Fidelity overhead for non-local measurements in variational quantum algorithms

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(Dated: May 17, 2022)

Measuring quantum observables by grouping terms that can be rotated to sums of only products of Pauli $\hat{z}$ operators (Ising form) is proven to be efficient in near term quantum computing algorithms. This approach requires extra unitary transformations to rotate the state of interest so that the measurement of a fragment’s Ising form would be equivalent to measurement of the fragment for the unrotated state. These extra rotations allow one to perform a fewer number of measurements by grouping more terms into the measurable fragments with a lower overall estimator variance. However, previous estimations of the number of measurements did not take into account non-unit fidelity of quantum gates implementing the additional transformations. Through a circuit fidelity reduction, additional transformations introduce extra uncertainty and increase the needed number of measurements. Here we consider a simple model for errors introduced by additional gates needed in schemes involving grouping of commuting Pauli products. For a set of molecular electronic Hamiltonians, we confirm that the numbers of measurements in schemes using non-local qubit rotations are still lower than those in their local qubit rotation counterparts, even after accounting for uncertainties introduced by additional gates.

I. INTRODUCTION

Measuring quantum observables is one of the bottlenecks of quantum variational algorithms.1 Here we consider quantum observables represented as a linear combination of Pauli products

$$\hat{O} = \sum_k c_k \hat{P}_k,$$

where $c_k$ are coefficients and $\hat{P}_k$ are tensor products of single-qubit Pauli operators. To measure an expectation value of $\hat{O}$ one needs to transform $\hat{O}$ into the Ising form $U^\dagger \hat{O} U = \hat{Z}$, where $\hat{Z}$ is a linear combination of Pauli products that contain only $\hat{z}$ operators for individual qubits. Finding such $\hat{U}$ for an arbitrary observable is challenging since it is equivalent to diagonalizing $\hat{O}$ in the computational basis. Fortunately, the expectation value of $\hat{O}$ can be obtained by summing the expectation values of simpler operators that can be easily transformed to their Ising forms ($\hat{Z}_n$):

$$\langle \Psi | \hat{O} | \Psi \rangle = \sum_n \langle \Psi | \hat{O}_n | \Psi \rangle = \sum_n \langle \Psi | \hat{U}^\dagger \hat{Z}_n \hat{U}^\dagger \hat{Z}_n | \Psi \rangle.$$ (2)

This is a partitioning approach to the measurement problem that was successfully applied in the variational quantum eigensolver (VQE).2 where $\hat{O}$ corresponds to the system Hamiltonian, $\hat{H}$. Even for a fixed observable there are usually numerous possible partitionings $\hat{O} = \sum_n \hat{O}_n$, where each partitioning involves its own set of unitary transformations $\hat{U}_n$. For all partitionings $\hat{U}_n$ should be straightforward to apply both on classical and quantum computers because one needs to know in advance $\hat{Z}_n$ operators for classical post-processing and be able to apply $\hat{U}_n$ to the quantum state $|\Psi\rangle$ before the measurement. The main quantity of interest that ranks partitionings in their efficiency is the total number of measurements required for achieving accuracy $\epsilon$ in estimating $\langle \Psi | \hat{O} | \Psi \rangle$, $N_m$. This number under the condition of optimal distribution of measurements between fragments $\hat{O}_n$ is

$$N_m = \left( \frac{1}{\epsilon} \sum_n \sqrt{\text{Var}_\Psi(\hat{O}_n)} \right)^2,$$ (3)

where $\text{Var}_\Psi(\hat{O}_n) = \langle \Psi | \hat{O}_n^2 | \Psi \rangle - \langle \Psi | \hat{O}_n | \Psi \rangle^2$ is the quantum variance for each operator fragment.3

Since one of the possible areas for demonstrating the quantum advantage is the electronic structure problem, for concreteness, here we focus on obtaining the expectation value of electronic Hamiltonians. There are multiple ways one can partition the Hamiltonian into diagonalizable fragments. For electronic Hamiltonians, there have been suggested two main approaches to partitioning using diagonalizable fragments in fermionic and qubit operator algebras. Recent comparisons of state-of-the-art techniques in the two categories shown that one can achieve a lower number of the measurements using techniques within the qubit operator algebra.4–6 These qubit techniques are based on partitioning of the Hamiltonian to sets of commuting Pauli operators.6–10

