Efficient quantum measurement of Pauli operators

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Estimating the expectation value of an observable is a fundamental task in quantum computation. Unfortunately, it is often impossible to obtain such estimates directly, as the computer is restricted to measuring in a fixed computational basis. One common solution splits the observable into a weighted sum of Pauli operators and measures each separately, at the cost of many measurements. An improved version first groups mutually commuting Pauli operators together and then measures all operators within each group simultaneously. The effectiveness of this depends on two factors. First, to enable simultaneous measurement, circuits are required to rotate each group to the computational basis. In our work, we present two efficient circuit constructions that suitably rotate any group of \(k\) commuting \(n\)-qubit Pauli operators using at most \(kn - k(k + 1)/2\) and \(O(kn/\log k)\) two-qubit gates respectively. Second, metrics that justifiably measure the effectiveness of a grouping are required. In our work, we propose two natural metrics that operate under the assumption that measurements are distributed optimally among groups. Motivated by our new metrics, we introduce SORTED INSERTION, a grouping strategy that is explicitly aware of the weighting of each Pauli operator in the observable. Our methods are numerically illustrated in the context of the Variational Quantum Eigensolver, where the observables in question are molecular Hamiltonians. As measured by our metrics, SORTED INSERTION outperforms four conventional greedy colouring algorithms that seek the minimum number of groups.

I. INTRODUCTION

Estimating the expectation value \(\langle O \rangle_\psi\) of an observable \(O\) on a quantum state \(|\psi\rangle\) is a fundamental task in quantum mechanical experiments. However, often there is no natural way to measure \(O\) directly and some indirect protocol is required. In particular, this is true of current quantum computers that can only measure each qubit in the computational basis defined, by convention, as eigenstates of the Pauli-Z operator.

One naive protocol, therefore, is to decompose \(O\) into a weighted sum of \(t\) Pauli operators (or Paulis) \(\{P_i\}_{i=1}^t\) and then measure each \(P_i\) separately. An extended version assembles the Paulis into \(N\) commuting subsets, or “groups”, given by

\[
C_i := \{P_{jk} \}_{j=1}^{m_i}, \quad i = 1, \ldots, N, \quad (1)
\]

for some \(m_i\). All Paulis in a group can then be measured at the same time, as any set \(C_j\) of commuting Paulis can be simultaneously diagonalised by a single unitary \(U\), so

\[
\langle P \rangle_\psi = \langle \Lambda(P) \rangle_U \psi, \quad \text{for all } P \in C_j, \quad (2)
\]

where \(\Lambda(P) := UPU^\dagger\) is diagonal in the computational basis. To measure all operators in \(C_j\) simultaneously, we first apply the unitary “rotation” \(U\) to \(|\psi\rangle\), then measure in the computational basis which yields a bitstring, \(z\), of measurements on each qubit, and finally, for each \(P \in C_j\), classically post-process \(z\) according to \(\Lambda(P)\) to infer \(\langle P \rangle_\psi\).

Expectation estimation features prominently as the quantum sub-routine of the Variational Quantum Eigensolver (VQE) algorithm [1], which has emerged as a leading candidate for exhibiting quantum advantage in the Noisy Intermediate Scale Quantum era [2]. VQE is a hybrid quantum-classical algorithm designed to find the ground state \([1, 3–9]\), or energy spectra \([10–15]\), of a physical or chemical system. The observable \(O\) in question is a Hamiltonian \(H\) on \(n\) qubits. In the context of quantum chemistry, \(H\) readily decomposes into a weighted sum of Paulis via, for example, the Jordan-Wigner [16], Bravyi-Kitaev [17], or Verstraete-Cirac [18] transformations.

The paper that introduced VQE [1] proposed measuring \(H\) according to the naive protocol above. However, this can be inefficient. For example, a second-quantised chemical Hamiltonian on \(n\) qubits decomposes into a very large number of Paulis that scales as \(n^4\). To remedy this problem, McClean et al. [3] proposed the extended protocol. The authors also argued using a toy example that, due to covariances between Paulis, optimally grouping \(C_j\) might not be the same as minimising the number of groups, \(N\). However, Ref. [3] did not propose strategies to obtain the commuting groups \(C_j\), neither did it show how to construct the rotation \(U\) that enables simultaneous measurement.

Recently, a series of papers [19, 23, 24] have appeared that together make good progress on both the grouping strategy and rotation construction problems. Our paper is in this same arena and attacks both problems.

First, we contribute two new methods for constructing Clifford rotation circuits \(U\) that enable simultaneous measurement of arbitrary \(C_j\), i.e., a group containing arbitrary commuting Paulis. Like Ref. [23], we approached the problem via the stabiliser formalism but have gone further to consider the case when \(C_j\) has any number \(k \leq n\) of independent Paulis. We show that the number of two-qubit gates in \(U\) can be reduced in a way that scales with \(k\). This is important because it is atypical for actual groupings to have exactly \(k = n\) independent Paulis and reducing the number of two-qubit gates is important, especially in the near-term [25, 39]. As far as we are aware, ours is the first paper to consider the \(k < n\) case ex-

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plicitly. Also, we emphasise the role classical post-processing can play in saving quantum resources.

More specifically, we introduce constructions “CZ” and “CNOT”. The CZ-construction builds on work by Van den Nest, Dehaene, and De Moor [40] in the graph-state literature to yield $U$ with a number of two-qubit gates, or “2q-size”, at most

$$u_{cz}(k, n) = kn - k(k + 1)/2.$$  

(3)

The CNOT-construction builds on our CZ-construction, and work by Aaronson and Gottesman [41] and Patel, Markov, and Hayes [42] to yield $U$ with 2q-size at most

$$u_{cnot}(k, n) = O(kn / \log k).$$  

(4)

We stress that $u_{cnot}$ and $u_{cz}$ are worst-case upper bounds. In practice, numerical simulations are needed to determine whether the CZ- or CNOT-construction is actually more efficient. We note that, in the case of $k = n$, our methods produce a two-qubit gate count scaling no worse than the previous best of $O(n^2)$ [23]. Other works, such as Ref. [23], Appendix A1, prove only that a Clifford $U$ exists, or demonstrate a worst-case gate count scaling that is worse than $O(n^2)$ [21]. Appendix B1, or present a method that cannot be used for arbitrary $C$ [22].

When considering the grouping strategy problem, we contribute two new but natural metrics, $R$ and $\hat{R}$, that quantify the performance of any given grouping. $R$ and $\hat{R}$ measure the ratio between the number of measurements required in the ungrouped case versus the grouped case to attain a fixed level of accuracy. The key novelty in these two metrics is that they assume measurements on the groups are distributed optimally to maximise accuracy, following Refs. [8, 43, 44]. The difference between them is that $R$ is state-dependent but $\hat{R}$ is designed to approximate $E[R]$ over the uniform spherical measure. Therefore, $R$ is more suitable for use given some knowledge of the underlying state $|\psi\rangle$, while $\hat{R}$ is more suitable otherwise.

We find it useful to prove that, for all $|\psi\rangle$, breaking a single commuting group into two never improves $R$ nor $\hat{R}$. More formally, let group $C_{a\cup b}$ be the disjoint union of groups $C_a$ and $C_b$; then

$$R(\{C_a, C_b\}) \geq R(\{C_{a\cup b}\}) \quad \text{for all } |\psi\rangle.$$  

(5)

This result is in direct contrast to the conclusion of the aforementioned toy example used by McClean et al. [3], and analysed in full in Ref. [23, Sec. 10.1], that breaking a group can be advantageous. The reason for the discrepancy is that we assume measurements are distributed optimally, whereas they assume measurements are distributed uniformly.

