Quantifying Fermionic Nonlinearity of Quantum Circuits

Shigeo Hakkaku,1,∗ Yuichiro Tashima,1,† Kosuke Mitarai,1,2,3,‡ Wataru Mizukami,1,2,3,§ and Keisuke Fujii1,2,4,5,¶

1Graduate School of Engineering Science, Osaka University, 1-3 Machikaneyama, Toyonaka, Osaka 560-8531, Japan
2Center for Quantum Information and Quantum Biology, Osaka University, 1-2 Machikaneyama, Toyonaka, Osaka 560-0043, Japan
3JST, PRESTO, 4-1-8 Honcho, Kawaguchi, Saitama 332-0012, Japan
4RIKEN Center for Quantum Computing (RQC), Hiroswa 2-1, Wako, Saitama 351-0198, Japan
5Fujitsu Quantum Computing Joint Research Division at QIQB, Osaka University, 1-2 Machikaneyama, Toyonaka 560-0043, Japan

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Variational quantum algorithms (VQA) have been proposed as one of the most promising approaches to demonstrate quantum advantage on noisy intermediate-scale quantum (NISQ) devices. However, it has been unclear whether VQA algorithms can maintain quantum advantage under the intrinsic noise of the NISQ devices, which deteriorates the quantumness. Here we propose a measure, called fermionic nonlinearity, to quantify the classical simulatability of quantum circuits designed for simulating fermionic Hamiltonians. Specifically, we construct a Monte-Carlo type classical algorithm based on the classical simulatability of fermionic linear optics, whose sampling overhead is characterized by the fermionic nonlinearity. As a demonstration of these techniques, we calculate the upper bound of the fermionic nonlinearity of a rotation gate generated by four-body fermionic interaction under the dephasing noise. Moreover, we estimate the sampling costs of the unitary coupled cluster singles and doubles (UCCSD) quantum circuits for hydrogen chains subject to the dephasing noise. We find that, depending on the error probability and atomic spacing, there are regions where the fermionic nonlinearity becomes very small or unity, and hence the circuits are classically simulatable. We believe that our method and results help to design quantum circuits for fermionic systems with potential quantum advantages.

I. INTRODUCTION

Quantum computers have attracted much attention because of their capability to solve classically intractable problems. Among them, the first industrial application is expected to be a quantum chemistry calculation, which uses quantum computers for simulating fermionic many-body systems. It has been predicted that a fault-tolerant quantum computer with about a million physical qubits can simulate both Fermi-Hubbard and molecular electronic structure Hamiltonians beyond classical approaches [1]. The application has also been anticipated for NISQ devices through the variational quantum eigensolver (VQE) [2–9].

It is essential to predict at what scale quantum computers can have advantages over classical ones for those applications. One way is to estimate the computational cost required for fault-tolerant quantum computers to simulate fermionic systems that are well beyond the reach of classical supercomputers [1, 10, 11]. However, this approach highly depends both on the objective system and algorithms employed in classical or quantum computers. As another approach, we can ask a question the other way around; given a quantum circuit that simulates a fermionic system, what is the cost of classical computation to simulate that circuit? If there exists a quantum advantage, at least such a quantum circuit has to be hard for a classical computer to be simulated.

One way to evaluate the classical simulatability of quantum circuits is to quantify the simulation cost of a specific quasiprobability-based simulator [12–17]. The central idea of quasiprobability simulators is to decompose a complex operator (operation) A over a discrete set of classically tractable operators (operations) \( \{ B_i \} \), i.e.,

\[ A = \sum_i \alpha_i B_i, \]

where the coefficients \( \{ \alpha_i \} \) are called “quasiprobability distribution”, and the L1 norm of the quasiprobability distribution \( \sum_i | \alpha_i | \) determines a sampling cost. Any set of operations that can be efficiently simulated by classical computers can be used as operators \( \{ B_i \} \) in a quasiprobability-based simulator. Over the past years, Clifford circuits have become a popular class of such channels. [13, 14, 16, 17].

