Measuring all compatible operators in one series of single-qubit measurements using unitary transformations

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The Variational Quantum Eigensolver approach to the electronic structure problem on a quantum computer involves measurement of the Hamiltonian expectation value. Formally, quantum mechanics allows one to measure all mutually commuting or compatible operators simultaneously. Unfortunately, the current hardware permits measuring only a much more limited subset of operators that share a common tensor product eigen-basis. We introduce unitary transformations that transform any fully commuting group of operators to a group that can be measured on current hardware. These unitary operations can be encoded as a sequence of Clifford gates and let us not only measure much larger groups of terms but also to obtain these groups efficiently on a classical computer. The problem of finding the minimum number of fully commuting groups of terms covering the whole Hamiltonian is found to be equivalent to the minimum clique cover problem for a graph representing Hamiltonian terms as vertices and commutativity between them as edges. Tested on a set of molecular electronic Hamiltonians with up to 50 thousand terms, the introduced technique allows for the reduction of the number of separately measurable operator groups down to few hundreds, thus achieving up to 2 orders of magnitude reduction. Based on the test set results, the obtained gain scales at least linearly with the number of qubits.

I. INTRODUCTION

Using quantum superposition and entanglement, quantum computers promise a new powerful route to solve problems that are exponentially hard for their classical counterparts. Even though quantum hardware advancements generated a surge of interest in developing new algorithms to solve these hard problems, we are still in the era of noisy intermediate scale quantum (NISQ) computing.\textsuperscript{1} One of the hallmarks of NISQ algorithms is hybrid quantum-classical optimization of parametrized quantum circuits. The Variational Quantum Eigensolver (VQE) approach is one of the most popular realizations of this idea for solving optimization problems by mapping their solution to lowest eigen-states of a particular Hamiltonian with a bounded spectrum.\textsuperscript{2–4} In this case, the optimization is simplified by the existence of the variational theorem that guarantees that any trial wavefunction will approach the solution from above. In VQE, the quantum computer prepares a trial wavefunction \( | \Psi(q) \rangle \) and estimates an expectation value for the target Hamiltonian \( \hat{H} = \langle \Psi(q) | \hat{H} | \Psi(q) \rangle \). The classical computer suggests a next trial wavefunction using results of expectation values based on previous wavefunctions.

One of the exponentially hard and thus attractive problems that is highly valuable for chemistry is the electronic structure problem.\textsuperscript{3–8} Its solution provides a route to predicting chemical properties and designing many new valuable compounds such as materials and drugs. It is formulated using the Born-Oppenheimer separation of nuclear variables as parameters for the electronic part of the time-independent molecular Schrodinger equation

\[ \hat{H}_e(R) | \Psi(R) \rangle = E_e(R) | \Psi(R) \rangle, \]

where \( \hat{H}_e(R) \) is the electronic Hamiltonian, \( R \) is the nuclear configuration of interest, and \( E_e(R) \) is the electronic energy. To treat this problem within the VQE framework it can be mapped to a qubit eigenvalue problem

\[ \hat{H}_q(R) | \Psi_q(R) \rangle = E_q(R) | \Psi_q(R) \rangle, \]

where \( \hat{H}_q(R) \) is the qubit Hamiltonian obtained from a second quantized form of \( \hat{H}_e(R) \)\textsuperscript{9} using one of the fermion-qubit mappings,\textsuperscript{10–14} and \( | \Psi_q(R) \rangle \) is the corresponding qubit wave-function. For a molecule, the qubit Hamiltonian is a linear combination

\[ \hat{H}_q(R) = \sum_I C_I(R) \hat{P}_I \]

of Pauli tensor products \( \hat{P}_I \) defined as

\[ \hat{P}_I = \prod_{i=1}^N \hat{\sigma}_i^{(I)}, \]

where \( \hat{\sigma}_i^{(I)} \) is one of the \( \hat{x}, \hat{y}, \hat{z} \) Pauli operators or the identity operator \( \hat{1} \) for the \( i \)-th qubit. The number of qubits, \( N \), is equal to the number of molecular spin-orbitals used in the second quantized form of the electronic Hamiltonian. Below, for simplicity, we will skip the nuclear configuration \( R \) but always assume its existence as a parameter.

Besides problems associated with devising low-depth circuits for accurate preparation of \( | \Psi_q \rangle \), the electronic structure problem poses another difficulty for VQE, namely estimation of the expectation value for the qubit Hamiltonian...
\[ \hat{H}_q \]. Note that in contrast to quantum simulators, in universal gate quantum computing, \( \hat{H}_q \) originated from \( \hat{H}_c \) is not physically implemented and does not correspond to the Hamiltonian of physical qubits. This makes its measurement a difficult task similar to the quantum tomography, with the only simplification that one needs to measure an \( O(N^4) \) subset of the total \( 4^N \) set of Pauli products.

Previously, the measurement problem has been addressed through grouping of Pauli products whose expectation value can be measured simultaneously. Owing to additivity of the total Hamiltonian expectation value such grouping allows the reduction of the number of separately measured operators. Considering that current hardware can only measure single-qubit operators and during the measurement the total wavefunction collapses to a tensor product state of one-qubit eigenstates of measured operators, only Pauli products that have a common tensor product eigen-basis (TPE) can be grouped together for simultaneous measurement. It was found to be possible to reformulate optimal grouping of terms based on their shared TPE as a graph minimum clique cover (MCC) problem. This reformulation gave a systematic approach to reduction of the total number of terms approximately three times from the total number of Hamiltonian terms.

TPE based grouping somewhat reduces the prefactor of the \( O(N^4) \) dependence for the number of measured groups but does not change the scaling. Recently another approach has been put forward: mean-field partitioning. Even though it gave some advantage compared to the TPE based partitioning, it requires introducing feed-forward measurement that has not yet become available in mainstream quantum hardware. Also, the assessment of mean-field partitioning is hindered by the absence of an optimal partitioning algorithm.

Here we propose a different approach: starting with groups of fully commuting terms we convert them into TPE sharing groups by introducing unitary transformations. The necessary unitary transformations are obtained analytically using an extension of symplectic geometry techniques developed by Bravyi et al. for tapering off qubits. In general, sizes of fully commuting groups in qubit Hamiltonians are much larger than those of TPE sharing groups, and the proposed technique allows for the scaling reduction of the number of simultaneously measurable groups, which significantly increases a range of molecular systems amenable to VQE studies on NISQ hardware.

\section{Theory}

\subsection{Tensor product eigen-basis sharing groups}

More insightful and practical criterion for grouping terms sharing TPE can be formulated using qubit-wise commutativity: two Pauli products are qubit-wise commutative if each single-qubit Pauli operator in one product commutes with its counterpart in the other product. Qubit-wise commutativity is a stricter condition than regular commutativity and thus can be considered as sufficient but not necessary for the latter. For example, \( \hat{x}_1 \hat{x}_2 \) and \( \hat{y}_1 \hat{y}_2 \) are both commutative and qubit-wise commutative, but \( \hat{x}_1 \hat{x}_2 \) and \( \hat{y}_1 \hat{y}_2 \) are only commutative.

