Hybrid quantum-classical algorithm for computing imaginary-time correlation functions

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New preprint

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Today's talk is based on

> **Hybrid quantum-classical algorithm for computing imaginary-time correlation functions**
>
> https://arxiv.org/abs/2112.02764

collaborator

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Computational materials science

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Density functional theory (DFT)

- Approximates the electronic quantum state with a single slater determinant.
- Success：Many semiconductors and metals
- Strong：Low computational cost ~$O(N^3)$ (N: #of orbitals).
- Weakness : strongly correlated electron systems
  (e.g. cuprate high-temperature superconductivity)

Quantum embedding theory (Dynamical mean-field theory)

- Focusing on a part of the whole system

- effective bath parameters are determined from the self-consistent condition:

- Physical quantities described by response functions are important. (single-particle excitation spectral functions or lattice spin susceptibility)

- In the field of quantum chemistry, density matrix embedding theory (DMET) are used.

- Why are multi-orbital and multi-atomic important?
  -->quantitative description of unconventional superconductivity

Dynamical mean-field theory (DMFT)

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- The biggest bottle neck: **quantum impurity problem (Computing Green's function)**
- Single impurity with few orbitals are the limit by classical methods: Quantum Monte Carlo , MPS/Tensor network
- Solving impurity models wit multi-orbital and multi impurity sites is a challenging task.

	$G(t)/G(\omega)$ **(Real)**	$G(\tau)/G(i\omega)$ **(Imaginary)**
Pros	Accurate description of spectral functions	Fewer bath sites
Cons	Many bath sites	Inaccurate description of spectral functions at high frequencies

Solving impurity problems with Quantum computer

Foult-tolerant quantum computer

- Algorithm based on Quantum phase estimation algorithm (~2015)
- Too much hardware resources

Quantum devices with limited hardware resources

- e.g.) Noisy Intermediate Scale Devices (NISQ)
  noisy quantum devices with ~100 qubits, about 100 depth (# of time steps)
- Need to calculate expectation value of the square of the Hamiltonian
  (H. Chen et *al*., arXiv :2105.01703v2)
- Efficient methods for computing imaginary-time Green's functions need to be explored
- Our work: new algorithm to compute the imaginary-time Green's function

Imaginary-time Green's function

Hamiltonian

$$H = \sum_{ij}^{N} t_{ij}\hat{c}_i^\dagger \hat{c}_j + \frac{1}{4}\sum_{ijkl} U_{ikjl}\hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_l \hat{c}_k - \mu \sum_i \hat{c}_i^\dagger \hat{c}_i,$$

$c_i / c_i^\dagger$: the creation and annihilation operators for the spin orbital i

Imaginary-time Green's function (GF)

$$G_{ab}(\tau) = -\theta(\tau)\left\langle \hat{c}_a(\tau)\hat{c}_b^\dagger(0)\right\rangle + \theta(\tau)\left\langle \hat{c}_b^\dagger(0)\hat{c}_a(\tau)\right\rangle, \tau = it, \hbar = k_{\mathrm{B}} = 1,$$

- At sufficiently low temperature T

$$G_{ab}(\tau) \underset{T\to 0}{=} \mp\left\langle \Psi_{\mathrm{G}} \left| \hat{A}_\pm e^{\mp(\mathcal{H}-E_{\mathrm{G}})\tau}\hat{B}_\pm \right| \Psi_{\mathrm{G}}\right\rangle, |\Psi_{\mathrm{G}}\rangle : \text{ground state}$$

$$A_+ = \hat{c}_a \text{ and } B_+ = \hat{c}_b^\dagger \text{ for } 0 < \tau < \frac{\beta}{2},$$

$$A_- = \hat{c}_b^\dagger \text{ and } B_+ = \hat{c}_a \text{ for } -\frac{\beta}{2} < \tau < 0$$

$$(\beta = 1/T)$$

Outline of our algorithm

- Introduce a fine mesh of τ in [-β / 2, β / 2]
- Then, compute $G_{ij}(\tau)$

For τ>0,

$$
\begin{aligned}
G_{ij}(\tau) &= -\operatorname{Tr}\left[e^{-\beta\hat{H}} c_i(\tau) c_j^\dagger(0)\right] / \operatorname{Tr}\left(e^{-\beta\mathcal{H}}\right) \\
&\simeq -\underbrace{\langle\Phi_G(0)|\, e^{-(\beta-\tau)\hat{H}}}_{\langle\Phi'_C|} c_i(0) \underbrace{e^{-\tau\hat{H}} c_j^\dagger(0)\, |\Phi_G(0)\rangle}_{|\Phi_C\rangle} / \left(e^{-\beta E_G}\right)
\end{aligned}
$$

