Multiband DMRG real time impurity solver

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- Real time: high resolution at all energies
- Can resolve multiplets in Hubbard bands
- As fast as CT-QMC (in cases checked)
- T=0
- no sign problems

- Hubbard, 2 bands
- SrVO$_3$, 3 bands
- SrMnO$_3$, 5 bands
- Off-diagonal interactions

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Outline

• Introduction and brief summary

• Matrix Product States (MPS): the formalism behind DMRG
  - Efficient representations of a state
  - Time evolution
  - Matrix Product Operators and DMRG

• FTPS: new impurity solver

• Results
  - SrVO$_3$ (3 bands)
  - SrMnO$_3$ (5 bands)
  - Extensions
DMFT: task of an impurity solver

• Band structure from DFT. Construct local Hamiltonian.

• Difficult task in DMFT cycle:

  Calculate Green's function for an Anderson impurity model

  \[ H_{AIM} = H_{loc} + \sum_k V_k \left( c_k^\dagger c_0 + h.c. \right) + \sum_k \epsilon_k n_k \]

“Star geometry” ↔ Wilson chain
Some current impurity solvers

• **Continuous Time Quantum Monte Carlo (CTQMC):**
  • Precise on imaginary axis
  • Analytic continuation → resolution problems, especially at larger energies
  • Can have sign problem and potentially convergence problems

• **Exact Diagonalization (ED) / Configuration interaction (CI):**
  • Exponential Hilbert space (e.g. $N_{\text{bath}} = 3$ for 3 bands)
  • Low resolution on real frequencies

• **Numerical Renormalization Group (NRG):**
  • Real axis, high resolution at very small energies
  • Low resolution at larger energies

• **Matrix Product States (MPS):**
  • DDMRG: high resolution but slow (separate calculation for every $\omega$)
  • Imaginary time: up to 6 orbitals, but few bath sites and low resolution
  • Real time → good resolution at all energies but multiband appeared expon. difficult
Matrix Product States (MPS)

• Formalism behind DMRG

• Very efficient representation of states of (mostly) one-dimensional systems:

\[ |\psi\rangle = \sum_{\{s_i\}} \underbrace{c_{s_1, \ldots, s_N}}_{=A_1^{s_1}A_2^{s_2}\cdots A_N^{s_N}} |s_1, s_2, \ldots, s_N\rangle \]

: Ansatz for coefficients: product of matrices

Graphical representation:

• Ground states by Density Matrix Renormalization Group (DMRG)

  Very precise, e.g. ground state energies exact up to 10 digits for chains of 100 sites

• Real time evolution, nonequilibrium physics, ...
Real time impurity solvers with MPS: strategy

- To obtain real frequency Green’s function:
  - Calculate ground state $|\psi_0\rangle$ of impurity model by DMRG
  - Time evolve excitation: $e^{iHt} c \, |\psi_0\rangle$
  - Calculate overlap: $G^<(t) = \langle \psi_0 | c^\dagger e^{iHt} c |\psi_0\rangle$
  - “Linear prediction”, Fourier transform $\rightarrow G(\omega)$

One band:

- Separate the spin-up and spin-down baths: (⇒ lower matrix dimensions)

```
spin-up bath      impurity      spin-down bath
```

- Large baths (O(100) sites) easily done
Real time impurity Solver with MPS: two bands

- Combine bands into bigger sites
- Works very well for 2 bands

Examples: DMFT spectrum of Hubbard model on Bethe lattice (Ganahl et al, 2015)

Sharp peaks (invisible in QMC): from interaction of doublon-holon pairs

(Lee, von Delft, Weichselbaum, PRL 2017, one-band model)

Problem: matrix dimensions $m$ multiply: computational effort $\sim m^3 \times n_{bands}$

$\Rightarrow$ no more than 2 bands feasible this way
New approach: Fork Tensor Product States (FTPS)

- Real time: high resolution at all energies
- Can resolve multiplets in Hubbard bands
- As fast as CT-QMC (in cases checked)
- $T=0$
- no sign problems

Example: 2 orbitals A, B:

