

Subspace-based local compilation of variational quantum circuits for large-scale quantum many-body simulation

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Simulation of quantum many-body systems is one of the most promising applications of quantum computers. It is crucial to efficiently implement the time-evolution operator as a quantum circuit to execute such simulations on near-term quantum computing devices with limited computational resources. However, standard approaches such as Trotterization sometimes require a deep quantum circuit, which is hard to implement on near-term quantum computers. Here, we propose a hybrid quantum-classical algorithm, called local subspace variational quantum compilation (LSVQC), for compiling the time-evolution operator of quantum many-body systems. The LSVQC performs a variational optimization to reproduce the action of the target time-evolution operator within a physically reasonable subspace. The optimization is performed for small local subsystems based on the Lieb-Robinson bound, which allows us to execute the cost function evaluation using small-scale quantum devices and/or classical computers. We demonstrate the validity of the LSVQC algorithm through numerical simulations of a simple spin-lattice model and an effective model of a parent compound of cuprate superconductors, Sr_2CuO_3 , constructed by the *ab initio* downfolding method. It is shown that the LSVQC achieves a 95% reduction of the circuit depth for simulating quantum many-body dynamics compared to the Trotterization at best while maintaining the same computational accuracy. We also demonstrate that the restriction to a subspace leads to a substantial reduction of required resources and improved accuracy compared to the case of considering the entire Hilbert space. Furthermore, we estimate the gate count needed to execute the quantum simulations using the LSVQC on near-term quantum computing architectures in the noisy intermediate-scale or early fault-tolerant quantum computing era. Our estimation suggests that the acceptable physical gate error rate for the LSVQC can be about one order of magnitude larger than that for the Trotterization.

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I. INTRODUCTION

Simulating quantum many-body systems is important in various fields of science such as condensed matter physics, nuclear physics, quantum chemistry, and materials science. For practical applications such as materials design and drug discovery, however, large-scale quantum simulations are necessary, which are hard tasks since the required resources for classical algorithms increase exponentially with increasing the system size. On the other hand, quantum computers generally realize such quantum simulations with exponentially fewer computational resources than classical computers. Hence, quantum simulation is expected to be one of the most promising applications to realize practical quantum advantage or quantum utility [1].

A crucial task in quantum simulation is implementing the time-evolution operator as a quantum circuit. This is not only a technique to simulate the dynamics of quantum many-body

systems according to the Schrödinger equation but also is an essential building block of various quantum algorithms such as quantum phase estimation [2–4]. A variety of algorithms have been developed to implement the time-evolution operator on quantum computers efficiently. The most common algorithm is the Trotterization [5], which allows us to implement the time-evolution operator most simply with analytically guaranteed precision. However, it often requires many quantum gates for practical applications beyond the capability of current or near-term quantum computers such as noisy intermediate-scale quantum (NISQ) devices [6]. Increased gate count in Trotterization is also problematic for ideal fault-tolerant quantum computers (FTQCs) since it causes a long computational time that hinders the practical use of quantum computers. More advanced algorithms such as the qubitization-based techniques [7] exhibit better asymptotic scaling of gate complexity than Trotterization. However, such techniques require many ancilla qubits and gate operations and are hence suitable only for long-term FTQCs.

For near-term NISQ devices, quantum-classical hybrid variational algorithms have been proposed to realize quantum simulation with shallow-depth quantum circuits. Some algorithms perform a variational optimization of parametrized quantum circuits (i.e., ansatz) to represent a time-evolved quantum state based on McLachlan's variational principle

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[8–12]. Another approach is variational quantum compiling algorithms [13–17] that aim to compile a Trotterized time-evolution circuit into a more easily implementable form. Although these variational algorithms potentially outperform the Trotterization-based approaches in small-scale quantum simulations, it is hard to scale up these algorithms to practically important large-scale quantum simulations because of their variational nature, which induces obstacles such as a barren plateau [18,19]. Considering the above difficulty of existing algorithms, it is necessary to develop a more sophisticated algorithm to implement the large-scale time-evolution operator on near-term quantum computers such as in the NISQ era. It is also important for early fault-tolerant quantum computers (early-FTQCs) [20–26], in which small-scale or partial quantum error correction is implemented but the number of logical qubits and circuit depth are still limited.

One possible route of designing algorithms to reduce implementation costs of quantum simulations is considering *subspace* relevant to the problem of interest. Indeed, various subspace-based algorithms have been devised to reduce the computational costs needed to perform quantum simulations on both classical and quantum computers [27]. In the electronic structure problems, the ground- and excited-state properties of quantum many-body systems can be approximately obtained by projecting the Schrödinger equation onto a subspace spanned by some physically relevant many-electron states. Diagonalization of such subspace-restricted Schrödinger equation is the basic idea of various near-term quantum algorithms to calculate eigenpairs of quantum many-body Hamiltonian such as quantum subspace expansion (QSE) [28,29], quantum equation of motion algorithm [30], quantum filter diagonalization (QFD) [31], multireference selected quantum Krylov (MRSQK) algorithm [32], quantum Lanczos algorithm [33], quantum power method [34], quantum selected configuration interaction (QSCI) [35,36], and so on. These methods mainly differ in the way of generating the basis states spanning the subspace. Subspace consideration is also important for simulating the time evolution of quantum systems. For example, it is shown that the analytical error bound of Trotterization is improved by considering the simulation of quantum states within a low-energy subspace [37]. Furthermore, diagonalizing time-evolution operators within a physically relevant subspace is a basic concept of some algorithms that aim to realize fast-forwarding time evolution on near-term quantum computers, e.g., subspace variational quantum simulator [38], fixed-state variational fast-forwarding (fsVFF) [17], and classical-quantum fast-forwarding [39].

In this paper, we propose a quantum-classical hybrid algorithm called local subspace variational quantum compilation (LSVQC). The LSVQC is a variant of the variational quantum compiling designed to compile the time-evolution operators of large-scale quantum many-body systems using small-scale near-term quantum devices and/or classical computers. The main advantages of the LSVQC over other variational algorithms are the following:

- (1) Reduction of requirement on the expressive power of the ansatz circuit to reproduce the time evolution.
- (2) Scalability to practically important large-scale quantum simulations.

These advantages stem from two features of the LSVQC, i.e., the *subspace-based compilation* and the *local compilation*. First, the LSVQC is performed to reproduce the action of the target time-evolution operator only within a physically relevant subspace (i.e., subspace-based compilation), which is designed based on the properties of physical quantities we wish to simulate. The subspace-based compilation is motivated by the fact that the time evolution of a quantum many-body state often stays within a small subspace in the entire Hilbert space such as low-energy subspace or specific symmetry sectors. In comparison with the case of full Hilbert space compiling, the subspace-based compiling leads to the reduction of the depth and number of parameters (i.e., expressive power) of the ansatz circuit required to accurately approximate the time evolution. It enhances the feasibility of quantum simulations on near-term quantum computers with a limited number of quantum gates and circuit depth. Second, the LSVQC performs the variational optimization for smaller-size local subsystems of the size $\mathcal{O}(L^0)$ or $\mathcal{O}(\log L)$ instead of the large-scale entire size- L system. The physics behind such local compilation protocol is the Lieb-Robinson (LR) bound [40], which dictates the universal causality of quantum many-body systems with local interactions. We formally derive the theoretical guarantee for the local compilation in a similar way as the local variational quantum compilation (LVQC), which was originally proposed in Ref. [41] and later extended to fermionic simulation in our previous work [42]. Note that the validity of such a local compilation protocol is intuitively nontrivial. Since the computationally hard large-scale optimization is replaced with a smaller-scale optimization requiring an ansatz circuit with low expressive power, the LSVQC is less susceptible to barren plateaus and is scalable to large-scale quantum simulations in contrast to other variational algorithms.

We demonstrate the validity of the LSVQC by performing numerical simulations of the one-dimensional (1D) Heisenberg model and an *ab initio* effective model of Sr_2CuO_3 [43–47], which is a quasi-one-dimensional strongly correlated material. It is demonstrated that the LSVQC allows us to accurately simulate quantum many-body dynamics using circuits shallower by about 90–95% than the Trotterization while maintaining accuracy. We also estimate the gate count needed to perform the quantum simulation of strongly correlated materials. The results suggest that the LSVQC significantly reduces the hardware requirement to execute the quantum simulation in the NISQ and early-FTQC era [20–26].

The rest of the paper is organized as follows. In Sec. II, we give an overview of the LSVQC algorithm. In Sec. III, we provide a theoretical formulation of the subspace-based compilation and some guidelines for subspace design. In Sec. IV, we derive a theorem that guarantees the local compilation protocol of the LSVQC. In Sec. V, we demonstrate the basic properties of the LSVQC by performing numerical simulations for the 1D Heisenberg model. In Sec. VI, we apply the LSVQC to quantum many-body dynamics simulations of the *ab initio* effective model of Sr_2CuO_3 . In Sec. VII, we perform resource estimation of the gate count and optimization cost for the strongly correlated materials simulations. Finally, we summarize our work in Sec. VIII.

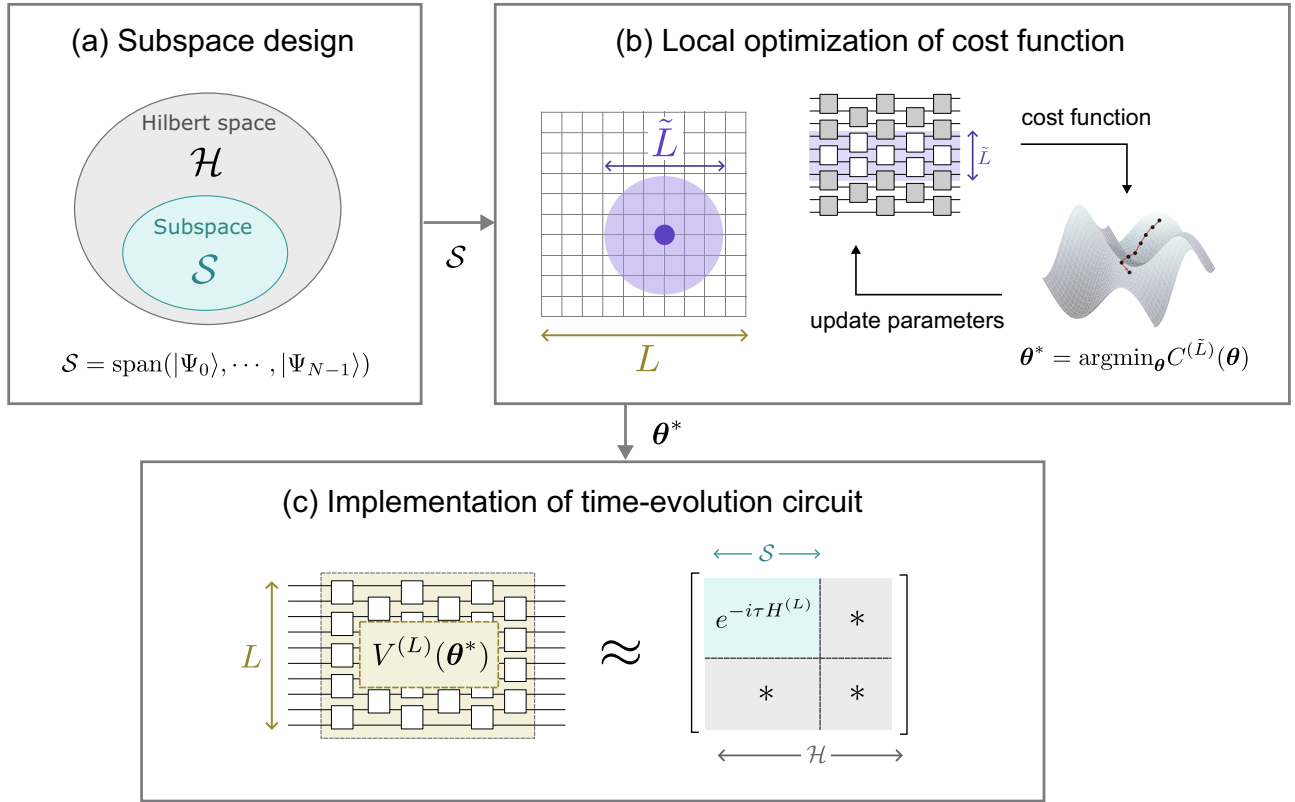


FIG. 1. Overview of the LSVQC algorithm. (a) First, we design a subspace $\mathcal{S}$ based on the properties of the physical quantities we aim to simulate. (b) Next, we perform variational optimization of a cost function $C^{(\tilde{L})}(\theta)$ defined on size- $\tilde{L}$ local subsystems, where $\tilde{L} \leq L$ with L being the entire system size. The cost function is evaluated using size- $\tilde{L}$ localized quantum circuits (represented as white two-qubit gates in the purple region). The optimization loop is executed on $\tilde{L}$ -qubit quantum computing devices and/or classical computers. Then, we obtain an optimal parameter set θ^* that minimizes the subsystem cost function $C^{(\tilde{L})}(\theta)$. (c) Finally, we implement an optimized ansatz $V^{(L)}(\theta^*)$ on an L -qubit quantum computing device. When the optimization is successfully converged, $V^{(L)}(\theta^*)$ approximates the action of the target time-evolution unitary $e^{-i\tau H^{(L)}}$ within the subspace $\mathcal{S}$.

II. OVERVIEW OF THE LSVQC ALGORITHM

In this section, we provide an overview of our LSVQC algorithm. The LSVQC aims to implement the time-evolution operator $e^{-i\tau H^{(L)}}$ for a L -qubit Hamiltonian $H^{(L)}$ with a fixed time τ . Specifically, the LSVQC compiles the target unitary $e^{-i\tau H^{(L)}}$ using an ansatz $V^{(L)}(\theta)$ as follows (see Fig. 1):

(i) Design a subspace $\mathcal{S}$ appropriate to physical quantities we aim to simulate. Here, we also specify a set of quantum circuits that prepare the basis states spanning the subspace.

(ii) Construct localized versions of the target time-evolution operator, ansatz, and state preparation circuits for local subsystems of size $\tilde{L} (\leq L)$. Then, variationally optimize a cost function defined on the local subsystems and find an optimal parameter set θ^* minimizing the cost function.

(iii) Construct an optimized ansatz circuit $V^{(L)}(\theta^*)$ on a L -qubit quantum computer using the optimal parameter set θ^* . The optimized circuit $V^{(L)}(\theta^*)$ approximates the time-evolution operator $e^{-i\tau H^{(L)}}$.

In step (i), the structure of the subspace is determined by details of the target physical quantities we aim to simulate. A guideline of the subspace design for some typical situations encountered in quantum many-body simulations is given in Sec. III B. In step (ii), the compilation size $\tilde{L}$, which typically

scales as $\mathcal{O}(L^0)$ or $\mathcal{O}(\log L)$, is estimated based on the LR bound as shown in Sec. IV. The optimization is executed by performing the Loschmidt echo test (LET) [14] using $\tilde{L}$ -qubit quantum devices (see Fig. 2 for the quantum circuit) and/or classical computers. The theoretical guarantee for the local compilation protocol is given in Sec. IV. Note that we can perform this local compilation protocol using only classical computers when the compilation size $\tilde{L}$ is sufficiently small such that the cost function can be easily calculated on classical computers. In this case, we can execute ideal optimization without physical and statistical errors inherent to quantum computers. When the optimization is successfully converged, the output quantum circuit $V^{(L)}(\theta^*)$ obtained in step (iii) accurately reproduces the action of the target time-evolution operator only within the subspace $\mathcal{S}$. In other words, the optimized circuit $V^{(L)}(\theta^*)$ returns a correct output state only when it is applied to a state belonging to the target subspace.

Here, we provide some comments on related works. The idea of subspace-based compiling is also employed in the fsVFF algorithm [17], which is a variant of the variational quantum compiling for fast-forwarding quantum simulation. However, the target cost function of the fsVFF, which is designed to realize subspace diagonalization of time-evolution unitary for various time steps, is different from that used

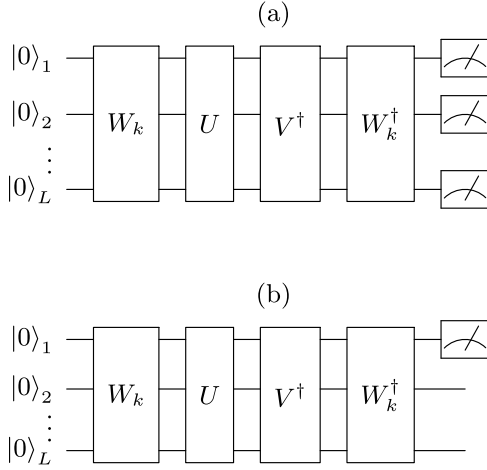


FIG. 2. (a) Quantum circuit for the LET. The probability of obtaining the measurement outcome in which all L qubits are in the $|0\rangle$ state is equal to $|\langle\Psi_k|V^\dagger U|\Psi_k\rangle|^2$. (b) Quantum circuit for the LLET. The probability of obtaining the measurement outcome in the j th qubit ($j = 1, 2, \dots, L$) is in the $|0\rangle$ state is equal to $\text{Tr}[\Pi_j \rho_k(U, V)]$ with ρ_k given by Eq. (5). Note that the figure is for $j = 1$.

in the LSVQC. Moreover, the fsVFF is valid only for fast-forwardable Hamiltonians, which belongs to a very restricted class of quantum many-body Hamiltonians [48–51]. In contrast, the LSVQC is a more general algorithm applicable to a broader class of Hamiltonians with the LR bound. Specifically, the LR bound exists in broad quantum many-body systems with finite-ranged, short-ranged, and long-ranged interactions in generic dimensions [52–59].

The local compilation protocol similar to the LSVQC is also adopted in the LVQC [41,42]. However, the LVQC is designed to compile the many-body time-evolution operators on the entire Hilbert space. Such full Hilbert space compiling is performed by optimizing a cost function related to the average gate fidelity, which is measured by the Hilbert–Schmidt test [13]. Since the Hilbert–Schmidt test uses maximally entangled Bell states, it requires qubits of twice the compilation size (i.e., $2\tilde{L}$ qubits) and many long-range CNOT gates connecting the Bell pairs (see Appendix F for details). This is problematic for near-term quantum devices, in which the number of qubits and qubit connectivity is highly restricted, and possibly causes large errors in evaluating the cost functions. On the other hand, the LET utilized in the LSVQC does not require doubling the number of qubits and long-range two-qubit gates connecting Bell pairs (see Fig. 2). Thus, compared to the LVQC, the LSVQC is more suitable for near-term quantum computers like NISQ devices or early-FTQCs, where the available number of qubits and gate operations are restricted. Furthermore, compared to the full Hilbert space compiling of the LVQC, we can expect that the subspace-based compiling of the LSVQC leads to a reduction of the expressive power of the ansatz needed to reproduce the time evolution of a specific physical quantity. In other words, the circuit depth and the gate count of the ansatz required for successful optimization of the LSVQC are smaller than those of the LVQC. We explain the details of the above advantages of the LSVQC in Sec. VII C.

III. FORMULATION FOR SUBSPACE-BASED COMPILATION

This section provides several formulations regarding the subspace-based compiling in the LSVQC algorithm.

A. Cost functions

We first introduce the cost function that we aim to minimize through the LSVQC algorithm. We compile the time evolution operator variationally into a low-depth quantum circuit within a N -dimensional subspace $\mathcal{S}$,

$$\mathcal{S} = \text{span}(|\Psi_0\rangle, \dots, |\Psi_{N-1}\rangle), \quad (1)$$

where $\{|\Psi_k\rangle\}_{k=0}^{N-1} \equiv B_{\mathcal{S}}$ are some basis states. Specifically, we impose that $B_{\mathcal{S}} = \{|\Psi_k\rangle\}_{k=0}^{N-1}$ is a linearly independent and nonorthogonal basis set for later convenience. To achieve this, we define the cost function

$$C_{\text{LET}}(U, V, B_{\mathcal{S}}) = 1 - \frac{1}{N} \sum_{k=0}^{N-1} |\langle\Psi_k|V^\dagger U|\Psi_k\rangle|^2, \quad (2)$$

where τ is a fixed time, $U = e^{-i\tau H^{(L)}}$ is the time evolution operator for a given L -qubit Hamiltonian $H^{(L)}$, and $V(\theta)$ is the ansatz quantum circuit with θ being a set of variational parameters. This cost function measures the overlap between the exact time-evolved state $U|\Psi_k\rangle$ and the ansatz state $V|\Psi_k\rangle$ averaged over the basis set spanning the subspace $\mathcal{S}$. The cost function C_{LET} becomes zero if and only if $U|\Psi_k\rangle = e^{i\varphi}V|\Psi_k\rangle$ for all k . Note that the global phase factor is independent of k owing to the linear independence and nonorthogonality of the basis states (see Appendix A for details). Hence, the time evolution of any states belonging to the subspace $\mathcal{S}$, which are described by linear combinations of the basis states, can be reproduced. We also assume that the basis states $\{|\Psi_k\rangle\}_{k=0}^{N-1}$ can be efficiently prepared on a quantum computer using a set of state preparation circuits $\{W_k\}_{k=0}^{N-1}$ as $|\Psi_k\rangle = W_k|0\rangle^{\otimes L}$. Then, the cost C_{LET} can be measured by performing the LET [14] on L -qubit quantum circuits shown in Fig. 2(a).

