

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

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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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- 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:

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

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

# Solving impurity problems with Quantum computer

## Fault-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  $\sim 100$  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

## Hamiltonian

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

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

## Imaginary-time Green's function (GF)

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

- At sufficiently low temperature  $T$

$$G_{ab}(\tau) \xrightarrow{T \rightarrow 0} \mp \left\langle \Psi_G \left| \hat{A}_\pm e^{\mp(\mathcal{H} - E_G)\tau} \hat{B}_\pm \right| \Psi_G \right\rangle, |\Psi_G\rangle : \text{ground state}$$

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

- 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。
- $N \rightarrow N+1 \rightarrow N$
- 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。
- $\beta$ : fictitious 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
- 複素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

R. Sakurai, W. Mizukami, H. Shinaoka,  
[arXiv:2112.02764](https://arxiv.org/abs/2112.02764)

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

For  $\tau > 0$ ,

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



## Preparation

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

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

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

- ◆ **Optimization:** parameter-shift rule

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

$$\frac{\partial \langle H(\theta) \rangle}{\partial \theta_i} = \frac{1}{2} \left( \langle H \left( \theta + \frac{\pi}{2} e_i \right) \rangle - \langle H \left( \theta - \frac{\pi}{2} e_i \right) \rangle \right)$$
$$(U(\boldsymbol{\theta}) = \prod_k e^{-i\theta_k P_k/2})$$

# STAGE2: Single-particle excitation

For  $\tau > 0$ ,

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

1. single-particle excited state

$$c_a^\dagger |\Psi_G\rangle = \frac{X_a - iY_a}{2} Z_{a-1} \dots Z_1 |\Psi_G\rangle$$

2. Prepare  $\left| \phi_{\text{EX}} \left( \vec{\theta}_{\text{EX}} \right) \right\rangle$  and  
measure  $\left\langle \phi_{\text{EX}} \left( \vec{\theta}_{\text{EX}} \right) \left| \hat{c}_a^\dagger \right| \Psi_G \right\rangle$

3. Minimize cost function:

$$|1 - \langle \Psi_{\text{EX}}(\vec{\theta}) | c_a^\dagger | \Psi_G \rangle|^2$$

4. Measure

$$c_1 = \left\langle \phi_{\text{EX}} \left( \vec{\theta}_{\text{EX}}^* \right) \left| c_a^\dagger \right| \Psi_G \right\rangle$$

# STAGE3: Imaginary-time evolution

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- The time-dependent Schrödinger equation

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

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

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

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

- From (1) and (2),

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

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

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

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

## Varuational Quantum Simulation (VQS)

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

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

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

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

## Direct VQS

$$\theta(\tau + \Delta\tau)$$

$$\simeq \operatorname{argmin}_{\vec{\theta}} \| | \phi(\vec{\theta}) \rangle - | \Psi(\tau) \rangle + \Delta\tau (\mathcal{H} - E_\tau) | \Psi(\tau) \rangle \|$$

$$= \operatorname{argmin}_{\vec{\theta}} \operatorname{Re} | \Delta\tau \langle \phi(\vec{\theta}) | H | \Psi(\tau) \rangle - (\Delta\tau E_\tau + 1) \langle \phi(\vec{\theta}) | \Psi(\tau) \rangle |$$

# STAGE4: Transition amplitude

transition amplitude

$$\langle \Psi_G | A_{\pm} | \Psi_{IM} \rangle$$

$$\rightarrow G(\tau) = -c_1 e^{\eta(\tau)} e^{\tau E_G} \langle \Psi_G | A_{\pm} | \Psi_{IM} \rangle$$

## 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  $\sim O(n^4)$

## Optimization

- A quasi-Newton method (BFGS method)

## Non-uniform mesh of $\tau$ 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

R. Sakurai, W. Mizukami, H. Shinaoka,  
[arXiv:2112.02764](#)

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

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

# Results : Four-site model

R. Sakurai, W. Mizukami, H. Shinaoka,  
[arXiv:2112.02764](https://arxiv.org/abs/2112.02764)

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

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



# Results : Fourier-transformed Green's function

R. Sakurai, W. Mizukami, H. Shinaoka,  
[arXiv:2112.02764](#)

- 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
- Our 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

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