Compact quantum circuit of variational quantum eigensolver for quantum impurity models

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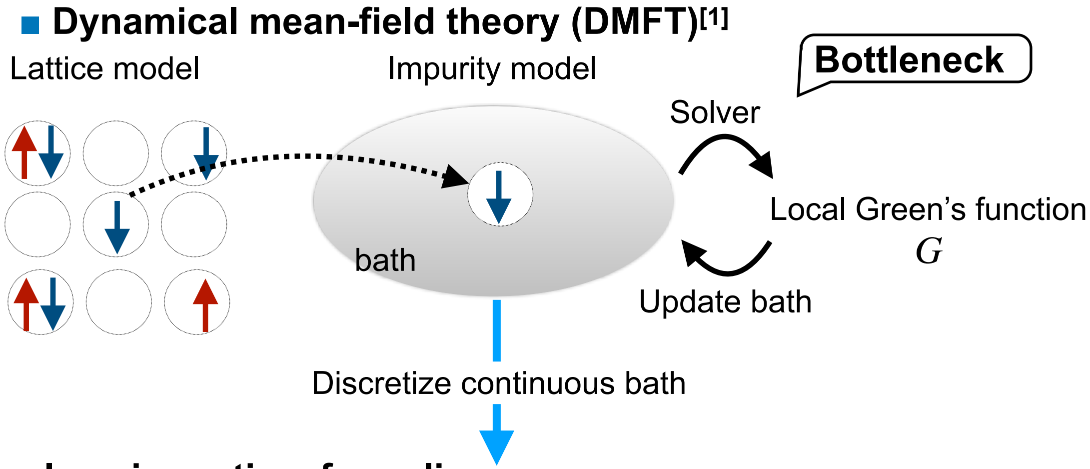
Take home message

- ⚠ Solving impurity models is the biggest bottleneck of DMFT.
- ⚠ VQA suffers from an increasing # of parameters with the # of orbitals.
- 💡 Compact quantum circuit for quantum impurity models

Introduction

Dynamical mean-field theory (DMFT)[1]



Lattice model

Impurity model

Bottleneck

Solver

Local Green's function G

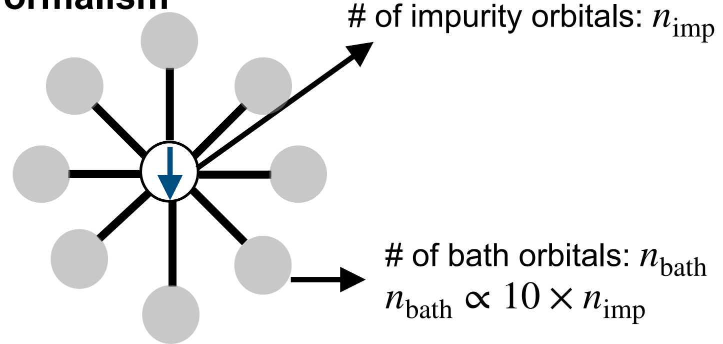
bath

Update bath

Discretize continuous bath

Imaginary-time formalism

→ fewer bath sites



# of impurity orbitals: n_{imp}

# of bath orbitals: n_{bath}

$n_{\mathrm{bath}} \propto 10 \times n_{\mathrm{imp}}$

e.g. Fe-based superconductor(LaFeAsO)[2]

$n_{\mathrm{orb}} = n_{\mathrm{imp}} + n_{\mathrm{bath}} \sim 40 + 332$

State-of-the-art "classical" simulation

Two-site impurity with three orbitals by MPS[3]

Quantum algorithms for impurity solver

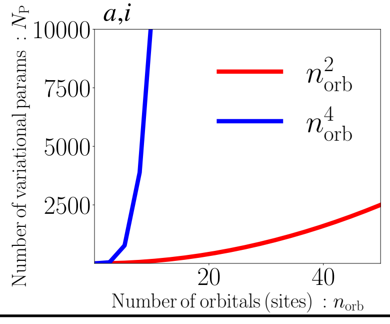
- Fault-tolerant QC[4]
- QC with limited hardware resources (*e.g.* NISQ devices)
  Variational quantum algorithms (VQA) for computing imaginary-time or frequency Green's functions $G(\tau)$[5], $G(i\omega)$[6]

Common problem: The number of variational parameters N_P in ansatz grows rapidly with the number of orbitals.

