Efficient evaluation of Pauli strings with entangled measurements

Ikkō Hamamura$^{1[a]}$ and Takashi Imamichi$^{2[b]}$

$^1$Kyoto University  
Department of Nuclear Engineering, Kyoto University, 6158540 Kyoto, Japan  
$^2$IBM Research – Tokyo  
19-21, Nihonbashi Hakozaki-cho, Chuō-ku, 103-8510 Tokyo, Japan.

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The advent of cloud quantum computing accelerates development of quantum algorithms. In particular, it is essential to study variational quantum-classical hybrid algorithms, which are executable on Noisy Intermediate-Scale Quantum (NISQ) computers. Evaluations of observables appear frequently in the variational quantum-classical hybrid algorithms for NISQ computers. By speeding up the evaluation of observables, we can realize a faster algorithm and save resources of quantum computers. The grouping of observables with separable measurements has been conventionally used, and the grouping with entangled measurements has also been proposed recently by several teams. In this paper, we demonstrate that entangled measurements enhance the efficiency of evaluation of observables both theoretically and experimentally by taking into account the covariance effect, which may affect the quality of evaluations of observables. We also propose using a part of entangled measurements for grouping in order to keep the depth of extra gates constant. Our proposed method is expected to be used in conjunction with other related studies. We hope that entangled measurements become crucial resources not only for joint measurements but also quantum information processing.

Keywords: Variational quantum eigensolver, entangled measurement, NISQ

I. INTRODUCTION

Researchers have been working to build a fault-tolerant quantum computer and quantum algorithms for years. Recently, the development of quantum computing has gained significant momentum. The main reason is the rise of the Noisy Intermediate-Scale Quantum (NISQ) computers$^{[1]}$ which have 50–100 qubits and quantum error corrections are not implemented yet. They have been developed with superconducting$^{[2]}$ and trapped ion$^{[3,4]}$ systems. Although the number of qubits is small and the fidelity of operations is not very high, programmable quantum computers have been released for not only researchers but also public users. For example, IBM released IBM Q Experience in 2016, Rigetti released Quantum Cloud Services (QCS) in 2018, and IonQ is going to start Quantum Cloud Service in 2019. Software stacks for NISQ computers have also been extensively developed such as Qiskit$^{[5]}$ by IBM, Forest$^{[6]}$ by Rigetti, and Cirq$^{[7]}$ by Google. Researchers are looking for killer applications for NISQ. Quantum chemistry is one of the biggest targets$^{[8–10]}$. Optimization problem$^{[11–13]}$ and machine learning$^{[14–17]}$ are also attractive applications. For finance, some algorithms are also discussed$^{[18–20]}$.

In this paper, we focus on Variational Quantum Eigensolver (VQE), which is a quantum-classical hybrid algorithm proposed by Peruzzo et al.$^{[8]}$ to compute eigenvalues and eigenvectors of matrices such as Hamiltonians. VQE has been applied to various problems such as quantum chemistry$^{[21]}$ and extensively studied because NISQ computers can handle only short-depth circuits and it is necessary to incorporate them with classical computers. Such hybrid algorithms are relatively robust to noise compared with full-quantum algorithms. See a review by McArdle et al.$^{[22]}$ for the details of VQE.

VQE minimizes the expectation value of the input operator by varying quantum state $|\psi(\theta)\rangle$ with parameters $\theta$. The expectation value of an operator $A$ with parameters $\theta$ can be denoted as $\langle A_\theta \rangle = \langle \psi(\theta) | A \psi(\theta) \rangle$. In quantum chemistry, an operator $A$ is usually a qubit Hamiltonian, mapped from a fermionic Hamiltonian of molecules. A qubit Hamiltonian can be written as a linear combination of tensor products of Pauli operators including the identity operator, i.e., $A = \sum_{i=1}^{n} a_i P_i$, where the tensor product of Pauli operators $P_i \in \{ \sigma^x, \sigma^y, \sigma^z, I \} ^{\otimes N}$ is called Pauli string. VQE minimizes the expectation value by applying optimization algorithms for classical computers:

$$\min_{\theta} \langle A_\theta \rangle = \min_{\theta} \langle \psi(\theta) | A \psi(\theta) \rangle$$

$$= \min_{\theta} \sum_{i=1}^{n} a_i \langle \psi(\theta) | P_i \psi(\theta) \rangle.$$  (2)
Quantum computers can evaluate the expectation values of Pauli strings $\langle \psi(\theta) | P_i \psi(\theta) \rangle$.

The quantum-classical hybrid algorithms require a large number of executions of quantum circuits to evaluate the expectation values of observables. According to Wecker et al. \(^{23}\), “the required number of measurements is astronomically large for quantum chemistry applications to molecules.” VQE consists of three nested iterations:

- Outer iteration: to update the parameters $\theta$ of quantum state $|\psi(\theta)\rangle$,
- Middle iteration: to evaluate the expectation value by taking the weighted sum of Pauli strings, and
- Inner iteration: to evaluate the expectation value of a Pauli string by sampling.

The inner iteration evaluates Pauli strings as an expectation value with multiple samples. This requires $O(\epsilon^{-2})$ samples for the statistical error $\epsilon$. In order to reduce the middle iteration, McClean et al. \(^{24}\) suggested a grouping of jointly measurable Pauli strings by sequential measurements. For a tensor product basis (TPB), Bravyi et al. \(^{25}\) have proposed the grouping, and Kandala et al. \(^{2}\) have used it in the experiments. In order to reduce the inner iteration, Wang et al. \(^{26}\) have proposed another theoretical approach.

In this paper, we focus on reducing the number of measurements in the middle iteration. If Pauli strings are commutative, these Pauli strings are compatible, that is, jointly measurable. Grouping by TPB can reduce the number of measurements in the middle iteration \(^{2,25}\). The incompatibility by TPB can be represented by a graph called Pauli graph. It is known that the grouping of Pauli strings can be reduced to the coloring problem of the Pauli graph. Although the graph coloring problem is NP-complete, we can apply heuristic algorithms to obtain groups of Pauli strings, e.g., the Largest Degree First Coloring (LDFC) algorithm.