Although the cost function C_{LET} is a natural quantity describing the difference between U and $V(\theta)$ within the target subspace $\mathcal{S}$, it suffers from the exponentially vanishing gradient (i.e., barren plateaus) for a large system size since C_{LET} is a global cost defined on the whole system [18,19]. To circumvent the barren plateau, we can alternatively use a local version of the cost function defined as

$$C_{\text{LLET}}(U, V, B_{\mathcal{S}}) = \frac{1}{L} \sum_{j=1}^L C_{\text{LLET}}^{(j)}(U, V, B_{\mathcal{S}}), \quad (3)$$

where

$$C_{\text{LLET}}^{(j)}(U, V, B_{\mathcal{S}}) = 1 - \frac{1}{N} \sum_{k=0}^{N-1} \text{Tr}[\Pi_j \rho_k(U, V, B_{\mathcal{S}})], \quad (4)$$

$$\rho_k(U, V, B_{\mathcal{S}}) = (\tilde{V}_k)^\dagger U |\Psi_k\rangle \langle \Psi_k| U^\dagger \tilde{V}_k. \quad (5)$$

In Eqs. (4) and (5), $\tilde{V}_k = V W_k$ and $\Pi_j = \mathbb{1}_1 \otimes \dots \otimes |0\rangle\langle 0|_j \otimes \dots \otimes \mathbb{1}_L$ is the projection operator for j th qubit ($j = 1, 2, \dots, L$). The local cost function C_{LLET} can be measured

on a quantum computer by performing the local Loschmidt echo test (LLET) [14] using a L -qubit quantum circuit shown in Fig. 2(b). Because the LLET only performs a local measurement at j th qubit to obtain $C_{\text{LLET}}^{(j)}$, the local cost function C_{LLET} avoids the barren plateau under the assumption of using a shallow-depth ansatz [17]. The local cost function C_{LLET} and global cost function C_{LET} are connected through the following inequality [13,14]:

$$C_{\text{LLET}} \leq C_{\text{LET}} \leq L \cdot C_{\text{LLET}}, \quad (6)$$

where we omitted the arguments (U, V) for brevity. From Eq. (6), we can safely say that $C_{\text{LLET}} = 0$ if and only if $C_{\text{LET}} = 0$. Therefore, we can alternatively minimize the local cost C_{LLET} instead of minimizing the global cost C_{LET} .

When the system size L is small enough and the target time evolution U can be efficiently implemented (e.g., using Trotterization), we can directly optimize the cost functions C_{LET} or C_{LLET} by performing the LET or LLET on L -qubit quantum devices. However, it becomes difficult to directly perform the LET or LLET on L -qubit quantum devices when the system size L becomes large. To address this, we adopt the LSVQC algorithm, which performs variational optimization on small local subsystems. In the LSVQC, not only measurement but also the size of the quantum circuit is localized in contrast to the LLET. In Sec. IV, we provide a theorem that guarantees such local optimization protocol.

B. Guideline for subspace design

Here, we provide a guideline for designing the subspace appropriate to typically encountered situations in quantum many-body simulations.

1. Dynamics of a fixed input state

One of the most common situations is simulating the dynamics of a physical observable A for a fixed input state $|\psi\rangle$ as

$$\langle A(t) \rangle_\psi = \langle \psi | e^{itH} A e^{-itH} | \psi \rangle, \quad (7)$$

where H is the Hamiltonian and t is a time. The input state $|\psi\rangle$ can be generally expanded in the energy eigenbasis as

$$|\psi\rangle = \sum_{m=1}^{N_{\text{eig}}} a_m |E_m\rangle, \quad (8)$$

where $\{|E_m\rangle\}_{m=1}^{N_{\text{eig}}}$ is a set of energy eigenstates, a_m is a nonzero complex coefficient, and $1 \leq N_{\text{eig}} \leq 2^L$. Then, the dynamics $\langle A(t) \rangle_\psi$ can be expressed as

$$\langle A(t) \rangle_\psi = \sum_{m,m'}^{N_{\text{eig}}} a_m^* a_{m'} e^{i(E_m - E_{m'})t} \langle E_m | A | E_{m'} \rangle. \quad (9)$$

Equation (9) indicates that the time evolution of $\langle A(t) \rangle_\psi$ is enclosed in the N_{eig} -dimensional subspace spanned by the energy eigenstates $\{|E_m\rangle\}_{m=1}^{N_{\text{eig}}}$. Thus, N_{eig} linearly independent states are required to perfectly learn the action of the time evolution e^{-itH} on the input state $|\psi\rangle$ [17,60]. From this fact, we naively expect that one appropriate choice of the subspace is the following Krylov subspace generated by the real-time

evolution,

$$\mathcal{S}_\psi(N_t) = \text{span}(\{U(t_n)|\psi\rangle\}_{n=0}^{N_t}), \quad (10)$$

where $U(t_n) \approx e^{-it_n H}$ is the approximate time-evolution operator, $t_n = n\Delta_t$ is a time step with some interval Δ_t , and N_t is an integer satisfying $0 \leq N_t \leq N_{\text{eig}}$. Although we can consider other subspaces (e.g., linear response subspace in Refs. [28,29]), we adopt the above Krylov subspace as a natural choice for quantum computers since the time-evolved states $\{U(t_n)|\psi\rangle\}$ can be prepared on quantum circuits with polynomial cost and controllable accuracy. Note that the real-time Krylov subspace is indeed utilized in other subspace-based quantum algorithms such as the QFD [31], MRSQK [32], and fsVFF [17]. The time-evolved states $\{U(t_n)|\psi\rangle\}$ in general form a linearly independent and nonorthogonal basis set except for very special parameter settings [17], and hence are appropriate for the LSVQC. Although the parameter N_t should be chosen to be equal to N_{eig} ideally, we allow $N_t < N_{\text{eig}}$ considering the common situations where only some eigenstates have dominant amplitudes. The value of N_{eig} can be estimated by computing the determinant of the Gramian matrix as proposed in Ref. [17].

Since the required number of quantum circuits for the LET or LLET increases with the dimension of the subspace, exponential growth of N_{eig} against the system size L is undesirable for efficient computation. Therefore, we only consider the case N_{eig} scales only polynomially with the system size L [17]. This is a reasonable assumption for many circumstances since many physically relevant quantum many-body states are confined within an exponentially small subspace of the entire Hilbert space [61]. Even when N_{eig} scales exponentially with the system size L , it is possible that the state $|\psi\rangle$ has a dominant overlap with only a small number of the energy eigenstates and we can set $N_t = \mathcal{O}(\text{poly}L)$ [17]. Note that such a subspace, spanned by a polynomial number of energy eigenstates, does not necessarily lie in a regime efficiently simulatable by classical computers when L is large. This is because classically simulating the dynamics within such an energy subspace requires diagonalizing the exponentially large Hamiltonian and expressing the time-evolution unitary and the input state $|\psi\rangle$ in the energy eigenstates $\{|E_m\rangle\}$.

We can implement the approximate time-evolution operator $U(t_n)$ by adopting the first-order Trotterization. We here note that, in near-term quantum computing devices, it is required that the depth of $U(t_n)$ is within the coherence time. In addition, the LSVQC itself requires that the depth of the state preparation circuits is shallow to ensure the local compilation theorem derived in Sec. IV [see Eq. (24) for details]. Considering these restrictions, we implement $U(t_n)$ as a single step Trotterized unitary for all t_n in numerical simulations in Secs. V and VI. Since such approximation generally causes a large Trotter error and leakage from the ideal Krylov subspace when t_n is large, a small value of t_n is desirable. On the other hand, the basis states in the Krylov subspace tend to be linearly dependent for small t_n since the unitary $U(t_n)$ approaches the identity operator. Such a situation is undesirable since the information on the ideal Krylov subspace is lost. Therefore, we choose a moderate value of t_n to balance the Trotter error and linear independence of basis states. We

demonstrate such a tradeoff in the numerical simulations in Sec. V.

2. Dynamics of correlation functions

Another common situation in quantum many-body physics is simulating the dynamical correlation function for a given quantum state $|\psi\rangle$,

$$\langle A(t)B \rangle_\psi = \langle \psi | e^{itH} A e^{-itH} B | \psi \rangle, \quad (11)$$

where A and B are some quantum mechanical operators (not necessarily Hermitian). For example, when A and B are fermionic annihilation and creation operators, respectively, $\langle A(t)B \rangle_\psi$ becomes the Green's function (GF), which is treated in Sec. VI. Equation (11) is regarded as a transition amplitude of the physical quantity A for the time-evolved states $e^{-itH}|\psi\rangle$ and $e^{-itH}B|\psi\rangle$. Thus, in the same spirit of the subspace (10), we can choose a real-time Krylov subspace for two states $|\psi\rangle$ and $B|\psi\rangle$ as a subspace appropriate for computing the dynamical correlation function $\langle A(t)B \rangle_\psi$. Specifically, such Krylov subspace is defined as

$$\mathcal{S} = \text{span}(\{U(t_n)|\psi\rangle, U(t_n)B|\psi\rangle\}_{n=0}^{N_t}), \quad (12)$$

where the definition of $U(t_n)$ and N_t are same with Eq. (10). In contrast to the subspace (10), the subspace (12) might not satisfy the requirement of linear independence and nonorthogonality depending on the details of the operators A and B . In such cases, we moderately change the choice of basis states to fulfill the linear independence and nonorthogonality conditions. An example of such transformation is shown in Sec. VIB for the GF. We note that a subspace similar to Eq. (12) is indeed used in Ref. [62] to perform the QSE for GF computation.

IV. LOCAL COMPILATION THEOREM

Here, we derive the *local compilation theorem* that guarantees the local optimization protocol in the LSVQC algorithm [procedure (b) in Fig. 1]. Similar to the discussion in Ref. [41], the local compilation theorem is derived in the following two steps:

(1) Local restriction of the target time-evolution operator by the LR bound.

(2) Local restriction of the ansatz and state preparation circuits based on the causal cone.

We consider the local restriction of not only the target time-evolution unitary and ansatz but also the state preparation circuit generating the subspace basis states. This is the main difference from the discussion of Ref. [41], in which only the local restriction of the target time-evolution unitary and ansatz is discussed.

First, we clarify the setup and notation. We consider quantum many-body Hamiltonian $H^{(L)}$ defined on a size- L lattice Λ (i.e., $L = |\Lambda|$),

$$H^{(L)} = \sum_{X \subseteq \Lambda} H_X, \quad (13)$$

where H_X denotes a term that nontrivially acts on a domain $X \subseteq \Lambda$. For simplicity of discussion, we only consider spin systems in this section although the extension to the fermionic

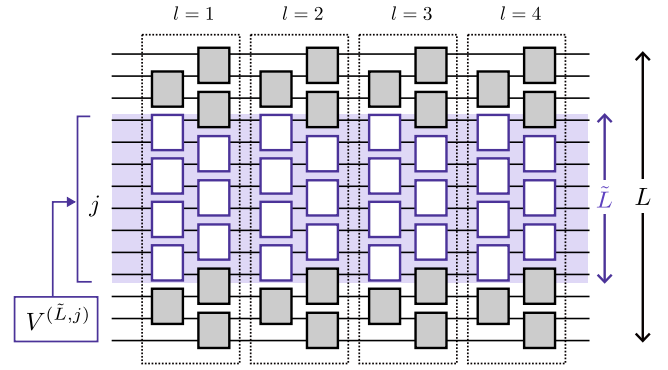


FIG. 3. Schematic illustration of the brickwork-structured ansatz $V^{(L)}(\theta)$ and its local restriction $V^{(L,j)}(\theta)$. The purple area represents the j -centered $\tilde{L}$ -size local domain $\Lambda^{(L,j)}$. Only white two-qubit gates contribute to the restricted ansatz $V^{(L,j)}(\theta)$.

Hamiltonian is straightforward (see Ref. [42]). We assume that $H^{(L)}$ consists of only local terms and finite-range interactions. This leads to the LR bound, which is formally expressed for any local observables $O_{X,Y}$ acting on domain $X, Y \subseteq \Lambda$ as follows [54]:

$$\|[(U^{(L)})^\dagger O_X U^{(L)}, O_Y]\| \leq C e^{-[\text{dist}(X,Y) - v|\tau|]/\xi}, \quad (14)$$

where $U^{(L)} = e^{-itH^{(L)}}$ for a fixed time τ , $\text{dist}(X,Y)$ is the distance between the domains, and $\|\cdot\|$ denotes the operator norm. The velocity v , length ξ , and constant C are determined by the properties of $H^{(L)}$ and irrespective of the system size L . The constant C typically linearly increases as a function of τ . For simplicity, we consider an ansatz $V^{(L)}(\theta)$ with a brick-wall structure (see Fig. 3),

$$V^{(L)}(\theta) = \prod_{l=1}^{d_V} \left[\left(\prod_{i=1}^{L/2} v_{2i-1,2i}^{(l)}(\theta_{2i-1}^{(l)}) \right) \times \left(\prod_{i=1}^{L/2-1} v_{2i,2i+1}^{(l)}(\theta_{2i}^{(l)}) \right) \right], \quad (15)$$

where d_V denotes the depth of the ansatz and $\theta = \{\theta_i^{(l)}\}_{i,l}$ is a set of variational parameters. The two-qubit gates $v_{i,i+1}^{(l)}$ acts nontrivially only on the sites i and $i+1$. We also impose the brick-wall structure on the state preparation circuits $W_k^{(L)}$ as

$$W_k^{(L)} = \prod_{l=1}^{d_{W_k}} \left[\left(\prod_{i=1}^{L/2} w_{2i-1,2i}^{(k,l)} \right) \left(\prod_{i=1}^{L/2-1} w_{2i,2i+1}^{(k,l)} \right) \right], \quad (16)$$

where d_{W_k} denotes the depth and $w_{i,i+1}^{(k,l)}$ acts nontrivially only on the sites i and $i+1$. Although we assume brick-wall structures to $V^{(L)}(\theta)$ and $\{W_k^{(L)}\}_{k=0}^{N-1}$ for simplicity, the local compilation theorem can be derived to other cases as long as these circuits have local structure.

Now, we proceed to the step (i). We define a local restriction of the Hamiltonian $H^{(L)}$ as

$$H^{(L',j)} = \sum_{X; X \subseteq \Lambda^{(L',j)}} H_X, \quad (17)$$

where $\Lambda^{(L',j)}$ is a j -centered L' -size lattice defined as

$$\Lambda^{(L',j)} = \{j' \in \Lambda | \text{dist}(j, j') \leq L'/2\}. \quad (18)$$

For the restricted Hamiltonian $H^{(L',j)}$, we define the corresponding time-evolution operator as

$$U^{(L',j)} = e^{-iH^{(L',j)}\tau} \otimes \mathbb{1}_{\Lambda \setminus \Lambda^{(L',j)}}. \quad (19)$$

The restricted time-evolution operator $U^{(L',j)}$ and the target time-evolution operator $U^{(L)} = e^{-i\tau H^{(L)}}$ is related by the following proposition.

Proposition 1 (Local restriction of the target time-evolution operator). Let us define the restriction size L' as

$$L' = 2(l_0 + r_H + v\tau + 2(d_V + \max_k d_{W_k})), \quad (20)$$

where r_H denotes the range of interaction, v is the LR velocity in Eq. (14), and l_0 is a tunable parameter. Here, we impose that the parameters τ , d_V , and d_{W_k} are chosen such that $L' < L$. Then, the local cost function $C_{\text{LLET}}^{(j),S}$ satisfies the following inequality:

$$C_{\text{LLET}}^{(j)}(U^{(L)}, V^{(L)}, B_S) \leq C_{\text{LLET}}^{(j)}(U^{(L',j)}, V^{(L)}, B_S) + \frac{1}{2}\epsilon_{\text{LR}}. \quad (21)$$

Here, the error term ϵ_{LR} scales as $\mathcal{O}(e^{-(l_0+R/2)/\xi})$ with $R = 4(d_V + \max_k d_{W_k})$. Thus, the approximation error ϵ_{LR} can be exponentially small by increasing the parameter l_0 (i.e., increasing the restriction size L').

Proposition 1 is justified by the LR bound (see Appendix B for the proof of Proposition 1). Based on Proposition 1, we can evaluate the local cost functions $C_{\text{LLET}}^{(j),S}(U^{(L)}, V^{(L)})$ in Eq. (4) by using the restricted time-evolution operator $U^{(L',j)}$ instead of the original time-evolution operator $U^{(L)} = e^{-i\tau H^{(L)}}$.

Next, we proceed to the step (ii). We define the locally restricted version of the ansatz $V^{(L)}(\theta)$ as

$$V^{(\tilde{L},j)}(\theta) = \prod_{l=1}^{d_V} \left[\left(\prod_{i \in \Lambda^{(\tilde{L},j)}} v_{2i-1,2i}^{(l)}(\theta_{2i-1}^{(l)}) \right) \times \left(\prod_{i \in \Lambda^{(\tilde{L},j)}} v_{2i,2i+1}^{(l)}(\theta_{2i}^{(l)}) \right) \right], \quad (22)$$

where $\prod'_{i \in \Lambda^{(\tilde{L},j)}}$ denotes the product over i such that the support of $v_{2i-1,2i}^{(l)}$ or $v_{2i,2i+1}^{(l)}$ is included in the domain $\Lambda^{(\tilde{L},j)}$ (see Fig. 3). Similarly, we define the local restriction of the state preparation circuits $\{W_k^{(L)}\}$ as

$$W_k^{(\tilde{L},j)} = \prod_{l=1}^{d_{W_k}} \left[\left(\prod_{i \in \Lambda^{(\tilde{L},j)}} w_{2i-1,2i}^{(l)} \right) \left(\prod_{i \in \Lambda^{(\tilde{L},j)}} w_{2i,2i+1}^{(l)} \right) \right]. \quad (23)$$

Then, $V^{(L)}(\theta)$ and $\{W_k^{(L)}\}$ appeared in Eq. (21) can be replaced by their locally restricted counterparts using the following proposition.

Proposition 2 (Local restriction of the ansatz and state preparation circuits). Let us set the compilation size $\tilde{L}(>L')$

such that

$$\tilde{L} \geq \max \left(\frac{L'}{2} + 2(d_V + \max_k d_{W_k}) + 1, L' + 4 \max_k d_{W_k} \right), \quad (24)$$

where L' is given by Eq. (20). Then, the following equality holds for the right-hand side of Eq. (21),

$$C_{\text{LLET}}^{(j)}(U^{(L',j)}, V^{(L)}, B_S) = C_{\text{LLET}}^{(j)}(\tilde{U}^{(L',j)}, V^{(\tilde{L},j)}, B_{\tilde{S}_j}). \quad (25)$$

Here, $\tilde{U}^{(L',j)}$ is the extension of $U^{(L',j)}$ to the $\tilde{L}$ -size domain $\Lambda^{(\tilde{L},j)}$,

$$\tilde{U}^{(L',j)} = e^{-i\tau H^{(L',j)}} \otimes \mathbb{1}_{\Lambda^{(\tilde{L},j)} \setminus \Lambda^{(L',j)}}. \quad (26)$$

$B_{\tilde{S}_j}$ denotes a basis set of a subspace $\tilde{S}_j$ spanned by the states generated by the locally restricted state preparation circuits $\{W_k^{(\tilde{L},j)}\}$, i.e.,

$$B_{\tilde{S}_j} = \{W_k^{(\tilde{L},j)}|0\rangle^{\otimes \tilde{L}}\}_{k=0}^{N-1}, \quad (27)$$

$$\tilde{S}_j = \text{span}(B_{\tilde{S}_j}). \quad (28)$$

Proposition 2 is derived based on the causal cone arising from the locality of the ansatz and state preparation circuits. The proof of Proposition 2 is given in Appendix B.

Combining Proposition 1 with Proposition 2, we arrive at the following local compilation theorem:

Theorem 1 (Local compilation theorem). We define the local subsystem cost function as

$$C^{(\tilde{L})}(\theta) = \frac{1}{L} \sum_{j=1}^L C_{\text{LLET}}^{(j)}(U^{(\tilde{L},j)}, V^{(\tilde{L},j)}(\theta), B_{\tilde{S}_j}). \quad (29)$$

When we achieve $C^{(\tilde{L})}(\theta^*) \leq \epsilon_{\text{opt}}$ for some optimal parameter set θ^* , the cost functions for the original L -size system are bounded as follows:

$$C_{\text{LLET}}(U^{(L)}, V^{(L)}(\theta^*), B_S) \leq \epsilon_{\text{opt}} + \epsilon_{\text{LR}}, \quad (30)$$

$$C_{\text{LET}}(U^{(L)}, V^{(L)}(\theta^*), B_S) \leq L(\epsilon_{\text{opt}} + \epsilon_{\text{LR}}). \quad (31)$$

The proof of Theorem 1 is provided in Appendix B. Based on Theorem 1, we can indirectly minimize the cost functions C_{LLET} or C_{LET} for the target L -size system by minimizing the local subsystem cost function $C^{(\tilde{L})}(\theta)$. This fact justifies the local optimization protocol of the LSVQC.

Theorem 1 is a general form of the local compilation theorem. On the other hand, we can modify the local compilation theorem into a form suitable for practical use. In Appendix C, we provide modified versions of the local compilation theorem for translation invariant systems and long-time dynamics simulation.

The appropriate choice of the compilation size $\tilde{L}$ depends on the purpose of the whole computation. If we aim to simulate the dynamics of global observables (i.e., observables acting on a large number of sites or whole lattice) with the accuracy ϵ , we need to achieve $C_{\text{LET}} = \mathcal{O}(\epsilon)$ at least. This indicates that the compilation size should be chosen to realize $L\epsilon_{\text{LR}} = \mathcal{O}(Le^{-(l_0+R/2)/\xi}) = \mathcal{O}(\epsilon)$. On the other hand, when we simulate the dynamics of some local observables (e.g., local particle density) with the accuracy ϵ , we only need

to realize $C_{\text{LLET}} = \mathcal{O}(\epsilon)$ since C_{LLET} quantifies the local accuracy of the time evolution. Then, the compilation size is determined to realize $\epsilon_{\text{LR}} = \mathcal{O}(e^{-(l_0+R/2)/\xi}) = \mathcal{O}(\epsilon)$. In summary, to achieve the accuracy ϵ for the dynamics simulation of global or local observables, the compilation size $\tilde{L}$ should be chosen as

$$\tilde{L} \geq \mathcal{O}(\xi \log(L^\alpha/\epsilon)) + r_H + v\tau + 2 \max_k d_{W_k} + \max \left(2d_V + 1, r_H + v\tau + 2 \max_k d_{W_k} \right), \quad (32)$$

where $\alpha = 1$ ($\alpha = 0$) for global (local) observables. Note that the LSVQC algorithm might work well even when the compilation size is set to be smaller than the right-hand side of Eq. (32) owing to the looseness of the expression of the LR bound given by Eq. (14). Indeed, we show such an example in Sec. VI.