	Unitary coupled cluster generalized singles and doubles (uCCGSD)[7]	*k*-unitary cluster jastrow (*k*-uCJ)[8]
N_P	$O\left((n_{\mathrm{imp}}+n_{\mathrm{bath}})^4\right)$	$O\left((n_{\mathrm{imp}}+n_{\mathrm{bath}})^2\right)$

uCCGSD
$$U(\vec{\theta}) = \prod_{a>i,b>j}^{n_{\mathrm{orb}}} \left\{ e^{\theta_{ij}^{ab}(c_a^\dagger c_b^\dagger c_j c_i - c_i^\dagger c_j^\dagger c_b c_a)} \right\} \prod_{a,i}^{n_{\mathrm{orb}}} \left\{ e^{\theta_i^a (c_a^\dagger c_i - c_i^\dagger c_a)} \right\}$$

k-uCJ
$$U(\vec{\theta}) = \sum_{i=1}^{k} [e^{\hat{K}_i} e^{\hat{J}_i} e^{-\hat{K}_i}]$$
$$\hat{J} = \sum_{jl}^{n_{\mathrm{orb}}} \theta_{jl} a_j^\dagger a_l^\dagger a_l a_j$$
$$\hat{K} = \sum_{jl}^{n_{\mathrm{orb}}} \sum_{\sigma=\uparrow,\downarrow} \theta_{jl} a_{j\sigma}^\dagger a_{l\sigma}$$



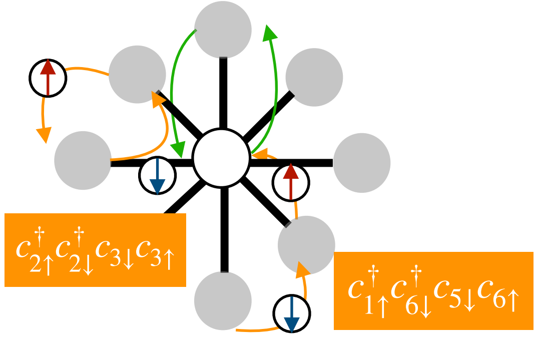
References

[1] G. Kotliar *et al.*, Rev. Mod. Phys. **78**, 865 (2006)
[2] H. Shinaoka *et al.,* Phys. Rev. B **103**, 045120 (2021)
[3] F. Alexander Wolf *et al.*, Phys. Rev. X **5**, 041032 (2015)
[4] B. Bauer *et al.*, Phys. Rev. X **6**, 031045 (2016)
[5] R. Sakurai *et al.*, Phys. Rev. Research **4**, 023219 (2022)
[6] H. Chen *et al.*, Phys. Rev. A **104**, 032405 (2021)
[7] J. Lee *et al.*, J. Chem. Theory. Comput. **15**, 1 (2019)
[8] Y. Kurashige *et al.*, J. Chem. Theory. Comput. **16,** 2 (2020)
[9] https://github.com/qulacs/qulacs

New "Sparse" ansatz

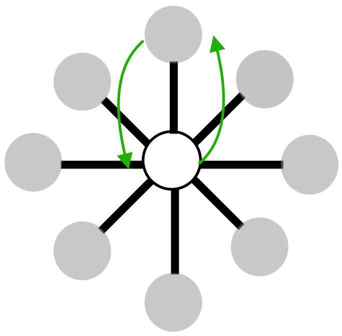
Assumption: Most two-particle excitation operators between bath sites do not contribute to the ground state significantly.

uCCGSD



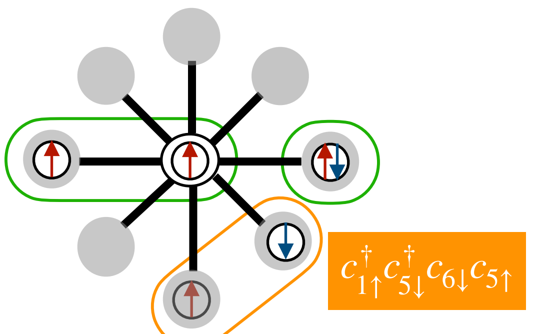
We **remove** operators with more than 3 bath orbitals.