In the conventional VQE scheme, \( \hat{H}_q \) is separated into sums of qubit-wise commuting (QWC) terms,

\[ \hat{H}_q = \sum_{n=1}^{M_{QWC}} \hat{A}_n, \]

\[ \hat{A}_n = \sum_{I} C_I^{(n)} \hat{P}_I^{(n)}, \]

where all \( \hat{P}_I^{(n)} \) within one \( \hat{A}_n \) group are qubit-wise commuting. Partitioning of \( \hat{H}_q \) in Eq. (5) allows one to measure all Pauli products within each \( \hat{A}_n \) term in a single set of \( N \) one-qubit measurements. For every qubit, it is known from the form of \( \hat{A}_n \), which Pauli operator needs to be measured. The advantage of this scheme is that it requires only single-qubit measurements, which are technically easier than multi-qubit measurements. Also, qubit-wise commutativity between terms provides a binary symmetric relation that is convenient for reformulation of optimal grouping as the MCC problem for a graph obtained by connecting \( \hat{H}_q \) Pauli products (vertices) that satisfy the qubit-wise commutativity relation. MCC is a partitioning of the Hamiltonian graph to the minimum number of fully connected (complete) subgraphs or cliques. The cliques represent terms that can be measured simultaneously.

The disadvantage of this scheme is that the Hamiltonian may require measuring too many \( \hat{A}_n \) terms separately (see Ref. 19 for examples, typically optimal partitioning of \( \hat{H}_q \) to QWC parts gives only reduction by a factor of 3 with respect to the total number of Pauli products in \( \hat{H}_q \)).

On the other hand, quantum mechanics allows us to determine eigenvalues of all mutually commuting operators at the same time. Therefore, potentially one can partition the Hamiltonian into groups of fully commuting terms

\[ \hat{H}_q = \sum_{n=1}^{M_C} \hat{H}_n, \]

\[ \hat{H}_n = \sum_{I} C_I^{(n)} \hat{P}_I^{(n)}, \]

and measure their expectation values. Clearly, because all QWC terms are also fully commuting the number of \( \hat{H}_n \) groups, \( M_C \), will not be larger than that for \( \hat{A}_n \) groups, \( M_{QWC} \). Moreover, Appendix A shows that the ratio between the numbers of Pauli products that commute and qubit-wise commute with an average Pauli product grows exponentially with the number of qubits. Two questions arise: 1) Is it possible to use the partitioning to fully commuting groups of terms in VQE without hardware modification?, and 2) How to find the optimal partitioning of the Hamiltonian to fully commuting groups of terms?
B. Unitary Transformations

To use more efficient partitioning in groups of fully commuting terms and keep the same single-qubit measurement protocol we introduce additional unitary transformations \( \{U_n\} \) that transform each fully commuting group \( \hat{H}_n \) into a QWC group, \( \hat{A}_n = U_n \hat{H}_n U_n^\dagger \). Note that \( \hat{A}_n \) are not necessarily the same QWC operators that appear in the QWC partitioning of \( \hat{H}_q \). Let us consider partitioning of the \( \hat{H}_q \) into fully commuting terms for the energy expectation value on a trial wavefunction \( \langle \Psi | \hat{H}_q | \Psi \rangle = \sum_n \langle \Psi | \hat{H}_n | \Psi \rangle \). (9)

By introducing resolutions of the identity \( \hat{U}_n^\dagger \hat{U}_n \) we can rewrite \( \hat{E} \) as

\[
\hat{E} = \sum_n \langle \Psi | \hat{U}_n^\dagger \hat{H}_n \hat{U}_n | \Psi \rangle = \sum_n \langle \Phi_n | \hat{A}_n | \Phi_n \rangle = \sum_n A_n, \tag{10}
\]

where we introduced the new wavefunctions \( |\Phi_n\rangle = \hat{U}_n |\Psi\rangle \) for which the QWC measurement of the \( \hat{A}_n \) group can be done in a regular manner. Since qubit-wise commutativity always implies full commutativity, introducing \( \hat{U}_n \) does not change the commutativity property of the \( \hat{H}_n \) set. Therefore, if we define \( \hat{U}_n \) and obtain \( \hat{A}_n \) groups, we can do QWC measurements of |\Phi_n\rangle wavefunctions that produce the expectation value of energy (see Fig. 1).

To accomplish this we use a somewhat extended idea of qubit tapering proposed by Bravyi et al.\textsuperscript{25} for the \( \hat{H}_n \) fragments. Bravyi et al. suggested a construction of unitary transformations applied to the whole qubit Hamiltonian that makes some of the qubit operators transform to the single Pauli operator \( \hat{x}_i \), which allows one to substitute \( \hat{x}_i \)'s by numbers and thus to remove them from consideration. For our purpose, we need to substitute all single-qubit operators within \( \hat{H}_n \) to a fixed single Pauli operator. This makes the transformed version of \( \hat{H}_n \) to have only QWC terms. Appendix B details the construction procedure for \( \hat{U}_n \) and also proves that such transformations always exist for linear combinations of commuting Pauli products. Another important aspect illustrated in Appendix B is efficiency of implementation of \( \hat{U}_n \) on both quantum and classical computers (see Fig. 1). This efficiency is guaranteed by the Gottesman-Knill theorem because \( \hat{U}_n \)'s can be expressed as a sequence of Clifford gates.\textsuperscript{26}

C. Illustrative Example

To illustrate the advantage of the new approach let us consider the model Hamiltonian \( \hat{H}_m = a \hat{x}_1 \hat{x}_2 + b \hat{z}_1 \hat{z}_2 \), clearly its parts commute and share eigenstates (i.e. Bell states)

\[
|\pm\rangle = \frac{1}{\sqrt{2}} (|\uparrow\uparrow\rangle \pm |\downarrow\downarrow\rangle) \tag{13}
\]

\[
|\mp\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle). \tag{14}
\]

These eigenstates give

\[
\hat{x}_1 \hat{z}_2 |\pm\rangle = (+1) |\pm\rangle \quad \hat{x}_1 \hat{x}_2 |\pm\rangle = (\pm 1) |\pm\rangle \tag{15}
\]

\[
\hat{z}_1 \hat{z}_2 |\mp\rangle = (-1) |\mp\rangle \quad \hat{x}_1 \hat{z}_2 |\mp\rangle = (\pm 1) |\mp\rangle \tag{16}
\]

and hence their eigenvalues for the model Hamiltonians are

\[
\langle |\pm\rangle | \hat{H}_m | |\pm\rangle = \pm a + b, \tag{17}
\]

\[
\langle |\mp\rangle | \hat{H}_m | |\mp\rangle = \pm a - b. \tag{18}
\]

