Calculation of the Green’s function on near-term quantum computers

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The Green’s function plays a crucial role when studying the nature of quantum many-body systems, especially strongly correlated systems. Although the development of quantum computers in the near future may enable us to compute energy spectra of classically intractable systems, methods to simulate the Green’s function with near-term quantum algorithms have not been proposed yet. Here, we propose two methods to calculate the Green’s function of a given Hamiltonian on near-term quantum computers. The first one makes use of a variational dynamics simulation of quantum systems and computes the dynamics of the Green’s function in real time directly. The second one utilizes the Lehmann representation of the Green’s function and a method which calculates excited states of the Hamiltonian. Both methods require shallow quantum circuits and are compatible with near-term quantum computers. We numerically simulated the Green’s function of the Fermi-Hubbard model and demonstrated the validity of our proposals.

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I. INTRODUCTION

The advent of a primitive but still powerful form of quantum computers, called noisy intermediate-scale quantum (NISQ) devices, is approaching [1]. NISQ devices have a few hundred to thousands of qubits under highly precise control but they are not fault tolerant. It is believed that the behavior of NISQ devices will soon reach a stage that one cannot simulate its dynamics using classical computers, due to exponentially increasing size of the Hilbert space with the number of qubits [2–6]. Therefore, many researchers expect that NISQ devices will exhibit supremacy over classical computers for some specific tasks, even though they cannot execute complicated quantum algorithms requiring a huge number of qubits and gate operations due to the erroneous nature of them [1].

One of the most promising tasks in which near-term quantum computers may outperform classical computers is quantum simulation, where one computes energy eigenvalues and/or eigenstates of a given quantum system. It enables us to calculate and predict properties of quantum many-body systems, which is of great importance to many fields such as quantum chemistry, condensed matter physics, and material science [7,8]. The most celebrated algorithm for quantum simulation on near-term quantum computers is the variational quantum eigensolver (VQE) [9–12], in which energy eigenstates and eigenenergies of the system are obtained based on the variational principle of quantum mechanics. Although the VQE was originally proposed for finding only the ground state, its extension to excited states was discussed in several recent works [13–17].

However, other important quantities to investigate quantum many-body systems other than eigenenergies and eigenstates have remained relatively disregarded in the recent development of near-term quantum algorithms, i.e., the Green’s function and the spectral function [18–20]. They are fundamental to study quantum many-body systems, especially strongly correlated systems; for example, in condensed matter physics, the spectral function tells us that the dispersion relation of quasiparticle excitations of a system, which gives crucial information on high-\(T_c\) superconductivity [21], magnetic materials [22], and topological insulators [23]. While several methods based on the Suzuki-Trotter decomposition of the time evolution operator [24,25] or quantum phase estimation [26–28] were already proposed to calculate the Green’s function on quantum computers (including general multipoint time correlation functions [29] used in gauge theories and nuclear physics [30–32]), they require a large number of qubits and gate operations which are hard to realize with near-term quantum computers.

In this paper, we propose two different algorithms for evaluating the Green’s function on near-term quantum computers. The first one takes advantage of the variational quantum simulation (VQS) algorithm [33–37] for an efficient calculation of the Green’s function in real time. We extend the original VQS algorithm in order to calculate the transition amplitude of general quantum operators between two different quantum states after time evolution. The second one is based on the Lehmann representation of the spectral function [18–20]. By calculating excited states of a given system and evaluating the transition amplitude of appropriate operators by using the subspace-search variational quantum eigensolver (SSVQE) [13] or the multistate contracted VQE (MCVQE) [16], one can compute

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the spectral function (hence the Green’s function). We confirm
the validity of our methods using numerical simulations of
the Fermi-Hubbard model, a model of strongly correlated
system. The extension of our methods to finite temperature
and general correlation functions is also discussed.

The rest of the paper is organized as follows. In Sec. II, we
briefly review the definition of the Green’s function and the
spectral function at zero temperature. In Sec. III, we propose a
method to calculate them by using the VQS algorithm. We
describe another method to calculate the Green’s function and
the spectral function as a simple application of the SSVQE
algorithm [13] and the MCVQE algorithm [16] in Sec. IV.
Section V is dedicated to demonstration of our methods
by performing numerical simulations calculating the spectral
functions of the two-site Fermi-Hubbard model. Section VI
discusses how the depth of the Ansatz for the VQS affects the
accuracy of numerical simulations. In Sec. VII, we discuss the
feasibility of implementing our proposed algorithms on near-
term quantum computers from the viewpoint of the number of
gate operations and their error rate required. We present the
extension of our methods to the finite-temperature Green’s
function in Sec. VIII. We discuss implications and possible
future directions of our results, and make a conclusion in
Sec. IX. Appendix A provides detailed resource estimations
of our algorithms. In Appendix B, we describe details of the
discussion in Sec. VII. Appendix C provides additional
numerical results, e.g., four-site Hubbard model simulation.
Appendix D gives details of the numerical simulations.

II. REVIEW OF THE GREEN’S FUNCTION AND THE
SPECTRAL FUNCTION AT ZERO TEMPERATURE

In this section, we briefly review definition of the Green’s
function at zero temperature for consistency [18–20].

Let us consider a fermionic system described by Hamiltonian
\( H \) which is composed of fermionic creation (anni-
hilation) operators \( c_{\sigma}, c_{\sigma}^\dagger \) where \( a \) is a label to specify the
fermionic mode. For example, \( a \) can be \((k, \sigma)\), where \( k \)
denotes the momentum and \( \sigma = \uparrow, \downarrow \) denotes the spin of the
fermion. The retarded Green’s function at zero temperature is
deﬁned as
\[
G_{ab}^R(t) = -i\Theta(t) \langle c_a(t)c_b^\dagger(0) + c_a^\dagger(0)c_b(t) \rangle_0,
\]
where \( \Theta(t) \) is the Heaviside step function, \( c_a(t) = e^{ith}c_a e^{-ith} \)
is the Heisenberg representation of the operator \( c_a \),
and \( \{ \cdots \}_0 = \{|G\} \cdots |G\} \) denotes the expectation value by
the ground state of the Hamiltonian \( |G\}. We employ the natural
unit where the Planck constant \( h \) and the Boltzmann constant
\( k_B = k_B = 1 \). For simplicity, throughout this paper we consider the Green’s function \( G_{ab}^R \) with \( a = b = (k, \uparrow) \),
namely, the Green’s function in the momentum space with
identical spin. We simply write
\[
G_{(k, \uparrow), (k, \uparrow)}^R(t) = G_{k}^R(t)
\]
in all other parts of the paper. We note that extension of
proposed methods in this study to the Green’s function with
general indices is straightforward.

The Green’s function is related to another important phys-
ical quantity to investigate quantum many-body systems,
namely, the spectral function \( A_k(\omega) \). It is defined through the
Fourier transform of \( G_{k}^R(\omega) \),
\[
G_{k}^R(\omega) = \int_{-\infty}^{\infty} dt e^{i(\omega + i\eta)t} G_{k}^R(t)
\]
\[
=: \int_{-\infty}^{\infty} d\omega' A_k(\omega') \frac{1}{\omega' - \omega + i\eta},
\]
where \( \eta \to +0 \) is a factor to assure the convergence of the
integral. The spectral function and the Green’s function \( G_{k}^R(\omega) \)
have a relation
\[
A_k(\omega) = -\pi^{-1} \text{Im} G_{k}^R(\omega).
\]
Finally, we introduce the Lehmann representation of the spec-
tral function which utilizes the energy eigenvalue \( E_n \) and
the eigenstate of the Hamiltonian \( |E_n\rangle \),
\[
A_k(\omega) = \sum_n \left( \frac{|\langle E_n|c_k^\dagger|G\rangle|^2}{\omega + E_G - E_n + i\eta} + \frac{|\langle E_n|c_k|G\rangle|^2}{\omega - E_G + E_n + i\eta} \right)
\]
where we call the first (second) term as particle (hole) part of
the spectrum function.

In Sec. III, we compute the spectral function by performing
the Fourier transformation to \( G_{k}^R(\omega) \) calculated by the VQS-
based method while we compute it by the Lehmann representa-
tion (6) with quantities calculated by the VQE-based method
in Sec. IV.

III. COMPUTATION OF GREEN’S FUNCTION WITH
VARIATIONAL QUANTUM SIMULATION

In this section, we ﬁrst review the VQS algorithm [33–36]
which calculates a quantum state after the time evolution by
a given Hamiltonian within parametrized Ansatz states. Next,
we propose the method to compute the Green’s function by
extending the original VQS algorithm.

A. Review of variational quantum simulation

Here we review the variational quantum real-time simul-
ation algorithm introduced in Ref. [33]. Let us consider an
Ansatz quantum state created by a parametrized quantum
circuit
\[
|\psi(\bar{\theta})\rangle = U(\bar{\theta})|\psi_0\rangle = U_{N_0}(\theta_{N_0}) \ldots U_{1}(\theta_{1}) \ldots U_{1}(\theta_{1})|\psi_0\rangle,
\]
where \( U_{i}(\theta_{i}) \) is some unitary gate with (real-valued)
parameter \( \theta_{i}, N_0 \) is the number of parameters, and \( |\psi_0\rangle \) is a reference state to create the
Ansatz state. We assume that \( U_{i}(\theta_{i}) \) is composed of a set of Pauli rotation gates \( e^{i\alpha^{(i)}P^{(i)}} \),
with a coefficient \( \alpha^{(i)} \) and a Pauli matrix \( P^{(i)} \), and other nonparametrized gates. For a
given initial state \( |\psi(0)\rangle \) and Hamiltonian \( H \), the VQS
algorithm ﬁnds the solution of the Schrödinger equation,
\[
\frac{d}{dt}|\psi(t)\rangle = -iH|\psi(t)\rangle,
\]
within the Hilbert space spanned by the Ansatz quantum
state \( \{|\psi(\bar{\theta})(t)\rangle\}_{\bar{\theta}} \). Specifically, the time evolution described
by Eq. (8) is mapped to the time evolution of parameters \( \theta(t) \). Al-
though there are several variational principles to map Eq. (8)
to the equations for $\theta(t)$ [38–40], we choose McLachlan’s variational principle [40] in this paper because it is the most stable and physically reasonable among them [34].