Informed by the mathematical form of $\hat{R}$, we contribute our new grouping strategy SORTED INSERTION. Unlike strategies used previously [19, 20, 23]. SORTED INSERTION is explicitly aware of the coefficients in the Pauli decomposition of an observable $O$. We present data showing SORTED INSERTION outperforming all four conventional greedy colouring algorithms that we tried, as measured by the metric $\hat{R}$. Our data also challenges the assumption that minimising the number of groups $N$ is optimal, as groupings with the smallest number of groups do not typically perform the best with respect to $\hat{R}$. Note that this does not logically contradict Eq. (5). We quantify the performance of SORTED INSERTION using the metric $\hat{R}$ for molecules ranging in size from hydrogen $H_2$, which requires two qubits, to hydrogen selenide $H_2Se$, which requires 38, finding that it leads to a 10 to 60 fold improvement in the number of measurements required. Note that we are defining a single measurement to consist of a measurement of all qubits, and so the number of measurements equals the number of ansatz state preparations.

Finally, we run SORTED INSERTION alongside our CZ-construction on molecules requiring up to 38 qubits to calculate the actual number of two-qubit gates required for real molecular systems. Our numerical results show that the typical number of two-qubit gates is fewer than the worst-case $u_{cz}(k, n)$ by a factor of 3.5.

II. ROTATION CONSTRUCTIONS

In this section, we assume familiarity of the reader with the stabiliser formalism, especially the 2n-bit binary representation of n-qubit Paulis [41, 45, 47]. We follow the convention that the upper and lower halves of the binary matrix encode $Z$ and $X$ operators respectively. This representation is reviewed in Appendix A. We also reserve symbols $I_m$ and $0_m$ for the $m \times m$ identity and all-zero matrices respectively.

Our starting point is a commuting group, $S'_{\text{start}}$, of $m$ Paulis which can be represented as a binary $2n \times m$ matrix $S'_{\text{start}}$. By Gaussian elimination on $S'_{\text{start}}$, we can form a $2n \times k$ matrix $S_{\text{start}}$ representing a set $S'_{\text{start}}$ of $k$ independent Paulis drawn from $S'_{\text{start}}$ where $k \leq \min(n, m)$. Our goal is to transform $S_{\text{start}}$, using certain allowed transformations, into a $2n \times n$ matrix $S_{\text{end}}$ where

$$S_{\text{end}} = \left( \begin{array}{c} I_n \\ 0_n \end{array} \right).$$  

(6)

Let $U$ denote the circuit consisting of 1q and 2q transformations in the order they were applied from $S_{\text{start}} \rightarrow S_{\text{end}}$. Then applying $U$ to any state $|\psi\rangle$, measuring in the computational basis, and classically post-processing allows us to measure $S'_{\text{start}}$ on $|\psi\rangle$ simultaneously.

The allowed set $\mathcal{T}$ of transformations on a binary $2n \times m$ matrix $S$ is, where $p$ ranges over all columns, $r$ ranges over all rows, and addition is mod 2:

1. 1q and 2q, one- and two-qubit quantum row operations, specifically:

- CZ on qubits $i$ and $j$:
  $$S_ip \leftarrow S_ip + S_{j+n,p},$$
  $$S_jp \leftarrow S_jp + S_{i+n,p}.$$  

- CNOT on control-qubit $i$ and target-qubit $j$:
  $$S_ip \leftarrow S_ip + S_{jp},$$
  $$S_{j+n,p} \leftarrow S_{j+n,p} + S_{i+n,p}.$$  

HADAMARD (H) on qubit $i$:
$S_{ip} \leftrightarrow S_{i+n,p}$.

PHASE (P) on qubit $i$:
$S_{ip} \leftrightarrow S_{ip} + S_{i+n,p}$.

2. cpp, classical post-processing:
- Products of eventual single-qubit computational-basis measurements:
right-multiply by invertible $m \times m$ matrix.
- Relabelling of qubits $i$ and $j$:
$S_{ip} \leftrightarrow S_{jp}$,
$S_{n+i,p} \leftrightarrow S_{n+j,p}$.

3. ext, basis extension.
- Addition of further stabiliser:
append new column $S_{r,m+1}$.

In the near term, operations in $T$ have different costs that can be justifiably ranked as “$2q \gg 1q > \text{cpp} > \text{ext} = 0$”. In the first inequality, cost can refer to either fidelity or gate-time [25–39]. Therefore, we have aimed to minimise the number of two-qubit gates, or “2q-size”, in the $U$ resulting from our constructions. This means, for example, we never perform the cpp row swap using a two-qubit SWAP.

In presenting our constructions, we shall refer to the commutativity condition, preserved under $T$, given by

$$S^T J_{2n} S = 0_n, \quad (7)$$

where $S$ is the $2n \times m$ matrix encoding the Paulis and

$$J_{2n} = \begin{pmatrix} 0_n & I_n \\ I_n & 0_n \end{pmatrix}, \quad (8)$$

We ignore any changes in sign of stabilisers under $T$ as this can be easily accounted for by classical post-processing. Readers interested in this and other details are referred to Appendix B where we work through our CZ-construction with a specific example.

A. CZ-construction

Important to our first approach is the special class of stabiliser states known as graph states. Consider any graph $G$ on $n$ vertices. The graph state $|\Phi_G\rangle$ is then defined by $n$ independent stabiliser generators

$$g_i = X_i \prod_{j \in \text{nbd}(i)} Z_j, \quad i = 1, \ldots, n, \quad (9)$$

where nbd($i$) is the set of neighbours of vertex $i$ in $G$. The binary representation of these stabilisers is

$$S_{\text{graph}} = \begin{pmatrix} A \\ n \end{pmatrix}, \quad (10)$$

where $A$, an $n \times n$ symmetric matrix with 0s on its diagonal, is exactly the adjacency matrix of $G$.

It is well-known that $|\Phi_G\rangle = VH^\otimes n |0^n\rangle$ where $V$ is a product of CZ gates and $H$ is the HADAMARD gate. More specifically, $V$ applies CZ between qubits $i$ and $j$ if and only if vertex $i$ neighbours $j$ in $G$.

Van den Nest, Dehaene, and De Moor [40] tell us that any stabiliser state can be transformed to a graph state by a product of single-qubit Clifford gates. It is therefore clear that we can transform any $S_{\text{start}}$ to $S_{\text{end}}$ via $S_{\text{graph}}$ using at most $n(n-1)/2$ two-qubit (CZ) gates, as this is the maximum number of edges on an $n$-vertex graph. The interesting question is whether we can do better by exploiting the potential low rank $k \leq n$ of $S_{\text{start}}$.

Our answer is in the affirmative and we now present an explicit and efficient algorithm that constructs $U$ with at most $u_{cz}(k,n) = kn - k(k+1)/2$ two-qubit gates.

$$S_{\text{start}} \xrightarrow{1q \text{ cpp}} \begin{pmatrix} A \\ B \end{pmatrix} \xrightarrow{\text{cpp}} \begin{pmatrix} C \\ D \\ I_k \\ F \end{pmatrix}$$

$$\xrightarrow{\text{ext}} \begin{pmatrix} C & D^T \\ D & 0_{n-k} \\ I_k & 0 \\ F & I_{n-k} \end{pmatrix} \xrightarrow{1q \text{ cpp}} \begin{pmatrix} E & D^T \\ D & 0_{n-k} \\ I_k & 0 \\ 0 & I_{n-k} \end{pmatrix} \xrightarrow{2q} S_{\text{end}}$$

FIG. 1. Reductions used in our CZ-construction.