If \( |\pm\rangle \) is set as a trial VQE wavefunction, a single-qubit measurement scheme cannot determine expectation values of \( \hat{z}_1 \hat{z}_2 \) and \( \hat{x}_1 \hat{x}_2 \) at the same time. This is easy to illustrate, by considering \( \hat{z}_1 \hat{z}_2 \) measurements, as it will collapse \( |\pm\rangle \) to either \( |\uparrow\uparrow\rangle \) or \( |\downarrow\downarrow\rangle \) with equal probabilities and an eigenvalue +1 for both outcomes. However, based on only \( \hat{z}_1 \hat{z}_2 \) measurements we will not be able to separate \( |\pm\rangle \) from \( |\mp\rangle \). On the other hand, expectation values of \( \hat{x}_1 \hat{x}_2 \) are uncertain after the \( \hat{z}_1 \hat{z}_2 \) measurement. Even though

\[
\langle |\uparrow\uparrow\rangle | \hat{x}_1 \hat{x}_2 | |\uparrow\uparrow\rangle = \langle |\downarrow\downarrow\rangle | \hat{x}_1 \hat{x}_2 | |\downarrow\downarrow\rangle = 0, \tag{19}
\]

there are nonzero variances for both wavefunctions. This is a result of a single-qubit projective measurement of \( |\pm\rangle \) that destroys the superposition and projects \( |\pm\rangle \) onto

\[
\hat{H}_m = \sum_{n=1}^{M_r} \hat{H}_n \quad \hat{A}_n = \hat{U}_n \hat{H}_n \hat{U}_n^\dagger \quad |\Psi\rangle = \hat{U} |0\rangle
\]
the $|\uparrow\rangle$ and $|\downarrow\rangle$ basis. The only way to obtain information on $\hat{x}_1 \hat{x}_2$ in the conventional single-qubit scheme is to start over and to measure $|\uparrow\rangle$ using $\hat{x}_1$ and $\hat{x}_2$ operators. This will produce the second set of data because measurement of $\hat{x}_1$ and $\hat{x}_2$ operators projects a wavefunction to a different basis

$$|\uparrow\rangle = \frac{1}{\sqrt{2}}(|\rightarrow\rangle + |\leftarrow\rangle),$$

(20)

where $\hat{x} |\rightarrow\rangle = +1 |\rightarrow\rangle$ and $\hat{x} |\leftarrow\rangle = -1 |\leftarrow\rangle$. In the case of $|\uparrow\rangle$ we will obtain two projections $|\rightarrow\rangle$ and $|\leftarrow\rangle$ both with eigenvalue +1, as previously the $z$ projections are uncertain after measuring $\hat{x}_1 \hat{x}_2$.

The new technique introduces a unitary transformation $\hat{U} = (\hat{x}_1 \hat{x}_2 + \hat{z}_1) (\hat{z}_1 \hat{x}_2 + \hat{x}_2)/2$ that modifies the model Hamiltonian into a QWC group

$$\hat{U} \hat{H}_n \hat{U}^\dagger = a \hat{z}_1 + b \hat{x}_2$$

(21)

Therefore, if we measure

$$\hat{U} |\uparrow\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle + |\downarrow\rangle) = |\rightarrow\rangle$$

(22)

on the QWC operator $a \hat{z}_1 + b \hat{x}_2$ we obtain $a + b$ in all instances with the wavefunction readout corresponding to $|\rightarrow\rangle$. Similarly, if $\hat{U} |\downarrow\rangle = |\rightarrow\rangle$ is measured for the QWC operator, we obtain the correct answer $-a + b$ in all cases with a single set of measurements.

D. Optimal partitioning of the Hamiltonian

Optimal partitioning for the qubit Hamiltonian to a minimal number of groups containing mutually commuting terms can be done exactly the same way as in the QWC partitioning. Regular commutativity can be also considered as a binary symmetric relation between Pauli products of the qubit Hamiltonian. This allows one to represent any qubit Hamiltonian as a graph with edges between commuting terms (vertices). As a simple illustration, one can consider the following model Hamiltonian

$$\hat{H}_q = \hat{z}_1 \hat{z}_2 + \hat{z}_1 \hat{z}_2 \hat{z}_3 + \hat{z}_1 \hat{z}_2 \hat{z}_4 + \hat{x}_3 \hat{x}_4 + \hat{y}_1 \hat{x}_3 \hat{x}_4 + \hat{y}_2 \hat{x}_3 \hat{x}_4,$$

(23)

whose commutativity graph is given in Fig. 2. Then, to determine how many terms can be measured at the same time, one needs to gather groups of terms that are commuting. In the graph representation, this means finding fully-connected sub-graphs or cliques. To optimize the measurement process we are interested in the minimum number of cliques, the MCC problem (Fig. 2, the middle panel)

$$\hat{H}_q = \hat{H}_1 + \hat{H}_2$$

$$\hat{H}_1 = \hat{z}_1 \hat{z}_2 + \hat{z}_1 \hat{z}_2 \hat{z}_3 + \hat{z}_1 \hat{z}_2 \hat{z}_4$$

(24)

$$\hat{H}_2 = \hat{x}_3 \hat{x}_4 + \hat{y}_1 \hat{x}_3 \hat{x}_4 + \hat{y}_2 \hat{x}_3 \hat{x}_4.$$  

(25)

This problem is NP-hard in general. Also, it is easy to see there are other clique covers possible (Fig. 2, the lower panel)

$$\hat{H}_q = \hat{H}_1' + \hat{H}_2' + \hat{H}_3'$$

(26)

$$\hat{H}_1' = \hat{z}_1 \hat{z}_2 + \hat{z}_3 \hat{x}_4$$

(27)

$$\hat{H}_2' = \hat{z}_1 \hat{z}_2 \hat{z}_3 + \hat{z}_1 \hat{z}_2 \hat{z}_4$$

(28)

$$\hat{H}_3' = \hat{y}_1 \hat{x}_3 \hat{x}_4 + \hat{y}_2 \hat{x}_3 \hat{x}_4.$$  

(29)

This solution contains larger number of cliques and thus is not optimal.

![Graph representation of commuting terms](image)

**FIG. 2.** Graph representation of commuting terms in the Hamiltonian Eq. (23) (upper panel), minimum clique cover of the graph (middle panel), non-minimum clique cover of the graph (lower panel).