"**Sparse**" uCCGSD



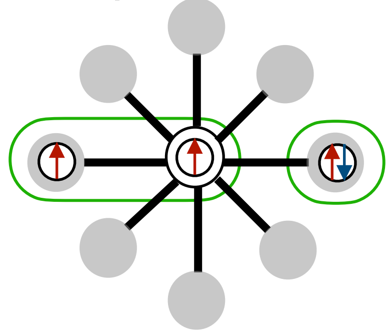
N_P	$O\left((n_{\mathrm{imp}})^4\right)$

k-uCJ



We **remove** operators between different bath site.

"**Sparse**" *k*-uCJ



$O\left(n_{\mathrm{imp}}^2\right)$, $\left(n_{\mathrm{bath}} \sim O(n_{\mathrm{imp}}\right)$

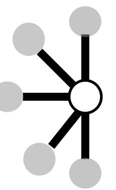
Numerical results

Numerical details

- Ground state calculation: Variational quantum eigensolver
- Qulacs[9] wrapped by julia
- Optimizer: BFGS

One impurity with five bath sites

$$H = U\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} - \mu \sum_{\sigma=\uparrow,\downarrow} \hat{n}_{1\sigma} - \sum_{k=2} \sum_{\sigma=\uparrow,\downarrow} V\left(\hat{c}_{1\sigma}^\dagger \hat{c}_{k\sigma} + \hat{c}_{k\sigma}^\dagger \hat{c}_{1\sigma}\right) + \epsilon_k \sum_{k=2} \sum_{\sigma=\uparrow,\downarrow} \hat{n}_{k\sigma}$$



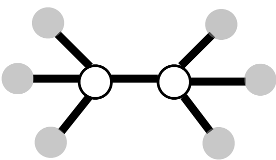
U = 4.0, μ = U / 2, t=1.0, $V \in [0.0, 1.0]$, $\epsilon_k = [-2, -1, 0, 1, 2]$

	Sparse uCCGSD (original)	Sparse *k*-uCJ (original)
N_P	**272** (1752)	**228** (288)

$\Delta = |E_{\mathrm{origi}}(V) - E_{\mathrm{sparse}}(V)| < O(10^{-4})$ ← Small influence on ground state!

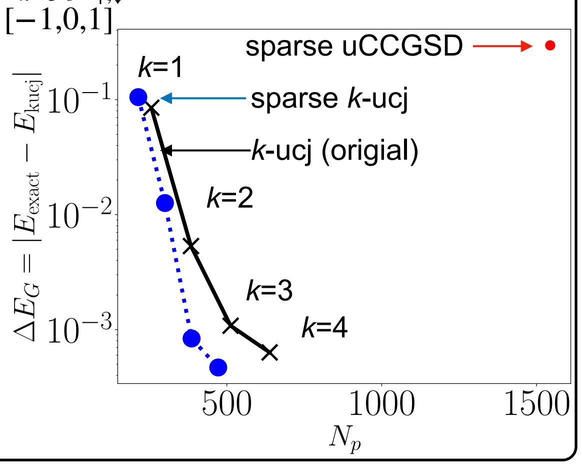
Two-site impurity with six bath sites

$$H = \sum_{i=1}^{2} U\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - \mu \sum_{i=1,2,\sigma=\uparrow,\downarrow} \hat{n}_{i\sigma} - \sum_{\sigma=\uparrow,\downarrow} t\left(\hat{c}_{1\sigma}^\dagger \hat{c}_{2\sigma} + \hat{c}_{2\sigma}^\dagger \hat{c}_{1\sigma}\right)$$
$$- \sum_{j=1,2} \sum_{k} \sum_{\sigma=\uparrow,\downarrow} V\left(\hat{c}_{j\sigma}^\dagger \hat{c}_{k\sigma} + \hat{c}_{k\sigma}^\dagger \hat{c}_{j\sigma}\right) + \epsilon_b \sum_{k=3} \sum_{\sigma=\uparrow,\downarrow} \hat{n}_{b\sigma}$$



U = 4.0, μ = U / 2, t = 1.0, V =0.5, $\epsilon_b = [-1, 0, 1]$

- Sparse *k*-ucj works for cluster impurity model.
- Sparse *k*-ucj outperforms sparse uCCGSD.



Future plan

- Computing spectral functions with moments expansion
- Effect of noise