V. NUMERICAL DEMONSTRATION FOR HEISENBERG SPIN CHAIN

Here, we demonstrate the basic properties of the LSVQC algorithm by performing a numerical simulation of a simple toy model. Specifically, we consider the 1D antiferromagnetic Heisenberg model

$$H^{(L)} = \sum_{j=1}^L (X_j X_{j+1} + Y_j Y_{j+1} + Z_j Z_{j+1}), \quad (33)$$

where we adopt the periodic boundary condition. We approximate the target time-evolution unitary $e^{-i\tau H^{(L)}}$ by applying the first-order Trotterization as

$$U^{(L)} = (e^{-i(\tau/r)H_{\text{even}}^{(L)}} e^{-i(\tau/r)H_{\text{odd}}^{(L)}})^r, \quad (34)$$

where the depth parameter r is set to be a large value $r = 100$. Note that we only need to implement a local restriction of $U^{(L)}$ to a compilation size $\tilde{L} (< L)$ in the optimization protocol of the LSVQC. $H_{\text{odd}}^{(L)}$ ($H_{\text{even}}^{(L)}$) represents the sum of terms connecting odd-even (even-odd) sites in $H^{(L)}$. To make clear correspondence with the discussion in Sec. IV, we adopt a brick-wall structure ansatz $V^{(L)}(\theta)$ given by Eq. (15). We parametrize the two-qubit gates $v_{j,j+1}(\theta_l)$ by the following symmetry-preserving form [41]

$$v_{j,j+1}(\eta, \zeta, \chi, \gamma, \phi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & e^{-i(\gamma+\zeta)} \cos \eta & -ie^{-i(\gamma-\chi)} \sin \eta & 0 \\ 0 & -ie^{-i(\gamma+\chi)} \sin \eta & e^{-i(\gamma-\zeta)} \cos \eta & 0 \\ 0 & 0 & 0 & e^{-i(2\gamma+\phi)} \end{pmatrix}, \quad (35)$$

in the basis of $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$. Here, $(\eta, \zeta, \chi, \gamma, \phi)$ is a set of variational parameters. $v_{j,j+1}(\theta_l)$ in the form of Eq. (35) preserves the total Z spin of the system, which is a symmetry of Eq. (33) [41]. We also impose the translational symmetry to the ansatz as $v_{j,j+1} = v_{j+2,j+3}$ for any $j \in \{1, 2, \dots, L\}$ under the periodic boundary condition. As a simple example, we aim

to simulate the dynamics of the following Néel state

$$|\psi_0\rangle = \prod_{j=1}^{L/2} X_{2j}|0\rangle^{\otimes L} = |1010 \dots 10\rangle. \quad (36)$$

For simplicity, we assume that the target physical quantity is not a correlation function like Eq. (11). In this case, we can utilize the Krylov subspace $\mathcal{S}$ given by Eq. (10) as a target subspace of the LSVQC.

Under the above setup, we numerically demonstrate the performance of the LSVQC algorithm. Since the Hamiltonian, the ansatz, and the state preparation circuits are all translationally invariant, we can apply the LSVQC based on Theorem 2 in Appendix C. We first estimate the compilation size $\tilde{L}$ based on Eq. (32). In the following, we fix the depth of the ansatz as $d_V = 2$ and execute the LSVQC to compile the time-evolution operator at $\tau = 0.1$. The range of the interaction of the Hamiltonian (33) is $r_H = 1$. The parameters v and ξ are in general $\mathcal{O}(1)$ and independent of the system size. Thus, $v\tau$ in Eq. (32) can be negligible when the time τ is chosen as a small value $\tau = 0.1$. Since $|\psi_0\rangle$ is just a computational basis state and the time-evolution operator in the Krylov subspace (10) is approximated by the single step Trotterization circuit, the depth of the state preparation circuits is $d_{W_k} = 1$. We set $\alpha = 0$ and use the LLET cost considering the simulation of local observables. Using these parameters, we can roughly estimate the proper compilation size as $\tilde{L} \gtrsim 8$. Therefore, we fix the compilation size as $\tilde{L} = 8$ and simulate the dynamics at size $L \geq 8$. The cost functions are minimized by using the Broyden-Fletcher-Goldfarb-Shanno (BFGS) method implemented in SciPy [63]. We start the optimization from the initial value θ_0 , which is chosen so that the initial ansatz $V^{(L)}(\theta_0)$ becomes equivalent to the same-depth Trotterization circuit (34) (i.e., $r = d_V = 2$). The quantum circuit simulation is performed using Qulacs [64].

First, we investigate how the subspace design influences the performance of the LSVQC. We quantify the accuracy of optimized ansatz by evaluating the state infidelity as

$$\bar{F}^{(L)}(t) = 1 - |\langle \psi_0 | V^{(L)}(\theta^*)^n | \psi_0 \rangle|, \quad (37)$$

where $t = n\tau$ and $n \in \mathbb{N}$. Figure 4 shows the time dependence of the state infidelity for $L = 16$ calculated by using the optimized ansatz $V^{(L)}(\theta^*)$ obtained by the LSVQC (colored markers). The results of the Trotterization with $r = d_V = 2$ (black dashed line) are also shown for comparison. The accuracy of the LSVQC is strongly affected by the parameters of the subspace (10). Enlarging the dimension of the subspace by increasing N_t from 0 to 5 with $\Delta_t = 0.1$, the state infidelity of the LSVQC gradually decreases and saturates at $N_t \simeq 4$ [Fig. 4(a)]. This suggests the time evolution of $|\psi_0\rangle$ can be accurately approximated by the LSVQC using a moderate number of basis states sufficient to describe the ideal Krylov subspace. Note that Δ_t is set to be a small value, $\Delta_t = 0.1$, and hence the effect of the Trotter error stated in Sec. III B is expected to be negligible. On the other hand, Fig. 4(b) shows that the accuracy of the LSVQC is maximized at some moderate value of Δ_t , i.e., $\Delta_t = 0.5$. This behavior can be understood as a consequence of the competition between the linear independence of the input states and the subspace leakage explained in Sec. III B. Increasing Δ_t increases the linear independence

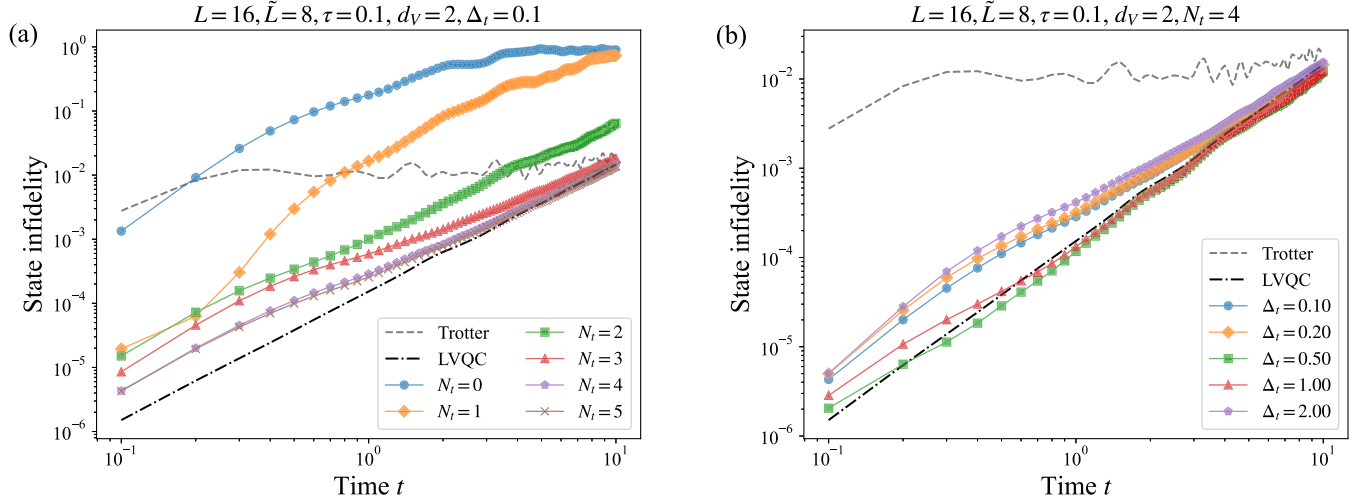


FIG. 4. State infidelity for the Néel state $|\psi_0\rangle$ with $L = 16$ as a function of the time $t = n\tau$ with $n \in \mathbb{N}$. The colored markers represent the results obtained by the LSVQC with (a) $\Delta_t = 0.1$, $N_t = 0, 1, \dots, 5$ and (b) $N_t = 4$, $\Delta_t = 0.1, 0.2, 0.5, 1.0, 2.0$. The gray dash-dotted line indicates the result obtained by the Trotterization. The LSVQC is performed for $\tilde{L} = 8$, $\tau = 0.1$, and $d_V = 2$.

of the input states, which is required to correctly learn the time evolution in the subspace as stated in the no-free-lunch theorem [60]. However, increasing Δ_t also induces leakage from the ideal subspace because of the large Trotter error. As a consequence of these two effects, the best performance of the LSVQC is obtained at some intermediate value of Δ_t as shown in Fig. 4(b). In the following numerical calculations, we choose the subspace parameters as $(N_t, \Delta_t) = (1, 0.5)$, which is an optimal parameter set found by computing the average state infidelity $\frac{1}{n} \sum_{n=1}^{100} \bar{F}(n\tau)$ for $N_t = 0, 1, \dots, 10$ and $\Delta_t = 0.1, 0.2, 0.5, 1.0, 2.0$.

Next, we demonstrate the circuit depth compression realized by the LSVQC. For convenience of the following discussion, we here define the depth compression rate as

$$R_{\epsilon}^{\text{LSVQC}} = \frac{D_{\epsilon}^{\text{trot}}}{D_{\epsilon}^{\text{LSVQC}}}, \quad (38)$$

where $D_{\epsilon}^{\text{LSVQC}}$ and $D_{\epsilon}^{\text{trot}}$ are the required circuit depth of the LSVQC and Trotterization to achieve some accuracy ϵ , respectively. The ratio $R_{\epsilon}^{\text{LSVQC}}$ measures how much the circuit depth can be reduced by employing the LSVQC compared to the Trotterization. When $R_{\epsilon}^{\text{LSVQC}} > 1$, depth compression compared to the Trotterization is realized by using the LSVQC.

In Fig. 5(a), we compare the size dependence of the state infidelity of LSVQC (green circles) and Trotterization (gray cross marks) as a function of the system size $L \geq \tilde{L} = 8$. To visualize the depth compression rate of the LSVQC against the Trotterization, we show the state infidelity of the Trotterization for various depth parameters r but the depth of the LSVQC is fixed to $d_V = 2$. We see that the state infidelity of the LSVQC is comparable to that of the Trotterization with $r = 40\text{--}50$ for all L . Hence, the depth compression rate can be estimated as $R_{\epsilon}^{\text{LSVQC}} \simeq 40/2 = 20$. In other words, the LSVQC realizes the simulation of this model using a circuit shallower by about 95% than the Trotterization while maintaining the accuracy. We also note that this result suggests

the robustness of the LSVQC for the extension of the system size under a fixed compilation size. The size-insensitive behavior is consistent with the local compilation theorem in Sec. IV, in which the bound of the compilation size does not directly depend on the system size L [see Eq. (24)]. In Fig. 5(b), we show that the state infidelity of the LSVQC gradually increases by increasing the simulation time step n . This is consistent with the fact that the approximation error of the LSVQC increases at a long-time scale as shown in Eq. (C8). This implies that we need to logarithmically enlarge the compilation size $\tilde{L}$ based on Eq. (C8) to achieve significant depth compression even at a long-time regime. We also note that ill-conditioning of Krylov basis (i.e., tendency of linear dependence of the Krylov basis for long-time regime [65]) may also contribute to the increased approximation error at the long-time regime. Such behavior might be alleviated by incorporating fast-forwarding techniques, based on the multi-reference Krylov subspace method [66], or by adopting a sophisticated fast-forwarding ansatz [17] for the circuit compilation. We leave these potential avenues for future research to improve the performance of the LSVQC.

VI. APPLICATION TO SIMULATION OF A STRONGLY CORRELATED MATERIAL MODEL

In this section, we apply the LSVQC to the simulation of a strongly correlated material model. Specifically, we aim to efficiently simulate a low-energy effective lattice model for strongly correlated electron materials (e.g., high-temperature superconductors) on quantum computers using the LSVQC. We use a technique of the classical materials simulation called the *ab initio* downfolding [67] to construct the effective low-energy model of strongly correlated electron materials. The *ab initio* downfolding is executed in the following three steps. The first step is the band structure calculation based on the density functional theory (DFT), which is executed using Quantum ESPRESSO package [68–70]. In the DFT calculation, we adopt the generalized gradient approximation

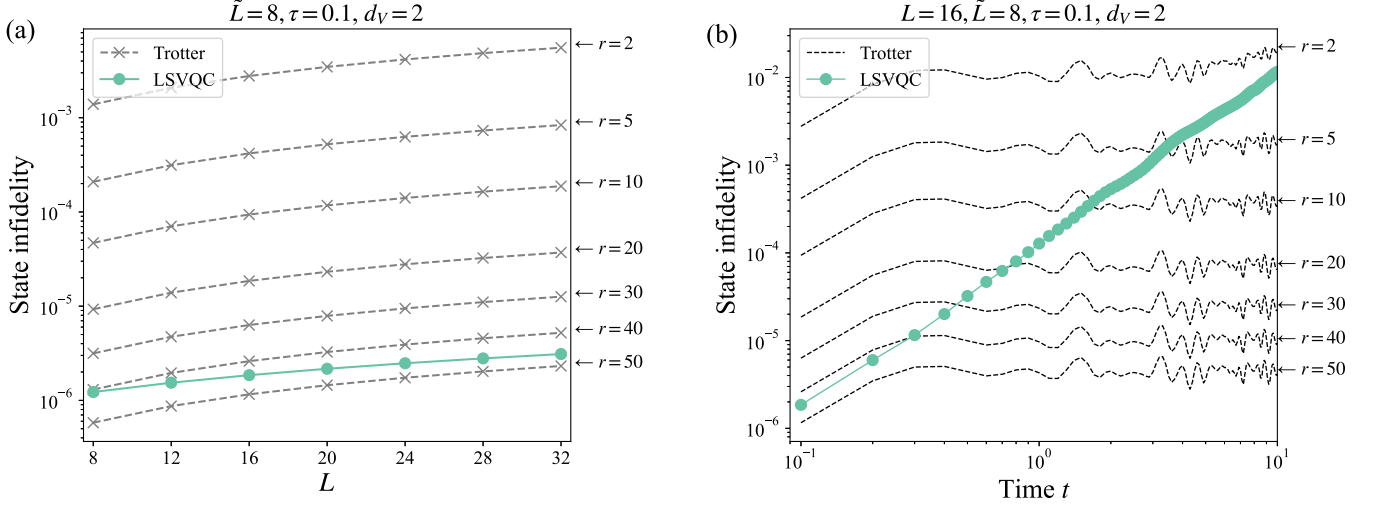


FIG. 5. Numerical demonstration of the depth compression in terms of the state infidelity for the Néel state $|\psi_0\rangle$. (a) The size dependence of the state infidelity for $L \geq 8$. (b) The state infidelity as a function of the time $t = n\tau$ for $L = 16$. The green circles show the state infidelity obtained by the LSVQC. The gray dashed lines or gray cross marks indicate the state infidelity of the Trotterization for various values of the depth parameter r . The LSVQC is performed for $\tilde{L} = 8$, $\tau = 0.1$, and $d_V = 2$.

by Perdew-Burke-Ernzerhof to the exchange-correlation functional [71] and norm-conserving pseudopotentials [72,73]. Second, we construct the orbital of the effective lattice model using the maximally localized Wannier function [74]. The third step is to calculate the effective Coulomb and effective exchange interactions by adopting the constrained random phase approximation [75] using the Wannier orbital obtained in the second step. The second and third steps are numerically executed using RESPACK package [76–81]. The effective lattice model obtained by the *ab initio* downfolding, which we call the “extended Fermi-Hubbard model” in the following, enables us to describe the low-energy physics of strongly correlated electron materials that cannot be captured by the DFT. More details are summarized in Appendix D.

We consider Sr_2CuO_3 as a benchmark material. Sr_2CuO_3 is a quasi-one-dimensional cuprate compound with strong electronic correlation mainly from Cu d orbitals [43–47]. The electronic correlation leads to various intriguing phenomena such as antiferromagnetism [43,44], and spin-charge separation [45,46]. Superconductivity is also reported in tetragonal hole-doped $\text{Sr}_2\text{CuO}_{3+\delta}$ [47]. Owing to the quasi-one-dimensional nature of the electronic structure, the *ab initio* downfolding for Sr_2CuO_3 generates a 1D extended Fermi-Hubbard Hamiltonian,

$$\begin{aligned}
 H^{(L)} = & -t_1 \sum_{i \in \Lambda} \sum_{\sigma=\uparrow, \downarrow} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + c_{i+1,\sigma}^\dagger c_{i,\sigma}) \\
 & - t_2 \sum_{i \in \Lambda} \sum_{\sigma} (c_{i,\sigma}^\dagger c_{i+2,\sigma} + c_{i+2,\sigma}^\dagger c_{i,\sigma}) \\
 & + U \sum_{i \in \Lambda} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i \in \Lambda} \sum_{\sigma} n_{i\sigma}, \quad (39)
 \end{aligned}$$

where $c_{i,\sigma}$ and $c_{i,\sigma}^\dagger$ are the annihilation and creation operator of an electron with spin $\sigma (= \uparrow, \downarrow)$ at site $i \in \Lambda = \mathbb{Z}_L = \{0, 1, \dots, L-1\}$, and $n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}$ is the particle number operator. The lattice Λ is defined under the periodic

boundary condition with $L = |\Lambda|$ being the total number of sites. We assume that L is an even integer in the following. The parameters t_1 , t_2 , U , and μ are the nearest-neighbor hopping integral, next-nearest-neighbor hopping integral, on-site Coulomb interaction, and chemical potential, respectively. Note that Eq. (39) contains the next-nearest-neighbor hopping term that is not included in the conventional Fermi-Hubbard model. The values of the parameters calculated by using RESPACK package [76–81] are summarized in Table I. Since there is only a single band around the Fermi energy in the DFT band structure of Sr_2CuO_3 [see Fig. 6(a)], the *ab initio* downfolding model (39) is described by using only a single Wannier orbital shown in Fig. 6(b).

In the quantum circuit simulation, we transform the fermionic Hamiltonian (39) into the qubit representation using the following Jordan-Wigner transformation [83]:

$$c_{i,\sigma} \mapsto \frac{1}{2}(X_{i_\sigma} + iY_{i_\sigma}) \prod_{k < i_\sigma} Z_{k_\sigma}, \quad (40)$$

$$c_{i,\sigma}^\dagger \mapsto \frac{1}{2}(X_{i_\sigma} - iY_{i_\sigma}) \prod_{k < i_\sigma} Z_{k_\sigma}, \quad (41)$$

where $(X_{i_\sigma}, Y_{i_\sigma}, Z_{i_\sigma})$ are the Pauli operators for i_σ th qubit. We allocate the qubits so that their indices satisfy $i_\uparrow = i (= 0, 1, 2, \dots, L-1)$ and $i_\downarrow = 2L-1-i (= 2L-1, 2L-2, \dots, L)$, and the total number of the qubits is $N_q = 2L$.

TABLE I. Parameters of the extended Fermi-Hubbard model for Sr_2CuO_3 obtained by the RESPACK package [76–81]. The value of the chemical potential μ is determined so that the origin of the Wannier-interpolated band structure coincides with that of the DFT band structure.

Parameters	t_1	t_2	U	μ
Value (eV)	0.532	0.0403	1.054	0.159

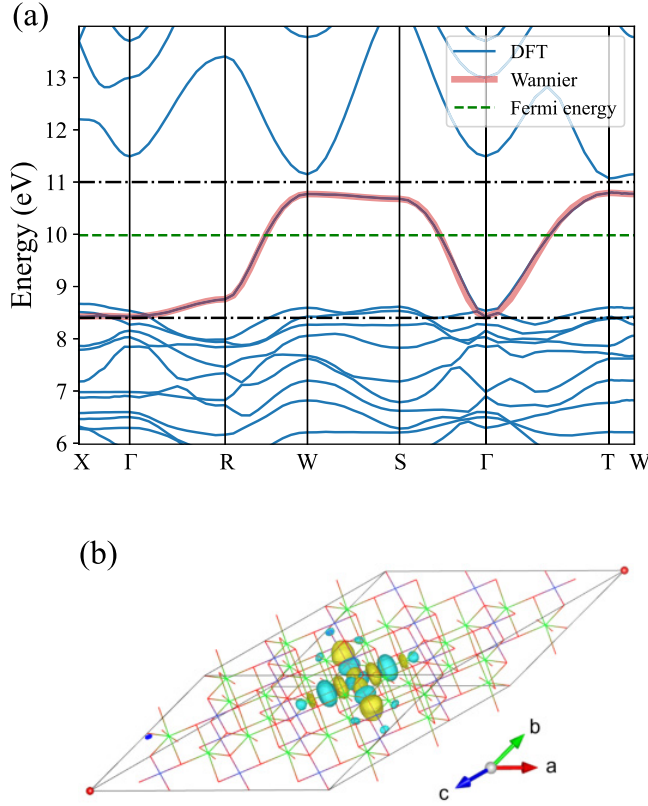


FIG. 6. (a) Band structure of Sr_2CuO_3 . The blue thin curves represent the DFT band structure calculated by using the Quantum ESPRESSO package, while the red bold curve is the Wannier-interpolated band structure. The green-dashed horizontal line indicates the Fermi energy. The Wannier orbitals are constructed using the band structure data in the energy window region, which is described by a region between the black dash-dotted horizontal lines. (b) Calculated Wannier function and the crystal structure of Sr_2CuO_3 (drawn by VESTA [82]). The blue and yellow isosurfaces indicate positive- and negative-value regions of the Wannier function. The green, blue, and red vertices express Sr, Cu, and O atoms, respectively.