In Fig. 1 we illustrate the sequence of reductions that allow us to reach $S_{\text{graph}}$, and so $S_{\text{end}}$, from $S_{\text{start}}$. We now describe the salient aspects of each step:

- $S_{\text{start}} \rightarrow S_1$. Following [41], Lemma 6, we can apply HADAMARD gates so that $B$ has rank $k$. By cpp row-swaps (relabelling of qubits), we can ensure that the first $k$ rows of $B$ have full-rank.
- $S_1 \rightarrow S_2$. Since the upper $k \times k$ submatrix of $B$ has full-rank, cpp column operations can reduce it to $I_k$.
- $S_2 \rightarrow S_3$. We can directly verify that the extension to $S_3$ is valid by Eq. (7). Clearly $S_3$ has full column-rank.
- $S_3 \rightarrow S_4 = S_{\text{graph}}$. Column operations can eliminate $F$, then PHASE gates can ensure $E$ has zeros on its diagonal. Importantly, $S_4$ represents a graph state $S_{\text{graph}}$.
- $S_4 \rightarrow S_{\text{end}}$. HADAMARD and CZ gates can implement this final reduction as discussed above. The maximum number of CZ gates required to map $S_4$ to $S_{\text{end}}$ equals the maximum number of off-diagonal 1s in the upper
half of $S_4$. When $n = k$, this is $n(n - 1)/2 = O(n^2)$. When $k \neq n$, this is $w_{cz}(k, n) = kn - k(k + 1)/2$ due to sparsity of the upper half of $S_4$ which traces back to the exact step from $S_3 \to S_4$.

Note that in step $S_4 \to S_{\text{end}}$, we can first try to reduce the upper half of $S_4$ by single-qubit gates before applying CZ. One way to do this is to reduce the number of edges in the graph whose adjacency matrix is specified by the upper half of $S_4$ by the so-called “local complementation” operation [40, 48, 49]. This corresponds precisely to reducing the number of CZ gates in our CZ-construction.

**B. CNOT-construction**

$$S_4 \xrightarrow{2q} \left( \begin{array}{cc} 0_k & D^T \\ D & 0_{n-k} \end{array} \right)$$

$$\xrightarrow{1q} \left( \begin{array}{cc} 0_k & D^T \\ D & 0_{n-k} \end{array} \right) \xrightarrow{2q} \left( \begin{array}{cc} I_k & D^T \\ D & I_{n-k} \end{array} \right)$$

$$\xrightarrow{3q} \left( \begin{array}{cc} I_k & D^T \\ D & I_{n-k} \end{array} \right)$$

$S_5 \quad S_6$

$S_7 \quad S_8$

$2q \to \left( \begin{array}{cc} D_1 M_1 \\ M_1 \end{array} \right)$

$\xrightarrow{c_{pp}} \left( \begin{array}{cc} I_k - D^T D & 0 \\ 0 & I_{n-k} \end{array} \right)$

$\xrightarrow{2q} \left( \begin{array}{cc} I_k - D^T D & 0 \\ 0 & I_{n-k} \end{array} \right)$

$\xrightarrow{c_{pp}} S_{\text{end}}$

**FIG. 2. Reductions used in our CNOT-construction starting at $S_4$ of our CZ-construction.**

We start from $S_4$ above which we reached without using two-qubit gates. Now, instead of using one block of CZ gates, we reduce to $S_{\text{end}}$ as shown in Fig. [2] using three blocks of CNOT gates:

- $S_4 \to S_5$. Note that $E$ must be symmetric by the commutativity condition given in Eq. (7). Then, following Ref. [41 Lemma 7], we can eliminate $E$ using single-qubit and $O(k^2/\log k)$ CNOT gates. This is accomplished by noting that any symmetric binary $E$ can be Cholesky decomposed as $E = \Lambda + M^T M$, with $\Lambda$ diagonal and $M$ invertible.

- $S_5 \to S_6$. Reduce $M$ to $I_k$ by column operations, then add $1$s on the top diagonal by phase gates.

- $S_6 \to S_7$. Now, the upper $n \times n$ matrix can be block-Cholesky decomposed as

$$\begin{pmatrix} I_k & D^T \\ D & I_{n-k} \end{pmatrix} = M_1^T D_1 M_1$$

where

$$M_1 := \begin{pmatrix} I_k & 0 \\ D & I_{n-k} \end{pmatrix}$$

$$D_1 := \begin{pmatrix} I_k - D^T D & 0 \\ 0 & I_{n-k} \end{pmatrix}$$

Next, we apply CNOT gates corresponding to $M_1$. The number of CNOT gates required here equals the number of row operations required to reduce $M_1$ to $I_n$. We find this is at most $u_{cz}(k, n) = O(kn/\log k)$ via arguments of Patel, Markov, and Hayes [42]. The proof is given in Appendix C.

- $S_7 \to S_8$. Multiply by $M_1^{-1}$ on the right.

- $S_8 \to S_{\text{end}}$. $I_k - D^T D$ is a $k \times k$ symmetric matrix and so can be again eliminated via the Cholesky decomposition using $O(k^2/\log k)$ CNOT gates.

Note that in the three steps $S_4 \to S_5$, $S_6 \to S_7$, and $S_8 \to S_{\text{end}}$, we have used blocks of CNOT gates. The method we used to synthesise these blocks is size-optimal [42, Lemma 1], but we could have alternatively used methods in Ref. [50], that built on Ref. [51], to achieve optimal space-depth tradeoff, where space refers to extra ancilla qubits.

To end our discussion of constructing rotation circuits, we briefly mention a third, ancilla-based construction with $2q$-size at most $kn$. This construction is well-known in the context of syndrome measurement [47] in quantum error correction but does not seem to have been mentioned in the context of measuring a Pauli decomposition of an observable, as in VQE. To measure $k$ commuting Paulis $\{P_i\}_{i=1}^k$, this “ancilla-construction” uses $k$ ancilla and involves $k$ consecutive blocks of generalised-CNOT gates, each targeted at a different ancilla. The controls in block $b \leq k$ are activated or deactivated by the $+1$ or $-1$ eigenstates of the single-qubit Paulis forming $P_b$ [52]. $k$ single-qubit measurements are performed on the ancilla at the end of each block to exactly give measurements of $P_b$. Unfortunately, this construction requires $k$ extra ancilla qubits and has worse worst-case $2q$-size than both of our constructions. However, it does serve as a simple way to see, a priori, that a $2q$-size scaling of $O(kn)$ is possible.