In this paper, we propose using entangled measurements in addition to TPB for the grouping of Pauli strings. Entangled measurements are measurements of entangled observable. Entangled observables are described by positive operator-valued measures which are not separable positive operator-valued measures. \(^{27}\) The advantage of using entangled measurements is that we can achieve a smaller number of groups; however, we need to add extra CNOT gates to construct a measurement circuit corresponding to the group, and they may affect the fidelity of the resulting expectation value. We thus study the properties of our grouping from both theoretical and experimental perspectives.

The contributions of this paper are as follows:

1. Grouping of Pauli strings with a part of entangled measurements,
2. Measurement strategy based on the sizes of groups to suppress the covariance effects,
3. Evaluation of the effect of the errors caused by additional CNOT gates, and
4. Proof-of-concept demonstration for a simple Hamiltonian on real quantum computers.

Recently, many research groups have discussed the efficient evaluation problem of Pauli strings \(^{28-35}\). We will discuss the differences in Section III.

II. RESULTS

A. Evaluation of Pauli strings

Let us consider the evaluation of the expectation values of observables. Target observables are mainly Hamiltonians, but not just them. Such observables of the multipartite qubit systems can be written as a linear combination of the Pauli strings $A = \sum_{i=1}^{n} a_i P_i$, where $a_i$ is a real number and $P_i$ is a $N$-qubit Pauli string. When the observables are not for the qubit systems, the Jordan-Wigner transformation for fermions or the Jordan-Schwinger transformation for bosons is useful to map the qubit systems from other systems. We describe the transformations for fermions in more detail. The second quantized fermionic Hamiltonian is described as

$$H = \sum_{ij} h_{ij} c_i^\dagger c_j + \frac{1}{2} \sum_{ijkl} h_{ijkl} c_i^\dagger c_j^\dagger c_k c_l,$$

where $h_{ij}$ is kinetic energy and potential energy, and $h_{ijkl}$ is interaction. Here, $c_i$ is an annihilation operator of the $i$-th fermion and $c_i^\dagger$ is a creation operator of the $i$-th fermion. There are three well-known transformations from fermionic systems to qubit systems: The Jordan-Wigner transformation \(^{36}\), that was originally proposed for lattice systems, Parity transformation, and Bravyi-Kitaev transformation \(^{37,38}\). Note that the difference between transformations will affect the results of grouping.
When one prepares a quantum state $|\psi\rangle$ in a quantum computer, the expectation value of an observable $A$ is $\langle A \rangle = \langle \psi | A | \psi \rangle$. We can evaluate the expectation values of Pauli operators. First, a measurement in the computational basis is available in a quantum computer. Then, by using single-qubit unitary rotation before the measurements, we can implement the measurements of other bases. Calculation $\langle A \rangle = \sum_{i=1}^{n} a_i \langle P_i \rangle$ gives the expectation value of $A$.

### B. Grouping Pauli strings with TPB

Some Pauli strings are simultaneously diagonalizable by the tensor product of basis $\{X, Y, Z\}$ where $X = \{|0\rangle \pm |1\rangle\}$, $Y = \{|0\rangle \pm i|1\rangle\}$, and $Z = \{|0\rangle \pm |1\rangle\}$. The sets of bases are called TPB sets. This implies that some Pauli strings that are simultaneously diagonalizable by TPB are jointly measurable by TPB. This fact also implies that such Pauli strings can be grouped and we can obtain the expectation values of the Pauli strings at the same time.

We introduce the Pauli graph $G = (V, E)$ of an observable $A = \sum_i a_i P_i$ as follows; nodes $V$ correspond to Pauli strings $P_i$, and edge $(u, v) \in E$ spans if Pauli strings $u$ and $v$ are not jointly measurable by TPB. Then, a coloring of the Pauli graph gives groups of the Pauli strings that are jointly measurable. For instance, Qiskit\(^3\) adopts the Largest Degree First Coloring (LDFC) algorithm, which first sorts the nodes in the descending order of degree and then assigns the smallest color number not used by its colored neighbors. It runs fast for practical graphs of interest and the number of the resulting groups is close to the lower bound by the max clique of the Pauli graph. See Table I for the details.

### C. Grouping with TPB and entangled measurements

Measurements by TPB are separable measurements. We propose taking advantage of entangled measurements. We introduce a new grouping approach of Pauli strings with not only TPB but also entangled measurements such as Bell measurements in order to reduce the number of measurements.

For example, the expectation values of $\sigma^x \sigma^z$, $\sigma^y \sigma^z$, and $\sigma^x \sigma^z$ cannot be obtained simultaneously from TPB measurements. It requires three types of measurements to compute the expectation values of $\sigma^x \sigma^z$, $\sigma^y \sigma^z$, and $\sigma^x \sigma^z$; however, these Pauli strings are jointly measurable by a Bell measurement (see Section IV.A for the details).

A simultaneous diagonalization provides a joint measurement using entangled observables. The incompatibility of Pauli strings can be checked by parity of the number of different Pauli operators $\sigma^x$, $\sigma^y$, and $\sigma^z$. One can make an extended Pauli graph based on this incompatibility and calculate the number of groups using the LDFC algorithm, where we call it “ALL” in Section II.E. We will actually calculate the number of groups using all measurements and LDFC later (see Table I). However, the computational cost of the circuit construction and the circuit depth increase according to the size of entanglements. Therefore, it may not be practical for NISQ computers to use all measurements due to the fidelity of operations of NISQ computers, especially multi-qubit operations.

To mitigate the drawback, we propose another approach to use a part of the entanglement of observables. It consists of two phases: choosing a set of entangled observables and grouping of Pauli strings with TPB and the set of entangled observables.