Here, we consider another popular class of classically simulatable circuits: fermionic linear optics (FLO) and matchgates [18–21]. These classes represent the dynamics of free fermions, generated by quadratic fermionic Hamiltonians. It represents a restricted class of quantum circuits in the sense that, in general, natural fermionic interactions are described by not only two-body but also four-body fermion operators. For example, the four-body interactions appear in quantum circuits tailored to simulate fermionic systems, such as unitary coupled clus-
define {simulate general fermionic interactions through FLO. We explain the quasiprobability method to satisfy or quantum advantages. We believe that our method and hydrogen chain can be simulated because of vanishing reasonable sampling cost. Furthermore, if \( p \) noise in quantum circuits for the hydrogen chain with the spaciolation from the results shows us that the noisy UCCSD ters obtained by full-vector simulations. A rough extrapolation from the results shows us that the noisy UCCSD quantum circuits for the hydrogen chain up to \( H_8 \) with several spacings using the optimized variational parameters obtained by full-vector simulations. A rough extrapolation from the results shows us that the noisy UCCSD quantum circuits for the hydrogen chain with the spacing of 0.8 Å at the error rate of the two-qubit dephasing noise \( p = 0.02 \) can be simulated up to \( H_2^2 \) within a reasonable sampling cost. Furthermore, if \( p = 0.03 \), the noisy UCCSD quantum circuit for the arbitrary-length hydrogen chain can be simulated because of vanishing fermionic nonlinearity. We believe that our method and results are helpful to design quantum circuits that simulate fermionic systems for potential quantum supremacy or quantum advantages.

II. FERMIonic NONLINEARITY OF QUANTUM CIRCUITS

A. Definition of fermionic nonlinearity

Here we briefly review the efficient simulatability of FLO before explaining the quasiprobability method to simulate general fermionic interactions through FLO. We define \( \{\hat{c}_i\}_{i=1}^{2n} \) as the Majorana fermion operators that satisfy

\[
\begin{align*}
\{\hat{c}_i, \hat{c}_j\} &= 2\delta_{ij}, \\
\hat{c}_i^\dagger &= \hat{c}_i, \\
\hat{c}_i^2 &= I.
\end{align*}
\]

The fermionic covariance matrix of a (unnormalized) mixed state \( \rho \) is defined as

\[
M_{ij} = \frac{i}{2} \frac{\text{Tr}(\rho [\hat{c}_i, \hat{c}_j])}{\text{Tr}(\rho)}.
\]

We call \( \rho \) a fermionic Gaussian state (FGS) iff its covariance matrix \( M \) satisfies \( MM^T = I \). An FGS is fully specified by the covariance matrix and the norm \( \Gamma = \text{Tr}(\rho) \). An operator \( G \) is called a fermionic Gaussian operator (FGO) iff it maps an FGS to an FGS by conjugation. An arbitrary FGO can be written in the form of \( \exp\left\{ \sum_{i<j} g_{ij}\hat{c}_i\hat{c}_j \right\} \). It is known that the evolution of an FGS under an FGO can be efficiently simulated on classical computers. See Refs. [20, 24] for the details.

We now describe a quasiprobability-based simulation method of general fermionic interactions via FLO. Given a non-FGO \( \mathcal{E} \) and a set of all possible trace-preserving FGOs \( \{S_i\} \), we seek to express \( \mathcal{E} \) as,

\[
\mathcal{E} = \sum_i q_i S_i = \sum_i p_i \|q\|_1 \text{sign}(q_i) S_i,
\]

where

\[
\|q\|_1 = \sum_i |q_i|, \quad p_i := \frac{|q_i|}{\|q\|_1}.
\]

\( p_i \) is a probability distribution because \( p_i \) is non-negative and sum to unity. If this decomposition can be made, we can simulate the non-FGO by sampling a trace-preserving FGO with probability \( p_i \) and multiplying the coefficient \( \|q\|_1 \text{sign}(q_i) \) to the results afterwards. The square of the L1 norm \( \|q\|_1 \) quantifies the classical simulation cost of this Monte-Carlo type simulation.