Even though the MCC problem is NP-hard, there are several heuristic algorithms that scale quadratically with the number of vertices and thus can be easily used for obtaining close to optimal solutions. Assessment of several such heuristic techniques is done in Ref. 19 for Hamiltonian graphs based on qubit-wise commutativity. Here, we will use the same heuristics as for the QWC grouping, and their descriptions can be found in Ref. 19 and original papers: Greedy Coloring (GC),27 Largest First (LF),28 Smallest Last (SL),29 DSATUR (DS),30 Recursive Largest First (RLF),31 Dutton and Brigham (DB),32 COSINE (C),33 Ramsey (R),34 Bron-Kerbosch-Tomita (BKT).35 All these heuristics except BKT have polynomial computational scaling with respect to the number of graph vertices.
TABLE I. The number of qubits ($N$), Pauli products in the qubit Hamiltonian (Total), QWC groups ($M_{QWC}$), and commuting groups produced by different heuristics (see their description in the text) for systems with up to 14 qubits. The STO-3G basis has been used for all Hamiltonians unless specified otherwise. BK and JW denote the Bravyi-Kitaev and Jordan-Wigner fermion-qubit transformations.

| Systems    | $N$ | Total | $M_{QWC}$ | GC | LF | SL | DS | RLF | DB | C | R | BKT |
|------------|-----|-------|-----------|----|----|----|----|-----|----|----|----|-----|
| H$_2$ (BK) | 4   | 15    | 3         | 2  | 2  | 2  | 2  | 2   | 2  | 2  | 2  | 2   |
| LiH (Parity) | 4   | 100   | 25        | 18 | 16 | 15 | 14 | 11  | 10 | 11 | 13 | 9   |
| H$_2$O (6-31G, BK) | 6   | 165   | 34        | 12 | 9  | 14 | 9  | 8   | 8  | 11 | 10 | 8   |
| BeH$_2$ (BK) | 14  | 666   | 172       | 33 | 32 | 34 | 27 | 29  | 23 | 33 | 38 | -   |
| BeH$_2$ (JW) | 14  | 666   | 203       | 30 | 37 | 36 | 25 | 28  | 24 | 33 | 41 | -   |
| H$_2$O (BK) | 14  | 1086  | 308       | 50 | 54 | 55 | 49 | 37  | 33 | 56 | 68 | -   |
| H$_2$O (JW) | 14  | 1086  | 322       | 53 | 50 | 56 | 48 | 43  | 33 | 53 | 64 | -   |

TABLE II. Comparison of RLF results for Bravyi-Kitaev (BK) and Jordan-Wigner (JW) transformed Hamiltonians: the number of cliques ($M_C$), their maximum size (Max Size) and standard deviation of their size distribution (STD). The total number of Hamiltonian terms (Total) is almost everywhere the same for JW and BK; for the last two systems, the JW numbers are in parenthesis.

| Systems    | $N$ | Total | $M_C$ | Max Size | STD  | $M_C$ | Max Size | STD  |
|------------|-----|-------|-------|----------|------|-------|----------|------|
| BeH$_2$ / STO-3G | 14  | 666   | 29    | 59       | 12.5 | 28    | 62       | 15.3 |
| H$_2$O / STO-3G | 14  | 1086  | 37    | 88       | 18.4 | 43    | 88       | 16.6 |
| NH$_3$ / STO-3G | 16  | 3609  | 126   | 92       | 15.3 | 130   | 98       | 15.6 |
| N$_2$ / STO-3G | 20  | 2951  | 68    | 128      | 26.0 | 76    | 128      | 25.1 |
| BeH$_2$ / 6-31G | 26  | 9204  | 168   | 264      | 39.8 | 163   | 312      | 46.8 |
| H$_2$O / 6-31G | 26  | 12732 | 231   | 192      | 29.7 | 235   | 192      | 26.3 |
| NH$_3$ / 6-31G | 30  | 52758 (52806) | 917  | 280      | 30.4 | 922   | 238      | 29.7 |
| N$_2$ / 6-31G | 36  | 34639 (34655) | 366  | 393      | 63.9 | 357   | 377      | 66.3 |
III. NUMERICAL STUDIES AND DISCUSSION

To assess the impact of grouping fully commuting terms we solve the MCC problem for graphs of qubit Hamiltonians constructed for several molecule/basis pairs (see Tables I and II). Details of generating these Hamiltonians are given in Supplementary Information.

According to Table I, the deviation between the minimum number of commuting cliques produced by different heuristics can reach up to 50%. Out of all heuristics the best results on the first three small Hamiltonians were produced by BKT, but because of exponential scaling it is not applicable to Hamiltonians larger than hundred terms. The next best approach is DB, but already for the 14-qubit systems it spends two orders of magnitude longer of time than RLF and thus has not been selected to investigate larger systems. Therefore, as for QWC grouping, RLF remains the algorithm of choice, being optimal in terms of computational time and yielding about 25% fewer cliques than the next-best heuristics.

Least-square fitting of the fully commuting clique numbers for RLF in Table II with \( N \) in the double logarithmic scale results in an \( N^3 \) dependence (Fig. 3). This is an \( N \)-fold reduction from the same dependence of the total number of terms in the studied Hamiltonians, \( N^4 \) (Fig. 3). As for maximum clique sizes and standard deviations of clique size distributions (Table II), they grow with rates slightly higher and lower than linear in \( N \), respectively. Separate analysis for the JW and BK transformations did not reveal any significant differences between groupings in Hamiltonians obtained with these transformations.

We have introduced a new method to reduce the number of measurements in the VQE approach to the electronic structure problem. The method is based on partitioning of the qubit Hamiltonian to the minimum number of groups whose terms are fully mutually commuting. By introducing additional unitary transformations each group can be transformed into a group of QWC terms that can be measured simultaneously.

The main advantage of the new technique is that it can reduce the number of simultaneously measurable terms to largest groups of compatible operators without the need for modification of the currently used measuring algorithms. For the considered examples of molecular electronic Hamiltonians the method produces at least \( N \)-fold reduction of the number of measurable groups compared to the previously used QWC grouping. An additional unitary transformation for each group introduces into a VQE circuit only \( 2N \) one-qubit gates and \( N \) multi-qubit Pauli product exponents that can be decomposed into a product of up to \( N^{1+log_2 3} \) two-qubit gates. Also, since these unitary transformations modify each Pauli product into another Pauli product they can be encoded using only Clifford gates on a quantum computer and performed efficiently on a classical computer according to the Gottesman-Knill theorem. Using their Clifford property, according to Ref. 36, the number of CNOT gates in circuits of the unitary transformations can be reduced to \( O(N^2/log(N)) \). In case when extra unitary transformations are not affordable due to limitations in circuit depth, the conventional method of grouping based on the QWC property is preferable, since it does not introduce any nonlocal gates.

Another possible application of the proposed technique is a systematic way to make nonlocal measurements required in mutually unbiased bases (MUB) quantum state tomography (QST). Generally, there is an exponential growth of measurements needed in QST, a naive approach would require \( 4^{N_q} - 1 \) measurements, while using QWC grouping would allow for the reduction to \( 3^{N_q} \). Introducing MUB is equivalent to considering fully commuting sets of Pauli strings, and requires only measurements of \( 2^{N_q} + 1 \) groups containing \( 2^{N_q} - 1 \) fully commuting Pauli strings. However, it is recognized that MUB-QST is challenging due to the entanglement present in MUB, and our unitary transformations allow one to present each of the \( 2^{N_q} + 1 \) groups as a QWC group and thus perform only local measurements.