Then, the qubit representation of Eq. (39) is obtained as

$$\begin{aligned}
 H^{(L)} = & -\frac{t_1}{2} \sum_{i=1}^L \sum_{\sigma=\uparrow,\downarrow} (X_{i+1\sigma} X_{i\sigma} + Y_{i+1\sigma} Y_{i\sigma}) \\
 & -\frac{t_2}{2} \sum_{i=1}^L \sum_{\sigma} (X_{i+2\sigma} Z_{i+1\sigma} X_{i\sigma} + Y_{i+2\sigma} Z_{i+1\sigma} Y_{i\sigma}) \\
 & + \frac{U}{4} \sum_{i=1}^L Z_{i\uparrow} Z_{i\downarrow} + \frac{1}{2} \left(\mu - \frac{U}{2} \right) \sum_{i=1}^L \sum_{\sigma} Z_{i\sigma}. \quad (42)
 \end{aligned}$$

We perform the LSVQC using the variational Hamiltonian ansatz (VHA) [84,85]. To construct the VHA, we divide the Hamiltonian (42) as

$$H^{(L)} = \sum_{m=1}^M c_m H_m^{(L)}, \quad (43)$$

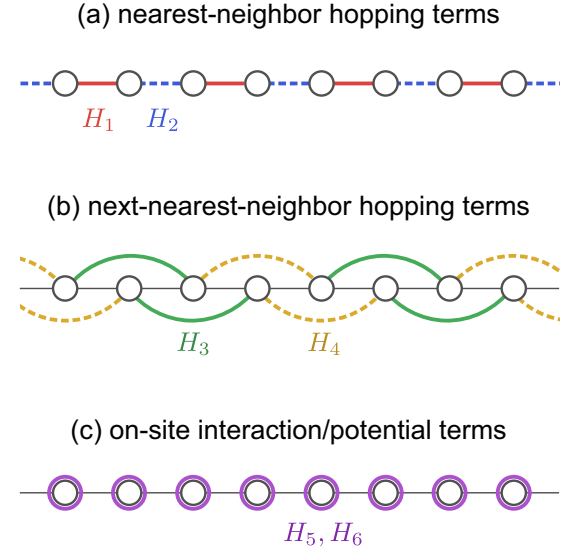


FIG. 7. Schematic illustration of the decomposition of the effective Hamiltonian for Sr_2CuO_3 . (a) Nearest-neighbor hopping terms H_1 (red-solid lines) and H_2 (blue dashed lines). (b) Next-nearest-neighbor hopping terms H_3 (green-solid lines) and H_4 (yellow-dashed lines). (c) On-site interaction terms H_5 and on-site one-body potential terms H_6 .

where each H_m is a sum of mutually commuting terms. The Hamiltonian (42) can be divided into the following six terms (i.e., $M = 6$):

$$H_1^{(L)} = \sum_{i \in \Lambda', \sigma} (X_{i+1\sigma} X_{i\sigma} + Y_{i+1\sigma} Y_{i\sigma}), \quad (44)$$

$$H_2^{(L)} = \sum_{i \in \Lambda', \sigma} (X_{i+2\sigma} X_{i+1\sigma} + Y_{i+2\sigma} Y_{i+1\sigma}), \quad (45)$$

$$H_3^{(L)} = \sum_{i \in \Lambda'', \sigma} (X_{i+2\sigma} X_{i\sigma} + Y_{i+2\sigma} Y_{i\sigma}) Z_{i+1\sigma}, \quad (46)$$

$$H_4^{(L)} = \sum_{i \in \Lambda'', \sigma} (X_{i+4\sigma} X_{i+2\sigma} + Y_{i+4\sigma} Y_{i+2\sigma}) Z_{i+3\sigma}, \quad (47)$$

$$H_5^{(L)} = \sum_{i \in \Lambda} Z_{i\uparrow} Z_{i\downarrow}, \quad (48)$$

$$H_6^{(L)} = \sum_{i \in \Lambda, \sigma} Z_{i\sigma}, \quad (49)$$

where $\Lambda' = (2\mathbb{Z})/L = \{0, 2, 4, \dots\}$ and $\Lambda'' = (4\mathbb{Z})/L \cup ((4\mathbb{Z})/L + 1) = \{0, 1, 4, 5, 8, 9, \dots\}$. Each term is schematically illustrated in Fig 7. The corresponding coefficients are explicitly given by $c_m = (-t_1/2, -t_1/2, -t_2/2, -t_2/2, U/4, (\mu - U/2)/2)$. Under the above decomposition, the VHA is defined as

$$V^{(L)}(\theta) = \prod_{l=1}^{N_L} \left[\prod_{m=1}^M e^{i\theta_{l,m} H_m^{(L)}} \right], \quad (50)$$

where $\theta = \{\theta_{l,m}\}$ is a set of $6N_L$ variational parameters. N_L denotes the number of layers corresponding to the circuit depth. In the same manner, we also define the first-order

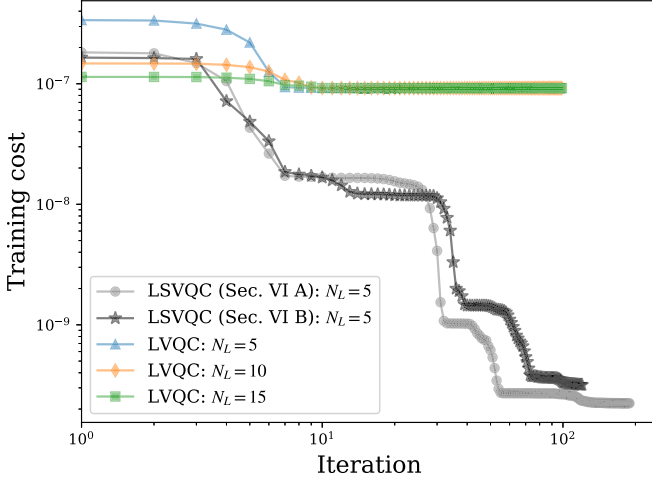


FIG. 8. History of optimization of the cost function of the LSVQC and LVQC for the extended Fermi-Hubbard model of Sr_2CuO_3 with $L = 8$. The cost functions are defined by Eqs. (29) and (F4) for LSVQC and LVQC, respectively. The compilation size is $\tilde{L} = 4$ for both the LSVQC and LVQC. The results of the LSVQC is obtained for two different subspace detailed in Secs. VIA and VIB using the VHA with $N_L = 5$.

Trotterization as

$$U_{\text{trot}}^{(L)}(t) = \left(\prod_{m=1}^M e^{i(t/r)c_m H_m^{(L)}} \right)^r, \quad (51)$$

where t denotes time. The target unitary of the LSVQC $e^{-itH^{(L)}}$ is approximated by the above Trotterization with a large depth $r = 100$. Note that it is not necessary to implement such a deep Trotter circuit on a large-scale L -qubit quantum device. Instead, we only need to implement a local restriction of $U_{\text{trot}}^{(L)}(t)$ to a small compilation size $\tilde{L} (< L)$ to perform the LSVQC algorithm.

Our numerical simulations are performed as follows. The number of sites is set to $L = 8$ ($N_q = 16$), which is the largest system size we could perform the exact classical simulation in our computational environment. The compilation size is set to $\tilde{L} = 4$ ($N_q = 8$), which is the smallest system size the next-nearest-neighbor hopping does not vanish. Although $\tilde{L} = 4$ might be too small compared with the rigorous compilation size given by Eq. (32), we expect that the LSVQC is applicable owing to the looseness of the LR bound. The optimization of the LSVQC is executed in the same way as that in Sec. V. We also execute the LVQC in the same setting for comparison (see Appendix F for details of the LVQC). The results of such cost function optimization are shown in Fig. 8. The subspace setting of the LSVQC is detailed in the following sections. For each subspace, the LSVQC's cost function converges to the optimal value of $\sim 10^{-10}$, which is about two orders of magnitude smaller than the initial value of the initial Trotterization. In contrast, the LVQC does not exhibit such a substantial reduction of the cost value from the initial Trotterization value even when the depth N_L is increased. This behavior reflects the improved trainability of the LSVQC, which is addressed in detail in Sec. VIIC 3.

A. Double occupation dynamics

First, we simulate the dynamics of a simple one-body local observable. Specifically, we consider the dynamics of the double occupation per site

$$\langle D(t) \rangle_{\psi_0} = \frac{1}{|\Lambda|} \sum_{i \in \Lambda} \langle \psi_0(t) | n_{i,\uparrow} n_{i,\downarrow} | \psi_0(t) \rangle, \quad (52)$$

where $|\psi_0(t)\rangle \equiv e^{-itH} |\psi_0\rangle$. The input state $|\psi_0\rangle$ is chosen as the ground state of the noninteracting Hamiltonian, which is obtained by setting $U = 0$ in Eq. (39). We obtain this state for the particle number $N_e = L = 8$ (i.e., half-filling) and total spin $S_z = 0$. Note that the Hamiltonian (39) preserves the particle number N_e and total spin S_z . The noninteracting ground state $|\psi_0\rangle$ can be efficiently prepared on a quantum circuit using the Givens rotation network [86]. We use OpenFermion package [87] to determine the Givens rotation angles. Note that the Givens rotation network circuit has a local circuit structure and satisfies the requirement of the LSVQC. At $t > 0$, the noninteracting ground state $|\psi_0\rangle$ is evolved under the interacting Hamiltonian (39). Since the double occupation $D = \sum_i n_{i,\uparrow} n_{i,\downarrow} / |\Lambda|$ does not commute with the interacting Hamiltonian (39), nontrivial behavior is expected under the time evolution.

We adopt the Krylov subspace given by Eq. (10) as a target subspace of the LSVQC. The parameters of the subspace are set to be $(N_t, \Delta_t) = (2, 0.5)$ based on a parameter search using the state infidelity such as in Sec. V. The depth of the VHA is fixed to $N_L = 5$. The compilation time is chosen as $\tau = 0.1$ in units where $\hbar = 1$ (i.e., the time unit is 0.658 fs). The long-time dynamics at $t = n\tau$ ($n \in \mathbb{N}$) is simulated by repeatedly applying the optimized circuit to the initial state $|\psi_0\rangle$.

In Fig. 9(a), we compare the results of the exact calculation (black line) and the LSVQC (green dots). We use the optimized ansatz circuit obtained by the cost function training shown in Fig. 8 for the LSVQC. The exact result is obtained by applying the exact time-evolution unitary $e^{-itH^{(L)}}$ to the input state $|\psi_0\rangle$ within a subspace with $N_e = 8$ and $S_z = 0$. We see that the LSVQC nicely reproduces the exact results in a wide range of time. To clarify the efficiency of the LSVQC in more detail, we assess the mean absolute error (MAE) of the double occupation as

$$\delta D_{\psi_0}(n\tau) = \frac{1}{n} \sum_{j=1}^n \left| \langle D(j\tau) \rangle_{\psi_0}^{\text{approx}} - \langle D(j\tau) \rangle_{\psi_0}^{\text{exact}} \right|, \quad (53)$$

where $\langle D(j\tau) \rangle_{\psi_0}^{\text{exact}}$ is the exact value of the double occupation, while $\langle D(j\tau) \rangle_{\psi_0}^{\text{approx}}$ is the approximate value of the double occupation calculated by using the LSVQC, LVQC, or Trotterization. In Fig. 9(b), we compare the MAE δD_{ψ_0} for the LSVQC (green circles), LVQC (brown diamonds), and Trotterization (gray dashed line). The LSVQC and LVQC are performed for the same compilation size $\tilde{L} = 4$ using the VHA with $N_L = 5$ (see Fig. 8 for the optimization history). We see that the MAE of the LSVQC is much smaller than that of the LVQC and comparable to the value of the Trotterization with $r = 60 - 80$. This means that the LSVQC achieves a significant depth compression against the Trotterization as $R_{\epsilon}^{\text{LSVQC}} \simeq 12 - 16$ [see Eq. (38) for the definition of $R_{\epsilon}^{\text{LSVQC}}$].

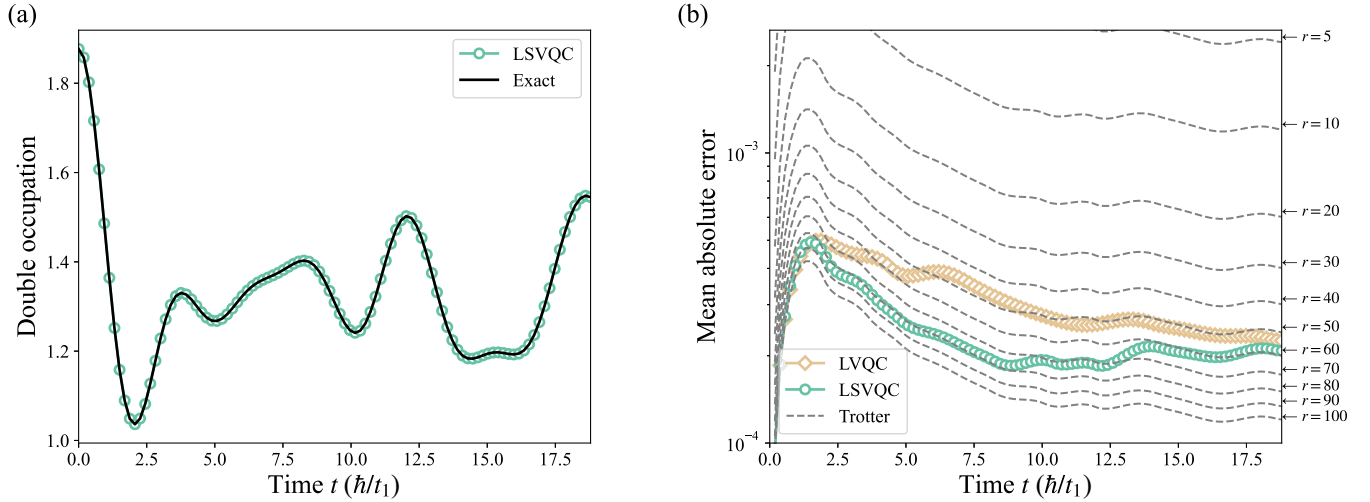


FIG. 9. (a) Double occupation dynamics of the extended Fermi-Hubbard model for Sr_2CuO_3 with $L = 8$. The green circles and the black solid line indicate the results obtained by the LSVQC and exact calculation, respectively. (b) MAE of the double occupation dynamics. The green circles (brown diamonds) represent the MAE of the LSVQC (LVQC). The gray dashed lines indicate the MAE of the Trotterization for various values of the depth parameter r . The LSVQC and LVQC are performed for $\tilde{L} = 4$, $\tau = 0.1$ (in the unit of $\hbar = 1$), and $N_L = 5$. The double occupation is calculated in the time domain $t \in [0, 10]$ with the time step $\tau = 0.1$ in the unit of $\hbar = 1$. The time t in the horizontal axis is shown in the $\hbar/t_1$ unit.

In addition, the LSVQC realizes a comparable or better depth compression ratio compared to the LVQC. This result supports the intuition behind the LSVQC, that subspace-based compiling achieves high accuracy compared to full Hilbert space compiling (e.g., LVQC) when using the same ansatz with limited expressive power.

B. Green's function

Next, we consider the simulation of real-time GF using LSVQC. Although the double occupation dynamics simulation in Sec VIA is a somewhat artificial setting, the GF is a crucial quantity for practical materials simulations, especially for studying strongly correlated electron materials like Sr_2CuO_3 .

We consider the retarded GF at zero temperature

$$G_{a,b}^R(t) = -i\Theta(t)\langle E_0 | \{e^{iHt} c_a e^{-iHt}, c_b^\dagger\} | E_0 \rangle, \quad (54)$$

where $\{A, B\} = AB + BA$ denote the anticommutator, $\Theta(t)$ is the Heaviside step function, $|E_0\rangle$ is the ground state of the Hamiltonian H , and c_a ($c_a^\dagger$) is annihilation (creation) operator of an electron with some index a specifying the fermionic mode. For our extended Fermi-Hubbard model (39), $a = (i, \sigma)$ with spin $\sigma = \uparrow, \downarrow$ and site index $i \in \Lambda = \{1, 2, \dots, L\}$. Hereafter, we consider only the spin-diagonal component of the GF because the target Hamiltonian is the spin-preserving. The GF in the momentum space is obtained by the Fourier transformation of Eq. (54) as

$$G_{\mathbf{k}\sigma}^R(t) = \frac{1}{|\Lambda|} \sum_{i,j \in \Lambda} e^{-i\mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)} G_{i\sigma, j\sigma}^R(t), \quad (55)$$

where $\mathbf{k}$ is the momentum and $\mathbf{r}_i$ denotes the coordinate vector describing the site i . Then, we can calculate the (single-

particle) spectral function as

$$A_{\mathbf{k}\sigma}(\omega) = -\frac{1}{\pi} \text{Im} \left[\int_{-\infty}^{\infty} dt e^{i(\omega + i\eta)t} G_{\mathbf{k}\sigma}^R(t) \right], \quad (56)$$

where $\eta(\rightarrow +0)$ is an infinitesimal positive number ensuring the convergence of the integral. From the spectral function, we obtain the density of states (DOS) as

$$\rho_\sigma(\omega) = \frac{1}{|\Lambda|} \sum_{\mathbf{k}} A_{\mathbf{k}\sigma}(\omega). \quad (57)$$

Here, we give some comments regarding the importance of the above quantities in condensed matter physics and materials science. The retarded GF plays an important role when studying the nonequilibrium transport phenomena based on the linear response theory [88–90]. For example, the electronic conductivity in strongly correlated materials can be calculated from the retarded GF using the Kubo formula [91]. The spectral function and DOS are crucial quantities describing the electronic structure of the strongly correlated materials. In experiments, the spectral function and DOS can be directly measured using spectroscopic techniques such as angle-resolved photoemission spectroscopy [92] and scanning tunneling spectroscopy [93].

Now, we introduce a subspace appropriate for the GF computation. Under the Jordan-Wigner transformation of Eqs. (40) and (41), the GF in Eq. (54) can be rewritten in the qubit representation as

$$\begin{aligned} G_{a,b}^R(t) = & -\frac{i}{2} \Theta(t) [\text{Re} \langle E_0 | e^{iH} \vec{X}_a e^{-iH} \vec{X}_b | E_0 \rangle \\ & + \text{Re} \langle E_0 | e^{iH} \vec{Y}_a e^{-iH} \vec{Y}_b | E_0 \rangle \\ & - i \text{Re} \langle E_0 | e^{iH} \vec{X}_a e^{-iH} \vec{Y}_b | E_0 \rangle \\ & - i \text{Re} \langle E_0 | e^{iH} \vec{Y}_a e^{-iH} \vec{X}_b | E_0 \rangle], \end{aligned} \quad (58)$$

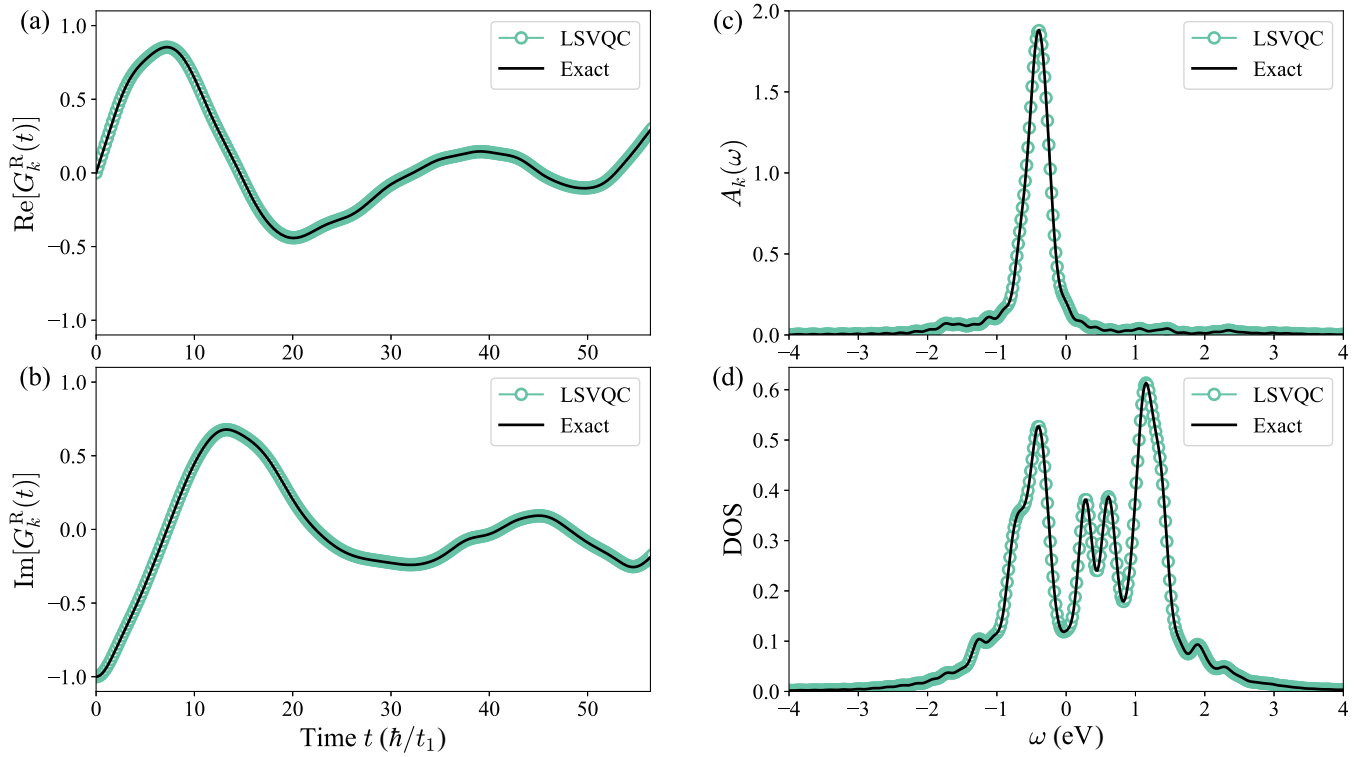


FIG. 10. (a) Real part and (b) imaginary part of GF, (c) spectral function $A_k(\omega)$, and (d) DOS of the extended Fermi-Hubbard model for Sr_2CuO_3 with $L = 8$. The green circles and the black-solid line indicate the results obtained by the LSVQC and exact calculation, respectively. The LSVQC is performed for $\tilde{L} = 4$, $\tau = 0.1$, and $N_L = 5$. We show the GF $G_k^R(t)$ and spectral function $A_k(\omega)$ for $\mathbf{k} = \pi/4$. The GF is calculated in the time domain $t \in [0, 30]$ with the time step $\tau = 0.1$ (in the unit of $\hbar = 1$). The spectral function and DOS are obtained by performing the Fourier transformation of the real-time GF with $\eta = 0.1$. The time t on the horizontal axis of (a) and (b) is shown in the $\hbar/t_1$ unit, while the frequency ω on the horizontal axis of (c) and (d) is shown in the electronvolt (eV) unit. Note that the results for the LVQC (shown in Fig. 11) almost coincide with the LSVQC results in the scale of this figure.