Due to differences in accuracy of performing one- and two-qubit transformations in quantum computers, it is convenient to distinguish two types of commutativity, general or full commutativity (FC) and a more restrictive qubit-wise commutativity (QWC). Two Pauli products qubit-wise commute only if every pair of corresponding single-qubit operators commute in them (e.g. $\hat{x}_1 \hat{y}_2 \hat{z}_3$ qubit-wise commutes with $\hat{x}_1 \hat{z}_3$ and does not qubit-wise
commute with \( \hat{y}_1\hat{z}_2\hat{z}_3 \). Measuring a linear combination of Pauli products that qubit-wise commute require only local (one-qubit) Clifford transformations (\( \hat{U}_n \)), while for the same task on commuting Pauli products one generally needs non-local (entangling) Clifford transformations. The main advantage of grouping schemes based on FC over QWC schemes is lower numbers of measurements required for estimating the Hamiltonian expectation values (Eq. (3)). However, estimates based on Eq. (3) do not account for additional uncertainties related to non-unit fidelities of gates that are required to introduce extra transformations needed for measurement, \( \hat{U}_n \). In this work, we investigate the extent to which these additional uncertainties reduce the advantage of the FC-based schemes over the QWC-based schemes in the number of measurements.

Classical shadow tomography (CST)\(^{11}\) has been proposed recently as an alternative to grouping of operator terms in measurable fragments for estimating the operator expectation value. CST techniques are based on learning about the expectation value of the operator by rotating the system with a random unitary transformation from a certain distribution and measuring the system in the computational basis. The obtained set of measurement results are projections (classical shadows) of the true system state. Expectation values of the operator for classical shadows can be calculated on a classical computer and averaged to reproduce the expectation value of the true system state. The Clifford group and its single-qubit subgroup distributions of unitaries have been used to draw random unitaries.\(^{11-15}\) Using the electronic structure Hamiltonians as examples of quantum observables, it was shown that for a single observable, CST schemes are generally inferior than grouping techniques in lowering the number of measurements required to estimate the expectation value.\(^{5,6}\) Therefore, here we consider the grouping methods to measurements but our analysis involving Clifford transformations can be extended to the CST schemes as well.

II. METHOD

A. Error Model

In both FC and QWC partitionings the electronic Hamiltonian in the qubit representation is partitioned to fragment Hamiltonians, \( \hat{H} = \sum_{j=1}^{N_q} \hat{H}_j \),

\[
\hat{H}_j = \sum_{j=1}^{M_q} a_j \hat{P}_j, 
\]

(4)

where \( \hat{P}_j \) are Pauli products, and \( \hat{P}_j \) within each \( \hat{H}_j \) commute or qubit-wise commute with each other. For all \( \hat{H}_j \), there are unitary transformations from the Clifford group \( \hat{U}_n \) so that \( \hat{H}_j = \hat{U}_n \hat{H}_j \hat{U}_n^\dagger \).

The VQE workflow can be separated in two parts: 1) preparing the state \( |\Psi\rangle = \hat{U} |0\rangle \) and 2) transforming \( |\Psi\rangle \) to the state that will be measured: \( |\Phi_n\rangle = \hat{U}_n |\Psi\rangle \). The total fidelity of the \( |\Phi_n\rangle \) state preparation \( F_n = pq_n \) is a product of fidelities for the preparation \( |\Psi\rangle \), \( p \), and of that for the additional measurement preparatory circuit \( \hat{U}_n, q_n \). FC and QWC schemes will be different in values of \( q_n \) and share the \( p \)-part. Since the total fidelity is multiplicative we assume that the common \( p \)-part also incorporates any noise contributions appearing due to projective measurements of all qubits. For the \( q_n \)-part, fidelities of one- and two-qubit gates are denoted as \( f_1, f_2 \), respectively. Thus, if \( G_{i,n} \) are the numbers of \( i \)-qubit gates for the \( \hat{U}_n \) circuit then \( q_n = f_1^{G_{1,n}} f_2^{G_{2,n}} \).

Due to non-unit gate fidelities in the state preparation we assume that instead of \( |\Phi_n\rangle \) one can only prepare the mixed state

\[
\rho_n = F_n |\Phi_n\rangle \langle \Phi_n| + \frac{(1 - F_n)}{d} I, 
\]

(5)

where \( d = 2^{N_q} \) is the dimension of the \( N_q \)-qubit space, and \( I \) is the identity operator in the \( d \)-dimensional space. In Eq. (5), it is assumed that there is no systematic bias and extra gates only contribute to probability of the depolarized component.