$\approx U-3J+\epsilon_0 \approx U-2J+\epsilon_0$

$\approx -\epsilon_0$

$\approx U+\epsilon_0$

SrVO$_3$ (3 bands)

Bauernfeind 2017, 2018
Matrix Product States
Matrix Product States

Outline:

• MPS representations of a state

• Time evolution

• Matrix Product Operators (MPO) and DMRG

Example: 1d Heisenberg spin chain (equivalent to 1d spinless fermions): 2 states per site

\[ \hat{H} = \sum_{i=1}^{L-1} \hat{H}_i \quad \text{with} \quad \hat{H}_i = \frac{J_{xy}}{2} \left[ S^+_i S^-_{i+1} + S^-_i S^+_ {i+1} \right] + J_z S^z_i S^z_{i+1} \]

\[ \Leftrightarrow \quad \hat{H}_i = t \left( c_j^\dagger c_{j+1} + \text{h.c.} \right) + V \left( \hat{n}_j - \frac{1}{2} \right) \left( \hat{n}_{j+1} - \frac{1}{2} \right) \]
MPS representation of a state

- Efficient parametrization of 1d states:

\[
|\psi\rangle = \sum_{\{s_i\}} \underbrace{c_{s_1, \cdots, s_N}}_{\text{MPS representation of a state}} |s_1, s_2, \cdots, s_N\rangle
\]

\[= A_1^{s_1} A_2^{s_2} \cdots A_N^{s_N} : \text{product of matrices} \]

Graphical representation:

Example: (product state)

\[
|\psi\rangle = \begin{array}{ccccccc}
\uparrow & \downarrow & \downarrow & \uparrow & \downarrow & \downarrow & \uparrow \\
1 & 2 & 3 & 4 & 5 & 6 & \\
\end{array}
\]

\[
j = \begin{array}{ccccccc}
0 & 0 & 1 & 0 & 1 & 0 & \\
\end{array}
\]

\[
A_j^\uparrow = \begin{array}{ccccccc}
0 & 1 & 0 & 0 & 0 & 1 & \\
\end{array}
\]

\[
A_j^\downarrow = \begin{array}{ccccccc}
1 & 1 & 0 & 0 & 0 & 1 & \\
\end{array}
\]
MPS representation of a state

**Example:** (singlet on 2 sites, entangled state)

\[ |\psi\rangle = \frac{1}{\sqrt{2}} \left( \begin{array}{c} 1 \\ 0 \end{array} \right) - \left( \begin{array}{c} 0 \\ 1 \end{array} \right) / \sqrt{2} \]

\[ A_j^\dagger = (1, 0), \quad \left( \begin{array}{c} 0 \\ 1 \end{array} \right) / \sqrt{2} \]

\[ A_j^\dagger_j = (0, 1), \quad \left( \begin{array}{c} 1 \\ 0 \end{array} \right) / \sqrt{2} \]

**Example:** (nonlocal singlet)

\[ |\psi\rangle = \frac{1}{\sqrt{2}} \left( \begin{array}{c} \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \end{array} \right) \]

\[ A_j^\dagger = 0, \quad 0, \quad (1, 0), \quad \left( \begin{array}{cc} 0 & 0 \\ 0 & 0 \end{array} \right), \quad \left( \begin{array}{cc} 0 & 0 \\ 0 & 0 \end{array} \right), \quad -\left( \begin{array}{c} 0 \\ 1 \end{array} \right) / \sqrt{2}, \quad 0, \quad 0 \]

\[ A_j^\dagger = 1, \quad 1, \quad (0, 1), \quad \left( \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right), \quad \left( \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right), \quad \left( \begin{array}{c} 1 \\ 0 \end{array} \right) / \sqrt{2}, \quad 1, \quad 1 \]
Main tool: Singular Value Decomposition (SVD)

• Every $m \times n$ matrix $M$ can be decomposed as
  
  $$\begin{bmatrix} M \end{bmatrix} = \begin{bmatrix} U & D & V^\dagger \end{bmatrix}$$

• $D$ is diagonal and contains $r$ positive singular values
  
  $$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_r > \lambda_{r+1} = 0 = \cdots = \lambda_N = 0 $$