**III. GROUPING STRATEGIES**

Now that we have demonstrated the construction of a rotation circuit for a group of generally commuting Paulis, we would like to quantify the advantage offered, in terms of use of the quantum computer, in assembling operators into such groups. We have a Hamiltonian, $H$, of the form

$$H = \sum_{i=1}^{N} H_i = \sum_{i=1}^{N} \sum_{j=1}^{m_i} a_{ij} P_{ij}$$

where $N$ is the number of groups of mutually commuting operators, $m_i$ is the number of operators in group $i$, $P_{ij}$ is the $j$th Pauli operator in the $i$th group and $a_{ij} \in \mathbb{R}$ is its coefficient.
Given $\epsilon$, let $M_a$ and $M_g$ be the minimal number of measurements required to attain an accuracy $\epsilon$ in the ungrouped and grouped (as per Eq. 14) cases respectively. Finding $M_a$ is a special case of finding $M_g$. To find $M_a$, we can solve the constrained optimisation problem that asks how a given number of measurements should be distributed in order to maximise accuracy. Following Ref. [8, 43, 44], we can use Lagrange multipliers to find

$$M_g = \left( \frac{1}{\epsilon} \sum_{i=1}^{N} \sqrt{\text{Var}[H_i]} \right)^2,$$  \hspace{1cm} (15)

where

$$\text{Var}[H_i] = \langle H_i^2 \rangle - \langle H_i \rangle^2.$$  \hspace{1cm} (16)

Since $M_a$ is just $M_g$ evaluated with every operator in its own group, we have

$$M_a = \left( \frac{1}{\epsilon} \sum_{i=1}^{N} \sum_{j=1}^{m_i} |a_{ij}| \sqrt{\text{Var}[P_{ij}]} \right)^2,$$  \hspace{1cm} (17)

where

$$\text{Var}[P_{ij}] = 1 - \langle P_{ij} \rangle^2.$$ \hspace{1cm} (18)

The ratio $R$, defined as

$$R := \frac{M_a}{M_g} = \left( \frac{\sum_{i=1}^{N} \sum_{j=1}^{m_i} |a_{ij}| \sqrt{\text{Var}[P_{ij}]} \sum_{i=1}^{N} \sqrt{\text{Var}[H_i]} }{\sum_{i=1}^{N} \sqrt{\text{Var}[H_i]} } \right)^2,$$  \hspace{1cm} (19)

therefore acts as a natural metric for the performance of a particular grouping under the assumption that measurements are distributed optimally. We prove as Claim 1 that combining two groups into one is always better with respect to $R$.

**Claim 1.** Consider two groups $C_a$ and $C_b$ of mutually commuting Paulis, where each Pauli is in at most one group. Suppose that it is possible to combine $C_a$ and $C_b$ into a single commuting group, called $C_{a,b}$. Let $R(\{C_a,C_b\})$ and $R(\{C_{a,b}\})$ denote the $R$ metric, as defined in Eq. (19), for the two groups separated and combined respectively. Then

$$R(\{C_a,C_b\}) \geq R(\{C_{a,b}\}).$$  \hspace{1cm} (20)

**Proof.** As $\sqrt{T}$ is a strictly increasing function for $f \in \mathbb{R}_{>0}$ and the numerator of $R$ is independent of the grouping, it is sufficient to consider only the size of denominator of $R$

$$\sum_{i=1}^{N} \sqrt{\text{Var}[H_i]}$$  \hspace{1cm} (21)

for the two cases. The variance of a single commuting group $C_i$ can be written as

$$\text{Var}[H_i] = \text{Cov}[H_i, H_i] = \sum_{j,k} a_{ij}^* a_{ik} \text{Cov}[P_{ij}, P_{ik}] = a^\dagger_i C a_i,$$  \hspace{1cm} (22)

where $C$ is the Hermitian and positive semi-definite covariance matrix for the state $|\psi\rangle$ and $a_i$ is a vector of the coefficients $a_{ij}$. $C$ is defined to have elements

$$C_{ij} := \text{Cov}[P_i, P_j] \quad \text{for all } P_i, P_j \in C_i, \hspace{1cm} (23)$$

where the covariance $\text{Cov}[P_i, P_j]$ is defined as

$$\text{Cov}[P_i, P_j] := \langle P_i P_j \rangle_{\psi} - \langle P_i \rangle_{\psi} \langle P_j \rangle_{\psi}. \hspace{1cm} (24)$$

Let us now turn our attention to the single and two group comparison. We define coefficient vectors $a$ and $b$, both of size $|C_{a,b}|$, which contain the coefficients of the operators contained within groups $C_a$ and $C_b$ respectively. If a Pauli operator is not present within $C_a$, the corresponding coefficient in $a$ will be zero, and similarly for $b$ and $C_b$. The combined group $C_{a,b}$ therefore has coefficients $a + b$. The contribution of the two separate groups to (22) is

$$\sqrt{a^\dagger C_{ab} a + \sqrt{b^\dagger C_{ab} b}}$$

$$= \sqrt{a^\dagger C_{ab} a + b^\dagger C_{ab} b}$$

$$= \sqrt{a^\dagger C_{ab} a + b^\dagger C_{ab} b + 2 \sqrt{(a^\dagger C_{ab} a)(b^\dagger C_{ab} b)}}, \hspace{1cm} (25)$$

where $C_{ab}$ is the $|C_{a,b}| \times |C_{a,b}|$ covariance matrix of the full set of operators contained within $C_{a,b}$. The contribution due to the single group is

$$\sqrt{(a + b)^\dagger C_{ab}(a + b)}$$

$$= \sqrt{a^\dagger C_{ab} a + b^\dagger C_{ab} b + a^\dagger C_{ab} b + b^\dagger C_{ab} a}$$

$$= \sqrt{a^\dagger C_{ab} a + b^\dagger C_{ab} b + 2 a^\dagger C_{ab} b}.$$  \hspace{1cm} (26)

Because $C_{ab}$ is positive semi-definite, we can define the semi-inner product $(a, b) := a^\dagger C_{ab} b$ [55, Example 1.1] and use the Cauchy-Schwarz inequality to find

$$(a^\dagger C_{ab} b)^2 \leq (a^\dagger C_{ab} a)(b^\dagger C_{ab} b). \hspace{1cm} (27)$$

Equality holds if and only if there exist $\alpha$ and $\beta \in \mathbb{C}$, such that not both are equal to 0 and $(\alpha a + \beta b, \alpha a + \beta b) = 0$ [55, Example 1.4]. Therefore, by comparison, (25) $\geq$ (26) and so

$$R(\{C_a, C_b\}) \geq R(\{C_{a,b}\}) \quad \text{for all } |\psi\rangle.$$  \hspace{1cm} (28)

Claim 1 shows that it is impossible to mitigate covariances by splitting groups and using the optimal measurement strategy. This is in contrast to Refs. [3, 23], who showed that it is possible using a sub-optimal measurement strategy. In Appendix D we re-do precisely their example using the optimal measurement strategy. Note that Claim 1 does not imply that the minimum number of groups is best, simply that it is never better to break a single group into two.
If all of the variances going into $R$ are replaced by their expectation values over the uniform spherical measure (see Ref. [54, Ch. 7]), we obtain another metric, $\hat{R}$, given by

$$
\hat{R} := \left( \frac{\sum_{i=1}^{N} \sum_{j=1}^{N} |a_{ij}|}{\sum_{i=1}^{N} \sqrt{\sum_{j=1}^{N} |a_{ij}|^2}} \right)^2.
$$

(29)

The derivation of $\hat{R}$ is given in Appendix B. The same proof as in Claim 1 can be used to show that breaking a group into two is never better when measured by $\hat{R}$; the only difference is the covariance matrix must be replaced by its expectation over the uniform spherical measure.

$\hat{R}$ is a particularly useful metric because it approximates $E[R]$ over the uniform spherical measure, but can be calculated analytically. A good grouping strategy maximises $\hat{R}$ by minimising the denominator. This is achieved by taking advantage of the concavity of the square root by placing the operators with the largest $|a_{ij}|^2$ coefficients in the same groups. Physically, this represents the optimal measurement scheme being able to direct many measurements towards a few groups with large variances. In the next paragraph, we propose a simple strategy for grouping operators motivated by this idea.

Given $H$, the strategy is to take each operator ordered by the absolute value of the coefficient, check if it can be placed in an existing group and, if not, start a new group. The groups are checked in order of creation. This is of complexity $nt(t-1)/2$ at worst, where we recall that $n$ is the number of qubits and $t$ is the number of Pauli terms in the Hamiltonian. We have named this strategy SORTED INSERTION.