McLachlan’s variational principle [40] maps Eq. (8) to the equation of motion of the parameters $\tilde{\theta}(t)$ by minimizing the distance between the exact evolution of the Schrödinger equation and the evolution of the parametrized Ansatz state under infinitesimal variation of time $\delta t$ [33]:

$$\min \delta \left\| \left( \frac{\partial}{\partial \delta t} + iH \right) |\psi(\tilde{\theta}(t))\rangle \right\|,$$

where $|||\psi||| = \langle \psi | \psi \rangle$ is the norm of $|\psi\rangle$. One can explicitly write the equation determining $\{\tilde{\theta}(t)\}$,

$$\sum_j M_{i,j} \tilde{\theta}_j = V_i,$$

where

$$M_{i,j} = \text{Re} \left( \frac{\partial \langle \psi(\tilde{\theta}(t)) | \partial \tilde{\theta}_j \rangle \frac{\partial \langle \psi(\tilde{\theta}(t)) | \partial \tilde{\theta}_i \rangle \partial \tilde{\theta}_j}{\partial \tilde{\theta}_j} \right),$$

$$V_i = \text{Im} \left( \langle \psi(\tilde{\theta}(t)) | H \frac{\partial \langle \psi(\tilde{\theta}(t)) | \partial \tilde{\theta}_j \rangle \partial \tilde{\theta}_j}{\partial \tilde{\theta}_j} \right).$$

for $i = 1, \ldots, N_\theta$. We note that the matrix $M$ and vector $V$ can be efficiently obtained by measurements of quantum circuits as described in Refs. [33,41].

Finally, from the solution of Eq. (10), one can evaluate the parameter at time $t + \delta t$ as $\tilde{\theta}(t + \delta t) \approx \tilde{\theta}(t) + \tilde{\theta}(t) \delta t$. By iterating this procedure from the initial parameters $\tilde{\theta}(0)$, we can obtain the time evolution of the parameters $\tilde{\theta}(t)$ and the quantum state $|\psi(\tilde{\theta}(t))\rangle$. We note that the VQS algorithm can be viewed as approximating the time evolution operator $U(t) = e^{-iHt}$ by the variational quantum circuit $U(\tilde{\theta}(t))$, although the approximation is valid only when the operators are applied for the initial state $|\psi(\tilde{\theta}(0))\rangle$: $U(\tilde{\theta}(t))$ is optimized to the chosen initial state $|\psi(\tilde{\theta}(0))\rangle$ and $U(\tilde{\theta}(t)) |\psi_1\rangle \neq e^{-iHt} |\psi_1\rangle$ for a different initial state $|\psi_1\rangle$ in general.

B. Computation of Green’s function

Now, we discuss how we can apply the VQS algorithm for evaluating the Green’s function. What we want to evaluate is the retarded Green’s function for $t > 0$: $G_k^R(t) = -i \langle G | e^{iHt} c_{k,\uparrow} e^{-iHt} c_{k,\downarrow}^\dagger | G \rangle + \langle G | c_{k,\downarrow}^\dagger e^{iHt} c_{k,\uparrow} e^{-iHt} | G \rangle \rangle$. (12)

The first and second terms can be evaluated similarly, so we focus on the first term.

First, we prepare the (approximate) ground state of a given Hamiltonian $H$ described by $N$ qubits on near-term quantum computers, by using the conventional VQE method [9–12] or the variational imaginary-time simulation algorithm [35,42]. We denote it as $|G\rangle = U_G |\psi_0\rangle$ with a unitary $U_G$ and a reference state $|\psi_0\rangle$. Next, we decompose the fermion operator $c_{k,\uparrow}$ into a sum of Pauli matrices [7,8,43–45],

$$c_{k,\uparrow} \rightarrow \sum_{n=1}^{N_\lambda} \lambda_n^{(k)} P_n, \quad c_{k,\downarrow} \rightarrow \sum_{n=1}^{N_\lambda} \lambda_n^{(k)} P_n,$$

for $k = 1, \ldots, N$. Then, $G_k^R(t)$ can be rewritten as

$$G_k^R(t) \approx \langle G | U_G \sum_{n=1}^{N_\lambda} \lambda_n^{(k)} P_n U_G^\dagger e^{-iHt} | G \rangle \rangle.$$
operator $U(t) = e^{-iHt}$ are different between two initial states $|G⟩$ and $|P_j⟩$. If we can construct the variational circuit $U(\tilde{θ}(t))$ which simultaneously approximates the time evolution operator for the initial states $|G⟩$ and $|P_j⟩$, we obtain

$$
⟨G|e^{iHt}P_j e^{-iHt}P_j|G⟩ 
\approx (G|U(\tilde{θ}(t)))^L P_U (\tilde{θ}(t)) P_j|G⟩.
$$

(18)

In this case, the quantum circuit for evaluating the term is significantly simplified as depicted in Fig. 2. We will now describe how to construct such variational quantum circuit which simultaneously approximates the time evolution operator for general multiple states.

Here, we consider the most general case where we have $L$ multiple initial states for the time evolution $⟨|ψ_l⟩|^L_{l=0}$. Let us consider a state with ancilla

$$
|Ψ₀⟩ = \frac{1}{\sqrt{L}} \sum_{l=0}^{L-1} |l⟩_a ⊗ |ψ_l⟩_s,
$$

(19)

where subscripts $a$ and $s$ denote the ancilla and the system of interest, respectively, and $\{|l⟩_a⟩\}$ is orthonormal state of the ancilla. We note that when $2^{k+1} < L ≤ 2^k$, $k$ ancilla qubits are needed. By using the VQS algorithm to the state $|Ψ₀⟩$ with the variational quantum circuit $I_a ⊗ U_s(\tilde{θ})$, we can construct the unitary operator $U_s(\tilde{θ}(t))$ which approximately behaves as the time evolution operator for $⟨|ψ_l⟩|^L_{l=0}$. To be more concrete, the Ansatz state for the VQS algorithm is

$$
|Ψ(\tilde{θ})⟩ := I_a ⊗ U_s(\tilde{θ})|Ψ₀⟩
= \frac{1}{\sqrt{L}} \sum_{l=0}^{L-1} |l⟩_a ⊗ |ψ_l(\tilde{θ})⟩_s,
$$

(20)

where we define $|ψ_l(\tilde{θ})⟩_s = U_s(\tilde{θ})|ψ_l⟩$. The $M$ matrix and $V$ vector in Eq. (11) become

$$
M_{i,j} = \text{Re}\left( \frac{∂⟨Ψ(\tilde{θ}(t))|∂ψ(l(\tilde{θ}(t)))⟩_s}{∂θ_i} \frac{∂⟨ψ(l(\tilde{θ}(t)))|∂ψ(l(\tilde{θ}(t)))⟩_s}{∂θ_j} \right)
= \frac{1}{L} \sum_{l=0}^{L-1} \text{Re}\left( \frac{∂⟨ψ(l(\tilde{θ}(t)))|∂ψ(l(\tilde{θ}(t)))⟩_s}{∂θ_i} \frac{∂⟨ψ(l(\tilde{θ}(t)))|∂ψ(l(\tilde{θ}(t)))⟩_s}{∂θ_j} \right)
$$

(21)

From this expression, one notices that this algorithm minimizes the average of $δ∥(\partial/\partial t + iH)ψ(\tilde{θ}(t))∥/l$ for $l = 0, \ldots, L – 1$. We also note that the algorithm itself can run without resorting to the ancilla because each summation in Eqs. (21) and (22) can be computed by a distinct quantum circuit: one can compute each term in different run of quantum computers and sum up them by classical computers. The advantage of using the ancilla is that we can compute $M$ and $V$ for exponentially increasing number of input states in terms of the number of ancilla qubits. For example, when $L = 4$ one should sum up results of four runs of quantum computers without the ancilla, whereas one run is necessary with the ancilla (accompanying with the drawback of the complicated quantum circuit). We remark that the evaluation of the transition amplitude between the time-evolved states $|ψ(l(\tilde{θ}(t)))⟩ = U(\tilde{θ})|ψ_l⟩$ requires some ancilla qubits in general such as Fig. 2.

In the case of calculation of the Green’s function, the initial states are $|ψ₀⟩ = |G⟩$ and $|ψ₁⟩ = |P_j⟩$. The Ansatz quantum state (20) for the VQS algorithm can be constructed by a quantum circuit shown in Fig. 3.

To sum up, the calculation of each term in Eq. (14), and consequently the Green’s function, with the VQS algorithm proceeds as follows:

1. Prepare the approximate ground state of a given Hamiltonian $H$ by conventional methods on near-term quantum computers, such as the VQE [9–12]. We denote the ground state as $|G⟩ = U_G|ψ₀⟩$.

2. Construct the variational quantum circuit $U(\tilde{θ})$ which approximates the time evolution $e^{-iHt}$ for two initial states $|G⟩$ and $|P_j⟩$. The VQS algorithm with the circuit shown in Fig. 3 will find such $U(\tilde{θ})$.