B. Estimator characteristics

Here we construct an estimator for \( \langle \Psi| \hat{H}_n |\Psi\rangle \) assuming that we only have access to measurement results for the density \( \rho_n \) (Eq. (5)) on the transformed fragment Hamiltonian, \( \hat{H}_n = \hat{U}_n^\dagger \hat{Z}_n \hat{U}_n \)

\[
\text{Tr}[\hat{Z}_n \rho_n] = F_n \langle \Phi_n| \hat{Z}_n |\Phi_n\rangle + F_n (1 - F_n) \text{Tr}[\hat{Z}_n]/d 
\]

\[
= F_n \langle \Phi_n| \hat{Z}_n |\Phi_n\rangle = F_n \langle \Psi| \hat{H}_n |\Psi\rangle, 
\]

(6)

where the second equality follows from the tracelessness of \( \hat{Z}_n \). Therefore, an estimator for \( \langle \Psi| \hat{H}_n |\Psi\rangle \), \( \hat{H}_n \), can be formulated as

\[
\hat{H}_n = \frac{\text{Tr}[\hat{Z}_n \rho_n]}{F_n}. 
\]

(8)

Its statistical variance can be obtained from the quantum variance of \( \text{Tr}[\hat{Z}_n \rho_n] \)

\[
\text{Var}(\hat{H}_n) = \frac{\text{Tr}[\hat{Z}_n^2 \rho_n]}{F_n^2} - \frac{\text{Tr}[\hat{Z}_n \rho_n]^2}{F_n^2}. 
\]

(9)

Next, we would like to connect the statistical variance of our estimator with the quantum variance of the fragment

\[
\text{Var}_q(\hat{H}_n) = \langle \Psi| \hat{H}_n^2 |\Psi\rangle - \langle \Psi| \hat{H}_n |\Psi\rangle^2. 
\]

This connection will elucidate a functional dependence of the estimator variance on fidelity contributions and the operator prop.
erties. Using $\rho_n$ form in Eq. (5) gives

$$\text{Var}(\bar{H}_n) = \frac{\langle \Psi | \hat{H}_n^2 | \Psi \rangle}{F_n} + \frac{1 - F_n}{dF_n^2} \text{Var}[\hat{Z}_n^2]$$

$$- \langle \Psi | \hat{H}_n | \Psi \rangle^2$$

$$= \text{Var}_p(\bar{H}_n) + \frac{1 - F_n}{F_n} \langle \Psi | \hat{H}_n^2 | \Psi \rangle$$

$$+ \frac{1 - F_n}{dF_n^2} \text{Var}[\hat{Z}_n^2].$$

(11)

Both terms additional to $\text{Var}_p(\bar{H}_n)$ in Eq. (11) are positive. $\text{Var}[\hat{Z}_n^2]/d$ can be further simplified as $\text{Tr}[\hat{Z}_n^2]/d = \sum_{j=1}^{M_n} a_j^2$ since any product of two different Pauli products is traceless. This gives the final expression for the estimator variance as

$$\text{Var}(\bar{H}_n) = \text{Var}_p(\bar{H}_n) + \frac{1 - F_n}{F_n} \langle \Psi | \hat{H}_n^2 | \Psi \rangle$$

$$+ \frac{1 - F_n}{F_n^2} \sum_{j=1}^{M_n} a_j^2.$$  

(12)

This expression allows us to formulate the minimal number of measurements for achieving $\epsilon$ accuracy with 66.7% probability as

$$N_m = \left( \frac{1}{\epsilon} \sum_n \sqrt{\text{Var}(\bar{H}_n)} \right)^2.$$  

(13)

Due to the relation $\text{Var}(\bar{H}_n) > \text{Var}_p(\bar{H}_n)$ for $p \neq 1$ or $q_n \neq 1$, $N_m$ will always be larger than its counterpart evaluated ignoring non-unit fidelity of gates.