The idea of introducing unitary transformations that change some Hamiltonian fragments to the sum of QWC terms without modification of the expectation value can be taken to the limit where the whole Hamiltonian is transformed by a single unitary operator to a QWC group, \( \hat{U} \hat{H} \hat{U}^\dagger = \hat{A} \). The maximum size of a QWC group is \( 2^N \), and thus such \( \hat{A} \) exists. This would allow one to measure the entire Hamiltonian in a single set of measurements; however, the complexity of \( \hat{U} \) is equivalent to that of the

![FIG. 3. Dependencies of the total number of the Hamiltonian terms (blue) and the number of fully commuting groups (red) on the number of qubits for the systems in Table II in the double log-scale. For the last two entries of Table II, the JW and BK results were averaged.](image)
original many-body problem. Yet, this example suggests that in the measurement process one is not limited by only groups of fully commuting terms and more general unitary transformations can be potentially devised to reduce the number of simultaneously measurable terms.

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NOTE ADDED:

After submission of this manuscript to arXiv we became aware of several new proposals addressing the measurement problem, which appeared within a week or two from each other.\textsuperscript{41–47}

APPENDIX A: COMMUTING AND QUBIT-WISE COMMUTING TERMS

Here, we illustrate that for an average Pauli product, in the full set of $4^N$ Pauli products, there is exponentially more commuting than qubit-wise commuting Pauli products. An average Pauli product can be thought as $\hat{e}_1\ldots\hat{e}_{N/4},\hat{\sigma}_{N/4+1}\ldots\hat{\sigma}_N$, where $\hat{e}_i$'s denote the identities on $i$-th qubits, $\hat{\sigma}_j$ are Pauli operators, and $N \mod 4 = 0$ for convenience. The number of QWC terms is

$$N_{\text{QWC}} = 4^{N/4}2^{3N/4} = 2^{5N/4}, \quad (30)$$

because in $\hat{e}_1\ldots\hat{e}_{N/4}$ one can substitute any identity by any Pauli operator without violating the QWC condition, which gives factor $4^{N/4}$, and in $\hat{\sigma}_{N/4+1}\ldots\hat{\sigma}_N$ one can substitute any $\hat{\sigma}$ by identity, which gives rise to factor $2^{3N/4}$. The number of terms commuting with the average Pauli product is

$$N_C = 4^N/2 = 2^{2N-1}. \quad (31)$$

Here we used the fact that the total number of Pauli products is $4^N$ and a half of them will be commuting with any non-constant Pauli product and another half will be anti-commuting. Therefore, the ratio $N_C/N_{\text{QWC}} = 2^{3N/4-1}$ grows exponentially with $N$.

APPENDIX B: DETAILS OF UNITARY TRANSFORMATIONS

Here we detail the construction of unitary transformations that produce QWC terms from any linear combination of fully commuting Pauli products. A few elements of this construction are taken from Bravyi et al.,\textsuperscript{25} but to keep the discussion uniform and self-contained we reproduce them here.

Unitary transformations

Let us consider construction of $\hat{U}_n$ for one of the Hamiltonian fragments $\hat{H}_n$ that contains mutually commuting Pauli products,

$$\hat{H}_n = \sum_I C_I \hat{P}_I, \quad [\hat{P}_I, \hat{P}_J] = 0. \quad (32)$$

Due to this commutativity and a mapping between the Pauli operator and symplectic linear vector spaces, it is possible to apply techniques developed by Bravyi et al.\textsuperscript{25} to find a set $\mathcal{T} = \{\hat{\tau}_1, \ldots, \hat{\tau}_n\}$ of $N$ mutually commuting Pauli products, which also commute with all terms of $\hat{H}_n$. Additionally, one can find a set $\mathcal{Q} = \{\hat{\sigma}_1, \ldots, \hat{\sigma}_N\}$ of single qubit Pauli operators $\hat{\sigma}_i$ for each $\hat{\tau}_i$ so that

$$\{\hat{\tau}_i, \hat{\sigma}_j\} = 0, \quad (33)$$

$$[\hat{\tau}_i, \hat{\tau}_j] = 0, \quad i \neq j \quad (34)$$

$$[\hat{\sigma}_i, \hat{\sigma}_j] = 0. \quad (35)$$

The unitary operation $\hat{U}_n$ that transforms $\hat{H}_n$ to its QWC form can be constructed as

$$\hat{U}_n = \prod_{i=1}^N \frac{1}{\sqrt{2}} (\hat{\tau}_i + \hat{\sigma}_i) \quad (36)$$

$$= \prod_{i=1}^N \hat{V}_i. \quad (37)$$

Here, each $\hat{V}_i$ takes $\hat{\tau}_i$ to the single-qubit Pauli operator $\hat{\sigma}_i$

$$\hat{V}_i^\dagger \hat{\tau}_i \hat{V}_i = \frac{1}{2} (\hat{\tau}_i + \hat{\sigma}_i) \hat{\tau}_i (\hat{\tau}_i + \hat{\sigma}_i) \quad (38)$$

$$= \frac{1}{2} (\hat{\tau}_i^3 + \hat{\tau}_i^2 \hat{\sigma}_i + \hat{\sigma}_i \hat{\tau}_i^2 + \hat{\sigma}_i \hat{\tau}_i \hat{\sigma}_i) \quad (39)$$

$$= \frac{1}{2} (\hat{\tau}_i + 2\hat{\sigma}_i - \hat{\tau}_i) = \hat{\sigma}_i. \quad (40)$$

where we used $\hat{\tau}_i^2 = \hat{\sigma}_i^2 = \hat{e}$ and anti-commutativity of $\hat{\tau}_i$ and $\hat{\sigma}_i$. The same effect on $\hat{\tau}_i$ will be from the full product of $\hat{V}_i$'s in $\hat{U}_n$, $\hat{U}_n^\dagger \hat{\tau}_i \hat{U}_n = \hat{\sigma}_i$, because $[\hat{V}_j, \hat{\tau}_i] = 0$ if $i \neq j$. Finally, using symplectic geometry techniques, it is possible to express every $\hat{P}_I$ from $\hat{H}_n$ as a product of $\hat{\tau}_i$'s up to a phase (essentially $\hat{\tau}_i$'s form a basis for elements of $\hat{H}_n$), and therefore, all $\hat{P}_I$'s can be transformed into products of $\hat{\sigma}_i$'s

$$\hat{U}_n^\dagger \hat{H}_n \hat{U}_n = \sum_I C_I \hat{U}_n^\dagger \hat{P}_I \hat{U}_n \quad (41)$$

$$= \sum_I C_I \hat{P}_I'. \quad (42)$$

where $\hat{P}_I'$ is a product of $\hat{\sigma}_i$ up to a phase. The procedures to obtain $\mathcal{T}$, $\mathcal{Q}$, and $\hat{P}_I$ expansions in terms of elements of $\mathcal{T}$ are detailed below.
FEW ELEMENTS OF SYMPLECTIC GEOMETRY

Before going to the procedures we would like to provide few elements of symplectic geometry essential for understanding these procedures.