3. Evaluate $⟨G|U(\tilde{θ})⟩P_U (\tilde{θ}) |P_j⟩$ by the quantum circuit shown in Fig. 2.

Finally, we present a detailed resource estimation about the number of required distinct runs of the quantum circuits for this algorithm in Appendix A.
IV. COMPUTATION OF GREEN’S FUNCTION WITH EXCITED-STATES SEARCH ALGORITHM

In this section, we describe another method to compute the Green’s function of a given quantum system. We compute the energy eigenstates and transition amplitudes of fermion operators by the algorithm based on the SSVQE method [13] and the MCVQE method [16], and take advantage of the Lehmann representation of the spectral function (6). We discuss two types of algorithms for calculating the excited states and the transition amplitudes. The first one is based on the SSVQE algorithm with different weights where one obtains the excited states directly on quantum computers, while the second one is based on the SSVQE algorithm with identical weights where some classical postprocessing after the use of quantum computers is required. The computation of the first algorithm is simpler than that of the second one, but the convergence of the algorithm is better for the second one in general. We note that the essential part of the algorithm described in this section is already discussed in Refs. [13,16], so our contribution will be application of it for calculation of the Green’s function.

A. Computation by SSVQE with different weights

Let us consider finding $K$ smallest eigenenergies and eigenstates of a given Hamiltonian. The SSVQE algorithm with different weights finds the variational quantum circuit $U(\tilde{\theta}^*)$ which makes input orthonormal states $|\psi_j\rangle_{j=0}^{K-1}$ into approximate eigenstates of $H$, $|\tilde{E}_j\rangle := U(\tilde{\theta}^*)|\psi_j\rangle$. The approximate eigenenergies are obtained as $\tilde{E}_j := \langle \tilde{E}_j | H | \tilde{E}_j \rangle = \langle \psi_j | U(\tilde{\theta}^*) H U(\tilde{\theta}^*) | \psi_j \rangle$. The algorithm performs this task by minimizing the cost function

$$C_0(\tilde{\theta}) = \sum_{j=0}^{K-1} w_j \langle \psi_j | U(\tilde{\theta}^*) H U(\tilde{\theta}^*) | \psi_j \rangle,$$

with respect to the parameters $\tilde{\theta}$, where $w_0 > \cdots > w_{K-1} > 0$ are weights which ensure the approximate eigenstates $|\tilde{E}_j\rangle_j$ have the ascending order $E_0 \leq \cdots \leq E_{K-1}$. After convergence of the classical minimization for $C_0(\tilde{\theta})$, one obtains optimal parameters $\tilde{\theta}^*$ and can compute $|\tilde{E}_j\rangle, |\tilde{E}_j\rangle_j$.

To compute the Lehmann representation of the spectral function (6), we also need the transition amplitude of the fermions $c_{k\lambda}, d_\lambda \dagger$, such as $\langle \tilde{E}_j | c_{k\lambda} \dagger | \tilde{E}_l \rangle$. In general, the evaluation of the transition amplitude between different quantum states needs a complicated quantum circuit, but in this case the evaluation will be done in a simple way due to the fact that $|\tilde{E}_j\rangle_j$’s are created from the same unitary gate $U(\tilde{\theta}^*)$. Specifically, if we can easily make superpositions of the input states $|\psi_j\rangle$ and $|\psi_j\rangle$, $\langle \tilde{E}_j | c_{k\lambda} \dagger | \tilde{E}_l \rangle$ can be evaluated by simply taking the expectation value of $c_{k\lambda}$ for several superpositions. To see this, first we map $c_{k\lambda}$ into qubit operators like Eq. (14) and decompose it into real part and imaginary part, $c_{k\lambda} = A_k + iB_k$, where $A_k$ and $B_k$ are Hermitian operators. Then, we have

$$\langle \psi_j | U(\tilde{\theta}^*) c_{k\lambda} \dagger U(\tilde{\theta}^*) | \psi_j \rangle = \langle \psi_j | U(\tilde{\theta}^*) A_k U(\tilde{\theta}^*) | \psi_j \rangle + i \langle \psi_j | U(\tilde{\theta}^*) B_k U(\tilde{\theta}^*) | \psi_j \rangle.$$

Each term can be evaluated by using $|\psi_j\rangle^\pm = U(\tilde{\theta}^*) (|\psi_j\rangle \pm |\psi_j\rangle) / \sqrt{2}$ and $|\psi_j\rangle^\pm = U(\tilde{\theta}^*) (|\psi_j\rangle \pm |\psi_j\rangle) / \sqrt{2}$ as

$$\text{Re}(\langle \psi_j | U(\tilde{\theta}^*) A_k U(\tilde{\theta}^*) | \psi_j \rangle) = \langle \psi_j^+ | A_k | \psi_j^- \rangle - \langle \psi_j^- | A_k | \psi_j^+ \rangle,$$

$$\text{Im}(\langle \psi_j | U(\tilde{\theta}^*) A_k U(\tilde{\theta}^*) | \psi_j \rangle) = \langle \psi_j^+ | A_k | \psi_j^- \rangle - \langle \psi_j^- | A_k | \psi_j^+ \rangle,$$

and similar equations for the $B_k$ term.

In typical situations, the input states are taken as simple states, e.g., computational basis, so preparing superpositions of them on quantum computers is not so difficult. Therefore, by substituting eigenenergies of Eq. (6) with $\tilde{E}_j$ and the transition amplitudes with $\langle \tilde{E}_0 | c_{k\lambda} \dagger | \tilde{E}_j \rangle$, we can evaluate the spectral function and the Green’s function accordingly.

B. Computation by SSVQE with identical weights

Next, we introduce another type of algorithm to obtain excited states and the transition amplitude between them. This algorithm combines the SSVQE algorithm with identical weights and the quantum subspace expansion method [17,46], and is essentially the same as the MCVQE algorithm [16].

The procedure of the algorithm is as follows. First, we prepare orthonormal input states $|\psi_j\rangle_{j=0}^{K-1}$, which are simple and easy to realize a superposition of them on quantum computers. Then, we minimize the cost function

$$C_1(\tilde{\theta}) = \sum_{j=0}^{K-1} \langle \psi_j | U(\theta^*) H U(\theta^*) | \psi_j \rangle,$$

with respect to parameters $\tilde{\theta}$, where $U(\tilde{\theta})$ is the Ansatz quantum circuit. After the optimization, the subspace spanned by $|\psi_j(\theta^*\rangle_{j=0}^{K-1}$ will be close to that spanned by the true $K$ eigenstates $|\psi_j\rangle_{j=0}^{K-1}$, where $\theta^*$ is the parameter after optimization. At this stage, $U(\theta^*)|\psi_j\rangle$ is generally the superposition of the excited states $|\psi_j\rangle_{j=0}^{K-1}$ and $\langle \psi_j | U(\theta^*) H U(\theta^*) | \psi_j \rangle$ is not a good approximation to the true eigenvalue $\tilde{E}_j$. Therefore, to obtain the eigenstates and eigenvalues of $H$, we solve the eigenvalue problem within the subspace spanned by $|\psi_j(\theta^*\rangle_{j=0}^{K-1}$,

$$\mathcal{H} \mathcal{V} = \mathcal{V} \mathcal{E},$$

where $\mathcal{H}_{i,j} = \langle \psi_i | U(\theta^*) H U(\theta^*) | \psi_j \rangle$, $\mathcal{V}$ is $K \times K$ matrix containing eigenvectors as its columns, and $\mathcal{E}$ is a diagonal matrix whose diagonal elements are eigenvalues. The approximate $m$th excited state $|\tilde{E}^m\rangle$ is expressed as

$$|\tilde{E}^m\rangle = \sum_j \mathcal{V}_{j,m} U(\theta^*) |\psi_j\rangle,$$

and the approximate eigenenergies appear as $\tilde{E}_j = \mathcal{E}_{j,j}$.

The transition amplitude $c_{m,n}^{(k)} = \langle \tilde{E}^m_{n} | c_{k\lambda} \dagger | \tilde{E}^n_{m} \rangle$ can be computed as

$$C_{m,n}^{(k)} = \sum_{j,j^*} \mathcal{V}_{j,m}^{*} \mathcal{V}_{j^*,n} \langle \psi_j | U(\theta^*) c_{k\lambda} \dagger U(\theta^*) | \psi_{j^*} \rangle.$$
\[ H = -t \sum_{\sigma \in \uparrow, \downarrow} (c_{i,\sigma} \sigma c_{i,\sigma} + \text{H.c.}) + U \sum_{i=1}^{2} c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger c_{i,\downarrow}^\dagger c_{i,\uparrow}^\dagger, \]

where \( t \) is a parameter characterizing hopping between the sites and \( U \) denotes the strength of the onsite Coulomb repulsion [47–49]. We set the hopping parameter \( t = 1 \) throughout this paper. We simulate two proposed protocols in Secs. III and IV by classical computers with the fast quantum circuit simulation library QULACS [50]. We use the Jordan-Wigner transformation [45] to map the fermionic Hamiltonian (30) into the qubit one with four qubits by using the library OPENFERMION [51].

A. Numerical simulation of the method based on variational quantum simulation

We calculate the real-time Green’s function of the model (30) at zero temperature by using the method described in Sec. III. First, we prepare the ground state of the model (30) by the standard VQE algorithm with a hardware-efficient-type Ansatz [10] depicted in Fig. 4. Then, we perform the VQS algorithm. As an Ansatz quantum state, we adopt the so-called variational Hamiltonian Ansatz [52,53] inspired by the Suzuki-Trotter decomposition of the time evolution operator \( e^{-itH} \). The variational Hamiltonian Ansatz is defined through

\[ H_{\text{qubit}} = \sum_{m} c_m P_m, \]

where \( P_m \) is a (multiqubit) Pauli matrix and \( c_m \) is a coefficient. An Ansatz state for the variational Hamiltonian Ansatz is given by \( |\psi(\theta)\rangle = U_{VH,A}(\theta)|\psi_0\rangle \), where

\[ U_{VH,A}(\theta) = \prod_{m,d} \left( \prod_{m} \exp \left( i\theta_m^{(d)} P_m \right) \right), \]

and \( n_d \) denotes the depth of the Ansatz. We note that we remove the identity operator from Eq. (31) when constructing the Ansatz. If the qubit representation of the Hamiltonian (31) has \( N_p \) terms (except for the identity operator), the number of parameters of the Ansatz will be \( N_p n_d \). In our simulation, \( N_p = 6 \) and we choose \( n_d = 8 \), so there are 48 parameters in the parametrized quantum circuit whereas general unitary operators on the system have \( (2^4)^2 = 256 \) parameters. Further details on numerical calculations are described in Appendix D.