The first phase is to choose entangled measurements (e.g., Bell measurements and omega measurement\(^3\)) (see Appendix A) and construct quantum circuits corresponding to the entangled measurements. This task can be done using simultaneous diagonalization as preprocessing. We can alternatively use other methods based on Clifford gates, which have been recently proposed\(^3\). Since quantum circuits can be generated in advance in this phase, the cost of circuit construction in the next phase can be reduced.

The second phase is to make groups of Pauli strings with TPB and the entangled measurements chosen in the first phase. One makes a Pauli graph in the same manner as TPB-based methods and sort the nodes in the descending order of degree. Then, one merges nodes if they are jointly measurable by TPB and the entangled measurements. Notice that this joint measurability depends on a merge history. If one merges nodes, it is determined to use the entangled measurement at particular positions of Pauli strings, and after that, one cannot change the measurement. The merged nodes correspond to the groups of measurements, and one can construct quantum circuits corresponding to the groups and perform the measurements. We name the grouping with TPB and Bell measurements “TPB+Bell”, the grouping with TPB and all 2-qubit measurements “TPB+2Q,” See Section IV.B for the details of the grouping algorithm, and see Section IV.A and Appendix A for 2-qubit entangled measurements.

Entanglement of observables could be considered as a resource of a joint measurement. In experiments with NISQ computers, available entangled measurements are limited due to the multi-qubit gate errors. Therefore, we need to consider algorithms with available measurements. For example, if one uses two qubit entangled measurements, only one entangler (e.g., CNOT gate) is required per each of qubits. Our proposal requires a constant depth of measurement circuits for fixed available entangled measurements. The advantage of our approach is that we can adjust the depth of the additional circuits for entangled measurements by considering errors of multi-qubit gates.
TABLE I: Comparison of numbers of groups. The clique sizes with ‘∗’ are the maximum. JW and BK are Jordan-Wigner and Bravyi-Kitaev transformations. TPB, TPB+BELL, TPB+2Q, and ALL denote the groupings using TPB, TPB and Bell measurements, TPB and all 2-qubit entangled measurements, and all measurements, respectively.

| Molecule Transformation | Number of groups | Clique size of Pauli graph |
|-------------------------|------------------|---------------------------|
|                         | No-grouping | TPB | TPB+Bell | TPB+2Q | ALL |
| LiH PAIRITY             | JW         | 631  | 136      | 42     | 42  | 35  | 130∗ |
|                         | BK         | 631  | 211      | 103    | 113 | 35  | 208∗ |
| BeH₂ PAIRITY            | JW         | 1150 | 215      | 59     | 59  | 58  | 200∗ |
|                         | BK         | 1150 | 341      | 199    | 200 | 58  | 335∗ |
| H₂O PAIRITY             | JW         | 1858 | 380      | 71     | 71  | 84  | 355∗ |
|                         | BK         | 1858 | 515      | 286    | 273 | 82  | 508∗ |
| NH₃ PAIRITY             | JW         | 4973 | 1052     | 127    | 127 | 117 | 994∗ |
|                         | BK         | 4973 | 1086     | 579    | 538 | 115 | 1040 |
| HCl PAIRITY             | JW         | 4427 | 906      | 154    | 153 | 110 | 844∗ |
|                         | BK         | 4427 | 1434     | 733    | 686 | 112 | 1413∗ |

D. Standard error caused by the grouping of Pauli strings

McClean et al. discussed covariance effects and, they illustrated that the additional covariance caused by a grouping may require more measurements. However, Kandala et al. numerically verified that the grouping with TPB has less errors than no-grouping does for some molecules. Note that the square of the error is in inverse proportion to the number of samples. We show mathematically that if the number of samples in each group is in proportion to the size of the group, the standard error of a grouping is smaller than that of no-grouping in Appendix B, where the total numbers of samples for the grouping and no-grouping are same.

E. Number of groups

We applied 4 types of grouping methods (one with TPB, one with TPB and Bell measurements, one with TPB and all 2-qubit entangled measurements, and one with all measurements) to molecules LiH, BeH₂, H₂O, NH₃, and HCl. We also computed the maximal clique numbers of Pauli graphs for TPB by applying MCQD algorithm. We ran MCQD on Intel Xeon E5-2690 CPU with 1-hour time limit and it found the maximum cliques for all Pauli graphs except NH₃ Parity and BK. Note that the Hamiltonians of the molecules are given in the previous study as ancillary files.

We compare the numbers of groups in Table I. The grouping with TPB achieved numbers of groups that are slightly larger than the clique sizes of the Pauli graphs. Note that the grouping with TPB cannot achieve less number of groups than the clique size because it is based on a coloring algorithm (see Eq. 64). On the other hand, the groupings using entangled measurements (TPB+Bell, TPB+2Q, ALL) achieved less numbers than the clique sizes. The grouping with TPB and 2-qubit entangled measurements (TPB+2Q) does not always have fewer numbers of groups than those by the grouping with TPB and Bell measurements (TPB+Bell). It implies that our heuristic algorithm cannot take full advantage of more choices of measurements. We also observe that the grouping with all measurements (ALL) does not always give the smallest number of groups among all methods. It implies that LDFC cannot obtain good solutions for the extended Pauli graphs. The number of groups depends on the type of transformations as well as the grouping methods. For example, for Jordan-Wigner transformation, TPB+Bell gives smaller numbers of groups for most molecules than groupings TPB and TPB+2Q do.