Operator-vector space mapping

To be able to use methods of symplectic geometry we introduce a mapping between $N$-qubit Pauli products and $2N$ symplectic vector space $\mathcal{F}$ over the $GF(2)$ field (also known as binary field $\mathbb{Z}_2$). Any Pauli product $\vec{P}$ corresponds to a binary vector $\vec{P}$ with $i^{th}$ and $(N+i)^{th}$ components defined as

$$ (\vec{P}_i, \vec{P}_{N+i}) = \begin{cases} (0, 1) & i^{th} \text{ qubit of } \vec{P} \text{ is } \hat{z} \\ (1, 0) & i^{th} \text{ qubit of } \vec{P} \text{ is } \hat{x} \\ (1, 1) & i^{th} \text{ qubit of } \vec{P} \text{ is } \hat{y} \\ (0, 0) & i^{th} \text{ qubit of } \vec{P} \text{ is } \hat{\epsilon}. \end{cases} \quad (43) $$

For example, for $N = 4$, $\vec{P} = \hat{x}_1\hat{y}_2\hat{z}_3\hat{\epsilon}_4$ is mapped to $\vec{P} = (1100; 0110)$, where the semicolon is put only for readability.

This mapping is convenient because commutativity between two Pauli products $[\vec{P}_1, \vec{P}_2] = 0$ corresponds to orthogonality between corresponding vectors, $[\vec{P}_1|\vec{P}_2] = 0$. The inner product $\langle \vec{P}_1|\vec{P}_2 \rangle$ between two vectors $\vec{P}_1$ and $\vec{P}_2$ is defined in a symplectic manner

$$ \langle \vec{P}_1|\vec{P}_2 \rangle = (\vec{P}_1, \vec{J}\vec{P}_2), \quad (44) $$

where $(,)$ is the normal Euclidian inner product and $\vec{J}$ is a symplectic metric matrix

$$ \vec{J} = \begin{bmatrix} 0_{N\times N} & 1_{N\times N} \\ 1_{N\times N} & 0_{N\times N} \end{bmatrix}. \quad (45) $$

Therefore, we will use commutation and orthogonality interchangeably. The symplectic inner product is bi-linear, and thus if $\vec{P}_1$ commutes with $\vec{P}_2$ and $\vec{P}_3$, then $\vec{P}_1$ is orthogonal to $\vec{P}_2 + \vec{P}_3$. Also anti-commutation $\{\vec{P}_1, \vec{P}_2\} = 0$ corresponds to $\langle \vec{P}_1|\vec{P}_2 \rangle = 1$.

Another useful correspondence is between results of addition of vectors and multiplication of Pauli product operators: $\vec{P}_1 + \vec{P}_2 = \vec{P}_3$ is equivalent to $\vec{P}_1 \cdot \vec{P}_2 = p\vec{P}_3$, where $p$ is a phase factor that has values $\pm 1, \pm i$ depending on single-qubit Pauli operators and their order in the $\vec{P}_1\vec{P}_2$ product.

Types of symplectic subspaces

Here we introduce a few types of symplectic subspaces that will be utilized to treat the fully commuting sets of operators. For a subspace $V$, the orthogonal complement will be denoted by $V^\perp$. The dimensionality of the two subspaces are connected by $\dim(V) + \dim(V^\perp) = 2N$.

while taking the complement twice returns the initial subspace, $(V^\perp)^\perp = V$. The examples below are given for $N = 2$, which corresponds to a $4$-dimensional symplectic vector space.

- $V$ is Isotropic $\iff V \subset V^\perp$. For example, $V = \text{span}\{(10; 00)\}$ is an isotropic subspace with the orthogonal complement

$$ V^\perp = \text{span}\{(10; 00), (01; 00), (00; 01)\}, \quad (46) $$

which contains $V$.

- $V$ is Coisotropic $\iff V^\perp \subset V$. For example, taking the $V^\perp$ of the previous example as $V$ one obtains a coisotropic subspace

$$ V = \text{span}\{(10; 00), (01; 00), (00; 01)\}, \quad V^\perp = \text{span}\{(10; 00)\}. \quad (47) $$

- $V$ is Lagrangian $\iff V = V^\perp$. For example,

$$ V = \text{span}\{(10; 00), (01; 00)\} = V^\perp. \quad (49) $$

A Lagrangian subspace is also the largest isotropic or the smallest coisotropic subspace.

Based on these examples it is clear that if $V$ is isotropic then $V^\perp$ is coisotropic, and $\dim(V) \leq N$, $\dim(V^\perp) \geq N$. It also can be proven that, for any isotropic space $V$, there exists Lagrangian subspace $L$ such that $V \subseteq L \subseteq V^\perp$, and $\dim(L) = N$. 48

PROCEDURES

A set of mutually commuting Pauli products from $\hat{H}_n$ is isomorphic to an isotropic subspace in the symplectic vector space of $2N$ dimensions. Thus, we can always find the Lagrangian subspace and its basis of $N$ orthogonal basis vectors. These basis vectors are mapped to the mutually commuting $\hat{\tau}_i$’s operators that also commute with all terms in $\hat{H}_n$.

Finding $\hat{\tau}_i$’s

Here we show how to find the $N$ mutually commuting operators $\hat{\tau}_i$’s that also commute with all terms in the group of Pauli terms $\hat{H}_n$.