• SVD is very useful to approximate a matrix by neglecting small singular values
  
  (e.g. image compression, signal compression; computational effort $O(\min(mn^2, m^2n))$

• SVD version with unitary matrices:
  
  $$M = \tilde{U} \tilde{D} \tilde{V}^\dagger$$

  $$\begin{bmatrix} M \end{bmatrix} = \begin{bmatrix} \tilde{U} & \tilde{D} & 0 0 0 \end{bmatrix} \begin{bmatrix} V^\dagger \\ \text{(rest)} \end{bmatrix}$$

  Lower rows of $\tilde{V}^\dagger$ do not contribute to $M$ because of the zeroes in $\tilde{D}$. They belong to the null space of $M$. 

Tool: Schmidt decomposition of a state

- Divide a system arbitrarily into parts A and B

- Generic state
  \[ |\Psi\rangle = \sum_{j,k} (c_{jk}) |j\rangle_A |k\rangle_B \]

- **SVD of the coefficients:**
  \[ (c_{jk}) = \tilde{U} \tilde{D} \tilde{V}^\dagger \]

- **→ basis transformation**
  \[ |A\rangle_\alpha := \sum_j \tilde{U}_{j\alpha} |j\rangle_A , \quad |B\rangle_\alpha := \sum_k (\tilde{V}^\dagger)_{\alpha k} |k\rangle_B \]

- **→ Schmidt decomposition**
  \[ |\Psi\rangle = \sum_{\alpha=1}^{\chi} (\lambda_\alpha) |A\rangle_\alpha |B\rangle_\alpha \]

  “diagonal” singular values \( \lambda_\alpha \)

  with \( \chi \leq \min(\dim(A), \dim(B)) \) and \( \sum_\alpha \lambda_\alpha^2 = 1. \)
Entanglement between subsystems A and B

- When operator $O$ acts only on A:

$$\langle \psi | \hat{O} | \psi \rangle = \sum_{\alpha \beta} \lambda_\alpha \lambda_\beta \langle B | A \rangle_\alpha \langle \hat{O} | A \rangle_\beta \langle B \rangle_\beta = \sum_\alpha \lambda_\alpha^2 \langle A | \hat{O} | A \rangle_\alpha$$

$$= \text{tr}_A \left( \hat{O} \sum_\alpha \lambda_\alpha^2 \langle A | A \rangle_\alpha \right)$$

$\hat{\rho}_A$: reduced density matrix $= \text{tr}_B \hat{\rho} \equiv \text{tr}_B |\psi\rangle \langle \psi|$  

- Von Neumann entanglement entropy between A and B:

$$S_A := - \text{tr}_A (\hat{\rho}_A \ln \hat{\rho}_A) = - \sum_\alpha \lambda_\alpha^2 \ln \lambda_\alpha$$

(depends only on $\lambda_\alpha$)

- Maximum possible value: $S_{A,max} = \ln \chi$ (when all $\lambda_\alpha$ are equal)

$\rightarrow$ need matrices up to dimension $\chi \approx \exp(S_A)$

- Examples:
  - Product state: $|\Psi\rangle = |\uparrow_A \uparrow_B\rangle = |\uparrow\rangle_A |\uparrow\rangle_B : S_A = 0 : \text{not entangled}$
  - Singlet: $|\Psi\rangle = \frac{1}{\sqrt{2}} \left( |\uparrow\rangle_A |\downarrow\rangle_B - |\downarrow\rangle_B |\uparrow\rangle_A \right) : S_A = \ln 2 : \text{max. entangled}$
**Exact MPS representation of a state**

- **General state:**
  \[ |\Psi\rangle = \sum_{s_1 \ldots s_L} c_{s_1 \ldots s_L} |s_1 \ldots s_L\rangle \]

- **First site: SVD**
  \[ c_{s_2 \ldots s_L} = \sum_{\alpha=1}^{2} \tilde{U}^{[1]}_{\alpha_1 s_1} \lambda^{[1]}_{\alpha_1} \tilde{V}^{\dagger}_{\alpha_1 s_2 \ldots s_L}(0) \]
  Also gives Schmidt decomposition between sites 1 and 2