Greedy colouring algorithms, as implemented in Ref. [19], require pre-generating the commutation graph which takes the same number of operations as the worst case scenario for SORTED INSERTION. The colouring algorithms then run on the graph adding their own complexity — see Table IV. Therefore, SORTED INSERTION’s worst case complexity is bounded by the best case complexity of greedy colouring algorithms, such as those we will compare it to in Sec. IV.

| Colouring Algorithm          | Time Complexity |
|-----------------------------|-----------------|
| Largest First               | $O(t^2)$        |
| Connected Sequential d.f.s. | $O(t^2)$        |
| DSATUR                      | $O(t^2 \log t)$|
| Independent Set             | $O(t^3)$        |

TABLE I. Time complexities of the greedy colouring algorithms we compare with SORTED INSERTION in Sec. IV after pre-generating the commutation graph [55].

IV. APPLICATION TO VQE

In this section, we present numerical results of the grouping method discussed in Sec. III along with the CZ-construction of Sec. II A to construct the rotation circuits for given commuting groups. In particular, we have applied our methods to the Hamiltonians of simple molecules so as to demonstrate their use in the context of VQE. The full results are given in Table IV with a subset shown in Table II. In all cases, we used OpenFermion [57] to obtain Hamiltonians in the STO-3G basis, at approximately the equilibrium geometry of the molecules, with the symmetry conserving Bravyi-Kitaev transformation [17, 58]. In order to reduce the number of two-qubit gates required, we considered qubits on which all operators in a group locally commute separately — a one-qubit rotation per locally commuting qubit is all that is required to do so.

In Fig. 3a, we plot the average group size against the number of qubits, $n$, for the molecular Hamiltonians. We can see that the average group size increases with increasing $n$, and the increase does not appear to be slowing down. We therefore conclude that our sorting method works well on systems of at least size $n = 38$. However, the key advantage of assembling a Hamiltonian into groups of mutually commuting operators is a reduction in the number of measurements required to obtain an energy expectation to a certain level of accuracy, and group size alone does not directly quantify this reduction. For a given Hamiltonian and quantum state, the reduction is instead given by $R$, as in Eq. (19).

We therefore calculated the value of $R$ for 100 different quantum states, generated using 100 random sets of ansatz parameters with a hardware efficient ansatz of depth 1, for the nine smallest molecular systems. We show the mean, minimum and maximum values for each molecule. In practice, the value of $R$ can at best be obtained approximately by making measurements on the quantum computer and so cannot be used to determine the expected advantage of a particular grouping a priori. The metric $\hat{R}$, given by Eq. (29), on the other hand, depends only on the coefficients of the terms in the Hamiltonian. From Table II we can see that $\hat{R}$ closely approximates the average of $R$ over many ansatz parameters, but can be calculated analytically without the need for simulations. In Fig. 3b, we show $\hat{R}$ as a function of the number of qubits for our full selection of molecules. We can see that it is highly molecule dependent, with systems of similar size having very different values.

The reduction in number of measurements required comes at the cost of applying additional quantum gates before the qubits are measured, the most costly of which are two-qubit gates. For the CZ-construction, we demonstrated in Sec. II A that the maximum number of additional two-qubit gates required for a group with $k$ independent terms is $nk - k(k + 1)/2$. We would like to know, in practice, how many additional two-qubit gates are required at a maximum, as this is the quantum resource that is most limiting. Assuming for a given Hamiltonian that at least one group has rank $n$, obtaining a measurement of all terms in a Hamiltonian on $n$ qubits may therefore require applying an additional $n(n-1)/2$ gates in a single circuit. However, for the molecules we have considered, we find that the largest number of two-qubit gates required is in fact far lower than this, typically by a factor of approximately 3.5, as can be seen in Fig. 3c.

Given the close relationship between the average value of $R$ and the value of $\hat{R}$, we propose using $\hat{R}$ as a metric for the
### TABLE II. A reduced set of results of the numerical simulations discussed in the main text, and shown in full in Table IV. For each molecule, we show a number of results related to the grouping of Hamiltonian terms, how the grouping reduces the number of measurements required using the metrics $R$ and $\hat{R}$, and the number of two-qubit gates in the resulting rotation circuits. Note that the mean value of $R$ and $\hat{R}$ are very similar.

| Molecule | $n$ qubits | $t$ Paulis | Grouping | Ratios $R$, $\hat{R}$ | Rotation Circuit $2q$-size |
|----------|-------------|-------------|-----------|-------------------------|--------------------------|
| $\text{H}_2$ | 2 | 4 | 2 | 2.00 | 1.50 | 1.09 | 1.93 | 4.60 | 1.76 | theory max: 0, true max: 0, mean: 0 |
| $\text{H}_3^+$ | 4 | 59 | 10 | 5.90 | 3.50 | 3.76 | 11.92 | 33.04 | 10.25 | 6 | 3 | 0.80 |
| LiH | 10 | 630 | 41 | 15.37 | 6.85 | 19.60 | 24.91 | 34.74 | 23.97 | 45 | 18 | 5.29 |
| OH$^-$ | 10 | 630 | 38 | 16.58 | 7.29 | 6.32 | 8.90 | 12.86 | 8.51 | 45 | 17 | 5.63 |
| HF | 10 | 630 | 39 | 16.15 | 6.97 | 6.07 | 8.57 | 12.27 | 8.21 | 46 | 16 | 5.74 |
| $\text{H}_2\text{O}$ | 12 | 1085 | 51 | 21.27 | 9.04 | 7.68 | 11.27 | 16.96 | 10.67 | 66 | 26 | 7.37 |
| BH$_3$ | 14 | 1584 | 66 | 24.00 | 10.36 | 17.21 | 20.93 | 32.13 | 20.05 | 91 | 26 | 9.56 |
| NH$_3$ | 14 | 3608 | 118 | 30.58 | 11.34 | 12.65 | 15.96 | 26.93 | 15.31 | 91 | 28 | 10.26 |
| CH$_4$ | 16 | 3887 | 123 | 31.60 | 13.39 | 16.96 | 21.63 | 29.33 | 20.27 | 120 | 45 | 16.75 |

### TABLE III. Comparison of the groupings produced by the greedy colouring algorithms “Largest First”, “Connected Sequential d.f.s.” (depth first search), “Independent Set” and “DSATUR” as implemented by the Python package NetworkX with our method SORTED INSERTION. For each method, the number of groups produced, $N$, and the metric $\hat{R}$ given by equation (29), are presented. The best or joint best methods are highlighted in bold for each molecule.