where $\vec{X}_a \equiv X_a Z_{a-1} \cdots Z_0$ and $\vec{Y}_a \equiv Y_a Z_{a-1} \cdots Z_0$ with $P_a \equiv P_{i_\sigma}$ for $a = (i, \sigma)$ and $P = X, Y, Z$. From Eq. (58), we see that the GF is described in the form of a dynamical correlation function as in Eq. (11). Thus, based on the subspace designing guideline described by Eq. (12), we can naively introduce the following subspace:

$$\begin{aligned} \mathcal{S}' = \text{span}(\{ & U_{\text{trot}}^{(L)}(t_n) | E_0 \rangle \\ & \cup \{ U_{\text{trot}}^{(L)}(t_n) R_{\vec{X}_j}(\phi) | E_0 \rangle \}_{j=0}^{N_q-1} \\ & \cup \{ U_{\text{trot}}^{(L)}(t_n) R_{\vec{Y}_j}(\phi) | E_0 \rangle \}_{j=0}^{N_q-1} \}_{n=0}^{N_t}), \end{aligned} \quad (59)$$

where $R_P(\phi) = e^{i\phi P}$ denotes the multi-qubit Pauli rotation gate with arbitrary angle ϕ and multi-qubit Pauli operator P . To ensure the nonorthogonality of the basis states, the angle ϕ is chosen as $0 < \phi < \pi/2$. The physical meaning of the above subspace can be well understood in the original fermionic representation. The ground state $|E_0\rangle$ is a state with a fixed particle number N_e because the Hamiltonian (39) preserves the particle number. Since the multi-qubit Pauli rotation gates $R_{\vec{X}_a}(\phi)$ and $R_{\vec{Y}_a}(\phi)$ correspond to the single-particle excitation operator $e^{i\phi(c_a + c_a^\dagger)}$ and $e^{-\phi(c_a - c_a^\dagger)}$ in the original fermionic representation, the above subspace consists of states with the particle number N_e and $N_e \pm 1$. This is consistent with the definition of the GF (54) that is described using only states with

the particle number N_e and $N_e \pm 1$. However, the subspace (59) cannot be directly applied to the LSVQC since the state preparation circuit is nonlocal because of the nonlocality of $R_{\vec{X}_a}(\phi)$ and $R_{\vec{Y}_a}(\phi)$. To circumvent this issue, we alternatively adopt the following subspace:

$$\begin{aligned} \mathcal{S} = \text{span}(\{ & U_{\text{trot}}^{(L)}(t_n) | E_0 \rangle \\ & \cup \{ U_{\text{trot}}^{(L)}(t_n) R_{X_j}(\phi) | E_0 \rangle \}_{j=0}^{N_q-1} \\ & \cup \{ U_{\text{trot}}^{(L)}(t_n) R_{Y_j}(\phi) | E_0 \rangle \}_{j=0}^{N_q-1} \}_{n=0}^{N_t}), \end{aligned} \quad (60)$$

Here, the nonlocal rotation gates $R_{\vec{X}_a}(\phi)$ and $R_{\vec{Y}_a}(\phi)$ are replaced to the local rotation gates $R_{X_a}(\phi)$ and $R_{Y_a}(\phi)$, respectively. Note that this replacement does not change the fermionic particle number of the basis states, and hence the subspace (60) is still physically reasonable to the GF computation. By setting $N_t = \mathcal{O}(\text{poly}(L))$, the dimension of the subspace (60) is bounded to polynomial of the system size as $(N_t + 1)(2L + 1) = \mathcal{O}(\text{poly}(L))$. We set $(N_t, \Delta_t) = (1, 0.5)$ and $\phi = 0.4\pi$ in following the numerical simulations.

Figure 10 shows the GF, spectral functions, and DOS obtained by the LSVQC and exact calculation. The ground state $|E_0\rangle$ is approximately prepared by the standard variational quantum eigensolver (VQE) [94] using the VHA with the depth $N_L = 5$. In the VQE calculation, the initial state is chosen as a noninteracting ground state prepared by the Givens

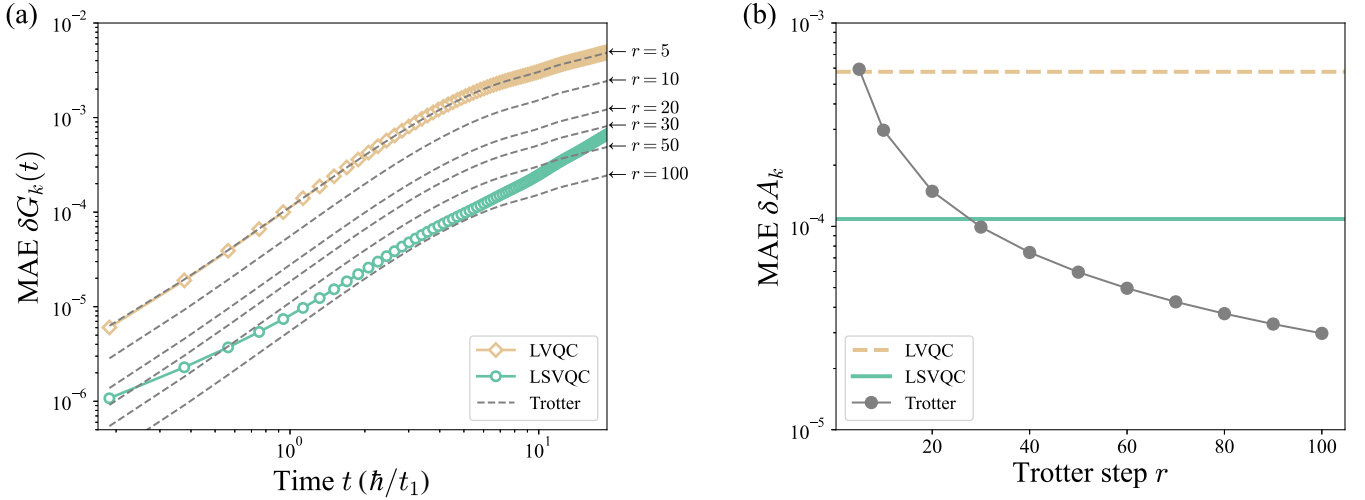


FIG. 11. (a) MAE of the GF $\delta G_k(t)$ for $\mathbf{k} = \pi/4$. The green circles (brown diamonds) represent the MAE of the LSVQC (LVQC). The gray dashed lines indicate the MAE of the Trotterization for various values of the depth parameter r . The time t in the horizontal axis is shown in the $\hbar/t_1$ unit. (b) MAE of the spectral function δA_k for $\mathbf{k} = \pi/4$. The green solid line (brown dashed line) represents the result of the LSVQC (LVQC). The gray dots indicate the MAE of the Trotterization as a function of the depth parameter r . The LSVQC and LVQC are performed for $\tilde{L} = 4$, $\tau = 0.1$, and $N_L = 5$. $\delta G_k(t)$ is calculated in the time domain $t \in [0, 30]$ with the time step $\tau = 0.1$ (in the unit of $\hbar = 1$). δA_k is calculated with $\eta = 0.1$, $\omega_0 = 5$ and $N_\omega = 250$.

rotation network [86]. The particle number of the ground state $|E_0\rangle$ is set to be the half-filling (i.e., $N_e = L = 8$). The LSVQC is performed to compile the time-evolution operator at $\tau = 0.1$ (see Fig. 8 for the cost function optimization), and the long-time dynamics at $t = n\tau$ ($n \in \mathbb{N}$) is obtained by repeatedly applying the optimized circuit to the VQE ground state. The exact GF is calculated by using the VQE ground state $|E_0\rangle$ and exact time-evolution unitary $e^{-itH^{(L)}}$, which is implemented as a sparse matrix within the subspace with the particle numbers $N_e = 8$, $N_e + 1 = 9$, and $N_e - 1 = 7$. From Fig. 10, we see that the exact GF, spectral function, and DOS are accurately reproduced by the LSVQC.

To see the superiority of the LSVQC compared to the Trotterization, we investigate the MAE of the GF

$$\delta G_k(n\tau) = \frac{1}{n} \sum_{j=1}^n |G_k^{\text{R,approx}}(j\tau) - G_k^{\text{R,exact}}(j\tau)|, \quad (61)$$

where $G_k^{\text{R,approx}}$ ($G_k^{\text{R,exact}}$) is the approximate (exact) value of the GF. Similarly, we define the MAE of the spectral function as

$$\delta A_k = \frac{1}{2N_\omega + 1} \sum_{j=-N_\omega}^{N_\omega} |A_k^{\text{approx}}(\omega_j) - A_k^{\text{exact}}(\omega_j)|, \quad (62)$$

where $\omega_j = j\omega_0/N_\omega$ ($j = -N_\omega, -N_\omega + 1, \dots, N_\omega$) is a discretized frequency point, and $2N_\omega + 1$ is the total number of the frequencies. In Fig. 11(a), we show the MAE of the GF δG_k at $\mathbf{k} = \pi/4$ for the LSVQC (green circles), LVQC (brown diamonds), and Trotterization (gray dashed lines). The LSVQC and LVQC are performed under the same condition with $\tilde{L} = 4$ and $N_L = 5$. The MAE δG_k of the LSVQC is much smaller than that of the Trotterization in a wide range of time, while the MAE of the LVQC is almost the same with the Trotterization (i.e., the LVQC fails to realize the depth compression against the Trotterization). Specifically, the LSVQC

achieves a MAE comparable to the value of the Trotterization with $r = 10-100$. Thus, the LSVQC succeeds in the depth compression against the Trotterization as $R_\epsilon^{\text{LSVQC}} \simeq 2-20$. The depth compression is especially significant in a short time regime. This behavior is consistent with the result in Fig. 4(b). As shown in Sec. V, the depth compression rate at a long-time regime will be improved by logarithmically increasing the compilation size $\tilde{L}$ based on Eq. (C8). Figure 11(b) shows the MAE of the spectral function δA_k at $\mathbf{k} = \pi/4$. We set $\omega_0 = 5$ and $N_\omega = 250$. The horizontal green solid (brown dashed) line indicates the MAE δA_k for the LSVQC (LVQC) at $N_L = 5$. We also show the result for the Trotterization as a function of the number of the Trotter step r . The MAE δA_k of the LSVQC (LVQC) is comparable to that of the Trotterization with $r \simeq 30$ ($r \simeq 5$). Thus, the LSVQC realizes the depth compression with $R_\epsilon^{\text{LSVQC}} \simeq 30/5 = 6$, while the LVQC fails to realize the depth compression (i.e., the depth compression rate of the LVQC is $5/5 = 1$). A remarkable point of the above results is that the LSVQC achieves a significantly better depth compression rate than the LVQC, although both the LSVQC and LVQC use the same ansatz. Similar to the results in Fig. 9, this result strongly supports the intuition behind the LSVQC. The subspace-based compiling of the LSVQC leads to high accuracy compared to full Hilbert space compiling (i.e., LVQC) when using the same ansatz with limited expressive power. Here, we note that the depth compression achieved against LVQC may vary depending on the specific problem parameters, such as the target Hamiltonian and physical quantity. Such dependence arising from the details of the problem will be further investigated in future work.

VII. RESOURCE ESTIMATION

Quantitative estimates of the computational resources required for executing quantum algorithms provide crucial information for determining the feasibility of practical

quantum computers. In this section, we discuss the utility of the LSVQC for large-scale quantum simulations from the viewpoint of computational resources. First, we estimate the gate count needed to simulate the dynamics of the two-dimensional (2D) Fermi-Hubbard model and extended Fermi-Hubbard models for some representative materials. Here, we estimate only the resources required to implement the time-evolution operator, as it consumes the most resources in quantum simulations. Next, we estimate the computational resource for the local compilation protocol. Based on the results, we discuss the utility of the LSVQC for near-term quantum computing architectures in the NISQ and early-FTQC era.

A. Method of gate count estimation

Here, we outline the procedure of our method to estimate the gate count for dynamics simulation. We first count the number of quantum gates needed to implement the time-evolution operator with an accuracy ϵ using the first-order Trotterization. It is realized by estimating the required Trotter step r based on the asymptotic scaling of the Trotter error bound. We employ two types of Trotter error bound, i.e., *worst-case* and *average-case* errors [95]. The worst-case Trotter error is quantified by the spectral (i.e., operator) norm corresponding to the largest singular value. Although the worst-case error analysis is rigorous, it sometimes overestimates the error for some input states [37,96–99] and gives estimates that are too pessimistic for practical applications. To address this, we also adopt the average-case Trotter error [95], which dictates the average error of the Trotterization for typical input states that appear in the context of quantum computing. Then, the required Trotter step for the (extended) Fermi-Hubbard model is estimated as

$$r_{\epsilon}^{\text{trout}} = \begin{cases} \mathcal{O}(L^2/\epsilon) & (\text{worst-case}) \\ \mathcal{O}(\sqrt{L}^2/\epsilon) & (\text{average-case}). \end{cases} \quad (63)$$

where L is the size of the lattice. In the following analysis, we asymptotically estimate $r_{\epsilon}^{\text{trout}}$ using Eq. (63) by setting the prefactor as 1 for simplicity.

Next, we heuristically estimate the gate count needed to achieve an accuracy ϵ using the LSVQC. To do this, we assume that the LSVQC realizes the depth compression over the Trotterization with $R_{\epsilon}^{\text{LSVQC}} > 1$ using the VHA [Eq. (50)], whose circuit structure is equivalent to the Trotterization. Since we cannot analytically estimate the depth compression ratio $R_{\epsilon}^{\text{LSVQC}}$ owing to the variational nature of the LSVQC, we empirically set the value of $R_{\epsilon}^{\text{LSVQC}}$ based on the numerical results. Specifically, we perform gate count estimation to simulate the time evolution of the (extended) Fermi-Hubbard model until moderate time $t = 1$ in units of the inverse of the hopping integral. The numerical results in Secs. V and VI (Figs. 9 and 11) demonstrates that the LSVQC achieves $R_{\epsilon}^{\text{LSVQC}} \simeq 10$ at such time scale. Based on this observation, we empirically set $R_{\epsilon}^{\text{LSVQC}} = 10$ in the following analysis. Note that the depth compression ratio $R_{\epsilon}^{\text{LSVQC}}$ may decrease for longer-time dynamics simulation as shown in our numerical results in Figs. 9 and 11. We also assume that $R_{\epsilon}^{\text{LSVQC}}$ is hardly affected by the system size because of the size insensitivity of the local compilation theorem [Eqs. (30) and (31)] and numer-

ical results in Sec. V (Fig. 5). Under these assumptions, the number of layers of the VHA N_L for the LSVQC is empirically estimated as

$$N_L = \begin{cases} \lfloor r_{\epsilon}^{\text{trout}}/R_{\epsilon}^{\text{LSVQC}} \rfloor & r_{\epsilon}^{\text{trout}}/R_{\epsilon}^{\text{LSVQC}} > 1 \\ 1 & r_{\epsilon}^{\text{trout}}/R_{\epsilon}^{\text{LSVQC}} \leq 1 \end{cases}. \quad (64)$$

1. NISQ devices

Under the above setup, we perform resource estimation for NISQ devices based on the capability of the error mitigation techniques. The error mitigation can be realized with a manageable sampling overhead when the total error in a quantum circuit is in the order of unity. For example, the probabilistic error cancellation can suppress the errors with a reasonable sampling overhead when $N_{\text{gate}} p_{\text{gate}} \lesssim 2$ [100], where N_{gate} is the number of gates and p_{gate} is the typical error rate of each gate operation. We here note that the single-qubit gate error rate p_{1q} is in general much smaller than the two-qubit gate error rate p_{2q} . Since two-qubit gates are the dominant source of errors, we impose $N_{2q} p_{2q} \leq 2$ as a condition of successful error mitigation in NISQ devices, where N_{2q} is the number of two-qubit gates in a given quantum circuit.

2. Early-FTQC devices

We also perform resource estimation for early-FTQC devices. Specifically, we consider the space-time efficient analog rotation quantum computing architecture (STAR architecture) proposed in Ref. [26] as a prototypical quantum computing architecture in the early-FTQC era. The STAR architecture realizes the universal quantum computation utilizing the fault-tolerant Clifford and analog rotation gates. The Clifford gates are executed in a fault-tolerant manner using the lattice surgery [101], while the analog rotation gates are performed directly utilizing a special magic state. The STAR architecture is suitable for the early-FTQC era since the T gate decomposition and magic state distillation, which are computationally expensive parts in the conventional FTQC architectures, are avoided.

In the STAR architecture, the logical error mainly originates from the analog rotation gates that are not fault-tolerant. This is in contrast to the NISQ devices in which the error rate of the single-qubit rotation gates is generally much lower than that of the two-qubit gates. In Ref. [26], the logical error rate from the analog rotation gates is obtained as

$$P_{L,\text{rotation}} = 4p_{\text{phys}}/15 + \mathcal{O}(p_{\text{phys}}^2), \quad (65)$$

where p_{phys} is the physical error rate. The above logical error from the analog rotation gates is mitigated by the probabilistic error cancellation [100], while the logical error from the Clifford gates can be negligible by taking a sufficiently large code distance. Therefore, we only count the number of analog rotation gates $R_Z(\theta) = e^{-i(\theta/2)Z}$ as a possible source of the logical error. Similar to the analysis for NISQ devices, we judge that the quantum simulation is executable on the STAR architecture when the success condition of the probabilistic error cancellation $N_{R_Z} P_{L,\text{rotation}} \leq 2$ [100] is satisfied. Here, N_{R_Z} is the number of analog rotation gates $R_Z(\theta)$ in a given logical quantum circuit. N_{R_Z} can be estimated by counting the number of terms in a given Hamiltonian since each term

produces a multi-qubit Pauli rotation gate (i.e., single analog rotation gate and some Clifford gates) in the Trotterization or VHA circuit.

B. Gate count estimation for quantum dynamics simulation

Here, we show the results of our gate count estimation to simulate the dynamics of the 2D Fermi-Hubbard model and extended Fermi-Hubbard models.

1. Fermi-Hubbard model

First, we show the results of resource estimation for the 2D Fermi-Hubbard model defined on a square lattice,

$$H = -t_{\text{hop}} \sum_{\langle i,j \rangle} \sum_{\sigma=\uparrow,\downarrow} (c_i^\dagger c_j + c_j^\dagger c_i) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \frac{U}{2} \sum_{i,\sigma} n_{i\sigma}, \quad (66)$$

where $\langle i, j \rangle$ denotes neighboring sites, t_{hop} is the hopping integral, U is the on-site Coulomb interaction, and the open boundary condition is adopted. We also impose the half-filling condition for simplicity. For quantum resource estimation, we consider Jordan-Wigner transformed qubit representation of the above fermionic Hamiltonian,

$$H = -\frac{t_{\text{hop}}}{2} \sum_{\langle i,j \rangle, \sigma} (X_{i\sigma} X_{j\sigma} + Y_{i\sigma} Y_{j\sigma}) \overleftrightarrow{Z}_{i\sigma, j\sigma} + \frac{U}{4} \sum_i Z_{i\uparrow} Z_{i\downarrow}, \quad (67)$$

where

$$\overleftrightarrow{Z}_{i\sigma, j\sigma} \equiv \begin{cases} Z_{i+1\sigma} Z_{i+2\sigma} \cdots Z_{j-1\sigma} & (i < j) \\ Z_{j+1\sigma} Z_{j+2\sigma} \cdots Z_{i-1\sigma} & (i > j). \end{cases} \quad (68)$$

In the above qubit representation, the qubits are ordered according to the so-called snake-shaped configuration as $i_\uparrow = i (= 1, 2, \dots, L)$ and $i_\downarrow = 2L + 1 - i (= 2L, 2L - 1, \dots, L + 1)$ [102].