- **Second site: SVD**
  \[ \lambda^{[2]}_{\alpha_2} \tilde{V}^{\dagger}_{\alpha_2 s_3 \ldots s_L} = \sum_{\alpha=1}^{4} \tilde{U}^{[2]}_{\alpha_1 s_2} \lambda^{[2]}_{\alpha_2} \tilde{V}^{\dagger}_{\alpha_2 s_3 \ldots s_L} \]
  with singular values \( \lambda_{\alpha} \)

- **After site j:**
  \[ |\Psi\rangle = \sum_{s_1 \ldots s_L} \sum_{\alpha_1}^{2} \sum_{\alpha_2}^{4} \sum_{\alpha_3}^{8} \cdots \tilde{U}^{[1]}_{s_1 \alpha_1} \tilde{U}^{[2]}_{(\alpha_1 s_2)\alpha_2} \cdots \tilde{U}^{[j]}_{(\alpha_{j-1}s_j)\alpha_j} \lambda^{[j]}_{\alpha_j} \tilde{V}^{\dagger}_{\alpha_j (s_{j+1} \ldots s_L)} |s_1 \ldots s_L\rangle \]

- **Rename U → A :**
  \[ \tilde{U}^{[1]}_{s_1 \alpha_1} \tilde{U}^{[2]}_{(\alpha_1 s_2)\alpha_2} \tilde{U}^{[3]}_{(\alpha_2 s_3)\alpha_3} \cdots =: A^{[1]}_{\alpha_1 s_1} A^{[2]}_{\alpha_1 \alpha_2} A^{[3]}_{\alpha_2 s_3} \cdots \]

- **→ Exact MPS:**
  \[ |\Psi\rangle = \sum_{s_1 \ldots s_L} \sum_{\{\alpha_i\}} A^{[1]}_{\alpha_1 s_1} A^{[2]}_{\alpha_1 \alpha_2} A^{[3]}_{\alpha_2 s_3} \cdots A^{[L]}_{\alpha_{L-1} s_{L-1}} A^{[L]}_{\alpha_{L-1} s_L} |s_1 \ldots s_L\rangle \]

- **But: maximum dimension** \( 2^{L/2} \) (?!?) in the middle (by doing SVD from left and from right)
  Really: matrix dimensions \( O(100) \) are enough! (see later)
• Write singular values explicitly, by defining matrices $\Gamma$:

$$A_{\alpha_{j-1} \alpha_j}^j s_j =: \lambda_{\alpha_{j-1} \alpha_j}^{j-1} \Gamma_{\alpha_{j-1} \alpha_j}^j s_j$$

and also

$$B_{\alpha_{j-1} \alpha_j}^j s_j =: \Gamma_{\alpha_{j-1} \alpha_j}^j s_j \lambda_{\alpha_{j-1} \alpha_j}^j$$

Provides Schmidt decomp. and reduced density matrix at any lattice bond

• Normalization: write $U^\dagger U = 1$ and $V^\dagger V = 1$ graphically:

$$\delta_{\alpha \beta} = \delta_{\alpha \beta}$$
Expectation value of a local operator

\[
\langle \Psi | \hat{O}^{[j]} | \Psi \rangle = \sum_{\{s\},\{s'\}} \langle s'_1 \ldots s'_L | \ldots \lambda^{*[j]} \Gamma^{*[j]} s'_j \lambda^{*[j-1]} \ldots \hat{O}^{[j]}_{s_j s'_j} \ldots \lambda^{[j-1]} \Gamma^{[j]} s_j \lambda^{[j]} \ldots | s_1 \ldots s_L \rangle
\]

Simplifies because of normalizations and becomes a local object
For 1d chains, **small** matrices are enough!