Step 1: Finding orthogonal basis vectors using Gaussian elimination: Gaussian elimination for all elements of $\hat{H}_n$ creates a basis of $V$ that is mutually commuting because the original terms are mutually commuting and their addition does not change this property. This basis forms isotropic space because all basis vectors are self-orthogonal and therefore can be thought as a part of the $V^\perp$ basis, hence, the condition $V \subseteq V^\perp$ is satisfied and $V$ is isotropic.
Then a new basis set of $M$ transform operators formation subspace that can be mapped directly to $N$ cannot find any new anti-commuting pairs, it will have $M$ to produce the procedure of orthogonalization of all \(\{\vec{c}\}_{k=1}^{M}\) by using a symplectic version of the Gram-Schmidt orthogonalization procedure. First, a pair of anti-commuting vectors is found. Using the enumeration freedom we can assume that this pair is formed by first two vectors: \((\vec{c}_1 | \vec{c}_2) = 1\). Then the other vectors are orthogonalized to the first two as follows

\[
\vec{c}_k = \vec{c}_k + (\vec{c}_k | \vec{c}_2) \vec{c}_1 + (\vec{c}_k | \vec{c}_1) \vec{c}_2, \quad k \in [3, M]
\]

so that

\[
(\vec{c}_1 | \vec{c}_k) = (\vec{c}_2 | \vec{c}_k) = 0.
\]

Then a new basis set of $M - 1$ vectors is formed, \(\vec{c}_1 \cup \{\vec{c}_k\}_{k=3}^{M}\). Note that there is a freedom in eliminating either \(\vec{c}_1\) or \(\vec{c}_2\) from the old basis. In the new basis, the only possible source of anti-commutativity is the \(\vec{c}_k\) subset, so the procedure for the search of an anti-commuting pair is repeated. Once the new pair is found the procedure of orthogonalization of all \(\{\vec{c}_k\}\) to that pair is repeated with elimination of one of the pair members to produce $M - 2$ basis vectors. Once the algorithm cannot find any new anti-commuting pairs, it will have $N$ mutually commuting basis vectors of the Lagrangian subspace that can be mapped directly to $\tau_i$’s.

**Finding $\tilde{\sigma}_i$’s**

Given a set of $\tilde{\tau}_i \in \mathcal{T}$, to build the unitary transformation $\tilde{U}_n$ [Eq. (36)] requires a set of single qubit Pauli operators $\tilde{\sigma}$ (i.e. $x_1$, $y_2$, $z_3$ etc.) satisfying

\[
(\tilde{\tau}_i | \tilde{\sigma}_j) = \begin{cases} 
1, & i = j \\
0, & i \neq j
\end{cases}
\]

(52)

\[
(\tilde{\sigma}_i | \tilde{\sigma}_j) = 0.
\]

(53)

Note that Eq. (53) requires that all $\tilde{\sigma}_i$’s correspond to different qubits. The resulting transformation $\tilde{U}_n$ will transform $\tilde{\tau}_i \rightarrow \tilde{\sigma}_i$.

For $\tilde{\tau}_1$, we have $N$ qubits available to define $\tilde{\sigma}_1$, so if $\tilde{\tau}_1$ has $\tilde{\sigma}_1$, $\tilde{\sigma}_1$ should be one of anti-commuting operators $\tilde{\sigma}_1$ or $\tilde{\sigma}_2$. To make the rest of $\tilde{\tau}_i$’s to commute with $\tilde{\sigma}_1$ we perform an orthogonalization step:

\[
\tilde{\tau}_k = \tilde{\tau}_k + (\tilde{\tau}_k | \tilde{\sigma}_1) \tilde{\sigma}_1, \quad k \in [2, N],
\]

so that $(\tilde{\tau}_k | \tilde{\sigma}_1) = 0$ is guaranteed, and the mutual commutation between $\tilde{\tau}_k$ is not changed. Then we find $\tilde{\sigma}_i$’s for the available qubits for the rest of $\tilde{\tau}_i$’s and after finding each $\tilde{\sigma}_i$ we do re-orthogonalization of $\{\tilde{\tau}_j\}_{j=i+1}^{N}$.

Let us prove the existence of $N \tilde{\sigma}_i$’s that can be found in the described process. We have already shown that it is straightforward to find the initial $\tilde{\sigma}_1$, let us consider some intermediate step, where $\mathcal{T}_A$ is a subset of $\mathcal{T}$ with $N_A$ elements for which $N_A \tilde{\sigma}_i$’s are found and are assigned to a $Q_A$ set. Then $\mathcal{T}_B = \mathcal{T}/\mathcal{T}_A$ is a complementary subset with the rest of $\tilde{\tau}_i$’s that are commuting with operators from both $\mathcal{T}_A$ and $Q_A$ sets. To continue the process we need to find a non-trivial (i.e. non-identity) qubit operator $\tilde{\sigma}'$ for a qubit that is not present in the $Q_A$ set but is in one of the elements of $\mathcal{T}_B$. Then, constructing the next $\tilde{\sigma}_{A+1}$ operator can be done by taking an operator that anti-commutes with $\tilde{\sigma}'$. To prove that this is possible we will show that such a non-trivial $\tilde{\sigma}'$ exists. Let us assume the contrary and arrive to a contradiction. Indeed, if all $\mathcal{T}_B$ elements have only trivial (i.e. identity) qubit operators for qubits higher than $N_A$, then they either must be all equal to the identity, which is a zero vector and cannot be a basis vector in the Lagrangian subspace, or they will not be able to commute with both $Q_A$ and $\mathcal{T}_A$ sets simultaneously, which is also a contradiction to the initial assumption about commutativity of $\mathcal{T}_B$ elements with the $Q_A$ and $\mathcal{T}_A$ sets.

**Obtaining expansions in $\tilde{\tau}_i$’s**

To apply the unitary operator $\tilde{U}_n$ in Eq. (36) to all Pauli products $\tilde{P}_i$’s in $\tilde{H}_n$, $\tilde{P}_i$’s need to be presented as products of $\tilde{\tau}_i$’s. Let $\tilde{P}$ be one of the Pauli products in $\tilde{H}_n$ for which sets $\mathcal{T}$ and $Q$ are found. Since the $\mathcal{T}$-set forms a basis in $L$ and the sum of the vectors can be mapped to a product of operators up to a phase, we can always find a subset, $K \subset \mathcal{T}$, so that

\[
\tilde{P} = p \prod_{\tilde{\tau}_k \in K} \tilde{\tau}_k,
\]

(55)

where $p$ is a phase that arises from multiplication between $\tilde{\tau}_k$. To find subset $K$ we solve a system of linear equations $A \vec{x} = \vec{b}$, where $A = [\tau_1, ..., \tau_N]$ is the $2N \times N$ binary matrix built out of $\tilde{\tau}_i$’s operators turned into corresponding vectors, and $\vec{b}$ is a symplectic vector representation of $\tilde{P}$. Indices of the binary vector $\vec{x}$ corresponding to nonzero entries give $k$ indices for $\tilde{\tau}_k$’s in $K$. We use the Gaussian elimination to solve for $\vec{x}$ in binary field $GF(2)$. This
representation makes transformation of each \( \hat{P} \) analytic

\[
\hat{U}_n^i \hat{P} \hat{U}_n = p \prod_{\hat{\tau}_k \in \mathcal{K}} \hat{U}_n^i \hat{\tau}_k \hat{U}_n = p \prod_k \hat{\sigma}_k. \tag{57}
\]

**Complexity of operations performed on a classical computer**

Finding the partitioning of the Hamiltonian into groups of all commuting terms uses the RLF heuristic that scales cubicly with the number of terms in \( \hat{H} \), the total number of terms in the Hamiltonian scales as \( O(N^4) \), and therefore, the total scaling of this step is \( O(N^4) \). In spite of the large degree, the pre-factor of this scaling is quite small.

