyond a certain number (>the limit of ED for $N_c=4$)
• Similar DOS at gap edge for $N_b \geq 12$, not for $N_b=8$.
• $(N_c, N_b) = (1, 9)$ and $(4, 12)$ are used
Single-site DMFT

- Spectral gap decreases linearly around the transition point and the slope is almost the same
- Phase diagram
  - Conventional Mott insulator
  - Metal
  - Coexistence region

\[
H = \sum_{\langle i,j \rangle} t_{ij} (c_i^\dagger c_j + \text{H.c.}) + \varepsilon_d \sum_{d \in \text{Cu}} n_d + (\varepsilon_d + \Delta) \sum_{p \in \text{O}} n_p + U \sum_{d \in \text{Cu}} n_{d \uparrow} n_{d \downarrow}
\]
Spatial correlation is included.

Categorized into three regions based on the slope:

- **Conventional Mott insulator**: Insulating in both single and four site DMFT
- **Magnetically correlated Mott insulator**:
  - Short ranged antiferromagnetic correlation opens a gap
  - Mott insulating behavior in \((0, \pi)\)-sector
- **Metal**: Spectral gap is zero
Experimental data: Optical conductivity of La$_2$CuO$_4$ [from Uchida et al. PRB 43, 7942 (1991)]

Theoretical data (this work): $U=8.0$eV, Vertex correction is included*

* N. Lin, E. Gull, and A. J. Millis, PRB 80, 161105 (2009)

- Experimentally relevant point is located in **MCMII** (Magnetically Correlated MI)
- Conductivity of gap edge is highly enhanced by short ranged AF correlations and the vertex correction solves a big difference between the experiment and the theory
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SUMMARY

• The CI solver enables us to add more bath orbitals in DMFT and check the convergence with respect to the number of bath orbitals.

• Application to the three band copper oxide model places the high-$T_c$ cuprates in the magnetically correlated Mott insulator (MCMI) of the phase diagram.

• Gap edge conductivity problem is solved by the vertex correction in 4-site DMFT. Intersite correlations play an essential role in the physics of high-$T_c$ cuprates.
THANK YOU!