We observe that the entangled measurements are effective to reduce the number of measurements of Pauli strings. However, there exist various errors on NISQ computers, and especially a two-qubit gate error is much larger than a one-qubit error in general. In the next section, we discuss the effect of additional CNOT gates introduced by entangled measurements.
F. Effect of additional CNOT gates

Entangled measurements require additional two-qubit gates. We evaluate the effect of additional CNOT gates for a Bell measurement in one of the simplest models, two-qubit antiferromagnetic Heisenberg model, whose Hamiltonian is given by

\[
H = \sigma^x \sigma^x + \sigma^y \sigma^y + \sigma^z \sigma^z,
\]

where we set the coupling constant to be 1 for simplicity. It is clear that these Pauli strings cannot be grouped by TPB but can be grouped by a Bell measurement. We compute the expectation value with the ground state using a noise model in Qiskit Aer and readout error mitigation in Qiskit Ignis. We assign 2000 samples to each group of no-grouping (3 groups) and 6000 samples to a group of the grouping by a Bell measurement (1 group). We assume that the one-qubit readout errors are \( p(1|0) = 0.01 \) and \( p(0|1) = 0.1 \), the one-qubit depolarizing error is 0.001. We simulated the expectation value of the Hamiltonian by varying the two-qubit depolarizing error. The row “No-grouping (raw)” denotes the expectation values with the standard error, where we did not apply the readout error mitigation. The rows of “Bell (raw)” and “Bell (mit)” denote the results with the readout error mitigation. The rows of “Bell (raw)” and “Bell (mit)” denote the results of the grouping of a Bell measurement with and without the readout error mitigation. We observe that the grouping with a Bell measurement achieved comparable expectation value with less standard error compared with no-grouping up to two-qubit error 0.010. The grouping with a Bell measurement results in worse expectation values with two-qubit error more than 0.010 because of the extra CNOT gate introduced by a Bell measurement. Note that we implemented our program with Qiskit Terra 0.7.2, Qiskit Aer 0.1.1, Qiskit Ignis 0.1.0, and Qiskit Aqua 0.4.1.

TABLE II: Simulation results of the expectation values and standard errors of the two-qubit antiferromagnetic Heisenberg model. We vary the two-qubit depolarizing error to evaluate the additional CNOT gate effects. “Bell” means the grouping with a Bell measurement. “(mit)” and “(raw)” denote results with and without readout error mitigation, respectively.

| Two-qubit error | 0 | 0.005 | 0.010 | 0.015 | 0.020 |
|-----------------|---|-------|-------|-------|-------|
| No-grouping (raw) | -2.318 ± 0.043 | -2.327 ± 0.042 | -2.313 ± 0.043 | -2.311 ± 0.043 | -2.293 ± 0.043 |
| No-grouping (mit) | -2.970 ± 0.008 | -2.971 ± 0.007 | -2.959 ± 0.009 | -2.957 ± 0.009 | -2.944 ± 0.011 |
| Bell (raw) | -2.227 ± 0.020 | -2.233 ± 0.020 | -2.207 ± 0.021 | -2.186 ± 0.021 | -2.153 ± 0.021 |
| Bell (mit) | -2.966 ± 0.005 | -2.987 ± 0.003 | -2.956 ± 0.005 | -2.929 ± 0.007 | -2.889 ± 0.008 |

We also evaluated additional CNOT gate effects using real quantum computers, IBM Q Tokyo and IBM Q Poughkeepsie (see Table III). Note that both IBM Q Tokyo and Poughkeepsie have 20 qubits. We picked up the pair of qubits with the best fidelity based on the property data of the devices when we executed the circuits. We observe that the grouping with a Bell measurement achieved comparable expectation value with less standard error compared with no-grouping. These experiments suggest that readout error has a significant influence (more than the additional two-qubit error).

TABLE III: The experiment of additional qubit gates using IBM Q Tokyo and IBM Q Poughkeepsie.

| Device name | Tokyo | Poughkeepsie |
|-------------|-------|--------------|
| No-grouping (raw) | -2.588 ± 0.034 | -2.313 ± 0.043 |
| No-grouping (mit) | -2.962 ± 0.010 | -2.889 ± 0.017 |
| Bell (raw) | -2.487 ± 0.017 | -2.432 ± 0.018 |
| Bell (mit) | -2.984 ± 0.003 | -2.983 ± 0.003 |

G. VQE with entangled measurements

We incorporate the grouping with Bell measurements into VQE to calculate the ground state energy of the two-qubit antiferromagnetic Heisenberg model, while we use the no-grouping as the baseline. We compare the numbers of circuits to be converged. We used \( R_y \) trial wave function with depth 1 as the variational form and the simultaneous perturbation stochastic approximation (SPSA) as the optimizer. We executed VQE algorithm with 40 iteration steps. We applied the readout error mitigation and calibrated the mitigation data every 10 iteration steps of VQE. We
fixed the number of executions of quantum circuits to 8192 samples, that is, the maximum number for a job of the IBM Q systems as of July 2019. See Fig. 1 for the results. The horizontal axis and the vertical axis represent numbers of quantum circuits performed and expectation values of the Hamiltonian, respectively. VQE with a Bell measurement has 1 circuits for each iteration, while VQE without grouping has 3 circuits for each iteration. We plot the standard error as well as the expectation values; but, the error bar is small enough to be buried in point. We observe that VQE with a Bell measurement required less circuits than VQE with no-grouping to converge. We will show more results and discuss them in Appendix C.

![Graph](image)

FIG. 1: Comparison of VQE with no-grouping and the grouping with a Bell measurement. The horizontal axis and the vertical axis represent numbers of quantum circuits performed and expectation values of the Heisenberg Hamiltonian, respectively. The graph legends plus and minus are used to optimize by SPSA algorithm. The black dashed line and the green one denote the exact ground state energy and the final result of VQE experiment, respectively.

III. DISCUSSION

In this paper, we discussed the efficient evaluation of Pauli strings with a part of entangled measurements. We propose reducing the number of groups of Pauli strings that are jointly measurable by utilizing both TPB and a part of entangled measurements. It is remarkable that the grouping using TPB and Bell measurements (TPB+Bell) has as few number of groups as the grouping using all measurements (ALL) for some molecules with the Jordan-Wigner transformation in Table I because the depth of the additional CNOT gates required for TPB+Bell is constant 1. Note that the grouping using all measurements were obtained by applying LDFC to the extended Pauli graph, the solutions may be suboptimal, and they can be improved with more sophisticated coloring algorithms. We also showed that if the number of samples in each group is in proportion to the size of the group, the standard error with grouping is always equal to or smaller than that with no-grouping.