To be more concrete, let us consider the expectation value of a two-body fermionic interaction \( c_{\mu} c_{\nu} \) with respect to \( \mathcal{E}(\rho) \) for an FGS state \( \rho \) and a non-FGO channel \( \mathcal{E} \). The desired quantity can be written as,

\[
\langle \hat{c}_\mu \hat{c}_\nu \rangle = \text{Tr}(\mathcal{E}(\rho) \hat{c}_\mu \hat{c}_\nu) = \sum_i p_i \|q\|_1 \text{sign}(q_i) \langle \hat{c}_\mu \hat{c}_\nu \rangle_{S_i},
\]

where

\[
\langle \hat{c}_\mu \hat{c}_\nu \rangle_{S_i} := \text{Tr}(S_i(\rho) \hat{c}_\mu \hat{c}_\nu).
\]

From Eq. (2), we can calculate the desired quantity \( \langle \hat{c}_\mu \hat{c}_\nu \rangle \) by sampling an index \( i \) with probability \( p_i \) and calculating \( \|q\|_1 \text{sign}(q_i) \langle \hat{c}_\mu \hat{c}_\nu \rangle_{S_i} \) efficiently, since \( \langle \hat{c}_\mu \hat{c}_\nu \rangle_{S_i} \) only involves an FGS and an FGO. Let \( N \) be the number of samples. Then, \( \|q\|_1 \text{sign}(q_i) \langle \hat{c}_\mu \hat{c}_\nu \rangle_{S_i} \) is an unbiased estimator of the desired quantity.
\[ \langle \hat{c}_\mu \hat{c}_\nu \rangle. \| q \| \text{sign}(q_i) \langle \hat{c}_\mu \hat{c}_\nu \rangle_G \] is bounded in the interval \([-\| q \|_1, \| q \|_1]\), and thus the Hoeffding inequality shows that to estimate \(\langle \hat{c}_\mu \hat{c}_\nu \rangle\) within additive error at most \(\epsilon\) with probability at least \(1 - \delta\), we must set the number of samples such that

\[ N \geq 2\| q \|^2 \frac{1}{\epsilon^2} \ln \frac{2}{\delta}. \]

Note that the expectation value of higher-order correlation function can be estimated in a similar way exploiting Wick’s theorem.

Having seen that \(\| q \|_1\) determines the sampling cost for simulations, we define the fermionic nonlinearity of a quantum channel \(\mathcal{E}\) as follows:

\[ W(\mathcal{E}) := \min_{\{q_i\}} \left\{ \| q \|_1 |\mathcal{E} = \sum_i q_i S_i \right\}. \tag{3} \]

\(W(\mathcal{E})\) quantifies the minimum number of samples to execute the Monte-Carlo type simulation of a quantum circuit with FLO. Moreover, fermionic nonlinearity is submultiplicative under composition, i.e., \(W(\mathcal{E}_2 \circ \mathcal{E}_1) \leq W(\mathcal{E}_2)W(\mathcal{E}_1)\). This property helps to estimate the upper bound of the sampling cost of an \(n\)-mode fermionic quantum channel when \(n\) is too large to calculate the fermionic nonlinearity directly. We prove the submultiplicativity in Appendix A.

### B. Concrete decomposition for four-body interactions

So far, we have assumed that there exists a decomposition of non-FGO in the form of Eq. (1). Here we consider how to explicitly calculate the decomposition and the fermionic nonlinearity of four-body fermionic interactions in the form of \(\exp(i\theta \hat{c}_i \hat{c}_j \hat{c}_k \hat{c}_l)\). This type of operators appears in the simulation of interacting fermions and in VQE ansatze such as the UCC ansatz [2], and its variant, Jastrow-type ansatz [4, 25], or Hamiltonian variational ansatz (HVA) [5, 23]. Without loss of generality, we consider the decomposition of the following operator,

\[ \mathcal{E}_{\text{rot}} = |\exp(-i\theta \hat{c}_1 \hat{c}_2 \hat{c}_3 \hat{c}_4)|, \]

where \([A]_{\rho} := A \rho A^\dagger\). This is because we can always perform transformation \(\hat{c}_i \to \hat{c}_1\), \(\hat{c}_j \to \hat{c}_2\), \(\hat{c}_k \to \hat{c}_3\), and \(\hat{c}_l \to \hat{c}_4\) by FGOs for mutually distinct indices \(i, j, k, \) and \(l\). The four-body fermionic interaction operator \(\hat{c}_1 \hat{c}_2 \hat{c}_3 \hat{c}_4\) can be mapped to a Pauli operator by the Jordan-Wigner transformation. It maps \(\hat{c}_k\) as follows.