Here we will consider the computational cost for finding \( \hat{U}_n \) for each of fully-commuting groups of terms in the Hamiltonian, \( \hat{H}_n \). Let \( n \) be the number of \( \hat{P}_l \) terms in \( \hat{H}_n \). Constructing \( \hat{U}_n \) requires the following procedures:

1) Finding \( N \hat{\tau}_i \)'s: The preliminary step involves representing \( n \hat{P}_l \)'s in the binary form, which scales as \( O(nN) \).

   **Step 1:** The Gaussian elimination applied to the binary matrix of \( \hat{P}_l \)'s (the matrix size is \( n \times 2N \)) costs \( O(nN^2) \).

   **Step 2:** Obtaining the null space after the Gaussian elimination costs \( O(N^3) \).

   **Step 3:** Constructing the Lagrangian subspace costs \( O(N^3) \) in CPU and \( O(N^2) \) in memory to save intermediate results of anti-commuting pairs.

2) Finding \( \hat{\sigma}_i \)'s: The orthogonalization step in Eq. (54) leads to \( O(N^3) \) scaling of \( \hat{\sigma}_i \)'s search because for each of \( N \hat{\tau}_i \)'s, a particular \( \hat{\sigma}_i \) can lead to modification of at most \( N \) other \( \hat{\tau}_i \)'s and each modification scales as \( O(N) \).

3) Expanding \( \hat{P}_l \)s in \( \hat{\tau}_i \)'s: Finding \( \hat{P}_l \) as a product of \( \hat{\tau}_k \) uses the Gaussian elimination, which costs \( O(N^3) \) for each element; there are \( n \) elements, so the total cost is \( O(nN^3) \). Computing the phase \( p \) in Eq. (55) for each \( \hat{P}_l \) requires \( O(N^2) \) multiplications since the number of \( \hat{\tau}_k \)'s scales as \( O(N) \) and each of them can have up to \( N \) Pauli operators. Thus, this part scales as \( O(nN^2) \) in total.

Considering all parts of the \( \hat{U}_n \) generation, the largest scaling is \( O(nN^3) \).

**Encoding unitary transformations on a quantum computer**

To put \( \hat{V}_i \)’s into a form acceptable for encoding on a quantum computer, we rewrite them as

\[
\hat{V}_i = (-i)e^{\frac{i}{2} \hat{\sigma}_i} e^{\frac{i}{2} \hat{\tau}_i} e^{\frac{i}{2} \hat{\sigma}_i}. \tag{58}
\]

It is straightforward to check that it is indeed an equality

\[
e^{\frac{i}{2} \hat{\sigma}_i} e^{\frac{i}{2} \hat{\tau}_i} e^{\frac{i}{2} \hat{\sigma}_i} = \frac{1}{2^{N^2/2}} (1 + i\hat{\sigma}_i)(1 + i\hat{\sigma}_i)(1 + i\hat{\sigma}_i)
\]

\[
= \frac{1}{2^{N^2/2}} (1 + i\hat{\sigma}_i + i\hat{\tau}_i - \hat{\sigma}_i \hat{\tau}_i)(1 + i\hat{\sigma}_i)
\]

\[
= \frac{1}{2^{N^2/2}} (1 + i\hat{\sigma}_i + i\hat{\tau}_i - \hat{\sigma}_i \hat{\tau}_i - \hat{\tau}_i \hat{\sigma}_i)
\]

\[
= \frac{i}{\sqrt{2}} (\hat{\tau}_i + \hat{\sigma}_i) = i\hat{V}_i, \tag{59}
\]

where to arrive at the last line we used anti-commutation between \( \hat{\tau}_i \) and \( \hat{\sigma}_i \).

In the worst case \( \hat{\tau}_i \) may involve all \( N \) qubits. We can decompose \( e^{\frac{i}{2} \hat{\tau}_i} \) into product of \( O(N^{\log_2 3}) \) two-qubit operations.49 Hence, \( \hat{U}_n \) [Eq. (36)] requires at most \( O(N^{1+\log_2 3}) \) one- and two-qubit gates. Moreover, note that \( \hat{U}_n \) transforms each Pauli product into another Pauli product and thus can be written as a sequence of Clifford gates.26 Aaronson and Gottesman36 found that for circuits containing only Clifford gates the number of CNOT gates can be bounded by \( O(N^2/\log(N)) \).

**Example: \( \text{H}_2 \) molecule**

We provide below a simple example of constructing the unitary transformation for one of two mutually commuting groups in the qubit Hamiltonian of \( \text{H}_2/\text{STO-3G} \). The BK transformed qubit Hamiltonian of \( \text{H}_2 \) contains the following mutually commuting group

\[
\hat{H}_1 = -0.4738 + 0.1412z_1 + 0.0558x_2z_0 + 0.0558y_2z_1y_0 + 0.0868z_2z_0 + 0.1425z_2z_1z_0 + 0.1489z_3z_1
\]

\[
+ 0.0558z_3x_2z_1x_0 + 0.0558z_3y_2z_1y_0 + 0.0868z_3z_2z_0 + 0.1425z_3z_2z_1z_0, \tag{60}
\]

The described procedures produce the following sets of \( T \) and \( Q \)

\[
T = \{ z_3, \hat{z}_1, \hat{y}_2y_0, \hat{x}_2\hat{x}_0 \} \tag{61}
\]

\[
Q = \{ \hat{x}_3, \hat{x}_1, \hat{x}_2, \hat{y}_0 \}, \tag{62}
\]

and the unitary operation

\[
\hat{U}_1 = 0.25x_3x_1x_0 + 0.25x_3x_1z_0 + 0.25x_3x_2x_0 + 0.25x_3x_2z_0
\]

\[
+ 0.25x_3x_2z_1y_0 + 0.25x_3y_2x_1 + 0.25x_3y_2z_1
\]

\[
- 0.25x_3z_2x_1z_0 - 0.25x_3z_2z_1x_0 + 0.25x_3z_1x_0
\]

\[
+ 0.25z_3z_0z_1 + 0.25z_3z_1x_0 + 0.25z_3z_2z_0
\]

\[
+ 0.25z_3y_2z_1 + 0.25z_3y_2z_1 - 0.25z_3z_2x_0 - 0.25z_3z_2z_0. \tag{63}
\]

The result of the transformation is a QWC group

\[
\hat{U}_1^\dagger \hat{H}_1 \hat{U}_1 = -0.4738 + 0.1412z_1 + 0.0558x_1y_0
\]

\[
- 0.0868y_2y_0 + 0.0558x_2x_1 - 0.1425x_2x_1y_0
\]

\[
+ 0.1489x_3x_1 + 0.0558x_3x_0 - 0.0868x_2x_0y_0
\]

\[
+ 0.0558x_3x_2x_1 - 0.1425x_3x_2x_1y_0. \tag{64}
\]
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