- In 1D, entanglement between “left” and “right” subsystem goes through a single bond
  → entanglement entropy $S$ is small, up to only $\ln$ (system size $N$) (**for ground states**)  
  → need only matrix dimensions $\chi = O(N) = O(100)$

- But excited states (time evolution) may need much more

- In higher dimensions: $S_{max} \sim L^{D-1} \rightarrow$ exponentially large matrices

- In practice, **truncate matrices** by discarding small singular values,  
  either to a maximum size (uncontrolled error),  
  or by limiting the “**truncated weight**” $t_w := \sum_\alpha \lambda_\alpha^2$ of the discarded directions to e.g. $10^{-10}$
### Time evolution

- H with nearest neighbor coupling: split
  \[ \hat{H} = \hat{H}_{\text{even}} + \hat{H}_{\text{odd}} = \sum_{j, \text{odd}} \hat{H}_j + \sum_{j, \text{even}} \hat{H}_j \]

  such that
  \[ e^{-i\hat{H}_{\text{even}}t} = \prod_{j, \text{even}} e^{-i\hat{H}_j t} \quad \text{and} \quad e^{-i\hat{H}_{\text{odd}}t} = \prod_{j, \text{odd}} e^{-i\hat{H}_j t} \]

  2-site operators

- Trotter-Suzuki:
  \[ e^{-i\hat{H}t} = \left( e^{-i\hat{H}_{\text{even}}\Delta t} e^{-i\hat{H}_{\text{odd}}\Delta t} e^{-i\hat{H}_{\text{even}}\Delta t} \ldots e^{-i\hat{H}_{\text{even}}\Delta t} \right) (1 + O(\Delta t)) \]

  (other operator sequences are possible)

- 2-site operators can be applied locally

- Matrix dimensions would double at each step → truncate back
Some real time evolutions (an aside)

- **Bound state propagation** of a $\uparrow\uparrow$ spin pair in Heisenberg groundstate ($J_z = 1.2$) (Ganahl PRL 2012)
  → dedicated cold atom experiment

- **Scattering** between a moving particle and a bound state of 10 particles, which is shifted left by 2 sites (Ganahl 2013)
  Later reproduced in Bethe ansatz (Vlijm, Ganahl 2015)
Matrix Product Operators (MPO) and DMRG

- Same approach as for states

\[ \hat{O} = \sum_{\{s_i\},\{s'_i\}} W^{s_1,s'_1} W^{s_2,s'_2} \ldots W^{s_L,s'_L} |s'_1, s'_2, \ldots, s'_L \rangle \langle s_1, s_2, \ldots, s_L | \]

Graphically:

- DMRG: find ground state. Sequentially optimize each MPS matrix A, by finding minimum \( \lambda \) of

\[ H^{\text{eff}}_i A[i] = \lambda A[i], \]

Graphically:
\[ H = \sum_{k\sigma} \epsilon_k n_{k\sigma} + \sum_{k\sigma} V_k (c_{0\sigma}^\dagger c_{k\sigma} + h.c.) + \sum_\sigma \epsilon_0 n_{0\sigma} + H_{int} \]

- Choose geometry and numbering

- Solution for MPOs (without \( H_{int} \))

\[
W_{1\uparrow} = \begin{pmatrix}
\epsilon_1 n_{1\uparrow} & 1 & V_1 c_{1\uparrow} & V_1 c_{1\uparrow}^\dagger
\end{pmatrix}
\]

\[
W_{k>1,\uparrow} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
\epsilon_k n_{k\uparrow} & 1 & V_k c_{k\uparrow} & V_k c_{k\uparrow}^\dagger \\
0 & 0 & p & 0 \\
0 & 0 & 0 & p
\end{pmatrix}
\]

with \( p = (-1)^n \) for fermion anticommutation
Impurity Solvers
Real time impurity solvers with MPS: strategy

To obtain real frequency Green's function:

- **Ground state** $|\psi_0\rangle$ of impurity model by DMRG
- **Time evolve** excitation: $e^{iHt} c |\psi_0\rangle$
- **Overlap**: $G^<(t) = \langle \psi_0| c^\dagger e^{iHt} c |\psi_0\rangle$
- “Linear prediction”, Fourier transform $\rightarrow G(\omega)$

One band:

- Separate the spin-up and spin-down baths: ($\Rightarrow$ lower matrix dimensions)

- Large baths (O(100) sites) easily done
Real time impurity Solver with MPS: two bands

- Combine orbitals into bigger sites
- Works very well for 2 bands

Examples: DMFT spectrum of Hubbard model on Bethe lattice (Ganahl et al, 2015)