\[ \hat{c}_{2k-1} = X_k \prod_{j<k} Z_j, \]

\[ \hat{c}_{2k} = Y_k \prod_{j<k} Z_j. \]

Hence, the fermionic interaction \(\mathcal{E}_{\text{rot}}\) can be rewritten as

\[ \mathcal{E}_{\text{rot}} = |\exp(i\theta Z \otimes Z)|. \]

Theoretically, the fermionic nonlinearity should be calculated using all possible FGOs. However, in practice, it is difficult to calculate the fermionic nonlinearity using all possible FGOs because the number of all possible FGOs is infinite. Therefore, here we calculate the upper bound of the fermionic nonlinearity using a discrete set of the FGOs. Below, we will omit the term “upper bound” if there is no risk of confusion.

We adopt the following trace-preserving fermionic Gaussian channels as the basis channels to decompose \(\mathcal{E}_{\text{rot}}\):

\[ \{ \{e^{\pm i\frac{\pi}{4}}Z\}, [I], [Z] \}^{\otimes 2} \cup \{ K_{1,\alpha}, K_{2,\alpha} |\alpha = \pm 1\} \]

\[ \cup \{ \{e^{\pm i\frac{\pi}{4}}G\} |G \in \{ XX, YY, XY, YX \} \}, \tag{4} \]

where

\[ K_{1,\alpha} := \left[ \frac{I + Z}{2} \otimes e^{i\alpha \frac{\pi}{4} Z} \right] + \left[ \frac{I - Z}{2} \otimes e^{-i\alpha \frac{\pi}{4} Z} \right], \]

\[ K_{2,\alpha} := \left[ e^{i\alpha \frac{\pi}{4} Z} \otimes \frac{I + Z}{2} \right] + \left[ e^{-i\alpha \frac{\pi}{4} Z} \otimes \frac{I - Z}{2} \right]. \]

The sets of the channels in Eq. (4), \(\{ \{e^{\pm i\frac{\pi}{4}}Z\}, [I], [Z] \}^{\otimes 2}\) and \(\{ K_{1,\alpha}, K_{2,\alpha} \}\), are adopted from Ref. [26], where the authors provided the way to simulate a two-qubit gate, such as \(\mathcal{E}_{\text{rot}}\), by sampling a single-qubit operation. Besides them, we add exp(\(\pm i\pi/4G\)) because they are the generators of FGOs and may be used for the decomposition. All of the elements in Eq. (4) are FGOs. Indeed, \(IZ, XX, XY, YX, YY, ZI\) can be rewritten as

\[ I_k Z_{k+1} = -i \hat{c}_{2k+1} \hat{c}_{2k+2}, \quad X_k X_{k+1} = -i \hat{c}_{2k} \hat{c}_{2k+1}, \]

\[ X_k Y_{k+1} = -i \hat{c}_{2k} \hat{c}_{2k+2}, \quad Y_k X_{k+1} = i \hat{c}_{2k-1} \hat{c}_{2k+1}, \]

\[ Y_k Y_{k+1} = i \hat{c}_{2k-1} \hat{c}_{2k+2}, \quad Z_k I_{k+1} = -i \hat{c}_{2k-1} \hat{c}_{2k}. \]

Thus the exponentials of these operators in Eq. (4) are FGOs. Moreover, the projective measurements in \(K_{i,\alpha}\) \((i = 1, 2)\) are FGOs [20].

We calculate the fermionic nonlinearity of \(\mathcal{E}_{\text{rot}}\) by solving the minimization problem in Eq. (3) using the basis channels in Eq. (4). To calculate fermionic nonlinearity, we use a convex-optimization solver CVXPY [27, 28].