Figure 12 shows the results for the NISQ devices. The gate count is estimated specifically for superconducting qubit devices using the results of Ref. [102]. Specifically, the number of single-qubit gates N_{1q} and two-qubit i SWAP gates N_{2q} needed to implement the Trotterization circuit of the Hamiltonian (67) on superconducting qubit devices is formally estimated as follows [102]:

$$N_{1q} = 3Lr_\epsilon^{\text{trot}}, \quad (69)$$

$$N_{2q} = (4L^{3/2} + 2L - 2\sqrt{L})r_\epsilon^{\text{trot}}. \quad (70)$$

Here, L is the number of sites and the gate count is obtained by adopting the FSWAP network [103]. The number of Trotter steps r_ϵ^{trot} is estimated using Eq. (63). The gate count for the LSVQC using the VHA with the depth N_L is obtained by replacing r_ϵ^{trot} with N_L in Eqs. (69) and (70). We set the accuracy $\epsilon = 0.01$ (i.e., 1% error) for both the worst-case and average-case error schemes. Note that the average-case error estimation produces computational resources about one order of magnitude smaller than that for worst-case error estimation. Unless otherwise mentioned, we discuss the resource requirement based on the average-case error estimation in the

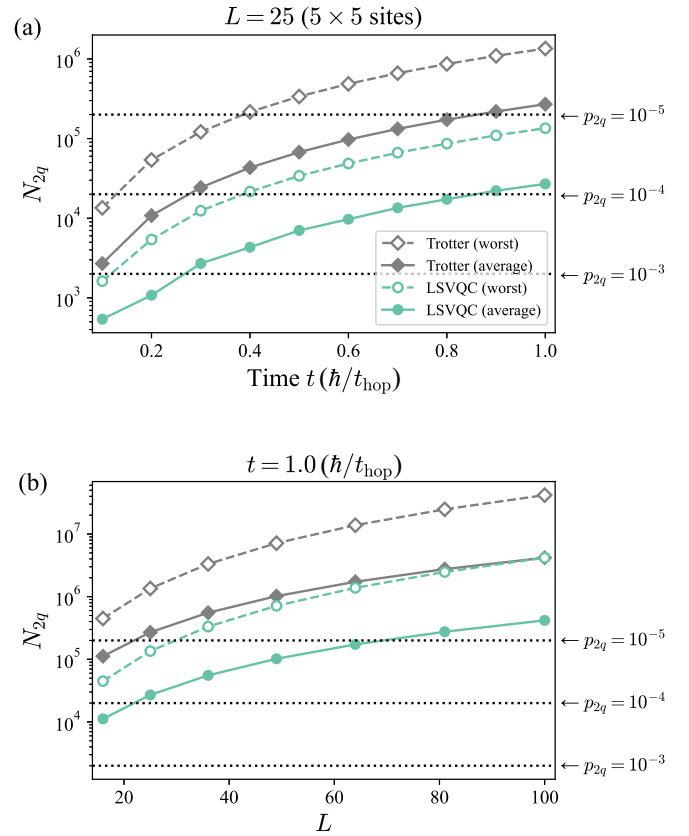


FIG. 12. Gate count of the 2D Fermi-Hubbard model for superconducting qubit NISQ devices. (a) Two-qubit gate count N_{2q} as a function of the simulation time t for $L = 5 \times 5$. (b) Two-qubit gate count N_{2q} as a function of the lattice size L for $t = 1.0$. The green filled (open) circles and gray filled (open) diamonds represent the results for the LSVQC and Trotterization in the average-case (worst-case) error scheme, respectively. The dotted-horizontal lines indicate the maximum two-qubit gate count allowed under two-qubit gate error rate $p_{2q} = [10^{-3}, 10^{-4}, 10^{-5}]$.

following. The horizontal dashed lines indicate the allowed maximum number of two-qubit gates for the physical error rate of $p_{2q} = [10^{-3}, 10^{-4}, 10^{-5}]$. In Fig. 12(a), we show that the two-qubit gate count N_{2q} for 5×5 site Fermi-Hubbard model (i.e., $L = 25$) as a function of simulation time t . The required gate resources increase with time t . Note that the simulation of quantum many-body systems using classical computers generally becomes difficult when $t \gtrsim 1$ in the unit of $\hbar/t_{\text{hop}}$ [104–106], where t_{hop} is the hopping parameter [see Eq. (66) for the definition of t_{hop}]. We see that the LSVQC (Trotterization) allows us to realize a quantum simulation of $t \simeq 1$ when the two-qubit gate error rate is $p_{2q} \simeq 10^{-4}$ ($p_{2q} \simeq 10^{-5}$). Figure 12(b) shows the size L dependence of the two-qubit gate count for $t = 1$. As a typical guideline, the quantum advantage is expected at around $L = 10 \times 10$ and $t = 1$ for the quantum dynamics simulation of the 2D Fermi-Hubbard model [104,105]. We see that the LSVQC (Trotterization) requires $p_{2q} \simeq 10^{-5}$ ($p_{2q} \simeq 10^{-6}$) to simulate a 10×10 site Fermi-Hubbard model. In summary, the acceptable two-qubit gate error rate of the LSVQC is about one order of magnitude larger than the Trotterization, although

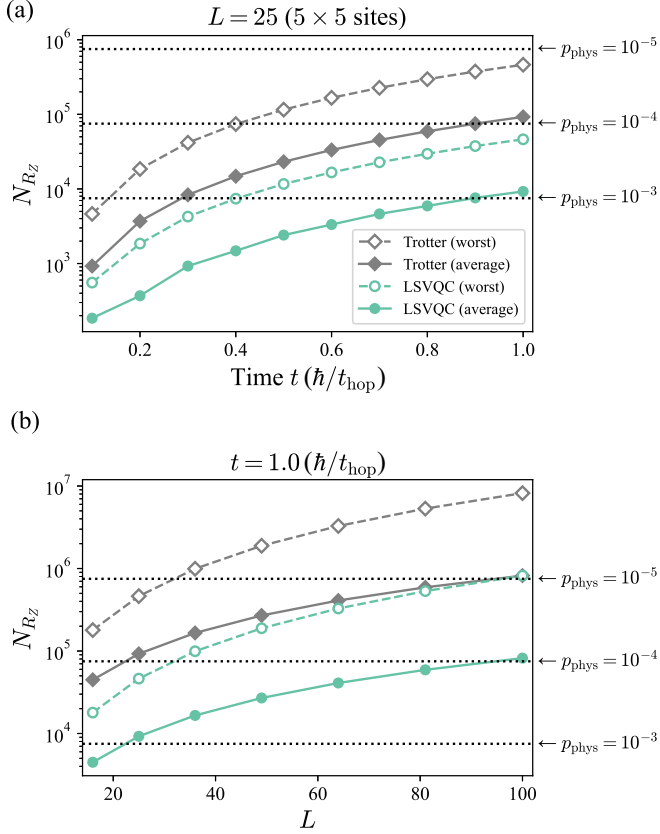


FIG. 13. Gate count of the 2D Fermi-Hubbard model for STAR architecture. (a) Analog rotation gate count N_{RZ} as a function of the simulation time t for $L = 5 \times 5$. (b) Analog rotation gate count N_{RZ} as a function of the lattice size L for $t = 1.0$. The green filled (open) circles and gray filled (open) diamonds represent the results for the LSVQC and Trotterization in the average-case (worst-case) error scheme, respectively. The dotted horizontal lines indicate the maximum analog rotation gate count allowed under physical error rate $p_{\text{phys}} = [10^{-3}, 10^{-4}, 10^{-5}]$.

hardware improvement is still necessary to achieve $p_{2q} \lesssim 10^{-4}$ in superconducting qubit devices.

Next, we perform resource estimation for the STAR architecture. From Eq. (67), the number of analog rotation gates [i.e., the number of terms in the Hamiltonian (67)] is counted as $9L - 8\sqrt{L}$. Hence, the total number of analog rotation gates in the Trotterization circuit is given by

$$N_{RZ} = (9L - 8\sqrt{L})r_{\epsilon}^{\text{tror}}. \quad (71)$$

The analog rotation gate count for the LSVQC using the VHA is obtained by replacing $r_{\epsilon}^{\text{tror}}$ with N_L [estimated by Eq. (64)] in Eq. (71). Figure 13(a) shows the analog rotation gate count needed to simulate the time evolution of 5×5 site Fermi-Hubbard model as a function of time t . The horizontal dashed lines indicate the maximum number of analog rotation gates available in the STAR architecture for the physical error rate of $p_{\text{phys}} = [10^{-3}, 10^{-4}, 10^{-5}]$. We see that the LSVQC realizes dynamics simulation of $t = 1$ at $p_{\text{phys}} \simeq 10^{-3}$, which is achievable on current quantum computing devices. On the other hand, the Trotterization requires $p_{\text{phys}} \lesssim 10^{-4}$ at $t = 1$. This is a remarkable improvement from the results for NISQ

devices (Fig. 12), in which the dynamics simulation of $t = 1$ and $L = 5 \times 5$ requires $p_{\text{phys}} \simeq 10^{-4}$ even if we utilize the LSVQC. In Fig. 13(b), we show the analog rotation gate count needed to simulate the time evolution of $t = 1$ as a function of the lattice size L . To simulate the 10×10 site model, the LSVQC (Trotterization) requires the physical error rate of $p_{\text{phys}} \simeq 10^{-4}$ ($p_{\text{phys}} \simeq 10^{-5}$). For both LSVQC and Trotterization, the acceptable physical error rate on the STAR architecture is about one order of magnitude larger than that on the NISQ devices. These results indicate that combining the LSVQC with the STAR architecture allows us to further mitigate the hardware requirement needed to realize large-scale quantum simulations. We note that the required number of physical qubits on the STAR architecture is generally much greater than that on NISQ devices. To create n logical qubits on the STAR architecture, at least $(1.5n + 5) \times 2d^2$ physical qubits are required for the code distance d [26] (e.g., 73 810 physical qubits are required for $L = 10 \times 10$ and $d = 11$). Strictly speaking, the code distance d should be carefully chosen considering the logical circuit depth under the lattice surgery [101]. This suggests that the LSVQC also allows us to reduce the number of physical qubits by reducing the required code distance. More detailed resource estimation considering such effects is left for future work.

2. Extended Fermi-Hubbard models

Next, we estimate the gate count for the extended Fermi-Hubbard models [Eq. (D1)] for some representative materials. We use the result of Ref. [107], in which the authors estimate the number of the single-qubit and two-qubit gates needed to implement a single Trotter step for the extended Fermi-Hubbard models of strongly correlated materials. Our contribution in this section is to show the gate count and acceptable gate error rate for the quantum dynamics simulation, not just to implement a single Trotter step.

Specifically, in the Ref. [107], the authors estimated the gate count N_{gate} as a function of the number of unit cells N_{cells} as

$$N_{\text{gate}} = \left(\sum_{i_{\text{int}}} N_{\text{terms/cell}}^{i_{\text{int}}} N_{\text{gates}}^{i_{\text{int}}} \right) N_{\text{cells}} + \frac{N_{\text{qubits/cell}}^2 N_{\text{cells}}^2 - 2N_{\text{qubits/cell}} N_{\text{cells}}}{2} N_{\text{gates}}^{\text{fswap}}, \quad (72)$$

where the fermionic modes are encoded to qubits using the Jordan-Wigner transformation and the FSWAP network is applied to deal with the nonlocal Pauli string. i_{int} is an index specifying the type of the interaction (i.e., hopping interaction, Coulomb interaction, and exchange interaction), $N_{\text{gates}}^{i_{\text{int}}}$ is the number of gates needed to implement the interaction operator specified by the index i_{int} , and $N_{\text{terms/cell}}^{i_{\text{int}}}$ is the number of interaction terms specified by the index i_{int} in the Hamiltonian. $N_{\text{gate}}^{\text{fswap}}$ is the gate count required for single FSWAP operation. $N_{\text{qubits/cell}}$ is the number of qubits per unit cell. Based on Eq. (72), we estimate the total number of gates needed to perform dynamics simulation as $N_{\text{gate}} N_L$ ($N_{\text{gate}} r$) using the LSVQC (Trotterization) with the circuit depth N_L (r). The values of $N_{\text{gates}}^{i_{\text{int}}}$, $N_{\text{terms/cell}}^{i_{\text{int}}}$, $N_{\text{gate}}^{\text{fswap}}$, and $N_{\text{qubits/cell}}$ are taken from the Ref. [107]. Specifically, the two-qubit (CNOT) gate

TABLE II. Gate counts of the extended Fermi-Hubbard models for $t = 0.1$ and $N_{\text{cells}} = 10$. The values enclosed in parentheses indicate the estimates based on the worst-case Trotter error bound.

Material	Qubits	Method	NISQ		STAR	
			CNOT	p_{2q}	R_Z	p_{phys}
(TMTSF) ₂ PF ₆	40	Trotter	$5.1 \times 10^4 (2.5 \times 10^5)$	$3.9 \times 10^{-5} (7.9 \times 10^{-6})$	$2.2 \times 10^4 (1.1 \times 10^5)$	$3.4 \times 10^{-4} (6.8 \times 10^{-5})$
		LSVQC	$1.3 \times 10^4 (2.5 \times 10^4)$	$3.4 \times 10^{-4} (6.8 \times 10^{-5})$	$5.5 \times 10^3 (1.1 \times 10^4)$	$1.4 \times 10^{-3} (6.8 \times 10^{-4})$
K ₃ C ₆₀	60	Trotter	$7.3 \times 10^4 (4.4 \times 10^5)$	$2.7 \times 10^{-5} (4.6 \times 10^{-6})$	$1.3 \times 10^4 (8.0 \times 10^4)$	$5.6 \times 10^{-4} (9.3 \times 10^{-5})$
		LSVQC	$1.5 \times 10^4 (4.4 \times 10^4)$	$1.4 \times 10^{-4} (4.6 \times 10^{-5})$	$2.7 \times 10^3 (8.0 \times 10^3)$	$2.8 \times 10^{-3} (9.3 \times 10^{-4})$
LaFeAsO	200	Trotter	$1.5 \times 10^6 (1.5 \times 10^7)$	$1.3 \times 10^{-6} (1.3 \times 10^{-7})$	$4.3 \times 10^5 (4.3 \times 10^6)$	$1.8 \times 10^{-5} (1.8 \times 10^{-6})$
		LSVQC	$1.5 \times 10^5 (1.5 \times 10^6)$	$1.3 \times 10^{-5} (1.3 \times 10^{-6})$	$4.3 \times 10^4 (4.3 \times 10^5)$	$1.8 \times 10^{-4} (1.8 \times 10^{-5})$
NiO	100	Trotter	$3.2 \times 10^6 (2.3 \times 10^7)$	$6.3 \times 10^{-7} (8.8 \times 10^{-8})$	$1.4 \times 10^6 (9.7 \times 10^6)$	$5.5 \times 10^{-6} (7.7 \times 10^{-7})$
		LSVQC	$4.5 \times 10^5 (2.3 \times 10^6)$	$4.4 \times 10^{-6} (8.8 \times 10^{-7})$	$1.9 \times 10^5 (9.7 \times 10^5)$	$3.9 \times 10^{-5} (7.7 \times 10^{-6})$
SrVO ₃	100	Trotter	$8.5 \times 10^5 (6.0 \times 10^6)$	$2.4 \times 10^{-6} (3.3 \times 10^{-7})$	$2.8 \times 10^5 (2.0 \times 10^6)$	$2.7 \times 10^{-5} (3.8 \times 10^{-6})$
		LSVQC	$1.2 \times 10^5 (6.0 \times 10^5)$	$1.7 \times 10^{-5} (3.3 \times 10^{-6})$	$4.0 \times 10^4 (2.0 \times 10^5)$	$1.9 \times 10^{-4} (3.8 \times 10^{-5})$

count for the NISQ devices in Table II is obtained based on Eq. (72). On the other hand, the analog rotation gate count N_{R_Z} for the STAR architecture is obtained by counting the number of terms in a given *ab initio* Hamiltonian in the same way as that for the Fermi-Hubbard model. Specifically, it is estimated as $N_{R_Z} = r N_{\text{terms/cell}}^{\text{int}} N_{\text{cells}}$ ($N_{R_Z} = N_L N_{\text{terms/cell}}^{\text{int}} N_{\text{cells}}$) for the Trotterization (LSVQC) with the depth r (N_L).

As a benchmark result, we count the gate resources required to perform a short-time dynamics simulation of time $t = 0.1$ with 1% accuracy. The number of unit cells N_{cells} is set to $N_{\text{cells}} = 10$ so that the number of qubits becomes on the order of 10^2 at maximum. Although $N_{\text{cells}} = 10$ may be too small for practical calculations, it is already in a region difficult to tackle with classical computers. The gate count and acceptable gate error rate are summarized in Table II. The column “NISQ” (“STAR”) indicates the resource estimates for NISQ devices (STAR architecture) based on the two-qubit CNOT gate count (analog rotation gate count). The acceptable error rate of the LSVQC is about one order of magnitude larger than the Trotterization for all materials in both “NISQ” and “STAR”. The LSVQC allows us to simulate organic compounds (TMTSF)₂PF₆ and K₃C₆₀ on NISQ devices with $p_{2q} \simeq 10^{-4}$. For the STAR architecture, more complex compounds such as LaFeAsO (iron-based superconductor) and SrVO₃ (perovskite oxide) are simulatable using the LSVQC when $p_{\text{phys}} \simeq 10^{-4}$. The above results suggest that the LSVQC has great utility for simulating the strongly correlated electron materials by combining it with a sophisticated quantum computing architecture like the STAR architecture.

C. Resource estimation for local compilation

Finally, we perform resource estimation for the local compilation protocol. Here, we compare the performance of the LSVQC with the LVQC [41,42], since both algorithms utilize local compilation though the procedure is different. The details of the LVQC are summarized in Appendix F.

1. Qubit count

First, we compare the qubit count needed to execute the local compilation. The cost function of the LVQC [Eq. (F4)] is measured by the local Hilbert-Schmidt test (LHST) [13], which is performed using $2\tilde{L}$ qubits for a $\tilde{L}$ -size local subsys-

tem (see Fig. 18 below). On the other hand, the cost function of the LSVQC [Eq. (29)] is measured by performing the LLET, which is realized using a $\tilde{L}$ -qubit circuit shown in Fig. 2(b). Therefore, the qubits required to evaluate the cost function of the LSVQC are about half as much as that of the LVQC. Note that the appropriate value of the compilation size $\tilde{L}$ is generally different for the LSVQC and LVQC because their local compilation protocol is based on distinct theoretical guarantees.

To clarify the impact of the qubit reduction of the LSVQC over the LVQC, we here compare the number of qubits required to perform the local compilation protocol, denoted as N_q^{lc} in the following. To reduce the computational cost of the variational optimization, it is desirable that N_q^{lc} is smaller than the number of qubits describing the entire system. Thus, we here define the condition of successful local compilation as $N_q^{\text{lc}} < L$. Figure 14 shows parameter regions where the local compilation succeeds as $N_q^{\text{lc}} < L$ for the 2D Fermi-Hubbard model. Specifically, we consider a situation in which local compilation using a classical computer. In Fig. 14, we only show regions where $N_q^{\text{lc}} \leq 36$ since we can currently simulate quantum circuits classically up to about 36 qubits systems [108]. For the LVQC (LSVQC), N_q^{lc} is estimated as $N_q^{\text{lc}} = 2\tilde{L}_{\text{LVQC}}$ ($N_q^{\text{lc}} = \tilde{L}_{\text{LSVQC}}$), where the prefactor 2 comes from the Bell measurement (see Appendix F for details). The compilation size $\tilde{L}_{\text{LVQC}}$ and $\tilde{L}_{\text{LSVQC}}$ are set to their approximate lower bounds, which are given by

$$\tilde{L}_{\text{LVQC}} = \log(L/\epsilon) + r_H + v\tau + 2d_V + 1, \quad (73)$$

$$\begin{aligned} \tilde{L}_{\text{LSVQC}} = & \log(L/\epsilon) + r_H + v\tau + 2 \max_k d_{W_k} \\ & + \max \left(2d_V + 1, r_H + v\tau + 2 \max_k d_{W_k} \right). \end{aligned} \quad (74)$$

Equations (73) and (74) are derived from Eqs. (F7) and (32) by setting the prefactor of the first term as 1 for simplicity, respectively. For the 2D Fermi-Hubbard model [Eq. (66)], $r_H = 1$ and $v \simeq 30.3$, where the value of the LR velocity v is estimated by using the result of Ref. [109] for $U/t_{\text{hop}} = 1$. Considering the Krylov subspace generated by the single-step Trotterized circuit such as adopted in Sec. V and VI, we set $d_{W_k} = 1$. The other parameters are set to $d_V = 2$ and $\epsilon = 10^{-2}$. Figure 14(a) shows that the local compilation of

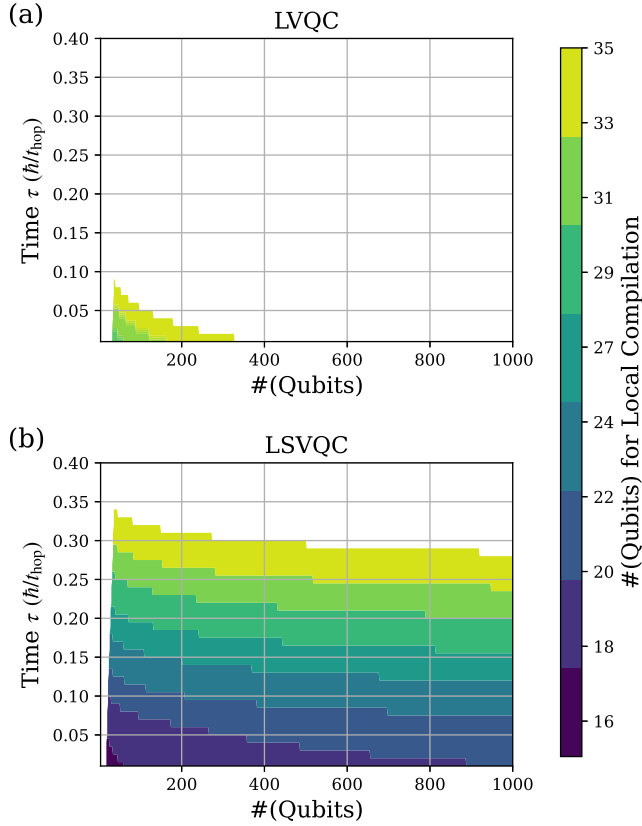


FIG. 14. Illustration of parameter regions where the local compilation can be performed with theoretical guarantees for (a) LVQC and (b) LSVQC. The color map shows the number of qubits required for the local compilation N_q^{lc} . The vertical and horizontal axis shows the time step τ and the qubit count for the entire system, respectively. The value of N_q^{lc} is estimated based on the LR velocity of the 2D Fermi-Hubbard model from Ref. [109].

the LVQC can be realized only for a tiny time step τ and a relatively small system. On the other hand, Fig. 14(b) demonstrates that LSVQC's local compilation holds for a significantly wider range of time steps and system sizes. For instance, the local compilation of the LVQC does not succeed for $L \geq 400$ (i.e., a lattice larger than 14×14 sites), while the LSVQC successfully performs the local compilation even when $L \geq 1000$ for a relatively large time step $\tau \simeq 0.3\hbar/t_{\text{hop}}$. This result demonstrates an improved scalability of the LSVQC over the LVQC, potentially allowing us to realize the utility-scale materials simulation using, e.g., the extended Fermi-Hubbard model with over 1000 qubits.