Public quantum computers are available as cloud service today. The time of computation is bounded by job time, we call it job bound. The time for a job is equal to the sum of waiting time and execution time. The execution time can be regarded as the execution time of the circuits included in the job. In other words, execution time is roughly proportional to the total number of circuits to be executed. Therefore, reducing the number of circuits in grouping contributes to the improvement of execution time.

In the present study, we implement the entangled measurements in the Heisenberg picture in the software layer. There are other possible candidates to implement joint measurements. The entangled measurements can be implemented in the hardware layer called joint readout. The joint readout may make our proposal more accurately and precisely. Direct or indirect sequential measurements also provide joint measurements.

In order to accelerate the iterations of VQE, several approaches have been discussed. An efficient partitioning by mean-field approach was proposed by Izmaylov et al. It requires feedforward measurements, which is not implemented in the current devices. However, once the feedforward is implemented, we may achieve better efficiency when it is used in combination with our methods. A sequential minimal optimization method reduces the outer iteration. It converges faster than previous optimizers and has no hyperparameter. Fermionic representability conditions are useful to reduce the middle iteration. Some efficiency improvements which do not relate to iterations were studied.
A remarkable property of the Bell measurement is that expectation values of \( \sigma \) we generate permutations of qubit positions and check if any of the entangled measurements can be applied to the quantum states. They discussed the case when an available gate set is limited to Clifford gates or single-qudit Clifford gates, while we discuss the case where available measurements are limited. The diagonalization by Clifford operators corresponds to all measurements, and the diagonalization by single-qubit Clifford corresponds to TPB. Yan et al.\(^{29}\) proposed a conversion method from groups of commuting Pauli strings into TPB using unitary transformations. Their unitary transformations were discussed in the Schrödinger picture; but, they used all measurements in the Heisenberg picture and proposed efficient circuit construction using Clifford gates. Gokhale et al.\(^{32}\) used entangled measurements to measure commuting Pauli strings and developed a circuit synthesis tool for joint measurement based on the stabilizer. Furthermore, their results have been demonstrated experimentally to compute the ground state energy of deuterium on the IBM Q Tokyo. Crawford et al.\(^{33}\) proposed taking into account coefficients of Pauli strings for the grouping to mitigate the covariance effect, while we propose adjusting the number of samples taking into account the sizes of groups. The linear reduction of the number of groups from \( O(N^4) \) to \( O(N^3) \) for molecular Hamiltonians has been proven in different ways.\(^{34,35}\) Izmaylov et al.\(^{30}\) and Huggins et al.\(^{31}\) developed a different method which does not use joint measurement of the Pauli strings. The anti-commute Pauli strings can be translated into a unitary matrix, and the expectation value of the unitary matrix can be estimated using a method such as Hadamard test.\(^{40}\) Huggins et al.\(^{31}\) were based on a decomposition of the two-electron integral tensor.

IV. METHODS

A. Entangled measurements

In this section, we introduce entangled measurements. Entanglement is a specific property of quantum theory and an essential concept in quantum information science and technology. Entanglement is originally defined for quantum states. Bell states are one of the maximally entangled states. Bell states are defined as follows:

\[
|\Phi^\pm\rangle = \frac{1}{\sqrt{2}} (|00\rangle \pm |11\rangle), \quad |\Psi^\pm\rangle = \frac{1}{\sqrt{2}} (|01\rangle \pm |10\rangle).
\]

Entanglement of states can be extended to observables. As entanglement of states can be detected by the violation of Bell-CHSH inequality\(^{27}\), an entanglement of observables can be detected by the violation of the dual Bell-CHSH inequality\(^{27}\). Measurements of entangled observable are called entangled measurements. Let us introduce examples of the entangled measurements. The first example of entangled measurements is Bell measurements defined as the projective measurements on Bell states. The Bell measurements are used in the quantum teleportation protocol\(^{55}\). A remarkable property of the Bell measurement is that expectation values of \( \sigma^x \otimes \sigma^x \), \( \sigma^y \otimes \sigma^y \), and \( \sigma^z \otimes \sigma^z \) can be calculated from the result of the Bell measurement. This property is based on the fact:

\[
\sigma^x \otimes \sigma^x = |\Psi^\pm\rangle \langle \Psi^\pm | + |\Phi^\pm\rangle \langle \Phi^\pm | - |\Psi^-\rangle \langle \Psi^- | - |\Phi^-\rangle \langle \Phi^- |,
\]

\[
\sigma^y \otimes \sigma^y = |\Psi^\pm\rangle \langle \Psi^\pm | + |\Phi^\pm\rangle \langle \Phi^\pm | - |\Psi^-\rangle \langle \Psi^- | - |\Phi^-\rangle \langle \Phi^- |,
\]

\[
\sigma^z \otimes \sigma^z = |\Phi^\pm\rangle \langle \Phi^\pm | + |\Phi^\mp\rangle \langle \Phi^\mp | - |\Psi^\pm\rangle \langle \Psi^\pm | - |\Psi^\mp\rangle \langle \Psi^\mp |.
\]

In order to implement the Bell measurement on a quantum computer, CNOT gate and Hadamard gate are required. The quantum circuit is shown in Fig. 2. We will describe other useful entangled measurements in Appendix A.