The results are shown in Fig. 1. Also the fermionic nonlinearity using the decomposition in Ref. [26] is shown in Fig. 1 to compare with our results. According to Fig. 1, the fermionic nonlinearity is the same as when one uses the decomposition in Ref. [26]. Also, we have confirmed that the generators exp(\(\pm i\pi/4G\)) for \(G \in \{ XX, XY, YX, YY \}\) do not contribute to the decomposition by examining the coefficients of the decomposition. Moreover, we have numerically checked that the fermionic nonlinearity does not decrease even if we add the basis channels whose rotation angles are changed from \(\pi/4\) to \(\pi/8\), or \(\pi/16\) in Eq. (4). Therefore, a measurement of a qubit in \(Z\) axis, \(\pm \pi/2\) rotations around the \(Z\) axis, and Pauli \(Z\) contribute significantly to the fermionic nonlinearity.
The blue circle illustrates the fermionic nonlinearity obtained as a function of the angle \( \theta \). The vertical axis shows the fermionic nonlinearity. The horizontal axis shows the angle \( \theta \).

Our decomposition
Mitarai-Fujii decomposition

FIG. 1. Fermionic nonlinearity of \( \mathcal{E}_{\text{rot}} = [e^{i\theta_1}e^{i\theta_2}e^{i\theta_4}] \) as a function of the angle \( \theta \). The horizontal axis shows the angle \( \theta \). The vertical axis shows the fermionic nonlinearity. The blue circle illustrates the fermionic nonlinearity obtained by the basis channels in Eq. (4). The orange triangle shows the fermionic nonlinearity obtained by the decomposition in Ref. [26].

FIG. 2. Fermionic nonlinearity of \( \mathcal{E}_{\text{noisy rot}} := \mathcal{N}_{\text{dep}} \circ \mathcal{E}_{\text{rot}} \) as a function of the angle \( \theta \) of \( \mathcal{E}_{\text{rot}} \) and the error rate \( p \) of the two-qubit dephasing noise \( \mathcal{N}_{\text{dep}} \). The horizontal axis shows the angle \( \theta \) of \( \mathcal{E}_{\text{rot}} \). The vertical axis shows the fermionic nonlinearity. The basis channels decomposing \( \mathcal{E}_{\text{noisy rot}} \) are shown in Eq. (4). The legend shows the error rate \( p \) of \( \mathcal{N}_{\text{dep}} \).

C. Fermionic nonlinearity of noisy channels and application to the VQE simulation

Next, we consider the fermionic nonlinearity of \( \mathcal{E}_{\text{rot}} \) being subject to noise:

\[
\mathcal{E}_{\text{noisy rot}} := \mathcal{N}_{\text{dep}} \circ \mathcal{E}_{\text{rot}},
\]

where \( \mathcal{N}_{\text{dep}} \) is the two-qubit dephasing noise

\[
\mathcal{N}_{\text{dep}} := (1 - p) [I \otimes Z] + \frac{p}{3} [I Z] + [Z I] + [Z Z])
\]

\( p \) is the error rate of the dephasing noise. Figure 2 shows the fermionic nonlinearity of \( \mathcal{E}_{\text{noisy rot}} \) as a function of the angle of \( \mathcal{E}_{\text{rot}} \) and the error rate of \( \mathcal{N}_{\text{dep}} \). We see that the fermionic nonlinearity decreases as the error rate of \( \mathcal{N}_{\text{dep}} \) increases. In addition, the smaller the rotation angle, the more easily the noise makes the fermionic nonlinearity unity, that is, such a noisy fermionic interaction becomes a probabilistic mixture of FGOs. One implication of these results is as follows. For VQEs of fermionic problems, if the Hartree-Fock approach is a good first-order approximation and hence fermionic nonlinearity of the ansatz stays small even after the optimization, such a quantum circuit is fragile against noise in the sense that it readily becomes simulatable by the proposed sampling method.