| Molecule | Largest First | Connected Sequential d.f.s. | Independent Set | DSATUR | SORTED INSERTION |
|----------|---------------|-----------------------------|-----------------|--------|------------------|
| $\text{H}_2$ | $N$ | $\hat{R}$ | $N$ | $\hat{R}$ | $N$ | $\hat{R}$ | $N$ | $\hat{R}$ | $N$ | $\hat{R}$ |
| $\text{H}_3^+$ | 10 | 4.86 | 10 | 10.25 | 10 | 10.30 | 9 | 4.10 | 10 | 10.25 |
| LiH | 39 | 23.87 | 45 | 23.33 | 30 | 5.72 | 29 | 10.47 | 41 | 23.97 |
| OH$^-$ | 40 | 8.27 | 41 | 8.41 | 21 | 3.00 | 28 | 3.23 | 37 | 8.51 |
| HF | 38 | 8.05 | 41 | 8.07 | 21 | 2.80 | 28 | 3.23 | 38 | 8.21 |
| $\text{H}_2\text{O}$ | 57 | 2.98 | 55 | 10.66 | 42 | 3.87 | 51 | 3.18 | 51 | 10.66 |
| BH$_3$ | 66 | 4.80 | 85 | 18.70 | 60 | 7.85 | 72 | 4.11 | 68 | 20.05 |
| NH$_3$ | 124 | 6.50 | 174 | 13.97 | 126 | 4.03 | 137 | 2.92 | 117 | 15.31 |
| CH$_4$ | 122 | 5.84 | 176 | 18.93 | 114 | 9.88 | 110 | 4.90 | 125 | 20.27 |
| O$_2$ | 62 | 13.62 | 85 | 19.95 | 42 | 6.79 | 52 | 7.91 | 67 | 20.23 |
| N$_2$ | 62 | 15.00 | 86 | 21.15 | 39 | 8.37 | 49 | 5.80 | 78 | 22.10 |
| CO | 124 | 20.70 | 155 | 20.67 | 89 | 6.03 | 106 | 4.55 | 128 | 21.31 |
| HCl | 117 | 2.16 | 141 | 10.29 | 98 | 3.52 | 104 | 2.04 | 123 | 10.36 |
| NaH | 121 | 8.78 | 181 | 12.40 | 149 | 3.44 | 145 | 3.65 | 135 | 12.90 |
| H$_2$S | 122 | 8.81 | 180 | 12.45 | 147 | 3.80 | 145 | 3.66 | 147 | 11.60 |
FIG. 3. The results of numerical simulations discussed in the text. We show (a) the average group size, (b) the value of \( \hat{R} \), given by Eq. (29), and (c) the ratio of the worst-case maximum number of two-qubit gates in a single rotation circuit to the actual number as a function of the number of qubits for a range of simple molecules. A subset of the data is shown in Table III, and the full data is shown in Table IV.

V. CONCLUSION

We have addressed two problems related to the efficient measurement of Pauli operators on a quantum computer. The first is how to synthesise rotation circuits that enable mutually commuting Paulis to be measured simultaneously, and the second is how to assemble a set of Paulis into groups in which they mutually commute.

We have contributed two rotation circuit constructions CZ and CNOT. The CZ-construction results in a maximum of \( u_{\text{cz}}(k,n) = kn - k(k + 1)/2 \) two-qubit gates while the CNOT-construction results in a maximum of \( u_{\text{cnot}}(k,n) = O(kn/\log k) \). On grouping Pauli operators, we contribute two natural metrics, \( R \) and \( \hat{R} \), that justifiably measure the effectiveness of a grouping. We also contribute a grouping strategy motivated by \( \hat{R} \) that we call SORTED INSERTION.

We have applied our theoretical work to the task of estimating energies of molecules in the context of VQE. We find that, for the CZ-construction, the largest number of two-qubit gates required is typically less than the theoretical worst-case by a factor of approximately 3.5. Comparison to other grouping methods shows that while SORTED INSERTION does not normally result in the smallest number of groups, it nearly always results in the best value of \( \hat{R} \).

VI. ACKNOWLEDGEMENT

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Appendix A: Binary representation

The Pauli group $\mathcal{P}_n$, on $n$-qubits is a group of $4^{n+1}$ elements defined by

$$\mathcal{P}_n = \{i^k \sigma_1 \otimes \cdots \otimes \sigma_n \mid \sigma_i \in \{I, X, Y, Z\}, k \in \{0, 1, 2, 3\}\}$$

(A1)

The binary representation, first introduced by Calderbank, Rains, Shor, and Sloane\cite{calderbank1996}, is a representation of $\mathcal{P}_n$ as binary vectors. In this representation, Paulis differing only in phase $i^k$ are represented in the same way.

Single-qubit Paulis are represented by 2-dimensional binary vectors, so that

$$\sigma_{00} := I \rightarrow (0, 0),$$
$$\sigma_{01} := X \rightarrow (0, 1),$$
$$\sigma_{10} := Z \rightarrow (1, 0),$$
$$\sigma_{11} := Y \rightarrow (1, 1).$$

(A2)

An $n$-qubit Pauli

$$\sigma_{u_1,v_1} \otimes \cdots \otimes \sigma_{u_n,v_n}$$

is then represented by the $2n$-dimensional binary vector

$$(u_1, \ldots, u_n, v_1, \ldots, v_n).$$

(A3)

In this representation, two $n$-qubit Paulis with binary vectors $a$ and $b$ commute if and only if

$$a^T J_{2n} b = 0,$$

where $J_{2n}$ denotes the $2n \times 2n$ matrix

$$J_{2n} := \begin{pmatrix} 0 & I_n \\ I_n & 0 \end{pmatrix}.$$  

(A4)

Given a set $S$ of $m$ $n$-qubit Paulis, we can write down a corresponding $2n \times m$ binary matrix $S$ where each column represents a Pauli. Then, from Eq. (A1), we deduce that all Paulis in $S$ mutually commute if and only if

$$S^T J_{2n} S = O_m,$$

(A5)

which recovers Eq. (7) in the main text. We say that the set $S$ of Paulis is independent if the matrix $S$ has rank $m$.

We shall often find it helpful to write $S$ in terms of its upper half $S^{(Z)}$ and lower half $S^{(X)}$, separated by a horizontal line for visual-aid, i.e.,

$$S = \begin{pmatrix} S^{(Z)} \\ S^{(X)} \end{pmatrix}.$$  

(A6)

The conjugation action of quantum gates on $S$ can be represented as transformations to the matrix $S$. For example, we document the transformations on $S$ that represent four common quantum gates. In the following, addition is mod 2 and $p$ ranges over all columns $\{1, \ldots, m\}$.

- **CZ on qubits $i$ and $j$:**
  $$S_{ip} \leftarrow S_{ip} + S_{i+n,p},$$
  $$S_{jp} \leftarrow S_{jp} + S_{i+n,p}.$$

- **CNOT on control-qubit $i$ and target-qubit $j$:**
  $$S_{ip} \leftarrow S_{ip} + S_{jp},$$
  $$S_{j+n,p} \leftarrow S_{j+n,p} + S_{i+n,p}.$$

- **HADAMARD (H) on qubit $i$:**
  $$S_{ip} \leftrightarrow S_{i+n,p}.$$

- **PHASE (P) on qubit $i$:**
  $$S_{ip} \leftarrow S_{ip} + S_{i+n,p}.$$

These rules can be directly verified by conjugating $X_i$, $Z_i$, $Z_j$ by the listed gates. They are also reproduced in Sec. III of the main text.