2. Gate count

The LHST of the LVQC requires $\tilde{L} + 1$ long-range CNOT gates connecting the Bell pairs. This is problematic for NISQ devices in which the available number of two-qubit gates and qubit connectivity are highly restricted. To clarify this point, let us consider NISQ devices with nearest-neighbor qubit connectivity such as the superconducting qubit devices. In such situations, a CNOT gate connecting k -nearest-neighbor qubits is implemented using $2(k - 1)$ SWAP gates (see Fig. 15). This SWAP network is implemented by $6(k - 1)$ nearest-neighbor

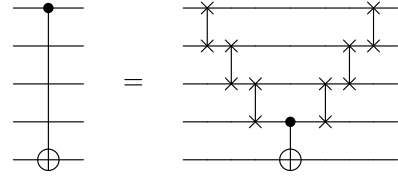


FIG. 15. Implementation of a k -nearest-neighbor CNOT gate using a nearest neighbor CNOT gate and SWAP gates. The figure shows the case of $k = 5$.

CNOT gates since a SWAP gate can be decomposed into three CNOT gates. Thus, the LHST circuit (Fig. 18 below) consumes additional $(6\tilde{L} - 5)(\tilde{L} + 1) = \mathcal{O}(\tilde{L}^2)$ nearest-neighbor CNOT gates to create the Bell pairs when the neighboring qubits in the figure are also geometrically neighbors. Here, we note that the local compilation needed to be executed on quantum devices only when $2\tilde{L} \gtrsim 36$, since we can classically simulate the LHST up to about 36 qubit systems [108]. For classically intractable regime $2\tilde{L} \gtrsim 36$, the additional CNOT gate count is about 2.0×10^3 , which already in the order of the maximum number of two-qubit gates $2/p_{2q}$ [100] for current NISQ devices with $p_{2q} \simeq 10^{-3}$. This indicates that the long-range CNOT gates in the LHST are the critical bottleneck for executing the LVQC on NISQ hardware, and the LSVQC is a more NISQ-friendly approach than the LVQC.

3. Trainability

Another important advantage of the local compilation of the LSVQC is the trainability of the cost function. As detailed in Sec. III, the LSVQC is designed to compile the time-evolution operator within a physically relevant N -dimensional subspace, where we assume $N = \mathcal{O}(\text{poly}L)$ for L -qubit systems. Thus, there is a large set of solutions to accomplish such compilation since the ansatz unitary can have an arbitrary action outside the subspace [see Fig. 1(c) for illustration]. In contrast, the LVQC performs the compilation to reproduce the target time-evolution on the full 2^L -dimensional Hilbert space. This implies that the solution set for the LSVQC is significantly larger than that of the LVQC, making it much more likely to find a good solution using a shallow-depth ansatz with limited expressive power. Such good trainability of the LSVQC is indeed observed in Fig. 8. It is shown that the LSVQC achieves a cost value of $\sim 10^{-10}$ after optimizing the five-layer ansatz. On the other hand, the cost value of the LVQC plateaus around $\sim 10^{-7}$ even though we increase the depth of the ansatz to 15 layers.

Using shallower depth ansatz has many important advantages. First, it is easy to implement a shallow-depth ansatz circuit on near-term quantum devices. Second, a shallow depth ansatz is less prone to barren plateaus. Specifically, it is known that the local cost functions such as those used in the LSVQC and LVQC avoid barren plateaus when the circuit depth is $\mathcal{O}(\text{poly}L)$ [18]. More specifically, the authors of Ref. [18] have formally derived that the variance of the gradient of such local cost functions scales as $\Omega(1/\text{poly}(n))$ when the circuit depth is $\mathcal{O}(\log(n))$ with n being the system size. Third, shallow-depth circuits require fewer cost function evaluations to compute the gradient for a gradient-based

optimization. For instance, the parameter shift rule [110] requires cost function evaluations proportional to the number of parameters (i.e., depth) of the ansatz.

VIII. DISCUSSION AND CONCLUSIONS

In this paper, we have developed the LSVQC algorithm for the resource-efficient simulation of large-scale quantum many-body systems on near-term quantum computers such as NISQ devices or early-FTQCs. The LSVQC performs the local optimization of the ansatz circuit to reproduce the action of the time-evolution operators within a subspace. The subspace is designed considering the properties of the target physical quantities that we aim to simulate. The local compilation is theoretically guaranteed by the LR bound and the locality of quantum circuits similarly to the LVQC. By restricting the range of optimization within a physically reasonable small subspace, the LSVQC allows us to accurately simulate the target physical quantities with fewer computational resources than does the Trotterization and LVQC.

The validity of the LSVQC has been demonstrated by numerical simulation using classical computers. Our numerical results for the 1D Heisenberg model show that the performance of the LSVQC is sensitive to the choice of the subspace and achieves a high accuracy under a proper subspace. It has also been clarified that the performance of the LSVQC is hardly altered by increasing the system size, which supports the scalability of the LSVQC to classically intractable large-scale quantum simulations. Furthermore, we have demonstrated that the LSVQC is effective in realistic materials simulations by performing quantum many-body dynamics simulations of the extended Fermi-Hubbard model of Sr_2CuO_3 . It has been shown that the required circuit depth to simulate quantum many-body dynamics using the LSVQC is about 1/20 of the Trotterization at best. The LSVQC also achieves significant depth compression against the LVQC specifically in the computation of the Green's function. Our heuristic resource estimation based on the above numerical results clarifies that the LSVQC allows us to relax the requirement on the gate error rate of quantum hardware to realize quantum simulations compared to that required by the Trotterization.

We here provide some comments about possible future directions. The performance of the LSVQC is highly influenced by the subspace and the ansatz circuit. Although we adopt the Trotterized Krylov subspace and VHA in this work, other subspaces and ansatzes might be more appropriate depending on the problem to which we wish to apply the LSVQC or on the performance of quantum computing hardware. A more detailed investigation of the dependence of the LSVQC on the choice of subspace and ansatz is one possible direction for future study. Another possible direction is a combined effort between the LSVQC and other sophisticated quantum computing techniques. In this work, we have briefly shown that the LSVQC achieves a significant relaxation of the requirement on the gate error rate when it is combined with the STAR architecture. Improvement of the LSVQC into a form suitable to the STAR architecture is left for future work. There is also a potential for further resource reduction in materials simulations by combining the LSVQC with some sophisticated

techniques that take into account detailed materials properties (e.g., a hybrid fermion-to-qubit mapping in Ref. [111]).

In conclusion, the LSVQC is a quantum-classical hybrid algorithm that enables us to efficiently implement the time-evolution operator of large-scale quantum many-body systems on near-term quantum computers. The superiority of the LSVQC over previously proposed methods has been clarified by numerical simulations of not only a simple toy model but also a realistic materials model based on the *ab initio* electronic structure calculation. We hope this work gives insight into the development of algorithms towards realizing practical materials simulation on near-term quantum computers.

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APPENDIX A: FAITHFULNESS OF COST FUNCTION FOR SUBSPACE-BASED COMPILING

Here, we show that the cost function C_{LET} given by Eq. (2) satisfies the faithfulness condition. In other words, we show that $C_{\text{LET}} = 0$ if and only if $U|\psi\rangle = e^{i\varphi}V|\psi\rangle$ for $\forall |\psi\rangle \in \mathcal{S} = \text{span}(\{|\Psi_k\rangle\}_{k=0}^{N-1})$ (For brevity, we describe $U^{(L)}$ and $V^{(L)}$ as U and V in this section). Here, the basis $\{|\Psi_k\rangle\}_{k=0}^{N-1}$ is assumed to be a linearly independent and nonorthogonal set of states.

First, we prove the forward direction. Since $0 \leq |\langle\Psi_k|V^\dagger U|\Psi_k\rangle|^2 \leq 1$ for all k , $C_{\text{LET}} = 0$ indicates that the action of V on $|\Psi_k\rangle$ coincides with the action of U on $|\Psi_k\rangle$ up to a nonzero phase factor $e^{i\varphi_k}$ as follows:

$$V|\Psi_k\rangle = e^{i\varphi_k}U|\Psi_k\rangle \text{ for } k \in \{0, 1, \dots, N-1\}. \quad (\text{A1})$$

In addition, when the basis states are linearly independent and nonorthogonal, the global phase factor $e^{i\varphi_k}$ is independent of k (i.e., $e^{i\varphi_k} = e^{i\varphi}$ for all k). To see this, following Ref. [17], let us consider two linearly independent and nonorthogonal states $|\Psi_0\rangle$ and $|\Psi_1\rangle$. Then, $|\Psi_1\rangle$ can be described as

$$|\Psi_1\rangle = c|\Psi_0\rangle + c_\perp|\Psi_0^\perp\rangle, \quad (\text{A2})$$

where $|c_\perp|^2 = 1 - |c|^2$, $|c|^2 > 0$, and $\langle\Psi_0|\Psi_0^\perp\rangle = 0$. From Eqs. (A1) and (A2), we obtain

$$\begin{aligned} e^{-i\varphi_1} &= \langle\Psi_1|V^\dagger U|\Psi_1\rangle \\ &= |c|^2\langle\Psi_0|V^\dagger U|\Psi_0\rangle + |c_\perp|^2\langle\Psi_0^\perp|V^\dagger U|\Psi_0^\perp\rangle \\ &= |c|^2e^{-i\varphi_0} + (1 - |c|^2)\langle\Psi_0^\perp|V^\dagger U|\Psi_0^\perp\rangle. \end{aligned} \quad (\text{A3})$$

Equation (A3) can be rewritten as

$$\begin{aligned} e^{-i\varphi_1} &= \langle\Psi_0^\perp|V^\dagger U|\Psi_0^\perp\rangle \\ &= |c|^2(e^{-i\varphi_0} - \langle\Psi_0^\perp|V^\dagger U|\Psi_0^\perp\rangle). \end{aligned} \quad (\text{A4})$$

Here, Eq. (A4) indicates that two vectors $\mathbf{v}_1$ and $\mathbf{v}_2$, which correspond to the left- and right-hand side on Eq. (A4) respectively, coincide on the complex plane. Since $|c|^2 > 0$, $|e^{-i\varphi_0}| = 1$, and $|\langle\Psi_0^\perp|V^\dagger U|\Psi_0^\perp\rangle| \leq 1$, the above condition is satisfied only when

$$e^{-i\varphi_0} = e^{-i\varphi_1} = \langle\Psi_0^\perp|V^\dagger U|\Psi_0^\perp\rangle. \quad (\text{A5})$$

Equation (A5) indicates that $e^{i\varphi_0} = e^{i\varphi_1}$. Repeating the above calculation for all pairs of basis states, we obtain $e^{i\varphi_k} = e^{i\varphi'_k} \equiv e^{i\varphi}$ for $\forall k, k' \in \{0, \dots, N-1\}$. Thus, $e^{i\varphi_k} = e^{i\varphi}$ for all k in Eq. (A1) since $\{|\Psi_k\rangle\}_{k=0}^{N-1}$ is defined as a linearly independent and nonorthogonal basis set. Here, we note that any state $|\psi\rangle$ belonging to the subspace $\mathcal{S}$ can be represented as a linear combination of $\{|\Psi_k\rangle\}_{k=0}^{N-1}$ as

$$|\psi\rangle = \sum_{k=0}^{N-1} c_k |\Psi_k\rangle. \quad (\text{A6})$$

From Eqs. (A1) and (A6), we obtain

$$V|\psi\rangle = \sum_{k=0}^{N-1} c_k e^{i\varphi_k} U|\Psi_k\rangle = e^{i\varphi} U|\psi\rangle, \quad (\text{A7})$$

where we used $e^{i\varphi_k} = e^{i\varphi}$. Therefore, $U|\psi\rangle = e^{i\varphi} V|\psi\rangle$ for $\forall |\psi\rangle \in \mathcal{S}$ if $C_{\text{LET}} = 0$.

The reverse direction is somewhat trivial. If $U|\psi\rangle = e^{i\varphi} V|\psi\rangle$ for $\forall |\psi\rangle \in \mathcal{S}$, then $U|\Psi_k\rangle = e^{i\varphi} V|\Psi_k\rangle$ for all k . This indicates that

$$|\langle \Psi_k | V^\dagger U | \Psi_k \rangle|^2 = |e^{i\varphi}|^2 = 1. \quad (\text{A8})$$

Inserting Eq. (A8) to the right-hand side of Eq. (2), we find $C_{\text{LET}} = 0$.

APPENDIX B: DERIVATION OF LOCAL COMPILATION THEOREM

In this Appendix, we provide details of the derivation of the local compilation theorem.

1. Proof of Proposition 1

Here, we provide a proof of Proposition 1. The proof is based on the LR bound. As a preliminary, we first modify the inequality of the LR bound given by Eq. (14). Let us consider a local operator $O_{X_{R,j}}$ acting on the R -size domain centered at the j th site, i.e., $X_{R,j} = \{j' \in \Lambda | \text{dist}(j, j') \leq R/2\}$. Then, the expression of the LR bound (14) can be rewritten in the following form [41,57]:

$$\begin{aligned} & \|(U^{(L)})^\dagger O_{X_{R,j}} U^{(L)} - e^{i\tau H^{(L',j)}} O_{X_{R,j}} e^{-i\tau H^{(L',j)}}\| \\ & \leq C' \int_{L'/2-r_H}^{\infty} dr e^{-(r-v\tau)/\xi}, \end{aligned} \quad (\text{B1})$$

where C' is a constant of $\mathcal{O}(\tau)$ independent of the system size. L' is determined such that $L'/2 - r_H$ is larger than $R/2$ (i.e., the radius of the support of $O_{X_{R,j}}$) and $H^{(L',j)}$ is the locally-restricted L' -size Hamiltonian given by Eq. (17). Using Eq. (B1), Proposition 1 is derived as follows:

Proof. From the definition in Eq. (4), the difference between $C_{\text{LET}}^{(j)}(U^{(L)}, V^{(L)}, B_S)$ and $C_{\text{LET}}^{(j)}(U^{(L',j)}, V^{(L)}, B_S)$ can

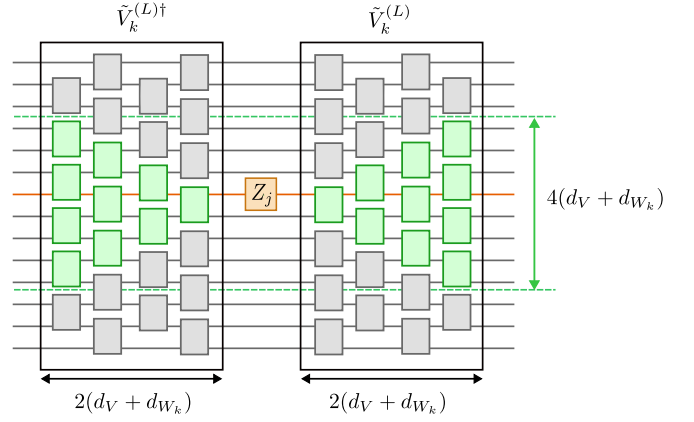


FIG. 16. Schematic illustration of the locality of the operator $O_{k,j} \equiv \tilde{V}_k^{(L)}(Z_j \otimes \mathbb{1}_{\bar{j}})(\tilde{V}_k^{(L)})^\dagger$. Only green two-qubit gates are active in $O_{k,j}$, while other gray two-qubit gates vanish by taking the contraction. Consequently, $O_{k,j}$ is a R_k -local operator with $R_k = 4(d_V + d_{W_k})$.

be written as follows $[\tilde{V}_k^{(L)} \equiv V^{(L)} W_k^{(L)}]$:

$$\begin{aligned} & |C_{\text{LET}}^{(j)}(U^{(L)}, V^{(L)}, B_S) - C_{\text{LET}}^{(j)}(U^{(L',j)}, V^{(L)}, B_S)| \\ & \leq \frac{1}{N} \sum_{k=1}^N |\langle \Psi_k | (U^{(L)})^\dagger \tilde{V}_k^{(L)} \Pi_j (\tilde{V}_k^{(L)})^\dagger U^{(L)} | \Psi_k \rangle \\ & \quad - \langle \Psi_k | (U^{(L',j)})^\dagger \tilde{V}_k^{(L)} \Pi_j (\tilde{V}_k^{(L)})^\dagger U^{(L',j)} | \Psi_k \rangle| \\ & \leq \frac{1}{2N} \sum_{k=1}^N \|(U^{(L)})^\dagger \tilde{V}_k^{(L)}(Z_j \otimes \mathbb{1}_{\bar{j}})(\tilde{V}_k^{(L)})^\dagger U^{(L)} \\ & \quad - (U^{(L',j)})^\dagger \tilde{V}_k^{(L)}(Z_j \otimes \mathbb{1}_{\bar{j}})(\tilde{V}_k^{(L)})^\dagger U^{(L',j)}\|, \end{aligned} \quad (\text{B2})$$

where we expanded the local projection operator Π_j as $\Pi_j = \frac{1}{2}(\mathbb{1}_j + Z_j) \otimes \mathbb{1}_{\bar{j}}$ with $\mathbb{1}_{\bar{j}} \equiv \mathbb{1}_1 \otimes \dots \otimes \mathbb{1}_{j-1} \otimes \mathbb{1}_{j+1} \otimes \dots \otimes \mathbb{1}_L$. Since we assume that the ansatz $V^{(L)}$ and the state preparation circuits $W_k^{(L)}$ are local such as in Eqs. (15) and (16), $\tilde{V}_k^{(L)}(Z_j \otimes \mathbb{1}_{\bar{j}})(\tilde{V}_k^{(L)})^\dagger$ is regarded as R_k -local operator with $R_k = 4(d_V + d_{W_k})$ (see Fig 16). Thus, we can apply Eq. (B1) to Eq. (B2) by setting $R \equiv \max_k R_k = 4(d_V + \max_k d_{W_k})$. This leads to the following inequality:

$$\begin{aligned} & |C_{\text{LET}}^{(j)}(U^{(L)}, V^{(L)}, B_S) - C_{\text{LET}}^{(j)}(U^{(L',j)}, V^{(L)}, B_S)| \\ & \leq \frac{C'}{2} \int_{L'/2-r_H}^{\infty} dr e^{-(r-v\tau)/\xi}. \end{aligned} \quad (\text{B3})$$

For D -dimensional lattice, the integral in Eq. (B3) is evaluated as follows [41,57]:

$$\int_{L'/2-r_H}^{\infty} dr e^{-(r-v\tau)/\xi} \leq C'' \left(\frac{L'}{2} - r_H \right)^{D-1} e^{-(L'/2-r_H-v\tau)/\xi}, \quad (\text{B4})$$

where C'' is a constant. Then, by describing L' as in Eq. (20), we obtain Eq. (21) from Eqs. (B3) and (B4). ■

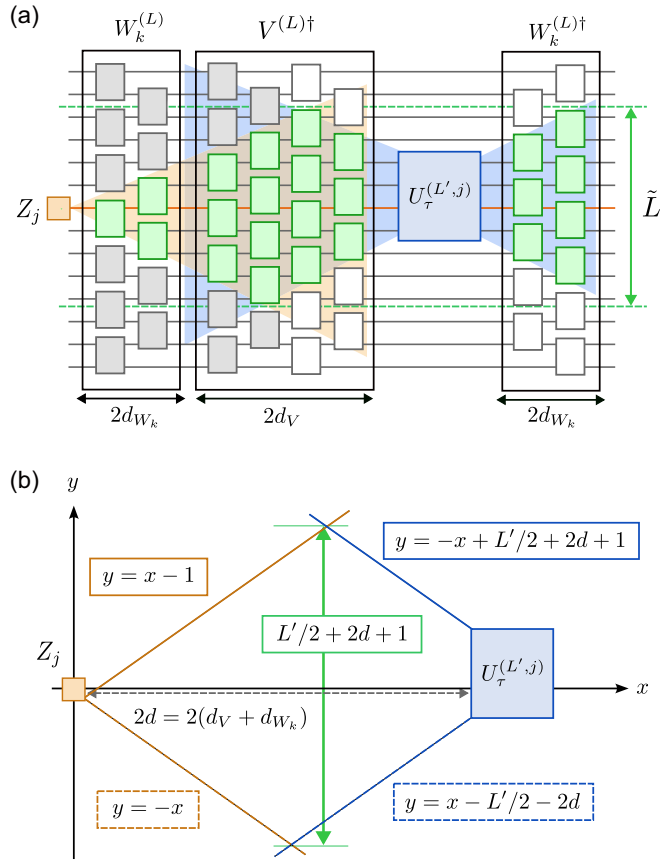


FIG. 17. (a) Schematic illustration of the causal cones in a quantum circuit to evaluate the local cost function $C_{\text{LLET}}^{(j)}(U^{(L',j)}, V^{(L)}, B_S)$. Only green two-qubit gates are active for computing the local cost function. The gray (white) two-qubit gates vanish by the contraction owing to the orange (blue) causal cone arising from the locality of the measurement operator (LR bound). (b) Schematic illustration of the estimation of the compilation size. A proper compilation size is estimated by considering an intersection of two causal cones geometrically.