To analyze more practical cases, we estimate the sampling cost of VQE that aims to obtain the ground state of the electronic Hamiltonian of the hydrogen chain \( H_m \). Such a Hamiltonian is often used to benchmark the performance of classical quantum chemistry simulations [29–37] and VQE [38] numerically. This is because it exhibits rich phenomena, including metal-insulator transitions, and one can benchmark methods in both strong and weak correlation regimes. In particular, the Hamiltonian of the hydrogen chain with the use of the STO-3G basis set has a connection with the Hubbard model; the large spacing of the hydrogen chain corresponds to the Hubbard model in the large coupling limit, and vice versa. As for VQE, the authors of Ref. [39] have demonstrated that their quantum computer can prepare the Hartree-Fock state of \( H_{12} \) using VQE, although their variational ansatz circuit is classically efficiently simulatable by FLO because the quantum circuit consists of two-body fermionic interactions. In the following numerical simulation, the Hamiltonians are generated by OpenFermion [40] and PySCF [41, 42] with the use of the STO-3G basis set, and then the Jordan-Wigner transformation maps them to qubit Hamiltonians, resulting in 2\( m \)-qubit Hamiltonian for an \( m \)-hydrogen chain \( H_m \). We take the Hartree-Fock (HF) state \( |\text{HF}\rangle \) as the reference state for the VQE.

We consider the UCC ansatz [43–48], which is a chemically inspired ansatz and often used in VQEs [2, 22]. In particular, we consider the UCCSD ansatz that only includes single and double excitations. The UCCSD ansatz is defined as

\[
U = e^{(T_1 - T_1^\dagger)} + (T_2 - T_2^\dagger),
\]

\[
T_1 := \sum_{a \in \text{virt}, i \in \text{occ}} t_{ai} \hat{a}_a \hat{a}_i^\dagger,
\]

\[
T_2 := \sum_{a,b \in \text{virt}, i,j \in \text{occ}} t_{abij} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_i \hat{a}_j,
\]

where \( \text{occ} \) and \( \text{virt} \) represent the sets of occupied and virtual orbitals, respectively, and \( t_{ai} \) and \( t_{abij} \) are vari-
tional parameters. Usually, the UCCSD is implemented as a quantum circuit by Trotter expansion of $U$:

$$
\hat{U} = \prod_{a \in \text{vir}, j \in \text{occ}} \exp \left( \frac{t_{a ij}}{N_{\text{trot}}} (\hat{a}_a^\dagger \hat{a}_i - \hat{a}_i^\dagger \hat{a}_a) \right) \prod_{a, b \in \text{vir}, i, j \in \text{occ}} \exp \left( \frac{t_{a b i j}}{N_{\text{trot}}} (\hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i - \hat{a}_j^\dagger \hat{a}_i^\dagger \hat{a}_b \hat{a}_a) \right)^{N_{\text{trot}}}
$$

In the following, we consider the UCCSD ansatz with $N_{\text{trot}} = 1$. Note that the fermion operator $\hat{a}_i$ is associated with the Majorana fermion operators $\hat{c}_{2i-1}, \hat{c}_{2i}$ as follows:

$$
\hat{c}_{2i-1} = \hat{a}_i + \hat{a}_i^\dagger, \\
\hat{c}_{2i} = -i (\hat{a}_i - \hat{a}_i^\dagger).
$$

Using this relation, a four-body interaction constituting $\hat{U}$ can be rewritten by the Majorana fermion operators as follows:

$$
e^{t_{a b i j}} (\hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_i \hat{a}_j - \hat{a}_j^\dagger \hat{a}_i^\dagger \hat{a}_b \hat{a}_a) \\
= e^{-\frac{t_{a b i j}}{8} \hat{c}_{2a-1} \hat{c}_{2b} \hat{c}_{2i-1} \hat{c}_{2j}} e^{-\frac{t_{a b i j}}{8} \hat{c}_{2a} \hat{c}_{2b-1} \hat{c}_{2i} \hat{c}_{2j-1}} e^{-\frac{t_{a b i j}}{8} \hat{c}_{2a} \hat{c}_{2b-1} \hat{c}_{2i-1} \hat{c}_{2j}} \\
= e^{-\frac{t_{a b i j}}{8} \hat{c}_{2a} \hat{c}_{2b-1} \hat{c}_{2i} \hat{c}_{2j-1}} e^{-\frac{t_{a b i j}}{8} \hat{c}_{2a} \hat{c}_{2b-1} \hat{c}_{2i-1} \hat{c}_{2j}} e^{\frac{t_{a b i j}}{8} \hat{c}_{2a} \hat{c}_{2b} \hat{c}_{2i} \hat{c}_{2j}}.
$$

We consider the sampling cost for simulating UCCSD circuits when each of the Majorana rotation gates in Eq. (5) are subjected to dephasing noise.