Appendix B: CZ-construction example

We walk through our CZ-construction for a specific example. In this example, we would like to obtain measurements simultaneously of a set $S'_{\text{start}}$ of six four-qubit Paulis given by

$$P_1 = Z_1 Z_2 Z_3 Z_4,$$
$$P_2 = X_1 X_2 Y_3 Y_4,$$
$$P_3 = Y_1 Y_2 X_3 X_4,$$
$$P_4 = Y_2 X_3,$$
$$P_5 = Y_1 X_4,$$
$$P_6 = X_1 Z_2 Z_3 Y_4.$$  

(B1)

We can represent these Paulis in a matrix $S'_{\text{start}}$ with

$$S'_{\text{start}} = \begin{pmatrix} 1 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 1 \end{pmatrix}.$$  

(B2)

By Gaussian elimination, we find the reduced row echelon form of $S'_{\text{start}}$ to be

$$\begin{pmatrix} 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$  

(B3)

The pivot columns are numbers 1, 2 and 4 which tells us that $P_1$, $P_2$ and $P_3$ are the three independent Paulis from which...
the remaining Paulis in $S'_{\text{start}}$ can be constructed. Therefore, we can write $S'_{\text{start}} = S_{\text{start}}R_0^{-1}$, where

$$
S_{\text{start}} := \begin{pmatrix}
1 & 0 & 0 \\
1 & 0 & 1 \\
1 & 1 & 0 \\
0 & 1 & 0 \\
0 & 1 & 1 \\
0 & 1 & 0
\end{pmatrix},
R_0^{-1} := \begin{pmatrix}
1 & 0 & 1 & 0 & 1 & 0 \\
0 & 1 & 1 & 0 & 1 & 1 \\
0 & 0 & 0 & 1 & 1 & 1
\end{pmatrix}.
$$

(B4)

Note that the inverse on $R_0^{-1}$ is purely notational. Now, the lower half $S_{\text{start}}^{(X)}$ of $S_{\text{start}}$ has column echelon form

$$
S_{\text{start}}^{(X)} = \begin{pmatrix}
1 & 0 & 0 \\
1 & 1 & 0 \\
1 & 1 & 0 \\
1 & 0 & 0
\end{pmatrix},
$$

(B5)

and so the first two rows are pivot rows. In order to give the lower half of $S_{\text{start}}$ a rank of $k = 3$, we therefore apply a HADAMARD to the rows corresponding to qubits 3 and 4 so that

$$
S_1 := Q_1S_{\text{start}} = \begin{pmatrix}
1 & 0 & 0 \\
1 & 0 & 1 \\
0 & 1 & 0 \\
0 & 1 & 1 \\
1 & 0 & 0 \\
1 & 1 & 0
\end{pmatrix}.
$$

(B6)

where

$$
Q_1 := \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0
\end{pmatrix}.
$$

(B7)

The lower half of $S_1$ now has rank 3, and performing Gaussian elimination on it, we find

$$
S_2 := Q_1S_{\text{start}}R_1 = \begin{pmatrix}
1 & 0 & 1 \\
0 & 1 & 1 \\
0 & 1 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1 \\
0 & 0 & 1
\end{pmatrix},
$$

(B8)

where

$$
R_1 = \begin{pmatrix}
0 & 1 & 0 \\
0 & 1 & 1 \\
1 & 1 & 0
\end{pmatrix}^{-1} = \begin{pmatrix}
1 & 0 & 1 \\
1 & 0 & 0 \\
1 & 1 & 0
\end{pmatrix}.
$$

(B9)

We now extend $S_2$ to a rank $n = 4$ matrix by adding a column that corresponds to a fourth Pauli $P_{\text{ext}}$. In the main text, this is the crucial ext step from $S_2 \rightarrow S_3$ which might have seemed fortuitous. In fact, ext was systematically obtained as follows.

To make our reasoning clearer, let us represent $S_2$ alternatively by the matrix

$$
P(S_2) := \begin{pmatrix}
Y & I & I & Z \\
I & Y & Z & I \\
Z & Z & X & X
\end{pmatrix},
$$

(B10)

where each row corresponds to a Pauli operator given by a column of $S_2$. Looking at the form of $P(S_2)$, we see that we can place $X$ in the 4th qubit position of $P_{\text{ext}}$ (and nowhere else) to ensure $P_{\text{ext}}$ is independent of the other Paulis. Then we observe that the left 3-by-3 sub-matrix of $P(S_2)$ has $X/Y$ on the diagonal and $I/Z$ everywhere else. This means we can place $I/Z$ in the other qubit positions of $P_{\text{ext}}$ depending on whether the $X$ in its 4th qubit position commutes with the 4th position terms of the other Paulis.

By this prescription, we find $P_{\text{ext}} = Z_1I_2I_3X_4$. Therefore $S_2$ is extended to

$$
S_3 := \begin{pmatrix}
1 & 0 & 1 & 1 \\
0 & 1 & 1 & 0 \\
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0
\end{pmatrix},
$$

(B11)

and

$$
Q_1S_{\text{start}}R_1 = S_3R_2^{-1},
$$

(B12)

where

$$
R_2^{-1} := \begin{pmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1 \\
0 & 0 & 0
\end{pmatrix}
$$

(B13)

Note that the inverse on $R_2^{-1}$ is also purely notational. The lower half of $S_3$ is full-rank and so we can take its inverse to find

$$
R_3 = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 1 & 1
\end{pmatrix}^{-1} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 1 & 1
\end{pmatrix},
$$

(B14)

and

$$
S_3R_3 = \begin{pmatrix}
1 & 0 & 1 & 1 \\
0 & 1 & 1 & 0 \\
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0
\end{pmatrix}.
$$

(B15)
Finally, we apply PHASE to qubits 1 and 2 so that

\[
S_4 = Q_2 S_3 R_3 = \begin{pmatrix}
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
1 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
0 & 1 & 0 & 0
\end{pmatrix},
\]  

where

\[
Q_2 = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 \\
\end{pmatrix}.
\]

\[S_4\] is of the form of a graph state and represents the following Paulis:

\[
\begin{align*}
\tilde{P}_1 &= X_1 I_2 I_3 Z_4, \\
\tilde{P}_2 &= I_1 X_2 Z_3 I_4, \\
\tilde{P}_3 &= I_1 Z_2 X_3 I_4, \\
\tilde{P}_4 &= Z_1 I_2 I_3 X_4.
\end{align*}
\]

We now have

\[S'_{\text{start}} = Q^{-1} S_4 R^{-1},\]

where

\[
Q^{-1} := Q_1^{-1} Q_2^{-1} = \begin{pmatrix}
1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0
\end{pmatrix}.
\]

and

\[
R^{-1} := R_3^{-1} R_2^{-1} R_1^{-1} R_0^{-1} = \begin{pmatrix}
0 & 1 & 1 & 0 & 1 & 1 \\
0 & 1 & 1 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 1 \\
1 & 1 & 0 & 0 & 0 & 1
\end{pmatrix}.
\]

The rotation circuit is shown in Fig. 4. Using \(Q^{-1}, S_4\) and \(R^{-1}\), we can work out that the phases for the six original operators are \((-1 + 1 + 1 - 1 - 1 - 1). Therefore, we can construct measurements of the original Pauli strings as follows:

- \(P_1\) from product of measurements of qubits 3 and 4,
- \(P_2\) from product of measurements of qubits 1 to 4,
- \(P_3\) from product of measurements of qubits 1 and 2,
- \(P_4\) from the negative of measurement of qubit 2,
- \(P_5\) from the negative of measurement of qubit 1,
- \(P_6\) from the negative product of measurements of qubits 1, 3 and 4.

Appendix C: Proof of \(O(kn/\log k)\)

We prove the following Claim \(\square\) via arguments of Patel, Markov, and Hayes \([42\). As acknowledged in Ref. [42], these arguments originate from the “Method of Four Russians” \([63\). Note that row operations correspond to CNOT gates, as explained in detail in Ref. \([42\).

Claim 2. Let \(M\) be a \(n \times n\) matrix with block form

\[
\begin{pmatrix}
I_k & A \\
0 & I_{n-k}
\end{pmatrix},
\]

where \(A\) is any \(k \times (n-k)\) matrix. Then \(O(kn/\log k)\) row operations suffice to reduce \(M\) to identity \(I_n\).

Proof. Let \(m\) be a constant we later choose. Partition \(A\) into \(l := (n - k)/m\) consecutive column-blocks \(A_i\), each containing \(m\) columns.