2. Proof of Proposition 2

Proposition 2 is derived based on the LR bound and causal cone of the quantum circuit structure. The proof is given as follows:

Proof. We consider the causal cone of quantum circuits used to compute the cost functions $C_{\text{LLET}}^{(j)}(U^{(L',j)}, V^{(L)}, B_S)$. From Eq. (4), we only need to focus on the $\text{Tr}[\Pi_j \rho_k(U^{(L',j)}, V^{(L)}, B_S)]$ term that can be schematically expressed in Fig. 17(a). There are two causal cones in the structure of $\text{Tr}[\Pi_j \rho_k(U^{(L',j)}, V^{(L)}, B_S)]$. The first causal cone is from the locality of the measurement operator Π_j , which is depicted as an orange region in Fig. 17(a). The gray two-qubit gates in Fig. 17(a) are inactive gates due to this causal cone since they are contracted to the identity gate. The second causal cone [blue regions in Fig. 17(a)] stems from the LR bound, i.e., the local restriction of the time-evolution operator. Considering this second causal cone, the white two-qubit gates can be contracted to the identity gate. Hence, only green two-qubit gates in Fig. 17(a) are relevant to evaluate $\text{Tr}[\Pi_j \rho_k(U^{(L',j)}, V^{(L)}, B_S)]$. This indicates we can

restrict the width of the quantum circuits $V^{(L)}$ and $W_k^{(L)}$ to some compilation size $\tilde{L}_k$ from L . By considering the intersection of two causal cones as shown in Fig. 17(b), we can estimate that the proper compilation size is given by

$$\tilde{L}_k = \max\left(\frac{L'}{2} + 2(d_V + d_{W_k}) + 1, L' + 4d_{W_k}\right). \quad (\text{B5})$$

When the compilation size $\tilde{L}$ is set to $\tilde{L} \geq \max_k \tilde{L}_k$ and satisfies Eq. (24), the locally restricted circuits $V^{(\tilde{L},j)}$ and $W_k^{(\tilde{L},j)}$ contain all active two-qubit gates. Thus, the term $\text{Tr}[\Pi_j \rho_k(U^{(L',j)}, V^{(L)}, B_S)]$ can be rewritten as

$$\begin{aligned} & \text{Tr}[\Pi_j \rho_k(U^{(L',j)}, V^{(L)}, B_S)] \\ &= \langle \Psi_k | (U^{(L',j)})^\dagger \tilde{V}_k^{(L)} \Pi_j (\tilde{V}_k^{(L)})^\dagger U^{(L',j)} | \Psi_k \rangle \\ &= \langle 0 | (W_k^{(\tilde{L},j)})^\dagger (\tilde{U}^{(L',j)})^\dagger V_k^{(\tilde{L},j)} W_k^{(\tilde{L},j)} \\ & \quad \times \Pi_j (W_k^{(\tilde{L},j)})^\dagger (V_k^{(\tilde{L},j)})^\dagger \tilde{U}^{(L',j)} W_k^{(\tilde{L},j)} | 0 \rangle. \end{aligned} \quad (\text{B6})$$

From Eq. (B6), we can derive Eq. (25). ■

3. Proof of Theorem 1

Theorem 1 (i.e., the local compilation theorem) is derived by combining Proposition 1 with Proposition 2 as follows:

Proof. From Eqs. (21) and (25), we obtain

$$\begin{aligned} & C_{\text{LLET}}^{(j)}(U^{(L)}, V^{(L)}, B_S) \\ & \leq C_{\text{LLET}}^{(j)}(\tilde{U}^{(L',j)}, V^{(\tilde{L},j)}, B_{S_j}) + \frac{1}{2} \epsilon_{\text{LR}}. \end{aligned} \quad (\text{B7})$$

Since the $H^{(L',j)}$ is a local restriction of $H^{(\tilde{L},j)}$ ($\tilde{L} \geq L'$), we can use Eq. (B1) by replacing $U^{(L)} \rightarrow U^{(\tilde{L},j)}$. Thus, by performing the same discussion with the proof of Proposition 1, we obtain

$$\begin{aligned} & C_{\text{LLET}}^{(j)}(\tilde{U}^{(L',j)}, V^{(\tilde{L},j)}, B_{S_j}) \\ & \leq C_{\text{LLET}}^{(j)}(U_\tau^{(\tilde{L},j)}, V^{(\tilde{L},j)}, B_{S_j}) + \frac{1}{2} \epsilon_{\text{LR}}. \end{aligned} \quad (\text{B8})$$

Combining Eqs. (B7) with (B8), we get

$$\begin{aligned} & C_{\text{LLET}}^{(j)}(U^{(L)}, V^{(L)}, B_S) \\ & \leq C_{\text{LLET}}^{(j)}(U_\tau^{(\tilde{L},j)}, V^{(\tilde{L},j)}, B_{S_j}) + \epsilon_{\text{LR}}. \end{aligned} \quad (\text{B9})$$

Taking the average of both sides of Eq. (B9) over j , we obtain Eq. (30). Equation (31) is straightforwardly derived from Eq. (30) using the relation between the global cost and local cost [Eq. (6)]. ■

APPENDIX C: EXTENSION OF LOCAL COMPILATION THEOREM

In this Appendix, we provide some modified versions of the local compilation theorem.

1. Translationally invariant systems

We first consider modifying the original local compilation theorem for translationally invariant systems. Let us consider the translationally invariant Hamiltonian $H^{(L)}$ under the periodic boundary condition. In this case, if both the ansatz

$V^{(L)}(\theta)$ and the state preparation circuits $\{W_k^{(L)}\}$ also exhibits translationally invariant structures, Theorem 1 can be simplified to the following theorem.

Theorem 2 (Local compilation theorem for translationally invariant systems). Suppose that we have an optimal parameter set θ^* such that

$$C_{\text{LLET}}(U^{(\tilde{L})}, V^{(\tilde{L})}(\theta^*), B_{\tilde{S}}) \leq \tilde{\epsilon}_{\text{opt}}, \quad (\text{C1})$$

with $B_{\tilde{S}} = \{W_k^{(\tilde{L})}|0\rangle_{k=0}^{\otimes \tilde{L}-1}\}$ and $\tilde{S} = \text{span}(B_{\tilde{S}})$. Here, $U^{(\tilde{L})} = e^{-i\tau H^{(\tilde{L})}}$, $V^{(\tilde{L})}(\theta)$, and $\{W_k^{(\tilde{L})}\}$ are translationally invariant. Then, the cost functions for the original L -size system are bounded as

$$C_{\text{LLET}}(U^{(L)}, V^{(L)}(\theta^*), B_S) \leq \tilde{\epsilon}_{\text{opt}} + \epsilon_{\text{LR}}, \quad (\text{C2})$$

$$C_{\text{LET}}(U^{(L)}, V^{(L)}(\theta^*), B_S) \leq L(\tilde{\epsilon}_{\text{opt}} + \epsilon_{\text{LR}}). \quad (\text{C3})$$

Proof. Since $U^{(L)}$, $V^{(L)}(\theta)$ and $\{W_k^{(L)}\}$ are assumed to be translationally invariant, the summands in Eq. (29) are independent of j . Although $U^{(\tilde{L},j)}$, $V^{(\tilde{L},j)}$ and $\{W_k^{(\tilde{L},j)}\}$ are not translationally invariant in general, we can recover the translational symmetry by padding some inactive gates at the boundary (see Fig. 5 in Ref. [41] for reference). This allows us to rewrite the summands in Eq. (29) to $C_{\text{LLET}}(U^{(\tilde{L})}, V^{(\tilde{L})}(\theta^*), B_{\tilde{S}})$, and hence the above theorem is justified. ■

2. Extension to long-time dynamics

We have derived the local compilation theorem for a fixed time τ in the main text. However, in practical applications, we usually compute long-time dynamics by repeatedly applying the optimized circuit $V^{(L)}(\theta^*)$ to some input states. Considering such situations, we explicitly provide a local compilation theorem for long-time dynamics simulation as follows:

Theorem 3 (Local compilation theorem for long-time dynamics). Suppose we aim to simulate long-time dynamics at $t = n\tau$ ($n \in \mathbb{N}$). Then, using ϵ_{opt} and ϵ_{LR} in Eqs. (30) and (31), the cost functions for the original L -size system for time $t = n\tau$ are bounded as

$$C_{\text{LLET}}((U^{(L)})^n, (V^{(L)}(\theta^*))^n, B_S) \lesssim n^2(\epsilon_{\text{opt}} + \epsilon_{\text{LR}}), \quad (\text{C4})$$

$$C_{\text{LET}}((U^{(L)})^n, (V^{(L)}(\theta^*))^n, B_S) \lesssim n^2 L(\epsilon_{\text{opt}} + \epsilon_{\text{LR}}). \quad (\text{C5})$$

Proof. The infidelity of a quantum state $|\Psi_k\rangle$ between V and U generally satisfies the following relation [17]:

$$\begin{aligned} 1 - |\langle \Psi_k | (V^\dagger)^n U^n | \Psi_k \rangle|^2 \\ \lesssim n^2 (1 - |\langle \Psi_k | V^\dagger U | \Psi_k \rangle|^2), \end{aligned} \quad (\text{C6})$$

where $n \in \mathbb{N}$. Applying the above relation to the definition of the global cost function C_{LET} [Eq. (2)], we obtain

$$\begin{aligned} C_{\text{LET}}(U_{n\tau}^{(L)}, (V^{(L)}(\theta^*))^n, B_S) \\ \lesssim n^2 C_{\text{LET}}(U^{(L)}, V^{(L)}(\theta^*), B_S). \end{aligned} \quad (\text{C7})$$

By combining Eqs. (C7) with (31), we obtain Eq. (C5). Then, Eq. (C4) is derived from Eqs. (C5) using the relationship between the global cost and local cost given by Eq. (6). ■

Based on Eqs. (C4) and (C5), when we want to achieve $C_{\text{LLET}, \text{LET}}(U_{n\tau}^{(L)}, (V^{(L)}(\theta^*))^n, B_S) = \mathcal{O}(\epsilon)$ for some accuracy

ϵ , we need to choose a compilation size $\tilde{L}$ as

$$\begin{aligned} \tilde{L} \gtrsim \mathcal{O}(\xi \log(n^2 L^\alpha / \epsilon)) + r_H + v\tau + 2 \max_k d_{W_k} \\ + \max \left(2d_V + 1, r_H + v\tau + 2 \max_k d_{W_k} \right). \end{aligned} \quad (\text{C8})$$

Equation (C8) indicates that the compilation size $\tilde{L}$ does not drastically increase as in increasing the simulation time, since it logarithmically increases as $\mathcal{O}(\log n)$ for the time step $n = t/\tau$.

APPENDIX D: AB INITIO DOWNFOLDING

In this Appendix, we describe details of the *ab initio* downfolding method [67]. As explained in Sec. VI, the *ab initio* downfolding is a technique to construct a low-energy effective lattice model for strongly correlated materials on the basis of maximally localized Wannier orbitals [74]. Specifically, the effective lattice model is obtained in the following form:

$$\begin{aligned} H = \sum_{n,m} \sum_{\sigma=\uparrow,\downarrow} t_{nm} c_{n\sigma}^\dagger c_{m\sigma} + \frac{1}{2} \sum_{n,m} \sum_{\sigma,\sigma'} U_{nm} c_{n\sigma}^\dagger c_{m\sigma'}^\dagger c_{m\sigma'} c_{n\sigma} \\ + \frac{1}{2} \sum_{n,m} \sum_{\sigma,\sigma'} J_{nm} (c_{n\sigma}^\dagger c_{m\sigma'}^\dagger c_{n\sigma'} c_{m\sigma} + c_{n\sigma}^\dagger c_{n\sigma'}^\dagger c_{m\sigma'} c_{m\sigma}), \end{aligned} \quad (\text{D1})$$

where n, m are the indices specifying the Wannier orbitals, $\sigma, \sigma' (= \uparrow, \downarrow)$ are the spin indices, and $c_{n\sigma}$ ($c_{n\sigma}^\dagger$) is the annihilation (creation) operator of an electron with the spin-orbital index $n\sigma$. t_{nm} is the one-body integral defined as

$$t_{nm} = \int d\mathbf{r} \psi_n^*(\mathbf{r}) H_0 \psi_m(\mathbf{r}), \quad (\text{D2})$$

where $\psi_n(\mathbf{r})$ is the n th Wannier orbital and H_0 is the noninteracting Kohn-Sham Hamiltonian obtained by the DFT. The integral in Eq. (D2) is taken over the crystal volume. U_{nm} and J_{nm} are the effective Coulomb and effective exchange interactions defined as,

$$U_{nm} = \iint d\mathbf{r} d\mathbf{r}' |\psi_n(\mathbf{r})|^2 W(\mathbf{r}, \mathbf{r}') |\psi_m(\mathbf{r}')|^2, \quad (\text{D3})$$

$$J_{nm} = \iint d\mathbf{r} d\mathbf{r}' \psi_n^*(\mathbf{r}) \psi_m(\mathbf{r}) W(\mathbf{r}, \mathbf{r}') \psi_m(\mathbf{r}')^* \psi_n(\mathbf{r}'), \quad (\text{D4})$$

where $W(\mathbf{r}, \mathbf{r}')$ is the screened Coulomb interaction obtained based on the constrained random phase approximation [75]. The parameters t_{nm} , U_{nm} , and J_{nm} are obtained by using the RESPACK package [76–81].

APPENDIX E: TROTTER ERROR BOUND

Here, we review details of the Trotter error bound used in the resource estimation in Sec. VII.

1. Worst-case error bound

Using the results of Ref. [112], the Trotter error bound in the worst-case scenario for the Hamiltonian $H = \sum_{\gamma=1}^{\Gamma} H_{\gamma}$ is expressed as

$$\|(U_1(t/r))^r - e^{-iHt}\| \leq \mathcal{O}(\alpha_{\text{comm}} t^2 / r), \quad (\text{E1})$$

where $U_1(t) = \prod_{\gamma=1}^{\Gamma} e^{-itH_{\gamma}}$ denote the first-order Trotter decomposition of the time evolution operator e^{-itH} , and α_{comm} is the commutator scaling factor given by

$$\alpha_{\text{comm}} = \sum_{\gamma_1, \dots, \gamma_{p+1}}^{\Gamma} \|[H_{\gamma_1}, \dots [H_{\gamma_p}, H_{\gamma_{p+1}}] \dots]\|, \quad (\text{E2})$$

Here, $\|\dots\|$ denotes the spectral norm. From Eq. (E1), the number of Trotter steps r needed to achieve the accuracy ϵ in the worst-case scenario can be estimated as

$$r = \mathcal{O}(\alpha_{\text{comm}} t^2 / \epsilon). \quad (\text{E3})$$

For the Fermi-Hubbard model, the coefficients α_{comm} asymptotically scales as $\alpha_{\text{comm}} = \mathcal{O}(L)$ [113] with L being the lattice size. We can expect the same scaling $\alpha_{\text{comm}} = \mathcal{O}(L)$ for the extended Fermi-Hubbard models owing to the similarity of the conventional Fermi-Hubbard model and the extended Fermi-Hubbard model obtained by the *ab initio* downfolding.

2. Average-case error bound

The average-case error captures the averaged error for some input states chosen randomly from an ensemble of quantum states $\mathcal{E} = \{(p_i, \psi_i)\}$, where p_i is the probability obtaining the state ψ_i . Formally, it is defined as

$$R(U_1(t), e^{-itH}) = \mathbb{E}_{\mathcal{E}}[\mathcal{D}(U_1(t)|\psi\rangle, e^{-itH}|\psi\rangle)], \quad (\text{E4})$$

where $\mathcal{D}(*, *)$ and $\mathbb{E}_{\mathcal{E}}[\dots]$ denote the distance measure and the expectation over the ensemble $\mathcal{E}$, respectively. From the results of Ref. [95], the average-case Trotter error bound (for the 1-design ensemble) is obtained as

$$R((U_1(t/r))^r, e^{-itH}) \leq \mathcal{O}(T_1 t^2 / r), \quad (\text{E5})$$

where

$$T_1 = \sum_{\gamma_1, \dots, \gamma_{p+1}}^{\Gamma} \frac{1}{\sqrt{d}} \|[H_{\gamma_1}, \dots [H_{\gamma_p}, H_{\gamma_{p+1}}] \dots]\|_F. \quad (\text{E6})$$

Here, $\|\dots\|_F$ denotes the Frobenius norm and $d = 2^n$ is the dimension of the Hilbert space of an n -qubit system. Thus, the Trotter step r needed to achieve the accuracy ϵ in terms of the average-case error is estimated as

$$r = \mathcal{O}(T_1 t^2 / \epsilon). \quad (\text{E7})$$

For an n -qubit nearest-neighbor Hamiltonian such as the Fermi-Hubbard model, the coefficient T_1 asymptotically scales as $T_1 = \mathcal{O}(\sqrt{n})$ [95]. Therefore, we expect $T_1 = \mathcal{O}(\sqrt{L})$ for the L -site Fermi-Hubbard and extended Fermi-Hubbard models in the main text.

APPENDIX F: BRIEF OVERVIEW OF LVQC

Here, we summarize the details of the LVQC algorithm [41,42]. The LVQC is designed to compile the time-evolution operator $U^{(L)} = e^{-itH^{(L)}}$ of L -qubit quantum many-body systems. In contrast to the LSVQC, the compilation of the LVQC is performed to reproduce the action of the time-evolution operator over the entire Hilbert space. Such full Hilbert space

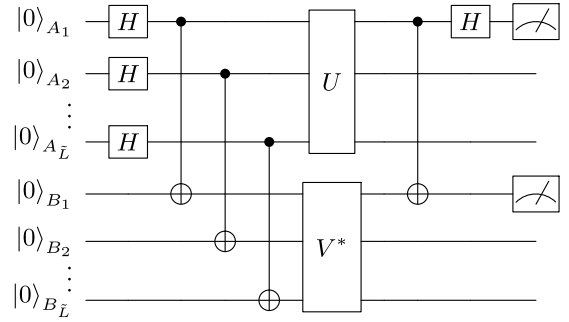


FIG. 18. Quantum circuit for the LHST. In this circuit, the probability of the qubits A_1 and B_1 are in the $|0\rangle$ state is equal to Eq. (F5) with $j = 1$.

compiling is realized by utilizing the following cost function:

$$C_{\text{HST}}(U^{(L)}, V^{(L)}) = 1 - \frac{1}{d^2} |\text{Tr}[(V^{(L)})^\dagger U^{(L)}]|^2, \quad (\text{F1})$$

where $d = 2^L$ is the dimension of the entire Hilbert space. $C_{\text{HST}} = 0$ is satisfied if and only if the full Hilbert space compiling succeeds as $U^{(L)} = e^{i\varphi} V^{(L)}$.

In the same spirit as the LSVQC, the LVQC indirectly minimizes the cost function C_{HST} by minimizing its localized counterpart. The local cost function of the LVQC is described by utilizing the Bell pair between copied systems A and B . The maximally entangled Bell state between A and B is given by

$$|\Phi_+\rangle_{AB} = \bigotimes_j |\Phi_+\rangle_{A_j B_j}, \quad (\text{F2})$$

$$|\Phi_+\rangle_{A_j B_j} = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)_{A_j B_j}, \quad (\text{F3})$$

where A_j and B_j denote the j th qubit of the system A and B , respectively. Then, the local cost function of the LVQC is defined as

$$C_{\text{LVQC}}^{(\tilde{L})}(\theta) = \frac{1}{L} \sum_{j=1}^L C_{\text{LHST}}^{(j)}(\tilde{U}^{(L',j)}, V^{(\tilde{L},j)}(\theta)), \quad (\text{F4})$$

where

$$C_{\text{LHST}}^{(j)}(U, V) = 1 - |\langle \Phi_+ |_{A_j B_j} (U \otimes V^*) | \Phi_+ \rangle_{AB}|^2. \quad (\text{F5})$$

In Eq. (F4), the $\tilde{U}^{(L',j)}$ and $V^{(\tilde{L},j)}$ are defined in the same way as in Sec. IV. Equation (F5) is measured by the LHST using a quantum circuit shown in Fig. 18. When we achieve $C_{\text{LVQC}}^{(\tilde{L})}(\theta^*) \leq \epsilon_{\text{opt}}$ for some optimal parameter set θ^* , the original cost function (F1) L -size system is bounded as

$$C_{\text{HST}}(U^{(L)}, V^{(L)}(\theta^*)) \leq L(\epsilon_{\text{opt}} + \frac{3}{4}\tilde{\epsilon}_{\text{LR}}), \quad (\text{F6})$$

where $\tilde{\epsilon}_{\text{LR}} = e^{-\mathcal{O}(l_0/\xi)}$ with a tunable parameter l_0 . Equation (F6) holds for the local Hamiltonian with the LR bound. If we want to realize $C_{\text{HST}} = \mathcal{O}(\epsilon)$, the compilation size $\tilde{L}$

should be chosen as

$$\tilde{L} \geq \mathcal{O}(\xi \log(L/\epsilon)) + r_H + v\tau + 2d_V + 1, \quad (\text{F7})$$

where the definition of each parameter is the same as that in the expression of the compilation size for the LSVQC [see Eq. (32)].

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