To understand why lower fidelities can be more detrimental for the QWC partitioning than for the FC one, it is instructive to rewrite $\text{Var}(\bar{H}_n)$ as

$$\text{Var}(\bar{H}_n) = \text{Var}_p(\bar{H}_n) + \frac{1 - F_n}{F_n} \sum_{i \neq j} a_i a_j \langle \Psi | \hat{P}_i \hat{P}_j | \Psi \rangle$$

$$+ (1 - F_n)(F_n^{-1} + F_n^{-2}) \sum_{j=1}^{M_n} a_j^2,$$  

(14)

where we partitioned the $\langle \Psi | \hat{H}_n^2 | \Psi \rangle$ term into the diagonal ($i = j$) and off-diagonal ($i \neq j$) parts. For lower fidelities the last term in Eq. (14) will dominate because of the $F_n^{-2}$ scaling. In the case where $F_n$ is dominated by the uniform reduction factor $p$, the estimator variance for each fragment can be approximated as

$$\text{Var}(\bar{H}_n) \approx \frac{(1 - p)}{p^2} \sum_{j=1}^{M_n} a_j^2.$$  

(15)

and the total number of measurements as

$$N_m \approx N_m^{(p)} = \frac{(1 - p)}{\epsilon^2 p^2} \left( \sum_n \sum_{j=1}^{M_n} a_j^2 \right)^2.$$  

(16)

Clifford group transformations do not change coefficients $a_j$, hence the total sum over all $a_j^2$ in all groups is a constant dependent on the system Hamiltonian rather than the partitioning approach. Clearly, this constant is partitioned to smaller parts in the QWC grouping than in the FC one. It is a general property of a square root function that $\sqrt{a + b} \leq \sqrt{a} + \sqrt{b}$ for real positive $a$ and $b$. Thus, if the total sum of $a_j^2$ is split into a larger number of smaller groups in QWC, and QWC $N_m^{(p)}$ will be larger than that for the FC scheme. This also follows from the fact that any QWC group is also FC group but not the other way around.

### III. RESULTS

We assess the difference in the number of measurements required in the FC and QWC schemes on a set of molecular electronic Hamiltonians. Details on the Hamiltonians are presented in Appendix A. Among various heuristics for grouping commuting Pauli products, we used the Sorted Insertion (SI) method because it generally outperforms other grouping techniques in the number of measurements. Since measurement circuits for $\hat{U}_i$ of the FC and QWC groups can be constructed using only Clifford group transformations, according to the Gottesman-Knill theorem these circuits can be implemented efficiently on both classical and quantum computers. For the FC grouping an asymptotically optimal scaling of $O(N_q^2/\log(N_q))$ in the number of 2-qubit entangling gates and single qubit rotations can be achieved. We have implemented this optimal circuit synthesis and optimization method in the Tequila program. The total number of CNOT, Hadamard and Phase gates for model systems averaged over measurable FC groups indeed follows the $O(N_q^2/\log(N_q))$ dependence according to Fig. 1.

Considering variety in fidelities of quantum gates available in different near term quantum computing architectures, we calculated $q_n$-parts of the total fidelity using two sets of 1- and 2-qubit gate fidelities. One set is based on the numbers from a recent work describing the Google superconducting quantum hardware, with $f_1 = 0.9938$ and $f_2 = 0.9984$. This set represents what is available on a contemporary superconducting qubit device. The second set is based on a projection that in the near future we will have quantum gates with $f_1 = 0.9999$ and $f_2 = 0.999$. The $p$-component of the total fidelity depends not only on gate fidelities but also on the state complexity, here, we would like to see the trend by evaluating the number of measurement estimates for $p = 1$, $p = 0.8$, and $p = 0.6$.

Table I provides the ratios of the measurement numbers required in the FC and QWC schemes. Ideal FC (FC-I) has always lower $N_m$ than that of QWC (QWC-I) except for $H_2$. The ratio between the numbers of measurements grows with the system size and reaches more than 20 for the largest system ($N_2$). When we introduce uncertainty related to non-unit fidelity of gates, the ra-
FIG. 1. An average number of gates ($N_g$) for measurement circuits of the FC scheme as a function of $N_q^2 / \log_{10}(N_q)$, where $N_q$ is the number of qubits. The averaging is done over measurable groups of the FC scheme for molecular systems described in Appendix A. The linear function $N_g = 0.72 N_q^2 / \log_{10}(N_q) + 21$ (red) has $R^2 = 0.997$.

tios decrease but in most cases indicate superiority of the FC scheme. This reduction in ratios is the consequence of generally lower fidelities ($F_n$) in FC groups compared to those of QWC groups because of a larger number of gates needed for measurements in the former. For small systems, H$_2$ and LiH, non-unit fidelity of gates lead to lower numbers of measurements for the QWC scheme (ratios $< 1$). Interestingly, accounting for the reduction of the circuit fidelity due to the $|\Psi\rangle$ state preparation ($p = 0.8$ and $p = 0.6$) increases the ratios for the small systems and even reverses the trend for H$_2$ and for LiH with the second set of gate fidelities. This detrimental effect of $p$ reduction on QWC $N_m$’s is attributed to the contribution of Eq. (16) that favours a smaller number of groups. The effect from Eq. (16) generally competes with other terms in Eq. (14) and is clearly seen in cases of H$_2$, LiH, and NH$_3$ (gate fidelities of a contemporary device). For the other systems, $p$ reduction leads to reduction of the ratios.