Side-peaks: (invisible in QMC): from interaction of doublon-holon pairs

(Lee, von Delft, Weichselbaum, PRL 2017, one-band model)

Problem: matrix dimensions $m$ multiply: computational effort $\sim m^3 \times n_{\text{orbital}}$

$\Rightarrow$ no more than 2 bands feasible this way
New approach: Fork Tensor Product States (FTPS)

- Separate the bands of the bath
  → small bath matrices

- Tree tensor network, bipartition at any bond
  → DMRG, Time Evolution etc. possible

- Tradeoff: Entanglement at impurity

- “Star geometry” (no Wilson chains):
  → lower entanglement, much faster

\[ V_k \left( c_k^\dagger c_0 + h.c. \right) + \epsilon_k n_k \]

Example: 2 orbitals A, B:

Tree tensor: see also Holzner et al, PRB 2010 (2 orbital NRG)
$$H = H_{\text{loc}} + H_{\text{bath}}$$

$$H_{\text{loc}} = \epsilon_0 \sum_{m\sigma} n_{m0\sigma} + H_{\text{DD}} + H_{\text{SF}} + H_{\text{PH}}$$

$$H_{\text{DD}} = U \sum_m n_{m0\uparrow} n_{m0\downarrow} + (U - 2J) \sum_{m' > m, \sigma} n_{m0\sigma} n_{m'0\bar{\sigma}} + (U - 3J) \sum_{m' > m, \sigma} n_{m0\sigma} n_{m'0\bar{\sigma}}$$

$$H_{\text{SF}} = J \sum_{m' > m} \left( c_{m0\uparrow}^\dagger c_{m0\downarrow} c_{m'0\uparrow}^\dagger c_{m'0\downarrow}^\dagger + \text{h.c.} \right)$$

$$H_{\text{PH}} = -J \sum_{m' > m} \left( c_{m0\uparrow}^\dagger c_{m0\downarrow}^\dagger c_{m'0\uparrow} c_{m'0\downarrow} + \text{h.c.} \right)$$

$$H_{\text{bath}} = \sum_{ml\sigma} \epsilon_l n_{ml\sigma} + V_l \left( c_{m0\sigma}^\dagger c_{ml\sigma} + \text{h.c.} \right),$$

$$H_{\text{free}} := H_{\text{bath}} + \epsilon_0 \sum_{m\sigma} n_{m0\sigma}$$

Bath parameters $\epsilon_l$, $V_l$ from arbitrary discretization ($\leftrightarrow$ energy resolution) of $\Delta(\omega)$
**FTPS: adapt methods**

- **SVDs:** combine tensor indices to get matrices → computational effort up to $O(m_i^3 m_B)$, where $m_i$: matrix dim. between impurities, $m_B$: matrix dim. to last bath site

- **Ground state:** construct MPOs (FTPOs) for $H$ and use DMRG
  Expensive: $O(m_i^3 m_B^3)$

**Time evolution:**

$$e^{-i\Delta t H} \approx \left( \prod_{m' > m} e^{-i \frac{\Delta t}{2} (H_{m,m'} + H_{m',m})} \right) e^{-i \frac{\Delta t}{2} H_m} e^{-i \Delta t H_m} e^{-i \frac{\Delta t}{2} H_m} \left( \prod_{m' > m} e^{-i \frac{\Delta t}{2} (H_{m',m} + H_{m,m'})} \right)$$

Construct and apply FTPOs for each time evolution operator (→ size up to 6 x 10)
Time evolution of bath

"Star geometry" ↔ Wilson chain

- Use star geometry
- Map onto chain → non-local hoppings (!)
- Treat by "moving impurity through bath and back"
- Achieve much smaller Trotter errors than in Wilson chain:
  → Bath evolution faster by factor 100 for same precision
Results
Results: SrVO$_3$

- 3 band model ($t_{2g}$ subspace), Kanamori-Hamiltonian
- Large bath (109 bath sites for each orbital-spin combination, converged)
- Time evolution up to 16eV$^{-1}$, T=0
- First: results with only density-density interactions:
  - Very good agreement with CTQMC (also on imaginary time axis)
  - FTPS only: 3-peak structure in upper Hubbard band
    