STAGE1: Ground-state calculation

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Preparation

- The hamiltonian need to be transformed to the qubit representation
  e.g.) Jordan-Wigner transformation

$$H \to \sum_p h_p S_p, S_p \in \{X, Y, Z, I\}^{\otimes m}$$

Variational Quantum Eigensolver (VQE) ------>

🔹 **Optimization**: parameter-shift rule

https://arxiv.org/pdf/1803.00745.pdf

$$\frac{\partial \langle H(\theta) \rangle}{\partial \theta_i} = \frac{1}{2}\left(H\left(\theta + \frac{\pi}{2} e_i\right)\right) - \left\langle H\left(\theta - \frac{\pi}{2} e_i\right)\right\rangle\Bigg)$$

$$(U(\boldsymbol{\theta}) = \prod_k e^{-i\theta_k P_k/2})$$

STAGE2: Single-particle excitation

For $\tau > 0$,

$$\hat{c}_a^\dagger \left|\Psi_{\mathrm{GS}}\right\rangle \simeq c_1 \left|\phi_{\mathrm{EX}}\left(\vec{\theta}_{\mathrm{EX}}\right)\right\rangle$$

1. single-particel excited state
   $c_a^\dagger \left|\Psi_G\right\rangle = \frac{X_a - iY_a}{2} Z_{a-1} \ldots Z_1 \left|\Psi_G\right\rangle$
2. Prepare $\left|\phi_{\mathrm{EX}}\left(\vec{\theta}_{\mathrm{EX}}\right)\right\rangle$ and measure
   $\left\langle \phi_{\mathrm{EX}}\left(\vec{\theta}_{\mathrm{EX}}\right) \left|\hat{c}_a^\dagger\right| \Psi_{\mathrm{G}} \right\rangle$
3. Minimize cost function:
   $|1 - \langle \Psi_{EX}(\vec{\theta}) | c_a^\dagger \left|\Psi_G\right\rangle|^2$
4. Measure
   $c_1 = \left\langle \phi_{\mathrm{EX}}\left(\vec{\theta}^*_{\mathrm{EX}}\right) \left|c_a^\dagger\right| \Psi_{\mathrm{G}} \right\rangle$

STAGE3: Imaginary-time evolution

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- The time-dependent Schrödinger equation

$$\frac{\mathrm{d}}{\mathrm{d}\tau}|\tilde{\Psi}(\tau)\rangle = -\left(H - E_\tau\right)|\tilde{\Psi}(\tau)\rangle$$

$$|\tilde{\Psi}(\tau)\rangle \equiv |\Psi(\tau)\rangle / \sqrt{\langle\Psi(\tau) \mid \Psi(\tau)\rangle}, E_\tau \equiv \langle\tilde{\Psi}(\tau)|H|\tilde{\Psi}(\tau)\rangle$$

- Prepare the following state on a quantum computer

$$|\tilde{\Psi}(\tau)\rangle = |\phi(\vec{\theta}(\tau))\rangle$$
$$|\Psi(\tau)\rangle = e^{\eta(\tau)}|\phi(\vec{\theta}(\tau))\rangle - (1)$$

- Introduce Norm $e^{\eta(\tau)}$:

$$\frac{\mathrm{d}}{\mathrm{d}\tau}|\Psi(\tau)\rangle = -H|\Psi(\tau)\rangle - (2)$$

- From (1) and (2),

$$\frac{d\eta(\tau)}{d\tau} = -E_\tau, (\eta \in \mathbb{R} \text{ and} \frac{\mathrm{d}\langle\Psi|\Psi\rangle}{\mathrm{d}\tau} = 0)$$

Question: How do we determine $\vec{\theta}(\tau)$ on a discrete mesh of τ ?

McLachlan's variational principal (A. McLachlan, Mol. Phys 8, 39-44 (1996))

$$\min \delta \left\| \left(\frac{\mathrm{d}}{\mathrm{d}\tau} + H - E_\tau\right) \mid \phi(\vec{\theta}(\tau))\rangle \right\|$$

STAGE3: Imaginary-time evolution

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Varuational Quantum Simulation (VQS)

$$\min \delta \left\| \left(\frac{\mathrm{d}}{\mathrm{d}\tau} + H - E_\tau \right) \mid \phi(\vec{\theta}(\tau)) \right\rangle \right\|$$

$$\sum_j A_{ij} \dot{\theta}_j = C_i$$

$$A_{ij} \equiv \mathcal{R} \frac{\partial \langle \phi(\vec{\theta})|}{\partial \theta_i} \frac{\partial |\phi(\vec{\theta})\rangle}{\partial \theta_j}, C_i \quad \equiv -\mathcal{R} \langle \phi(\tau)| \mathcal{H} \frac{\partial |\phi(\vec{\theta})\rangle}{\partial \theta_i}$$

$$\vec{\theta}(\tau + \Delta\tau) \simeq \vec{\theta}(\tau) + A^{-1} \vec{C} \Delta\tau$$

