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

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New preprint

R. Sakurai, W. Mizukami, H. Shinaoka,
arXiv:2112.02764

Today's talk is based on following preprint

> **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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- 密度汎関数理論 (DFT)の概略とその問題点についてまとめる
- 単一のスレーター行列で物質の電子状態を近似
- 多くの半導体、金属の電子状態の記述は成功
- 強相関だと量子的な重ね合わせやエンタングルメントの増加により、DFT単体では記述が難しい

Dynamical mean-field theory (DMFT)

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

$$G_{\mathrm{imp}} = G_{\mathrm{loc}}^{\mathrm{lattice}} \equiv \sum_{\boldsymbol{k}} \frac{1}{i\omega_n - (\epsilon_{\boldsymbol{k}} - \mu) - \Sigma}$$

- The biggest bottle neck: **quantum impurity problem (Computing Green's function)**
- Classical methods: Quantum monte carlo, Tensor network
- Solving impurity models wit multi-orbital and multi impurity sites is challenging task

Solving impurity problems with Quantum computer

Foult-tolerant quantum computer

- Quantum phase estimation algorithm
- It assumes fault-tolerant QC

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

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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

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

$A_+ = \hat{c}_a$ and $B_+ = \hat{c}_b^\dagger$ for $0 < \tau < \frac{\beta}{2}, A_- = \hat{c}_b^\dagger$ and $B_+ = \hat{c}_a$ for $-\frac{\beta}{2} < \tau < 0, (\beta = 1/T)$

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- 実例として、ハバードアトムなどのグリーン関数の図を見せる(上のスライド）)
- 指数関数
- 数式との対応づける。
- N --> N+1 --> N
- 虚時間が
- Non-uniform なメッシュの図
- correction vectorの先行研究と何が非自明なのか。
- β: fictious temperature
- 応答関数で記述される物理量（スペクトル関数とか格子スピン感受率）が物性では重要
- DMFT
- 複数不純物クラスターの低温での計算は困難。
- 将来的に、量子で
- 有限温度の

Outline of our algorithm

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

For τ>0,

$$G_{ij}(\tau) = -\operatorname{Tr}\left[e^{-\beta\hat{H}} c_i(\tau) c_j^\dagger(0)\right] / \operatorname{Tr}\left(e^{-\beta\mathcal{H}}\right)$$

$$\simeq -\underbrace{\langle\Phi_G(0)|\, e^{-(\beta-\tau)\hat{H}}}_{\langle\Phi'_C|} c_i(0) \underbrace{e^{-\tau\hat{H}} c_j^\dagger(0)\, |\Phi_G(0)\rangle}_{|\Phi_C\rangle} / \left(e^{-\beta E_G}\right)$$

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

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

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

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:
   $\left|1 - \left\langle \Psi_{EX}(\vec{\theta}) | c_a^\dagger \left|\Psi_G\right\rangle \right|^2$
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)
  (Nooijen, Marcel. 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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$$\mathcal{H} = U\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} - \mu \sum_{\sigma=\uparrow,\downarrow} \hat{n}_{1\sigma} - V \sum_{\sigma=\uparrow,\downarrow} \left(\hat{c}^{\dagger}_{1\sigma}\hat{c}_{2\sigma} + \hat{c}^{\dagger}_{2\sigma}\hat{c}_{1\sigma} \right) + \epsilon_b \sum_{\sigma=\uparrow,\downarrow} \hat{n}_{2\sigma}$$

- 79 sparse sampling points
- Non-diagonal componet also can be computed

Results : Four-site model

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

- At half-filling
- 70 sparse sampling points + adaptive construction of the mesh

Results : Fourier-transformed Green's function

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- We use irbasis (N. Chikano *et al*., Comput. Phys. Commun. **240**, 181 (2019))
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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