    Not resolved by MaxEnt

CPU time for one DMFT iteration:
FTPS: 80h, CTQMC: 32h
SrVO$_3$: multiplet in upper Hubbard band

- FTPS can resolve multiplets
- Related to atomic energies

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<th>state</th>
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$\approx U - 3J + \varepsilon_0 \approx U - 2J + \varepsilon_0$

$\approx -\varepsilon_0$

$\approx U + \varepsilon_0$

Excitations in N=3 Sector
SrVO$_3$: upper Hubbard band for different J

- Interactions $\Rightarrow$ broadened and shifted peaks

- Can be described by effective $J_{\text{eff}} \neq J$
  
  $J= 0.5 \text{ eV} \rightarrow J_{\text{eff}} = 0.59(6) \text{ eV}$  
  $J= 0.6 \text{ eV} \rightarrow J_{\text{eff}} = 0.66(3) \text{ eV}$  
  $J= 0.7 \text{ eV} \rightarrow J_{\text{eff}} = 0.72(2) \text{ eV}$

- Central peak almost constant
**SrVO$_3$: full rotational symmetry**

Include spin flip and pair hoppings

Only affect $N=2$ sector →
Hole excitation and quasi particle peak do not change

Different multiplets due to different atomic eigenstates/eigenenergies.

Energy differences $2J$ and $3J$
SrMnO$_3$

- 3 electrons in Mn-3d orbitals. Mott Insulator with $|GS\rangle \approx |\uparrow, \uparrow, \uparrow\rangle + |\downarrow, \downarrow, \downarrow\rangle$

- DFT-DOS:

  - $e_g$ orbitals largely above $E_F$ $\rightarrow$ “unoccupied”
  - Is $e_g$ important?

  - Strong hybridizations with oxygen p-states in lower Hubbard band

  $\rightarrow$ Use wide energy window [-10eV, 5eV] for Wannier projection
  - GS then mixes N=3 and N=4 sectors

- DMFT: $t_{2g}$ only
SrMnO$_3$: $t_{2g}$ and $e_g$ orbitals

- Full 5-band calculation (U=6.0, J=0.8)

DMFT: $t_{2g}$ plus $e_g$

$e_g$ high spin
$e_g$ low spin
$\omega$ (eV)

$A(\omega)$

$t_{2g}$ "double occ."

Gap determined by $e_g$

$t_{2g}$ only

$U=5$ eV, $J=0.7$ eV

$\omega$ (eV)
SrMnO$_3$: $t_{2g}$ and $e_g$ orbitals

- Full 5-band calculation ($U=6.0$, $J=0.8$)

- $e_g$ is important:
  - determines the gap
  - creates 3-peak structure above $E_F$
    (not resolved by CTQMC)

DMFT: $t_{2g}$ plus $e_g$

Comparison to CTQMC

FTPS: 700 CPU-h, CTQMC: 600 CPU-h
SrMnO$_3$: $t_{2g}$ and $e_g$ orbitals

- Full 5-band calculation ($U=6.0$, $J=0.8$)

- $e_g$ is important:
  - determines the gap
  - creates 3-peak structure above $E_F$
    (not resolved by CTQMC)

DMFT: $t_{2g}$ plus $e_g$

Comparison to experiment

3-peak structure visible in experiment

Gap determined by $e_g$

J.-S. Kang et al., PRB 78, 054434 (2008)
Conclusions

- **FTPS: real time impurity solver for DMFT**
  - Efficient: comparable to CTQMC
  - $T=0$
  - Large baths, no analytic continuation $\rightarrow$ high resolution at all energies

- **5-orbital calculations possible**
  - Can resolve multiplets in upper Hubbard band
  - SrMnO$_3$: three-peak structure $e_g t_{2g} e_g$ is also visible in experiment

- **Outlook:**
  - Non-diagonal baths, without sign problem (in preparation)
  - Nonequilibrium (in preparation) $\rightarrow$ next talk by Martin Eckstein
  - Better resolution than CT-QMC even at low energies (25meV) (→ M. Rumetshofer)

- **Limitations:**
  - Single site (so far)
  - No black box yet
  - ....