Direct VQS

$$\begin{aligned}
&\theta(\tau + \Delta\tau) \\
&\simeq \underset{\vec{\theta}}{\mathrm{argmin}} \| |\phi(\vec{\theta})\rangle - |\Psi(\tau)\rangle + \Delta\tau \left(\mathcal{H} - E_\tau \right) |\Psi(\tau)\rangle \| \\
&= \underset{\vec{\theta}}{\mathrm{argmin}}\, \mathrm{Re} \mid \Delta\tau \langle \phi(\vec{\theta})| H |\Psi(\tau)\rangle - \left(\Delta\tau E_\tau + 1 \right) \langle \phi(\vec{\theta}) \mid \Psi(\tau) \rangle
\end{aligned}$$

STAGE4: Transition amplitude

transition amplitude

$\langle \Psi_{\mathrm{G}} | A_{\pm} | \Psi_{\mathrm{IM}} \rangle$

-->$G(\tau) = -c_1 e^{\eta(\tau)} e^{\tau E_{\mathrm{G}}} \langle \Psi_{\mathrm{G}} | A_{\pm} | \Psi_{\mathrm{IM}} \rangle$

Numerical Details

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Ansatz

- Unitary coupled cluster with generalized singles and doubles (UCCGSD)
  (M. Nooijen, Phys. Rev. Lett. **84**, 2108 (2000),
  J. Lee, *et al*., Journal of chemical theory and computation **15**, 311 (2019))
- $U(\boldsymbol{\theta}) = \prod_{i,j,a,b=1}^{n} \left\{ e^{\theta_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i - \theta_{ij}^{ab} a_i^\dagger a_j^\dagger a_b a_a} \right\} \prod_{a,i=1}^{n} \left\{ e^{\theta_i^a a_a^\dagger a_i - \theta_i^a a_i^\dagger a_a} \right\}$
- N_p : # of the parameters ~ $O\left(n^4\right)$

Optimization

- A quasi-Newton method (BFGS method)

Non-uniform mesh of τ in $[-\beta/2, \beta/2]$ ($\beta = 1000$)

- A sparse mesh generated according to the intermediate-representation (IR) basis.
  (J. Li *et al*., PRB **101**, 035144 (2020))

Results: Dimer model

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

- U=1,μ=1/2, V=1, ϵ_b=1
- At half-filling
- #of parameters: 104
- 79 sparse sampling points
- Non-diagonal componet also can be computed

Results : Four-site model

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$$H = U\hat{n}_{0\uparrow}\hat{n}_{0\downarrow} - \mu \sum_{\sigma=\uparrow,\downarrow} \hat{n}_{0\sigma} - \sum_{k=1}^{3} \sum_{\sigma=\uparrow,\downarrow} V_k \left(\hat{c}^{\dagger}_{0\sigma} \hat{c}_{k\sigma} + \hat{c}^{\dagger}_{k\sigma} \hat{c}_{0\sigma} \right) + \epsilon_k \sum_{k=1}^{3} \sum_{\sigma=\uparrow,\downarrow} \hat{n}_{k\sigma}$$

- value of parametes is obtained by DMFT calculation
- At half-filling
- #of parameters: 1568
- 70 sparse sampling points + adaptive construction of the mesh

Results : Fourier-transformed Green's function

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- We use a library called「irbasis」 (N. Chikano *et al*., Comput. Phys. Commun. **240**, 181 (2019))
- Fourier-transformed Green's function (Matsubara Green's function) $G_{ab}(\mathrm{i}\nu) = \int_0^\beta \mathrm{d}\tau e^{\mathrm{i}\nu\tau} G_{ab}(\tau)$

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Conclution

- New hybrid quantum classical algorithm for computing imaginary-time Green's functions by applying the VQS
- Out algorithms efficiently computes GF using non-uniform mesh based on IRbasis
- No need to calculate expectation value of the square of the Hamiltonian
  (H. Chen et *al*., arXiv :2105.01703v2)
- The hardware cost for transition amplitude may be high for NISQ devices 😢

future plan

1️⃣**Simulation under realistic noise model**: 2 qubit error
2️⃣**Ansatz for impurity models**: tensor decomposition, topology of impurity models