The result is shown in Fig. 5. The VQS algorithm nicely reproduces the exact dynamics (the panels in left and center columns), and the spectral function (right columns). These figures illustrate the possibility of the VQS algorithm proposed in this study to calculate the Green’s function. In Sec. VI, dependence of the results on the depth of the Ansatz is analyzed. Furthermore, numerical simulations for \( n_d = 4 \) and the four-site Fermi-Hubbard model are presented in Appendix C. One can see that numerical results for \( n_d = 4 \) have almost the identical performance compared to the case of \( n_d = 8 \); therefore, depending on strength of physical noises, the choice of \( n_d = 4 \) may be recommended to avoid accumulation of physical errors.

B. Numerical simulation of the method based on excited-state search

Next, we numerically simulate the method described in Sec. IV. We adopt the symmetry-preserving Ansatz [54] drawn in Fig. 6, which preserves the total number of particles in the system. We use the SSVQE algorithm with identical weight and calculate five energy eigenstates of the model (30). As input states, we simply choose the computational basis states with desired particle number: to calculate the particle (hole) part of the spectrum function, we choose \(|\psi_0\rangle = |0011\rangle\) for the ground state, \(|\psi_1\rangle = |0001\rangle, |\psi_2\rangle = |0010\rangle, |\psi_3\rangle = |0100\rangle, |\psi_4\rangle = |1000\rangle\) for the first excited state \(|\psi_1\rangle = |0111\rangle, |\psi_2\rangle = |1011\rangle, |\psi_3\rangle = |1101\rangle, |\psi_4\rangle = |1110\rangle\) for the excited states.

Figure 7 shows the result of numerical simulation. The SSVQE algorithm almost perfectly reproduces the exact result obtained by exact diagonalization.

VI. DEPENDENCE OF ACCURACY OF THE VARIATIONAL QUANTUM SIMULATION ON DEPTH OF THE ANSATZ

In this section, we provide a systematic analysis on how the accuracy of the numerical simulations of the variational quantum simulation (VQS) in Sec. V depends on the depth \( n_d \) of the Hamiltonian Ansatz [Eq. (32)]. We run numerical
CALCULATION OF THE GREEN’S FUNCTION … PHYSICAL REVIEW RESEARCH 2, 033281 (2020)

FIG. 5. Numerical simulation of the VQS algorithm to compute the Green’s function in real time $G_k(t)$ [(a), (b), (d), (e)] and the spectral function [(c), (f)] for the model (30) of $U = 3$ [(a)–(c)] and $U = 6$ [(d)–(f)]. The time step is taken as $dt = 0.1(0.03)$ for $U = 3(6)$. The exact spectral function is calculated by the exact dynamics of the Green’s function in real time from $t = 0$ to 100 with step $dt = 0.1$. We take $\eta = 0.2$ for the calculation of the spectral functions.

simulations for $n_d = 4, 5, \ldots, 10$ under the same conditions as in Fig. 5.

To see the accuracy of the simulations quantitatively, we calculate the mean absolute error (MAE) of the spectrum function at $k = \pi$ in the region of $\omega \in [-5, 5]$,

$$\Delta_E(k) = \frac{1}{2N_\omega + 1} \sum_{n=-N_\omega}^{N_\omega} \left| A_{\text{exact}}(k, \omega = \frac{5n}{N_\omega}) - A_{\text{VQS}}(k, \omega = \frac{5n}{N_\omega}) \right|,$$

(33)

where $2N_\omega + 1$ is the total number of data points and $A_{\text{exact(VQS)}}(k, \omega)$ is the spectrum function calculated by exact diagonalization (VQS). We take $N_\omega = 5000$. Interestingly, as seen from Fig. 8, the MAE decreases with the inverse of the depth of the Ansatz. This dependence reminds us of the Suzuki-Trotter decomposition of the time evolution operator, i.e.,

$$U(t) = e^{-\i H_{ptot} t} \approx U_{n_d}^\text{tro}(t) = \left( \prod_m e^{-\i H_{rd} t_{rd}} \right)^{n_d}$$

(34)

with the error of $O(t^2/n_d)$, where we have used the notation in Eq. (31). In Fig. 8, we also show the MAE of the spectrum function calculated by the dynamics obtained from the approximate time evolution operator (34) with the same time step and duration used for the VQS. The MAE for this case exhibits $1/n_d$ dependence as expected, but the values of the MAE are much larger than those for the VQS; the slope of the fit of the MAE with $1/n_d$ is about six times smaller for the VQS ($1.820/0.285 \approx 6.4$). The result shown in Fig. 8 not only provides an estimation of errors in the VQS calculation when the Ansätze with various depths are used, but also illustrates the practical advantage of employing the VQS compared with the Suzuki-Trotter decomposition of the time evolution operator which has the same-depth quantum circuit.

VII. FEASIBILITY OF QUANTUM ALGORITHMS ON NEAR-TERM QUANTUM COMPUTERS

In this section, we discuss the feasibility of implementing our proposed algorithms on near-term quantum computers. Let us consider 25 sites two-dimensional Fermi-Hubbard model on a square lattice, whose exact simulation requires 50 qubits and is almost intractable for classical computers. The

FIG. 6. (Top) Definition of the symmetry-preserving Ansatz [54] used for the demonstration of the SSVQE algorithm with identical weight. (Bottom) Definition of the $A$ gate. Here, $R(\theta, \phi)$ is defined as $R(\theta, \phi) = R_x(\theta + \pi/2)R_z(\phi + \pi)$, where $R_x(\theta) = e^{\i \theta/2}$ and $R_z(\phi) = e^{\i \phi/2}$.
model is defined as
\[ H_{2d} = -t \sum_{(i,j),\sigma} \epsilon_i \sigma_i^{\dagger} c_j \sigma + H.c. + U \sum_i \epsilon_i \sigma_i^{\dagger} \sigma_i \sigma_i^{\dagger} \sigma_i , \]  
where \((i,j)\) runs nearest-neighbor sites on a square lattice and \(\sigma = \uparrow, \downarrow\) denotes the spin. Based on the argument in Ref. [55], using the Hamiltonian Ansatz [Eq. (32)] with the Jordan-Wigner transformation, we need \(N_{\text{gate}} \approx 1000\) two-qubit gates per depth of the Ansatz when we employ the rotation \(Z\) gate and partial swap gates as elementary gates. Although near-term quantum computers contain inevitable noise in gate operations, the technique of quantum error mitigation [56,57] can suppress errors and recover noiseless results with a reasonable overhead when the error rate per gate \(\epsilon_{\text{gate}}\) satisfies \(N_{\text{gate}} \epsilon_{\text{gate}} \lesssim 2\), where \(N_{\text{gate}}\) is the number of gates. Therefore, when we adopt the Hamiltonian Ansatz of two depths as an Ansatz quantum circuit for the VQS or the SSVQE, we need at least 2/2000 = 0.1% for the error rate of two-qubit gates, which has been achieved in current experimental setups [58,59]. We note that the error of single-qubit gate is ignored here because it is negligible compared with that of two-qubit gate. Only a few additional controlled operations in the VQS-based algorithm introduced in Sec. III are also neglected. In addition, for the VQS-based algorithm, gates for the unitary \(U_G\) which prepares the ground state of the system must be taken into account. The more detailed argument has been made in Appendix B.

**VIII. EXTENSION TO FINITE-TEMPERATURE GREEN’S FUNCTION**

Here, we discuss the extension of our proposed methods to the Green’s function at finite temperature. For finite temperature \(T > 0\) or inverse temperature \(\beta = 1/T < \infty\), the retarded Green’s function is defined as
\[
G_k^R(t; \beta) = \frac{1}{Z(\beta)} \sum_n e^{-\beta E_n} G_{k,n}^R(t),
\]
where \(Z(\beta) = \text{Tr}(e^{-\beta H})\),
\[
G_{k,n}^R(t) = -i \Theta(t) \langle E_n \vert e^{iHt} c_k^{\dagger} e^{-iHt} c_k \vert E_n \rangle
+ \langle E_n \vert c_k^{\dagger} e^{iHt} c_k e^{-iHt} \vert E_n \rangle,
\]
where \(|E_n\rangle\) and \(E_n\) denote the eigenstates and eigenvalues of Hamiltonian \(H\), respectively. The corresponding spectral function is
\[
\tilde{G}_k^R(\omega; \beta) = \int_{-\infty}^{\infty} dt e^{i\omega t+i\eta y} G_k^R(t; \beta),
\]
\[
A_k(\omega; \beta) = \frac{1}{Z(\beta)} \sum_{n,m} e^{-\beta E_n} \left( \frac{|\langle E_n \vert c_k^{\dagger} \vert E_m \rangle|^2}{\omega + E_m - E_n + i\eta} + \frac{|\langle E_n \vert c_k \vert E_m \rangle|^2}{\omega - E_m + E_n + i\eta} \right).
\]

**A. Variational quantum simulation for Green’s function at finite temperature**

Equation (36) can be evaluated on quantum computers by combining the VQS method and the thermofield double...
technique which purifies the Gibbs state of the system. The procedure is essentially the same as the finite-temperature version of the density matrix renormalization group method [60,61]. We note that several methods based on the typicality in Hilbert spaces of chaotic quantum systems at finite temperature [62–64] might also be combined with the VQS algorithm.