B. Grouping Algorithm

We propose a heuristic algorithm of grouping Pauli strings by TPB and a part of entangled measurements in a greedy way. We first make a Pauli graph as the grouping with TPB does and then merge nodes with high degrees if they are jointly measurable by given entangled measurements. In order to check whether a pair of Pauli strings, we generate permutations of qubit positions and check if any of the entangled measurements can be applied to the position. The number of resulting groups depends on the order of measurements to be applied in Algorithm 2. We let \( E = \{ \text{Bell, TPB} \} \) for ‘TPB+Bell’ and \( E = \{ \text{Bell, Omega-XX, Omega-YY, Omega-ZZ, Chi, TPB} \} \) for ‘TPB+2Q’ in the experiments of Section II E. See Algorithm 1 and 2 for the details of the algorithm and Appendix A for the definitions of the omega and chi measurements.
Algorithm 1  Greedy grouping of Pauli strings with available measurements

1: Input: observable \( A = \sum_{i=1}^{n} a_i P_i \), a set of measurements \( E = \{ \mathcal{E}_1, \ldots, \mathcal{E}_l \} \). Note that each Pauli string has length \( N \) and the measurements may include both TPB and entangled measurements.
2: Make a Pauli graph \( G \) of Pauli strings \( \{ P_i \} \) based on TPB.
3: Sort the nodes in the descending order of degree on \( G \) and let them be \( \{ v_1, \ldots, v_n \} \)
4: Initialize the assignment of measurements \( M_i \) of all nodes \( v_i \).
5: for \( i = 1, \ldots, n \) do
6: if \( v_i \) is already merged, skip it.
7: for \( j = i + 1, \ldots, n \) do
8: if \( v_j \) is already merged, skip it.
9: if \( v_i \) and \( v_j \) are jointly measurable by \( M_i \) and \( E \) (see Algorithm 2) then
10: Merge \( v_j \) to \( v_i \) and update \( M_i \).
11: end if
12: end for
13: end for
14: Return the merged nodes as the groups of observables.

Algorithm 2  Greedy assignment of measurements

1: Input: a pair of Pauli strings \( (v_i, v_j) \), a set of measurements \( E \), current assignment of measurements \( M_i \) for \( v_i \).
2: Note that \( M_i \) represents a set of measurements and the qubits associated with the measurements, e.g., first qubit to be measured by \( \sigma_x \) and second and fourth qubits to be measured by \( \sigma_y \).
3: Return fail if any qubit of \( v_j \) is not compatible with \( M_i \).
4: Let \( U \) be the set of positions of qubits that \( M_i \) does not cover.
5: Remove positions of qubits from \( U \) where \( v_i \) and \( v_j \) have common Pauli operators.
6: while \( U \neq \emptyset \) do
7: for \( \mathcal{E} \in E \) do
8: for \( p \in \text{permutation of } U \) with the length of measurement \( \mathcal{E} \) do
9: if both \( v_i \) and \( v_j \) are compatible with \( \mathcal{E} \) at position \( p \) then
10: Update \( M_i \) with \( \mathcal{E} \) at position \( p \).
11: Update \( U \) by removing \( p \).
12: Go to line 6.
13: end if
14: end for
15: end for
16: Return fail.
17: end while
18: Return \( M_i \).

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The first example of entangled measurements, Bell measurements, is shown in Section IV A. The second example of entangled measurements is an omega measurement that is a projective measurement on omega states introduced in the board game Entanglion developed by IBM Research. Omega states are defined as

\[ \Omega^{0Y} = \frac{1}{2} |00\rangle + \frac{1}{2} |01\rangle - \frac{1}{2} |10\rangle + \frac{1}{2} |11\rangle, \]  
\[ \Omega^{1Y} = -\frac{1}{2} |00\rangle + \frac{1}{2} |01\rangle + \frac{1}{2} |10\rangle + \frac{1}{2} |11\rangle, \]  
\[ \Omega^{2Y} = \frac{1}{2} |00\rangle + \frac{1}{2} |01\rangle + \frac{1}{2} |10\rangle - \frac{1}{2} |11\rangle, \]  
\[ \Omega^{3Y} = \frac{1}{2} |00\rangle - \frac{1}{2} |01\rangle + \frac{1}{2} |10\rangle + \frac{1}{2} |11\rangle. \]  

Here, we note that omega states are described as omega-YY states because there are other omega states introduced later. We can get the expectation values of \( \sigma^y \otimes \sigma^y \), \( \sigma^z \otimes \sigma^z \), and \( \sigma^x \otimes \sigma^x \) from an omega-YY measurement, since the following identity holds:

\[ \sigma^y \otimes \sigma^y = \frac{1}{2} \left( |00\rangle \langle 00| + |01\rangle \langle 01| + |10\rangle \langle 10| - |11\rangle \langle 11| \right), \]  
\[ \sigma^z \otimes \sigma^z = \frac{1}{2} \left( |00\rangle \langle 00| + |01\rangle \langle 01| + |10\rangle \langle 10| - |11\rangle \langle 11| \right), \]  
\[ \sigma^x \otimes \sigma^x = \frac{1}{2} \left( |00\rangle \langle 00| + |01\rangle \langle 01| - |10\rangle \langle 10| - |11\rangle \langle 11| \right). \]  

Circuit implementation of an omega-YY measurement is shown in Fig. 3.
An omega-XX measurement is a joint measurement of observables $\sigma^x \otimes \sigma^x$, $\sigma^+ \otimes \sigma^-$, and $\sigma^y \otimes \sigma^x$. This is derived from the following identities:

$$\sigma^z \otimes \sigma^z = |\Omega_0^{ZZ}\rangle \langle \Omega_0^{ZZ}| + |\Omega_1^{ZZ}\rangle \langle \Omega_1^{ZZ}| - |\Omega_0^{ZZ}\rangle \langle \Omega_1^{ZZ}| - |\Omega_1^{ZZ}\rangle \langle \Omega_0^{ZZ}|,$$

$$\sigma^x \otimes \sigma^y = |\Omega_0^{Z\bar{Z}}\rangle \langle \Omega_0^{Z\bar{Z}}| + |\Omega_0^{Z\bar{Z}}\rangle \langle \Omega_0^{Z\bar{Z}}| - |\Omega_0^{Z\bar{Z}}\rangle \langle \Omega_0^{Z\bar{Z}}| - |\Omega_0^{Z\bar{Z}}\rangle \langle \Omega_0^{Z\bar{Z}}|,$$

and

$$\sigma^y \otimes \sigma^x = |\Omega_0^{Z\bar{Z}}\rangle \langle \Omega_0^{Z\bar{Z}}| + |\Omega_0^{Z\bar{Z}}\rangle \langle \Omega_0^{Z\bar{Z}}| - |\Omega_0^{Z\bar{Z}}\rangle \langle \Omega_0^{Z\bar{Z}}| - |\Omega_0^{Z\bar{Z}}\rangle \langle \Omega_0^{Z\bar{Z}}|. $$