The sampling cost of a UCCSD quantum circuit can be given by the upper bound of the fermionic nonlinearity, which can be calculated by the product of the fermionic nonlinearity of the four-body fermionic interactions. Note that, as mentioned before, the HF states used as the reference states are FGSs; therefore, there are no sampling costs due to the input states. We use the optimized variational parameters of error-free UCCSD quantum circuits, calculated by the full-vector simulations performed with Qulacs [49].

Figure 3 shows the upper bound of fermionic nonlinearity of the UCCSD quantum circuit as a function of the length $m$ of the hydrogen chains $H_m$ and the error rate of the dephasing noise at different spacings of the hydrogen atoms. In the case of 0.5 Å and 0.8 Å, the Hamiltonian for the hydrogen chain embodies a weakly correlated electronic system. In contrast, the Hamiltonian in the case of 1.5 Å provides a strongly correlated electronic system. From Fig. 3, we find that the fermionic nonlinearity is smaller when the spacing of the hydrogen chain is smaller. This reflects that an HF state is a good approximation of the ground state when the spacing is small.

Finally, we discuss the size of the hydrogen chain that can be simulated within one day using $10^6$ CPU cores.

Suppose that we want to estimate the expectation value of the Hamiltonian $H$ for the hydrogen chain within an additive error $\epsilon = \|H\|_{\text{op}} \times 10^{-3}$, with a success probability of at least $1 - \delta = 1 - 10^{-2}$, where $\|A\|_{\text{op}}$ is the operator norm of $A$. Assuming that each core takes at most 1 ms to calculate one sample of a quasi-probability distribution, a UCCSD quantum circuit whose fermionic nonlinearity is upper-bounded by $3 \times 10^3$ could be simulated within one day. We estimate the fermionic nonlinearity for $m > 8$ using the geometrical mean of fermionic nonlinearity of $W(E_{\text{noisy rot}})$ in the noisy UCCSD quantum circuit at $m = 8$, $W(E_{\text{noisy rot}})_{m=8}$. Let $N_4$ be the number of four-body Majorana operators in $\hat{T}_2 - \hat{T}_2^\dagger$. We estimate the upper bound of fermionic nonlinearity of $H_m (m > 8)$ by

$$
W(E_{\text{noisy rot}})_{m=8}^{N_4}.
$$

At $p = 0.02$ and the spacing of 0.8 Å, $W(E_{\text{noisy rot}})_{m=8}$ is 1.00012. Therefore, we estimate the UCCSD circuits for hydrogen chains under such conditions can be simulated up to $m = 22$ if this mean stays at the same level at
larger $m$. Furthermore, we find $W(\mathcal{E}_{\text{noisy rot}})_{m=8} = 1$ if $p \geq 0.03$ and the spacing is less than $0.8 \text{Å}$, or if $p \geq 0.07$ and the spacing is $1.5 \text{Å}$. We hence expect that the UCCSD circuits under such conditions can be simulated for arbitrary $m$.

Note that the energy expectation value obtained from simulations of noisy UCCSD circuits is slightly biased from the true value (HF$|U^1HU|\text{HF}$). If we allow such a bias, we can take an alternative approach; we can utilize the classical coupled cluster (CC) theory to simulate UCC circuits. It is known that the CC theory can simulate up to large UCC systems with a small perturbative error when $t_{abij}$ (and $t_{ai}$) are small (i.e., small rotation angles $\theta$). The conventional CC can be solved in polynomial time using a non-variational projection method, assuming the Hartree-Fock state to be a good reference wave function. If this assumption holds, the accuracy of the non-variational CC is almost as good as that of variational UCC [50, 51]. An established way to diagnose the correctness of the premise is by examining the magnitude of the parameters of the CC wave function [52–57]. According to the rule of thumb in the classical CC, the maximum $t_{abij}$ is about 0.1 or less in the region where non-variational CC works well [57]. Besides, in systems where classical CC fails, the maximum $t_{abij}$ tends to be larger than 0.15 [57]. Our UCC calculations show that for $m = 8$, the maximum $t_{abij}$ is about 0.08 when the distance between the hydrogens is 0.8 Å and about 0.18 when the distance is 1.5 Å. Therefore, our results are in line with the empirical trend in classical computing.