Let us consider a $N$-qubit “environment” system (denoted by subscript $e$) in addition to the original $N$-qubit system of interest (denoted by subscript $s$). First, we prepare a state $|\Phi_0\rangle$ which satisfies $\text{Tr}_e(|\Phi_0\rangle\langle\Phi_0|) = I$. For example, we choose $|\Phi_0\rangle = \frac{1}{\sqrt{2^N}} \sum_{i=0}^{2^N-1} |\hat{\phi}_i\rangle \otimes |\hat{i}\rangle$, where $|\hat{\phi}_i\rangle \otimes |\hat{i}\rangle$ is the computational basis of the system and environment. By using the method of variational imaginary-time evolution introduced in Ref. [34], one can obtain the state $|\Phi(\beta)\rangle \approx Z(\beta)^{-1/2}e^{-\beta H/2}|\Phi_0\rangle$. Namely, the variational imaginary-time evolution for the total system with the “Hamiltonian” $H \otimes I_e$ and the variational quantum circuit drawn in Fig. 9 will produce $|\Phi(\beta)\rangle$. We note that $|\Phi(\beta)\rangle$ satisfies

$$\text{Tr}_e(|\Phi(\beta)\rangle\langle\Phi(\beta)|) \approx \frac{1}{Z(\beta)} e^{-\beta H}. \quad (38)$$

Next, we perform the same VQS algorithm for the Green’s function at zero temperature by replacing $|G\rangle$ with $|\Phi(\beta)\rangle$. It will bring out the variational quantum circuit on the original system $U_s(\vec{\theta})$ satisfying

$$\langle\Phi(\beta)\rangle U_s(\vec{\theta}) P_{j}^{s} U_s(\vec{\theta}) P_{j}^{s} |\Phi(\beta)\rangle \nonumber$$

$$\approx \langle\Phi(\beta)\rangle e^{iH t_j} P_{j}^{s} e^{-iH t_j} P_{j}^{s} |\Phi(\beta)\rangle \nonumber$$

$$= \frac{1}{Z(\beta)} \sum_n e^{-\beta E_n} \langle E_n | e^{iH t_j} P_{j}^{s} e^{-iH t_j} P_{j}^{s} | E_n \rangle, \quad (39)$$

where superscript of the Pauli operator $P_{j}^{s}$ implies that it only acts on the system $s$. In Fig. 10, we show the Ansatz quantum circuit to construct the unitary gate $U_s(\vec{\theta}(t))$. By substituting the above quantity into Eq. (36), we can evaluate (each term of) $G_{ik}(t; \beta)$.

We finally remark on another way to evaluate Eq. (36) based on the VQS algorithm. It is possible to obtain several approximate eigenenergies $|\hat{E}_n\rangle_{n=1}^{K}$ and eigenstates $|\hat{E}_n\rangle_{n=1}^{K}$ of the system by the SSVQE or MCVQE algorithm, and to perform the VQS algorithm in Sec. III for each obtained eigenstate $|\hat{E}_n\rangle$. The result approximates $G_{ik}^{0}(t)$ in Eq. (36), so substituting it as well as $E_n$ into Eq. (36) will give the Green’s function at finite temperature (with truncating the summation up to $n = K$). This type of the algorithm does not need the environment qubits, but the number of energy eigenstates $K$ to evaluate the Green’s function with fixed accuracy would exponentially increase as the size of the system and the inverse temperature $\beta$.

B. Computing Green’s function at finite temperature with excited-states search method

Extension of the algorithm in Sec. IV to the finite-temperature Green’s function is rather simple. Since we already introduce a way to evaluate the quantity $|\langle E_n | H_k | E_m \rangle|^2$, putting them into Eq. (37) gives the spectral function at finite temperature with truncating the summation up to $n = K$, where $K$ is the number of eigenstates obtained by the excited-states search algorithms. Again, this method also has a potential problem of the exponentially increasing number of eigenstates required to compute the Green’s function with fixed accuracy.

IX. DISCUSSION AND CONCLUSION

In this paper, we proposed two methods for calculating the Green’s function compatible with NISQ hardwares. One of the proposed methods uses the conventional VQE to prepare a ground state, and directly calculate the real-time retarded Green’s function for the obtained ground state by the VQS algorithm. We introduced a method for constructing a variational quantum circuit which acts as the time evolution operator for multiple initial states simultaneously, and makes the quantum circuit for computation of the Green’s function significantly shallower. Note that this method can be straightforwardly applied to evaluation of the linear response function [65] expressed as

$$\phi_{BA}(t-t') = i \langle B(t-t') A(0) \rangle_0,$$

$$B(t-t') = e^{iH(t-t')} Be^{-iH(t-t')}, \quad (40)$$

where $A$ is an observable coupled to external field, for example, magnetic moment or charge density, $B$ an observable to be measured. The other proposed method evaluates the transition amplitude of the fermion operators between energy eigenstates of the system by exploiting either the SSVQE or MCVQE method, and computes the spectral
function and the Green’s function with the use of the Lehmann representation.

In numerical simulation for the Green’s function at zero temperature, both methods successfully reproduced the spectral function of the two-site Fermi-Hubbard model. We here discuss possible causes to hinder or deteriorate the performance of the methods for general large systems. For the first method by the VQS algorithm, the choice of the Ansatz for the real-time evolution is crucial: once the variational quantum state is out of the correct trajectory in the Hilbert space, it is rare that the state returns to it. Therefore, the Ansatz has to be chosen carefully so that the simulated quantum state has remained in a correct trajectory. As for the second method by the excited-states search methods, it is in general unclear how many excited states are required to reach the desired precision of the Green’s function. It will possibly grow exponentially as the inverse temperature $\beta$ and the size of the system $N$. We leave the investigation of these problems and further comparison of two methods proposed in this study to future work.

Since the Green’s function is fundamental to study the nature of quantum systems, we believe our study will extend the possibility to utilize near-term quantum computers in condensed matter physics, quantum chemistry, and materials science.

Note added in proof. Recently, a paper discussing calculation of the Green’s function with NISQ devices appeared [66]. The method used in that paper is based on the Lehmann representation of the Green’s function, and the authors calculated excited states of the system by performing the VQE with penalty terms which are proportional to the overlaps between previously found low excited states [14,15].

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APPENDIX A: RESOURCE ESTIMATION OF THE ALGORITHM BASED ON THE VARIATIONAL QUANTUM SIMULATION

In this Appendix, we discuss the number of distinct runs of quantum circuits required to implement our algorithm based on the VQS introduced in Sec. III. We first show that the error of the Green’s function can be upper bounded by a product of the operator norm of observables involved in the Green’s function and the trace distance between the ideal time-evolved state and the state computed by the VQS. Next, based on the argument in Ref. [33], we discuss the errors of the real-time Green’s function and clarify two sources of error: algorithmic error and implementation error. Finally, we estimate the number of total distinct runs of quantum circuits needed to achieve a certain accuracy in computing the Green’s function in the frequency domain, i.e., the spectral function.

1. Relationship between the error of the Green’s function and the trace distance

   a. Difference of expectation values of an observable between two states

First, we prove the difference of expectation values of an observable $M$ for two distinct quantum states (density matrices) $\rho$ and $\sigma$ can be upper bounded by the product of the operator norm of $M$ and the trace distance of the two states. It follows that

$$\text{Tr}[M(\rho - \sigma)] = \sum_k m_k \text{Tr}[E_k(\rho - \sigma)]$$

$$\leq \sum_k |m_k| |\text{Tr}[E_k(\rho - \sigma)]|$$

$$\leq \sum_k \|M\| |\text{Tr}[E_k(\rho - \sigma)]|$$

$$= 2\|M\| D(\rho, \sigma),$$  \hspace{1cm} (A1)

where $\|M\|$ is an operator norm of $M$ (the largest singular value of $M$), and $M = \sum_k m_k E_k$ is the spectral decomposition of $M$ ($m_k$ is an eigenvalue of $M$ and $E_k$ is the corresponding projector). We used $|\text{Tr}[E_k(\rho - \sigma)]| \leq |\text{Tr}[E_k(\rho - \sigma)]|$ [67] and $\sum_k E_k = I$.

   b. Error of the Green’s function as the trace distance of the ideal state and the trial state

Next, we show the trace distance between the exact state after time evolution and the state obtained by the VQS gives the upper bound of the error of the calculated Green’s function in our algorithm. For simplicity, we only consider $t > 0$.

Let us introduce two wave functions as

$$|\Psi(\tilde{\theta}(t))\rangle = \frac{1}{\sqrt{2}} (|0\rangle_a \otimes U(\tilde{\theta}(t))|G\rangle_s + |1\rangle_a \otimes U(\tilde{\theta}(t))P_j|G\rangle_s),$$  \hspace{1cm} (A2)

$$|\Phi(t)\rangle = \frac{1}{\sqrt{2}} (|0\rangle_a \otimes e^{-iHt}|G\rangle_s + |1\rangle_a \otimes e^{-iHt}P_j|G\rangle_s),$$  \hspace{1cm} (A3)

where a subscript $a$ denotes an ancilla qubit and $|G\rangle_s$ is the ground state of the system.