An omega-XX measurement is a joint measurement of observables $\sigma^x \otimes \sigma^z$, $\sigma^+ \otimes \sigma^z$, and $\sigma^y \otimes \sigma^z$. This is derived from the following identities:

$$\sigma^x \otimes \sigma^x = |\Omega_0^{XX}\rangle \langle \Omega_0^{XX}| + |\Omega_1^{XX}\rangle \langle \Omega_1^{XX}| - |\Omega_0^{XX}\rangle \langle \Omega_1^{XX}| - |\Omega_1^{XX}\rangle \langle \Omega_0^{XX}|,$$

$$\sigma^y \otimes \sigma^z = |\Omega_0^{XX}\rangle \langle \Omega_0^{XX}| + |\Omega_1^{XX}\rangle \langle \Omega_1^{XX}| - |\Omega_0^{XX}\rangle \langle \Omega_1^{XX}| - |\Omega_1^{XX}\rangle \langle \Omega_0^{XX}|,$$

$$\sigma^z \otimes \sigma^y = |\Omega_0^{XX}\rangle \langle \Omega_0^{XX}| + |\Omega_1^{XX}\rangle \langle \Omega_1^{XX}| - |\Omega_0^{XX}\rangle \langle \Omega_1^{XX}| - |\Omega_1^{XX}\rangle \langle \Omega_0^{XX}|.$$ 

Circuit implementations of an omega-ZZ measurement and an omega-XX measurement are shown in Fig. 4.

The fifth example is a chi measurement. A chi measurement is a joint measurement of $\sigma^x \otimes \sigma^y$, $\sigma^y \otimes \sigma^z$, and $\sigma^z \otimes \sigma^x$. 

FIG. 3: Quantum circuit of an omega-YY measurement.
Let us define the following states:

\[
|X_0\rangle = \frac{1}{2} |00\rangle + \frac{1}{2} |01\rangle + \frac{i}{2} |10\rangle - \frac{i}{2} |11\rangle, \\
|X_1\rangle = \frac{1}{2} |00\rangle + \frac{1}{2} |01\rangle - \frac{i}{2} |10\rangle + \frac{i}{2} |11\rangle, \\
|X_2\rangle = \frac{1}{2} |00\rangle - \frac{1}{2} |01\rangle + \frac{i}{2} |10\rangle + \frac{i}{2} |11\rangle, \\
|X_3\rangle = -\frac{1}{2} |00\rangle + \frac{1}{2} |01\rangle + \frac{i}{2} |10\rangle + \frac{i}{2} |11\rangle.
\]  

(A22) (A23) (A24) (A25)

A chi measurement is a projective measurement of these states because following identity holds:

\[
\sigma^x \otimes \sigma^y = -|X_0\rangle \langle X_0| + |X_1\rangle \langle X_1| + |X_2\rangle \langle X_2| - |X_3\rangle \langle X_3|,
\]

\[
\sigma^y \otimes \sigma^z = |X_0\rangle \langle X_0| - |X_1\rangle \langle X_1| - |X_2\rangle \langle X_2| - |X_3\rangle \langle X_3|,
\]

\[
\sigma^z \otimes \sigma^x = |X_0\rangle \langle X_0| + |X_1\rangle \langle X_1| - |X_2\rangle \langle X_2| - |X_3\rangle \langle X_3|.
\]

(A26) (A27) (A28)

Circuit implementation of a chi measurement is shown in Fig. 5. Here, we use a one-pulse gate $U_2$ defined in Qiskit Terra. $U_2$-gate has two parameters $\phi$ and $\lambda$. The matrix representation of $U_2$-gate is

\[
\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & e^{i\lambda} \\ e^{i\phi} & -e^{i\lambda} \end{pmatrix}
\]

(A29)

In the Fig. 5, the parameters of $U_2$-gate are given by $\phi = 0$ and $\lambda = \frac{\pi}{2}$.

There are entangled measurements with three or more qubits for joint measurement of Pauli strings and they can be realized as similar formulations; however, we used only two-qubit entangled measurements in our experiments. This is because large quantum circuits are required for multipartite entangled measurements in general and it seems difficult to execute such circuits on current quantum computers due to errors.
Appendix B: Error derived from grouping

1. Theoretical analysis of the covariance effects by grouping

We assume that observables are given by the following weighted sum of Pauli strings:

\[ A = \sum_{i=1}^{n} a_i P_i \]  

(B1)

where \( a_i \) is a real number and \( P_i \) is a Pauli string. In this section, let us consider the standard error derived from grouping of Pauli strings. Let a grouping divide \( n \) Pauli strings into \( K \) sets \( s_1, s_2, \ldots, s_K \). Then, the equality

\[ A = \sum_{k=1}^{K} \sum_{i \in s_k} a_i P_i, \]  

(B2)

holds by definition. If the number of samples for group \( s_k \) is \( S_k \), the standard error is given by

\[ \epsilon_G = \sqrt{\sum_{k=1}^{K} \frac{\text{Var} \left( \sum_{i \in s_k} a_i P_i \right)}{S_k}}, \]  

(B3)

\[ = \sqrt{\sum_{k=1}^{K} \frac{\sum_{(i,j) \in s_k \times s_k} a_i a_j \langle (P_i - \langle P_i \rangle)(P_j - \langle P_j \rangle) \rangle}{S_k}}. \]  

(B4)

When the case of no-grouping, that is, \( |s_k| = 1 \), the standard error is

\[ \epsilon_{NG} = \sqrt{\frac{1}{S} \sum_{i=1}^{n} a_i^2 \langle (P_i - \langle P_i \rangle)^2 \rangle}, \]  

(B5)

where we assume that \( S_k = S \) for simplicity using a constant positive integer \( S \). This error does not contain the covariance effects.