Our results indicate that, to demonstrate the quantum supremacy or quantum advantages with the UCCSD ansatz, one has to choose target Hamiltonians that exhibit strong electronic correlations and execute the quantum circuits with sufficiently low error rates. Note that even if the gate error of a device is 1%, the effective physical error rate of the two-qubit dephasing noise in $\mathcal{E}_{\text{noisy rot}}$ would be much higher because, in general, the noise on the entangling gates to simulate non-local fermionic two-body or four-body rotations by physically allowed operations accumulates.

We note that we have discussed the classical simulatability of noisy UCCSD ansatz using the optimized variational parameters obtained by the error-free simulations and found that, under certain circumstances, they become classically simulatable. In such cases, even if sophisticated error mitigation and optimization strategies allowed us to perform the VQE successfully, we cannot achieve a quantum advantage because the resulting circuit can be simulated classically.

### III. CONCLUSION

In this work, we propose a quasiprobability-based simulation algorithm using FLO and quantify its simulation cost by establishing the corresponding measure, fermionic nonlinearity $W(\mathcal{E})$. The sampling cost of the quasiprobability-based simulator is proportional to $W(\mathcal{E})^T$. As an example, we calculate the upper bound of fermionic nonlinearity of the noisy rotation gate generated by a four-body Majorana fermionic operator, which often appears in the parametrized quantum circuits in VQE. We find that the fermionic nonlinearity increases as the rotation angle becomes larger and decreases as the error rate of the dephasing noise increases. Based on the above observation, we discuss the simulatability of the quantum circuits for quantum chemistry with our proposed method. We estimate the sampling costs of the noisy UCCSD quantum circuits for the hydrogen chain, and discuss whether they can be simulated within one day when $10^6$ CPU cores are available. We find that the UCCSD circuits with the dephasing error rate $p = 0.02$ for hydrogen chains with the spacing of 0.8 Å can be simulated up to $H_{22}$. Furthermore, if $p \geq 0.03$, the noisy UCCSD circuits for hydrogen chain of arbitrary length with the same spacing can be simulated. Although this numerical result is pessimistic, it stimulates to investigate or design another VQE ansatz that retains quantumness against noise with the use of our results and method.

Our work leaves several open questions. Although we use the basis channels based on Ref. [26] to decompose the four-body Majorana fermionic interaction, there may exist more optimal basis channels. It is an interesting and nontrivial problem to choose the optimal discrete set of FGOs to decompose a given non-FGO. We formulate the classical simulatability of a quantum circuit for fermionic Hamiltonians in the channel picture, but it is also of great interest to establish such a formulation in the state picture, which should be compatible with the results shown in Ref. [58].

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### Appendix A: Submultiplicativity of Fermionic Nonlinearity

Let us prove the submultiplicativity of fermionic nonlinearity: $W(\mathcal{E}_1 \circ \mathcal{E}_2) \leq W(\mathcal{E}_1)W(\mathcal{E}_2)$. Let $\mathcal{E}_1$ and $\mathcal{E}_2$ have decompositions over all possible trace-preserving FGOs.
\{S_i\}

We consider the composition of both channels

\[\mathcal{E}_1 \circ \mathcal{E}_2 = \sum_{i,j} x_i y_j S_i \circ S_j.\]

Since the composition of FGOs is also an FGO, this gives a decomposition of \(\mathcal{E}_1 \circ \mathcal{E}_2\) over FGOs. Taking the absolute sum, we have

\[\sum_{i,j} |x_i y_j| \leq \left(\sum_i |x_i|\right) \left(\sum_j |y_j|\right) = W(\mathcal{E}_1) W(\mathcal{E}_2).\]

Therefore, \(W(\mathcal{E}_1 \circ \mathcal{E}_2) \leq W(\mathcal{E}_1) W(\mathcal{E}_2)\).

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