In our algorithm based on the VQS, the Green’s function is calculated based on the following decomposition [Eq. (14) in the main text]:

$$G_{ij}^k(t) = \sum_{i,j} \lambda_i^{(k)} \lambda_j^{(k)} \langle G|e^{-iHt}P_j e^{-iHt}P_i G\rangle$$

$$\equiv \sum_{i,j} \lambda_i^{(k)} \lambda_j^{(k)} G_{ij}^{(0)}(t).$$  \hspace{1cm} (A4)
The quantity $G_{ij}^{(0)}(t)$ is approximated by

$$G_{ij}(\tilde{\theta}(t)) \equiv \langle \Psi(\tilde{\theta}(t)) | X_a | \Psi(\tilde{\theta}(t)) \rangle + i \langle \Psi(\tilde{\theta}(t)) | Y_a | \Psi(\tilde{\theta}(t)) \rangle,$$

where the measurement of $X_a$ and $Y_a$ correspond to the cases we set $\phi = 0, \pi/2$ in Fig. 2 in the main text, respectively. By using Eq. (A1), the error of this approximation is upper bounded as

$$\epsilon_{i,j} \equiv | \tilde{G}_{i,j}(\tilde{\theta}(t)) - G_{i,j}^{(0)}(t) | \leq 2 \sqrt{2} D(\Phi(0)), | \Phi(t) \rangle + \frac{\sqrt{2}}{\sqrt{N_m}}.$$

where $\tilde{G}_{i,j}(\tilde{\theta}(t))$ is an experimentally obtained value of $G_{i,j}(\tilde{\theta}(t))$ according to Eq. (A5) and we denote the trace distance between two pure states $| \phi \rangle \langle \phi |$ and $| \phi' \rangle \langle \phi' |$ as $D(\phi, \phi')$. The second term in the right-hand side indicates the shot noise, where $N_m$ is the number of measurements for $X_a$ and $Y_a$. Finally, we can describe the error of the Green’s function as follows:

$$e^R = \sum_{i,j} | \lambda_i^{(k)} | \lambda_j^{(k)} | \epsilon_{i,j} \leq \sum_{i,j} | \lambda_i^{(k)} | \lambda_j^{(k)} \left( 2 \sqrt{2} D(\Phi(0)), | \Phi(t) \rangle \right) + \frac{\sqrt{2}}{\sqrt{N_m}} = \alpha \left( 2 D(\Phi(0)), | \Phi(t) \rangle \right) + \frac{1}{\sqrt{N_m}}.$$

where $\alpha = \sqrt{2} \sum_{i,j} | \lambda_i^{(k)} | \lambda_j^{(k)}$.

### 2. Algorithmic and implementation errors

We now analyze sources of errors of the real-time Green’s function in this subsection and clarify two of main contributions of them: algorithmic and implementation errors. According to Ref. [33], we can upper bound the trace distance between the ideal time-evolved state and the simulated state by the VQS as

$$D(\Phi(0)), | \Phi(t) \rangle + \sum_{n=1}^{N_{exp}} D(U| \Phi(\tilde{\theta}(n-1)\delta t)), | \Phi(n\delta t) \rangle,$$

where $T$ is the time to be simulated, $U$ is the exact time evolution operator of small time step $\delta t$ described as $U = \exp(-iH\delta t)$, and $N_{exp} = T/\delta t$ is the number of time steps. The first term corresponds to the state preparation error of the ground state via the variational quantum eigensolver (VQE), which we denote as $\epsilon_\delta = D(\Phi(0)), | \Phi(t) \rangle$. The second term, which accumulates an error for each time step, can be decomposed into two types of errors: algorithmic and implementation errors. Algorithmic errors contain error due to imperfection of the Ansatz approximating the trial state and one due to a finite time step. Implementation errors are caused by physical errors stemming from the noisy nature of near-term quantum computers and the shot noise. We assume physical errors can be ignored because they can be suppressed by using quantum error mitigation techniques [56,57,68–71], i.e., we consider only the shot noise as the implementation error. By using the triangle inequality, it follows that

$$D(U| \Phi(\tilde{\theta}(n-1)\delta t)), | \Phi(\tilde{\theta}(n\delta t)) \rangle \leq D(U| \Phi(\tilde{\theta}(n-1)\delta t)), | \Phi(0)) \rangle + D(U| \Phi(\tilde{\theta}(n\delta t)) \rangle, | \Phi(0) \rangle \rangle.$$

where $| \Phi(0) \rangle$ denotes the state without implementation errors. The first term in the right-hand side corresponds to the algorithmic error and the second term does to the error for the implementation error for each time step. We denote these errors $\delta \epsilon_A(n)$ and $\delta \epsilon_I(n)$, respectively.

#### a. Algorithmic error

The algorithmic error can be written as [33]

$$\delta \epsilon_A(n) \equiv D(U| \Phi(\tilde{\theta}(n-1)\delta t)), | \Phi(0)) \rangle \rangle = \Delta_n^{(2)} \delta t^2 + \Delta_n^{(3)} \delta t^3 + O(\delta t^4).$$

where

$$\Delta_n^{(2)} = \langle \delta \Phi(\tilde{\theta}(n\delta t)) | \delta \Phi(\tilde{\theta}(n\delta t)) \rangle - \langle | \delta \Phi(\tilde{\theta}(n\delta t)) | \Phi(\tilde{\theta}(n-1)\delta t)) | \rangle^2;$$

$$| \delta \Phi(\tilde{\theta}(n\delta t)) \rangle \rangle = -iH | \Phi(\tilde{\theta}(n-1)\delta t)) \rangle - \sum_k \delta_{n}^{(0)} \delta \Phi(\tilde{\theta}(n-1)\delta t)) \rangle = \delta \Phi(\tilde{\theta}(n\delta t)) \rangle = \frac{\partial}{\partial \theta_k} \delta \Phi(\tilde{\theta}(n\delta t));$$

$$\Delta_n^{(3)} = \| H \| \| H^2 \| + \frac{1}{3} \| H^3 \| + \frac{1}{3} \| \frac{d \delta t}{d t} \| \| \frac{d \delta t}{d t} \|^2 + \| \frac{d \delta t}{d t} \|^2 + \frac{1}{3} \| \frac{d \delta t}{d t} \|^2 + \frac{1}{3} \| \frac{d \delta t}{d t} \|^2 + \frac{1}{3} \| \frac{d \delta t}{d t} \|^2 + \frac{1}{3} \| \frac{d \delta t}{d t} \|^2,$$

the matrix norm $\| . \|$ is induced by the vector norm, the operator $d/dt$ is defined as $d/dt = \dot{\theta}(t) \cdot \partial / \partial \theta$, and $\delta t \equiv I_e \otimes U(\tilde{\theta}(t))$ is the unitary circuit consisting of the Ansatz [Eq. (20)]. The term proportional to $\Delta_n^{(3)}$ stems from limited representative
capability of the Ansatz state $|Ψ(\vec{θ})\rangle$ approximating the true state. The term proportional to $\Delta_n^{(3)}$ is, on the other hand, due to a finite time step $\delta t$. Therefore, the total accumulation of algorithmic errors from $t = 0$ to $T$ is

$$
\epsilon_A = \sum_{n=1}^{N_{\text{step}}} \delta \epsilon_A(n) \lesssim \sqrt{\Delta_{\max}^{(2)} T} + \sqrt{\Delta_{\max}^{(3)} \delta t},
$$

(A12)

where $\Delta_{\max}^{(2)} = \max_n \Delta_n^{(2)}$ and $\Delta_{\max}^{(3)} = \max_n \Delta_n^{(3)}$. The first term in the right-hand side does not depend on the time step $\delta t$ because this is the error caused by imperfections of the Ansatz to represent the quantum state after the time evolution, whereas the second term can be suppressed by taking the small time step.

Here, we also show another important property of our algorithm based on the VQS. By denoting $|Ψ(\vec{θ}(t))\rangle$ as $|Ψ(\vec{θ}(t))\rangle = \frac{1}{\sqrt{2}}(|\psi_1(\vec{θ}(t))\rangle + |\psi_2(\vec{θ}(t))\rangle)$ for simplicity, we have

$$
\Delta_n^{(2)} = \frac{1}{2} \langle (\delta ψ_1(\vec{θ}(n\delta t))) | ψ_1(\vec{θ}(n\delta t)) \rangle + \langle (\delta ψ_2(\vec{θ}(n\delta t))) | ψ_2(\vec{θ}(n\delta t)) \rangle - \frac{1}{2} \text{Re} \langle (\delta ψ_1(\vec{θ}(n\delta t))) | ψ_1(\vec{θ}(n\delta t)) \rangle \langle ψ_2(\vec{θ}(n\delta t)) | ψ_2(\vec{θ}(n\delta t)) \rangle,
$$

(A13)

where

$$
\Delta_n^{(2)} = \frac{1}{2} \langle (\delta ψ_1(\vec{θ}(n\delta t))) | ψ_1(\vec{θ}(n\delta t)) \rangle - \frac{1}{2} \text{Re} \langle (\delta ψ_1(\vec{θ}(n\delta t))) | ψ_1(\vec{θ}(n\delta t)) \rangle \langle (\delta ψ_2(\vec{θ}(n\delta t))) | ψ_2(\vec{θ}(n\delta t)) \rangle.
$$

(A14)

From the expression above, one can see that $\Delta_n^{(2)}$ for $|Ψ\rangle$ is not just a mean of $\Delta_n^{(2)}$ for $|ψ_1\rangle$ and $|ψ_2\rangle$ but also includes the term $\delta t = \frac{1}{2} \langle (\delta ψ_1 | ψ_1) \rangle - \frac{1}{2} \langle (\delta ψ_2 | ψ_2) \rangle$. This term, $\delta t_{\text{alg}}$, indicates that the algorithmic error due to the insufficient Ansatz increases when we want to find a unitary operator to evolve two input states simultaneously, compared with finding different unitaries for each state. The term $\delta t_{\text{alg}}$ clarifies the drawback of our algorithm to find a unitary which simultaneously approximates the time evolution operator for multiple states.