We propose that the number of samples in each group is in proportion to the size of the group, i.e., \( S_k = |s_k| S \), where the total numbers of samples for no-grouping and grouping are same. Let us compare the standard error without grouping \( \epsilon_{NG} \) and that with grouping \( \epsilon_G \) as follows:

\[ \epsilon_G^2 = \sum_{k=1}^{K} \frac{\sum_{(i,j) \in s_k \times s_k} a_i a_j \langle (P_i - \langle P_i \rangle)(P_j - \langle P_j \rangle) \rangle}{S_k}, \]  

(B6)

\[ = \frac{1}{S} \sum_{k=1}^{K} \frac{\sum_{(i,j) \in s_k \times s_k} \langle (a_i P_i - \langle a_i P_i \rangle)(a_j P_j - \langle a_j P_j \rangle) \rangle}{|s_k|}, \]  

(B7)

\[ \leq \frac{1}{S} \sum_{k=1}^{K} \frac{\sum_{(i,j) \in s_k \times s_k} \sqrt{\langle (a_i P_i - \langle a_i P_i \rangle)^2 \rangle \langle (a_j P_j - \langle a_j P_j \rangle)^2 \rangle}}{|s_k|}, \]  

(B8)

\[ \leq \frac{1}{S} \sum_{k=1}^{K} \frac{\sum_{(i,j) \in s_k \times s_k} \left[ \langle (a_i P_i - \langle a_i P_i \rangle)^2 \rangle + \langle (a_j P_j - \langle a_j P_j \rangle)^2 \rangle \right]}{2|s_k|}, \]  

(B9)

\[ = \frac{1}{S} \sum_{k=1}^{K} \sum_{i \in s_k} \langle (a_i P_i - \langle a_i P_i \rangle)^2 \rangle, \]  

(B10)

\[ = \epsilon_{NG}^2, \]  

(B11)

where we applied the Cauchy–Schwarz inequality to the first inequality [B8] and the AM–GM inequality to the second inequality [B9]. As a result, we obtain the following theorem:

**Theorem 1.** The standard error of grouping is less or equal to that of no-grouping, that is, the inequality

\[ \epsilon_G \leq \epsilon_{NG}, \]  

(B12)

holds.
2. Numerical experiment

Here, we study the two-qubit antiferromagnetic Heisenberg model, which is described as

\[ H = J(\sigma^x\sigma^x + \sigma^y\sigma^y + \sigma^z\sigma^z), \]

with \( J > 0 \). We assume \( J = 1 \) for simplicity. A variance of this Hamiltonian is

\[ \text{Var}[H]_{NG} = \text{Var}[\sigma^x\sigma^x] + \text{Var}[\sigma^y\sigma^y] + \text{Var}[\sigma^z\sigma^z], \]

if one performs measurements \( \sigma^x\sigma^x \), \( \sigma^y\sigma^y \), and \( \sigma^z\sigma^z \) independently. If one performs a joint measurement (Bell measurement), a variance of the Hamiltonian is

\[ \text{Var}[H]_G = \text{Var}[\sigma^x\sigma^x + \sigma^y\sigma^y + \sigma^z\sigma^z] = \text{Var}[\sigma^x\sigma^x] + \text{Var}[\sigma^y\sigma^y] + \text{Var}[\sigma^z\sigma^z] + 2\text{Cov}[\sigma^x\sigma^x, \sigma^y\sigma^y] + 2\text{Cov}[\sigma^y\sigma^y, \sigma^z\sigma^z] + 2\text{Cov}[\sigma^z\sigma^z, \sigma^x\sigma^x]. \]

We numerically compute the square of standard errors for Pauli strings and grouped Pauli strings using a Bell measurement. We prepare 10000 random states by Haar random unitary and calculate the standard errors. The number of running circuit is 500 samples per Pauli strings for no-grouping (3 groups) and 1500 samples per sets for a Bell measurement (1 group). The average of the squared standard errors of no-grouping is 0.00479, and that of the grouping with a Bell measurement is 0.00159. This numerical result shows that the grouping with Bell measurement has less standard error. See Fig. 6 for the distributions. The distribution for the grouping with a Bell measurement is interesting because the values are concentrated around the upper bound, while this characteristic is not seen in the case of the grouping with TPB (see Fig. S5. in Supplementary information of Kandala et al [2]). It might be an intrinsic property of the grouping with entangled measurements.

![Graph](image_url)

(a) The square of the standard error for Pauli strings (no-grouping) is \( \text{Var}[H]_{NG}/500 \). We run 500 samples per each of measurements.

(b) The square of the standard error for Pauli strings (grouping by a Bell measurement) is \( \text{Var}[H]_G/1500 \). We run 1500 samples of the Bell measurement.

FIG. 6: Comparison of distributions of the square of standard errors. Both of values are computed for 10000 random states. From Theorem [1] the values on the left are greater than those on the right for the same quantum state.

Appendix C: Convergence of VQE on real quantum computers

We executed VQE on quantum computers several times (including the result in Section II G) and plot the results in Fig. [7]. In the experiments of VQE, it took from several minutes to several hours to run a circuit on the quantum computers depending on the waiting time of the job queue. Thus, the experiments took a long time to execute all circuits. The results depend on the device conditions and the condition may change during the waiting time. Although the energy failed to converge in a few experiments, they converged faster with the proposed method than the baseline in the cases where both methods converged.

In some cases, the energy went down once and then went up again. Thus, the converged values are not always the minimum. This implies that SPSA is not robust enough to the noise, and we need to try more optimizers to find...
FIG. 7: Experimental results of VQE on quantum computers. In the labels, ‘pok’ and ‘tokyo’ denote that the experiments were conducted on IBM Q Poughkeepsie and IBM Q Tokyo, respectively. The optimizer SPSA outputs plus and minus values; but, we plot only the mean value of plus and minus. The label ‘average’ is the average of all cases. These experiments were performed from June 4th to July 14th in 2019.

robust one. We also need to save the states of the optimizer as the checkpoint and go back to the checkpoint if we detect such fluctuation.