IV. CONCLUSIONS

Using a simple unbiased depolarization error model we have derived an estimation for the number of measurements needed in the VQE measurement schemes involving local and non-local qubit transformations. Considering realistic fidelities for current and near future superconducting quantum processors and using the implementation of the non-local unitary transformations minimizing the number of CNOT gates, it was found that the non-local scheme based on grouping commuting Pauli products generally requires fewer measurements than the corresponding local scheme based on grouping of qubit-wise commuting Pauli products. Due to a larger number of additional gates the advantage of the non-local scheme decreases with reduction in gate fidelities. Another trend is that the advantage from the FC scheme is diminished even further if one accounts for the fidelity reduction due to the state preparation circuit. However, lowering of the state preparation fidelity can also exhibit an interesting opposite trend that favors the FC scheme because it has a smaller number of groups. Overall, we found that for all systems larger than LiH (in the STO-3G basis) the number of measurements needed in the FC scheme is lower than that in the QWC scheme even with accounting for all uncertainties introduced by non-unit gate fidelities.

ACKNOWLEDGEMENTS

A.F.I. acknowledges financial support from the Google Quantum Research Program, Early Researcher Award, and Zapata Computing Inc. This research was enabled in part by support provided by Compute Ontario and Compute Canada.
TABLE I. Ratios of the number of measurements $N_m$ to achieve $\epsilon = 1 \times 10^{-3}$ Hartree accuracy in the energy expectation value (with 66.7% probability) assuming the optimal distribution of measurements for individual fragments. Two partitioning methods are considered: FC and QWC. Three gate fidelity sets are used: ideal, unit fidelities (−I); fidelities available on a contemporary device, set 1 (−C); and near future fidelities, set 2 (−F).

| Systems  | $N$ | $H_2$ | LiH | BeH$_2$ | H$_2$O | NH$_3$ | N$_2$ |
|----------|-----|-------|-----|---------|-------|--------|------|
| $N_m(QWC-C)/N_m(FC-C)$ | 0.965 | 0.602 | 1.91 | 1.15 | 1.20 | 1.67 |
| $N_m(QWC-F)/N_m(FC-F)$ | 0.993 | 0.990 | 4.54 | 2.72 | 4.17 | 14.1 |
| $N_m(QWC-I)/N_m(FC-I)$ | 1.00 | 1.08 | 5.51 | 3.24 | 5.30 | 23.2 |
| $N_m(QWC-C)/N_m(FC-C)$ | 1.04 | 0.912 | 1.37 | 1.14 | 1.18 | 1.24 |
| $N_m(QWC-F)/N_m(FC-F)$ | 1.06 | 1.11 | 1.68 | 1.36 | 1.75 | 2.12 |
| $N_m(QWC-C)/N_m(FC-C)$ | 1.09 | 0.979 | 1.29 | 1.15 | 1.20 | 1.20 |
| $N_m(QWC-F)/N_m(FC-F)$ | 1.10 | 1.16 | 1.55 | 1.33 | 1.65 | 1.85 |

Appendix A: Details of Hamiltonians

Qubit Hamiltonians were generated using the STO-3G basis and the Bravyi-Kitaev (BK) transformation. The nuclear geometries for the Hamiltonians are $R(H - H) = 1\text{Å}$ ($H_2$), $R(Li - H) = 1\text{Å}$ (LiH), $R(Be - H) = 1\text{Å}$ with collinear atomic arrangement (BeH$_2$), $R(O - H) = 1\text{Å}$ with $\angle HOH = 107.6^\circ$ ($H_2O$), $R(N - H) = 1\text{Å}$ with $\angle HNH = 107^\circ$ (NH$_3$), and $R(N - N) = 1\text{Å}$ (N$_2$). To collect more data points for circuit gate complexity in Table I, additional qubit Hamiltonians were generated using the 6-31G basis and the BK transformation for BeH$_2$, H$_2$O, NH$_3$, and N$_2$ with the same nuclear geometries as in the STO-3G case.

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