However, as seen in numerical simulation in Sec. V, we successfully reproduced the real-time Green’s functions of the two-site Fermi-Hubbard model, which implies that the effect of $\delta t_{\text{alg}}$ can be made small. In general, the cost for employing different unitaries for multiple states and the circuit like in Fig. 1 is much larger than employing a single unitary and the circuit like in Fig. 2.

### b. Implementation error

The implementation error is caused by the shot noise and gives errors in the solution of Eq. (10) in the main text:

$$
M\hat{θ} = \mathcal{V},
$$

(A15)

where

$$
M_{i,j} = \text{Re} \left. \left( \frac{\partial \langle Ψ(\vec{θ}) | Ψ(\vec{θ}) \rangle}{\partial θ_i} \right) \right|_{\vec{θ} = \vec{θ}(n\delta t)},
$$

(A16)

$$
V_j = \text{Im} \left. \left( Ψ(\vec{θ}) | H \frac{\partial \langle Ψ(\vec{θ}) |}{\partial θ_j} \right) \right|_{\vec{θ} = \vec{θ}(n\delta t)}.
$$

(A17)

At each time step, the matrix $M$ and the vector $V$ are obtained by measuring outputs of appropriate quantum circuits [33,41], which include the shot noise. We denote error-free values of the matrix $M$ and the vector $\mathcal{V}$ as $M_0$ and $\mathcal{V}_0$, and observed values of them as $M_0 + \delta M$ and $\mathcal{V}_0 + \delta \mathcal{V}$, respectively. The solution of Eq. (A15) calculated by $M_0$ and $\mathcal{V}_0$ is denoted by $\hat{θ}_0$ and the one calculated by $M_0 + \delta M$ and $\mathcal{V}_0 + \delta \mathcal{V}$ as $\hat{θ}_0 + \delta \hat{θ}$. In the first order of $\delta M_0$ and $\delta \mathcal{V}_0$, it follows

$$
\delta \hat{θ} \approx M_0^{-1} \delta \mathcal{V} - M_0^{-2} \delta M \mathcal{V}_0,
$$

(A18)

and we thus have

$$
\|\delta \hat{θ}\| \lesssim \|M_0^{-1}\|\|\delta \mathcal{V}\| + \|M_0^{-1}\|^2 \|\mathcal{V}_0\| \|\delta M\|.
$$

(A19)
Since we consider only the shot noise, \( \| \delta \vec{V} \| \) and \( \| \delta M \| \) can be described as
\[
\| \delta M \| \approx \frac{\Delta M}{\sqrt{N_r}}, \\
\| \delta \vec{V} \| \approx \frac{\Delta \vec{V}}{\sqrt{N_r}},
\]
where \( N_r \) is the number of shots to evaluate \( M \) and \( \vec{V} \). When we denote the derivative of the state \( |\Psi(\vec{\theta})\rangle \) as
\[
\frac{\partial |\Psi(\vec{\theta})\rangle}{\partial \theta_k} = \sum_{i=1}^{N_{rA}} g_{k,i} \otimes (U_N \ldots U_{k+1} P_k U_{k-1} \ldots U_1) |\Psi(\vec{\theta})\rangle,
\]
where \( g_{k,i} \) is a complex number and \( P_k \) is a Pauli operator [recalling that we have assumed the \( \text{Ansatz} \) has the form of Eq. (7) in the main text], \( \Delta M \) can be written as
\[
\Delta M = 2 \sqrt{\sum_{k,j} \left( \sum_{i,j} |g_{k,i} g_{k,j}|^2 \right)}. 
\]
Similarly, \( \Delta \vec{V} \) is written as
\[
\Delta \vec{V} = 2 \sqrt{\sum_k \left( \sum_{i,j} |g_{k,i} h_{k,j}|^2 \right)}. 
\]
where the Hamiltonian is written as \( H = \sum_j h_j P_j \) with \( P_j \) being a Pauli operator and \( h_j \) a coefficient.

In Ref. [33], the implementation error is shown to be approximated as
\[
\delta \epsilon_I(n) \equiv D(\Psi(\vec{\theta}(n\delta t))), |\Psi(0)\rangle(\vec{\theta}(n\delta t))) 
= \sqrt{\delta \vec{V}^T B \delta \vec{V} \delta t^2 + O(\delta t^3)} \lesssim \| B \| \| \delta \vec{V} \| \delta t 
\lesssim \sqrt{\| B \|} \frac{\Delta \vec{V}}{\sqrt{N_r}} \delta t,
\]
where \( \Delta \vec{V} = \| M_0^{-1} \delta \vec{V} + \| M_0^{-1} \| \| V_0 \| \Delta M \) and
\[
B_{i,j} = \frac{\partial (\Psi(\vec{\theta}((n-1)\delta t)))}{\partial \theta_i} \frac{\partial (\Psi(\vec{\theta}((n-1)\delta t)))}{\partial \theta_j} - \frac{\partial (\Psi(\vec{\theta}((n-1)\delta t)))}{\partial \theta_i} \frac{\partial (\Psi(\vec{\theta}((n-1)\delta t)))}{\partial \theta_j} \times (\Psi(\vec{\theta}((n-1)\delta t))) \frac{\partial (\Psi(\vec{\theta}((n-1)\delta t)))}{\partial \theta_j}.
\]
Finally, the total implementation error will be
\[
\epsilon_I \equiv \sum_{n=1}^{N_{\text{step}}} \delta \epsilon_I(n) \leq \sqrt{\| B \|_{\max} \frac{\Delta \vec{V}^{(\text{max})}}{\sqrt{N_r}} \delta t},
\]
where the superscript and subscript “max” on \( \| B \| \) and \( \Delta V \) represent the maximum value for \( n = 1, \ldots, N_{\text{step}} \).

3. Resource estimation

a. Evaluation of the error of the real-time Green’s function and the resource estimation

From Eqs. (A7), (A12), and (A26), the error of the computed Green’s function by our algorithm based on the VQS reads as
\[
\epsilon^R \leq \alpha \left( 2(\epsilon_I + \epsilon_A) + \frac{1}{\sqrt{N_m}} \right) 
= \alpha \left[ 2(\epsilon_I + \sqrt{\Delta^{(2)} T} + \sqrt{\Delta^{(3)} \delta t T}) 
+ \sqrt{\| B \|} \frac{\Delta \vec{V}}{\sqrt{N_r}} \right] + \frac{1}{\sqrt{N_m}}),
\]
where we omitted the subscript and superscript “max” for simplicity. The first and second terms in the right hand correspond to the state preparation error and the (part of) algorithmic error, respectively. Both stem from imperfections of the \( \text{Ansatz} \) to represent the ideal quantum state to be simulated and the analysis of them is not straightforward; e.g., it depends on details of the system (Hamiltonian) and/or the \( \text{Ansatz} \) as well as the optimization method used for the VQE. We leave them for future work. On the other hand, the third, fourth, and fifth terms in the right-hand side can be suppressed by employing sufficiently small time step \( \delta t \) and the large number of shots \( N_r, N_m \) for measuring the quantum circuits. Those terms represent the algorithmic error due to a finite time step, the implementation error, and the shot noise in evaluating the Pauli matrices involved in the Green’s function, respectively.

Let us evaluate the size of time step \( \delta t \) and the number of shots \( N_r, N_m \) so as to bound each term in the right-hand side of Eq. (A27). To upper bound the third term by \( \epsilon_A \), we need the time step
\[
\delta t = \frac{\epsilon_A^2}{4 \alpha^2 \Delta^{(3)} T^2}. 
\]
It means that the number of time steps will be
\[
N_{\text{step}} = \frac{T}{\delta t} = \frac{4 \alpha^2 \Delta^{(3)} T^3}{\epsilon_A^2}. 
\]
To upper bound the fourth term by \( \epsilon_I \), we need to set the number of shots to evaluate the matrix \( M \) as
\[
N_r = \frac{4 \alpha^2 \| B \| T^2}{\epsilon_I^2}. 
\]
Similarly, if we want to upper bound the fifth term by \( \epsilon_m \), it is required
\[
N_m = \frac{\alpha^2}{\epsilon_m^2}. 
\]
Finally, let us count the number of distinct runs of the quantum circuits to obtain the Green’s function and discuss its dependence on the required error bound to the Green’s function. The number of shots (distinct runs of quantum circuit) to populate matrix \( M \) and \( V \) matrix is at most \( N_0^2 N_0^2 + N_0 N_H N_D \), where \( N_0 \) is the number of parameters (the number of elements of \( \vec{\theta} \)), \( N_H \) is the number of terms of the Hamiltonian, and \( N_D \) is
maxi  N_{\text{site}}). Hence, the number of distinct runs of the quantum
circuits to obtain the Green’s function will be
\[ N_{\text{tot}} = N_{\text{step}} \times N_c \times (N_c^2 N_D^2 + N_c N_H N_D) + N_c \times N_m \]
\[ = \frac{16\alpha^4 \|B\| \Delta^{(3)} T^5}{\epsilon^2} (N_c^2 N_D^2 + N_c N_H N_D) + \frac{N_c \alpha^2}{\epsilon^2}, \quad \text{(A32)} \]
where \( N_c \) is the number of the Pauli matrices in which we expand the electron creation operator \( c_i \) [see Eq. (13) in the main text]. This is one of the main results for the resource estimation for calculating the Green’s function based on the VQS, although this number is a very loose, or pessimistic, estimation.

We note that further simplification may be possible when we set \( \epsilon_A = \epsilon_l = \epsilon_m = \epsilon / 3 \), i.e., we set the total error of the Green’s function to \( \epsilon \), ignoring the errors originating from imperfections of the Ansatz:
\[ N_{\text{tot}} = \frac{1296\alpha^4 \|B\| \Delta^{(3)} T^5}{\epsilon^4} (N_c^2 N_D^2 + N_c N_H N_D) + \frac{9N_c \alpha^4}{\epsilon^2} \]
\[ \approx \frac{1296\alpha^4 \|B\| \Delta^{(3)} T^5}{\epsilon^4} (N_c^2 N_D^2 + N_c N_H N_D). \quad \text{(A33)} \]
We will use this relationship in the next section.

b. Evaluation of the error of the Green’s function in frequency domain and the resource estimation

The Green’s function in frequency domain is defined as
\[ \tilde{G}^R_k(\omega) = \int_0^{\infty} e^{i\omega t} G^R_k(t) dt \quad (\eta \rightarrow +0), \quad \text{(A34)} \]
and its imaginary part \( \text{Im} \tilde{G}^R_k(\omega) \) gives the spectrum function. Suppose the Hamiltonian of interest has the energy spectrum \( \{E_{\min}, \ldots, E_{\max}\} \), where \( E_{\min} \) (\( E_{\max} \)) is the minimal (maximum) energy. We assume all energies are positive, \( E_{\min} > 0 \), without loss of generality. According to the sampling theorem, to avoid aliasing in \( \tilde{G}^R_k(\omega) \), we need to sample the real-time Green’s function \( G^R_k(t) \) with over twice the maximum frequency contained in it. It means that we need to have the time step
\[ \delta t \leq \frac{1}{2f_{\max}} = \frac{1}{E_{\max}/\pi}, \quad \text{(A35)} \]
where \( f_{\max} = E_{\max}/2\pi \) is the maximum frequency of the real-time Green’s function, in the VQS algorithm. It is important to note that this bound is consistent with regard to the required accuracy to the real-time Green’s function while the step time shown in Eq. (A28) depends on it, so we adopt Eq. (A28) as the time step to be considered. Meanwhile, the necessary evolution time \( T_0 \) to obtain information of the lowest-frequency component is \( T_0 = 2\pi/E_{\min} \).

In our simple numerical integration scheme, the real-time Green’s function is sampled at \( t = 0, \delta t, \ldots, T_0 \). The Green’s function in frequency domain is approximated as
\[ \tilde{G}^R_k(\omega) \approx \int_0^{T_0} e^{i(\omega + \eta)t} G^R_k(t) dt \quad (\eta \rightarrow +0) \]
\[ \approx \sum_{n=0}^{N_{\text{step}}} G^R_k(n\delta t)e^{i\omega t}\delta t + O(\delta t), \quad \text{(A36)} \]
where \( N_{\text{step}} = T_0/\delta t \) is the total number of time steps for simulation. We note that the first term in the last line is \( O(\delta t^3) \).

When the errors of all data \( \{\tilde{G}^R_k(n\delta t)\}_{n=0}^{N_{\text{step}}} \) are bounded by \( \tilde{\epsilon} \), the error of the imaginary part of \( \tilde{G}^R_k(\omega) \) can be upper bounded as
\[ \delta (\text{Im}[\tilde{G}^R_k(\omega)]) \leq N_{\text{step}} \cdot \tilde{\epsilon} \cdot \delta t = \tilde{\epsilon} T_0. \quad \text{(A37)} \]
The same argument can be made for the real part. Therefore, if we want to set total accuracy of \( \tilde{G}^R_k(\omega) \) to \( \epsilon \), i.e., we should take \( \tilde{\epsilon} = \epsilon / T_0. \) In that case, the total number of measurements [Eq. (A32)] will be
\[ N_{\text{tot}} = \frac{1296\alpha^4 \|B\| \Delta^{(3)} T_0^9}{\epsilon^4} (N_c^2 N_D^2 + N_c N_H N_D) \]
\[ = (2\pi)^9 \times 1296\alpha^4 \|B\| \Delta^{(3)} \frac{\epsilon^4}{N_{\text{min}}^2 N_c^2} (N_c^2 N_D^2 + N_c N_H N_D). \quad \text{(A38)} \]
Conversely, when the time step \( \delta t \) is fixed and takes only errors related to \( \delta t \) into account, the error of the Green’s function in frequency domain is
\[ \delta (\text{Im}[\tilde{G}^R_k(\omega)]) \sim 2\alpha T_0^{3/2} \sqrt{\Delta^{(3)} \delta t}. \quad \text{(A39)} \]

APPENDIX B: DETAILS OF DISCUSSION ON THE FEASIBILITY OF OUR ALGORITHMS IN SEC. VII

In this Appendix, we provide details of the discussion on the feasibility of our proposed algorithms in Sec. VII based on Ref. [55]. We take the two-dimensional Hubbard model [Eq. (35) in the main text] of \( N_{\text{site}} \) sites with the open boundary condition as an example. By applying the Jordan-Wigner transformation, the Hamiltonian will have the form of \( H = \sum_j h_j P_j \), where \( h_j \) is real coefficient and \( P_j \) is Pauli matrices. The Hamiltonian Ansatz is defined as [Eq. (32) in the main text]
\[ \prod_{d=1}^{n_d} \left( \prod_j \exp (i\theta_{j}^{(d)} P_j) \right), \quad \text{(B1)} \]
where \( n_d \) is the depth of the Ansatz and \( \theta_{j}^{(d)} \) is a parameter to be optimized in the Ansatz. In Ref. [55], it is shown that the number of single-qubit gates and two-qubit gates to implement the single-depth \((n_d = 1)\) Hamiltonian Ansatz of this model is
\[ N_{\text{single}} = 4N_{\text{site}}^2 + 7N_{\text{site}} - 4\sqrt{N_{\text{site}}}, \]
\[ N_{\text{two}} = 8N_{\text{site}}^2 + N_{\text{site}} - 4\sqrt{N_{\text{site}}}, \quad \text{(B2)} \]
with assuming \( \alpha / \lambda \) rotation gate and the partial swap gate as elementary single- and two-qubit operations. Therefore, the total number of gates is \( n_d(N_{\text{single}} + N_{\text{two}}) \). By putting \( n_d = 1 \) and \( N_{\text{site}} = 25 \) as in the main text, we obtain \( N_{\text{single}} \approx 650, N_{\text{two}} \approx 1000 \). Alternatively, when we set \( n_d = N_{\text{site}} \), the total number of gates is \( N_{\text{single}} \approx 16 400 \), \( N_{\text{two}} \approx 2600 \). In this case, the tolerable error rate for quantum error correction, \( N_{\text{gate}} \epsilon_{\text{gate}} \lesssim 2 \), gives \( \epsilon_{\text{gate}} = 8 \times 10^{-2}\% \) even if we consider only the two-qubit gates. This value indicates that the further improvement of two-qubit gate fidelity is required.
FIG. 11. Numerical simulation of the VQS algorithm to compute the Green’s function in real time $G_0^R(t)$ [(a), (b), (d), (e)] and the spectral function [(c), (f)] for $n_d = 4$ and the model (30) of $U = 3$ [(a)–(c)] and $U = 6$ [(d)–(f)]. The time step is taken as $dt = 0.1(0.03)$ for $U = 3(6)$. The exact spectral function is calculated by the exact dynamics of the Green’s function in real time from $t = 0$ to 100 with step $dt = 0.1$. We take $\eta = 0.2$ for the calculation of the spectral functions.

APPENDIX C: ADDITIONAL SIMULATION RESULTS

Here, we show additional numerical results. The results for $n_d = 4$ are presented in Fig. 11. We can see that the results are almost identical with the result of $n_d = 8$ in Fig. 5 in the main text although the peaks of the spectral function are slightly smeared.

Furthermore, we present results of the variational quantum simulation (VQS) for four-site Fermi-Hubbard model for further convincing the readers of the feasibility of our algorithm.

The Hamiltonian of the four-site Fermi-Hubbard model is defined as

$$H = - \sum_{i=1,2,3,4,\sigma=\uparrow,\downarrow} \left( c_i^\dagger c_{i+1,\sigma} + H.c. \right) + U \sum_{i=1}^{4} c_i^\dagger c_i c_{i+1}^\dagger c_{i+1} - \frac{U}{2} \sum_{i=1,2,3,4,\sigma=\uparrow,\downarrow} c_i^\dagger c_i c_{i,\sigma}. \quad (C1)$$

FIG. 12. Numerical simulation of the VQS algorithm to compute the Green’s function in real time $G_0^R(t)$ (a) and the spectral function (b) of the four-site Fermi-Hubbard model (C1) of $U = 6$. The Hamiltonian Ansatz (32) of the depth $n_d = 16$ is used and the time step is taken as $dt = 0.03$. The exact spectral function is calculated by the exact dynamics of the Green’s function in real time from $t = 0$ to 100 with step $dt = 0.1$. We take $\eta = 0.4$ for the calculation of the spectral functions.
Simulating this model requires eight qubits, so it is closer to the current experiments of the near-term quantum computers. We employ the Hamiltonian Ansatz (32) of the depth $n_d = 16$ which has 320 parameters (the number of Pauli terms in the Hamiltonian except for the identity operator is $N_p = 20$). The result of the numerical simulation of the VQS is displayed in Fig. 12, which well reproduces the exact result. While only uses real 320 parameters to simulate the dynamics for computing the Green’s function by using the VQS algorithm in Sec. III.

**APPENDIX D: DETAILS ON NUMERICAL SIMULATION**

For the numerical calculation in Sec. III, we evaluate the derivatives appearing in Eq. (11) by numerical differentiation by taking $\delta \theta_i = 10^{-4}$ for all parameters $\theta_i$ of the Ansatz quantum state. We solve Eq. (10) by minimizing $\| M \hat{\theta} - \vec{V} \|$ by using numpy.linalg.lstsq function implemented in Python library NUMPY [72] with neglecting the singular values of $M$ smaller than $10^{-8}$. The size of the time step $dt$ is taken so small that there is no significant change in the final result when decreasing $dt$.

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