Start at \(A_1\) and eliminate any duplicate rows using at most \(k\) row operations. There then remain at most \(2^m\) unique rows in \(A_j\) which can be eliminated by at most \(m2^{m-1}\) row operations that add rows from \(I_{n-k} A_1\) is now zero.

For each of \(A_2, \ldots, A_l\) perform the same operation as was done to \(A_1\). \(M\) then becomes

\[
\begin{pmatrix}
B & 0 \\
0 & I_{n-k}
\end{pmatrix},
\]

where \(B\) is some \(k \times k\) matrix that must be invertible. \(B\) can then be row-reduced to \(I_k\) using \(O(k^2/\log k)\) by the result of Ref. [42].

The total number \(N\) of row operations is therefore

\[
N = (k + m2^{m-1}) \frac{n-k}{m} + O\left(\frac{k^2}{\log k}\right).
\]

Choosing \(m = \alpha \log k\), we find

\[
N = \frac{k(n-k)}{\alpha \log k} + \frac{k^2(n-k)}{2} + O\left(\frac{k^2}{\log k}\right),
\]

which is \(O(kn/\log k)\) provided \(\alpha < 1\). \(\square\)
Appendix D: Example to demonstrate that combining two groups into one reduces $R$

Consider the example in Ref. [3, 23] where we consider measuring the energy, given by Hamiltonian

$$H = -XX - YY + ZZ + ZZ + ZZ$$  \hfill (D1)

on the state $|\psi\rangle = |01\rangle$. For these Paulis, the covariance matrix is

$$C = \begin{pmatrix}
1 & 1 & 0 & 0 \\
1 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix}.$$  \hfill (D2)

The covariance between the non-commuting operators in the upper right and lower left blocks is not defined. We have set them to equal zero for convenience (highlighted in bold).

First, we consider grouping the Paulis into

$$\{-XX, -YY, ZZ\}, \{IZ, ZI\}.$$  \hfill (D3)

For these groups of Paulis, the coefficient vectors are given by

$$a = \begin{pmatrix}
-1 \\
-1 \\
1 \\
0
\end{pmatrix}, \quad c = \begin{pmatrix}
0 \\
0 \\
1 \\
1
\end{pmatrix}.$$  \hfill (D4)

The number of measurements to achieve an accuracy of $\epsilon$ is

$$M_g = \frac{1}{\epsilon^2} \left( \sqrt{a^\dagger Ca} + \sqrt{c^\dagger Cc} \right)^2$$

$$= \frac{1}{\epsilon^2} \left( \sqrt{4} + \sqrt{0} \right)^2$$

$$= \frac{4}{\epsilon^2}. \hfill (D5)$$

Now, let us consider breaking up the first group into

$$\{-XX\}, \{-YY, ZZ\}.$$  \hfill (D6)

In this case, the coefficient vectors are

$$a = \begin{pmatrix}
-1 \\
0 \\
0 \\
0
\end{pmatrix}, \quad b = \begin{pmatrix}
0 \\
-1 \\
1 \\
0
\end{pmatrix}, \quad c = \begin{pmatrix}
0 \\
0 \\
1 \\
1
\end{pmatrix}.$$  \hfill (D7)

The number of measurements required to attain an accuracy $\epsilon$ is therefore

$$M_g = \frac{1}{\epsilon^2} \left( \sqrt{a^\dagger Ca} + \sqrt{b^\daggerCb} + \sqrt{c^\daggerCc} \right)^2$$

$$= \frac{1}{\epsilon^2} \left( \sqrt{1} + \sqrt{1} + \sqrt{0} \right)^2$$

$$= \frac{4}{\epsilon^2}. \hfill (D8)$$

Therefore, under the optimal measurement strategy it is not preferable to break the $\{-XX, -YY, ZZ\}$ group into $\{-XX\}$ and $\{-YY, ZZ\}$. In this specific example we have equality because for $\alpha = -\beta$ we have $\langle \alpha a + \beta b, \alpha a + \beta b \rangle = 0$.

Appendix E: Derivation of $\hat{R}$ formula

Claim 3. For $R$ as defined in Eq. (19), if all variances and covariances are replaced with their expectation value over uniform spherical distribution, we obtain a new metric, $\hat{R}$, given by

$$\hat{R} = \left( \frac{\sum_{i=1}^{N} \sum_{j=1}^{N} |a_{ij}|^2}{\sum_{i=1}^{N} \sqrt{\sum_{j=1}^{N} a_{ij}^2}} \right)^2 \hfill (E1)$$

Proof. The variance of a single Pauli operator is

$$\text{Var}[P_i] := 1 - \langle P_i \rangle^2. \hfill (E2)$$

The expectation of this variance for all $P_i \neq I$ is

$$\mathbb{E}[\text{Var}P_i] = 1 - \mathbb{E}[\langle P_i \rangle^2]$$

$$= 1 - \int \langle \langle \psi | P_i | \psi \rangle \rangle^2 \, d\psi \hfill (E3)$$

$$= 1 - \alpha_n,$$

where $\alpha_n := 1/(2^n + 1)$, with $n$ the number of qubits, is independent of $P_i$ [54, Exercise 7.3]. Trivially, $\text{Var}[I] = 0$. In addition, it was shown in Ref. [23] that

$$\mathbb{E}[\text{Cov}[P_i, P_j]] = 0, \hfill (E4)$$

for all $P_i \neq P_j$. Simple substitution of these results yields Eq. (E1). $\square$
Appendix F: Full numerical results

In this Appendix, we present the results of the numerical simulations discussed in the main text.

| Molecule | \( n \) qubits | \( t \) Paulis | Grouping | Ratios \( R, \hat{R} \) | Rotation Circuit 2q-size |
|----------|----------------|--------------|----------|----------------|--------------------------|
| \( \text{H}_2 \) | 2 | 4 | 2 | 2.00 | 1.50 | 1.09 | 1.93 | 4.60 | 1.76 | 0 | 0 | 0 |
| \( \text{H}_2^+ \) | 4 | 59 | 10 | 5.90 | 3.50 | 3.76 | 11.92 | 33.04 | 10.25 | 6 | 3 | 0.80 |
| \( \text{LiH}^- \) | 10 | 630 | 41 | 15.37 | 6.85 | 19.60 | 24.91 | 34.74 | 23.97 | 45 | 18 | 5.29 |
| \( \text{OH}^- \) | 10 | 630 | 38 | 16.58 | 7.29 | 6.32 | 8.90 | 12.86 | 8.51 | 45 | 17 | 5.63 |
| \( \text{HF} \) | 12 | 1085 | 51 | 21.27 | 9.04 | 7.68 | 11.27 | 16.96 | 10.67 | 66 | 26 | 7.37 |
| \( \text{BH}_3 \) | 14 | 1584 | 66 | 24.00 | 10.36 | 17.21 | 20.93 | 32.13 | 20.05 | 91 | 26 | 9.56 |
| \( \text{NH}_3 \) | 14 | 3608 | 118 | 30.58 | 11.34 | 15.96 | 26.93 | 15.31 | 7.37 |
| \( \text{CH}_4 \) | 16 | 3887 | 123 | 31.60 | 16.39 | 16.96 | 21.63 | 29.33 | 20.27 | 120 | 45 | 17.65 |
| \( \text{O}_2 \) | 18 | 2238 | 67 | 33.40 | 13.48 | - | - | - | - | 20.23 | 153 | 44 | 21.57 |
| \( \text{N}_2 \) | 18 | 2950 | 78 | 37.82 | 13.91 | - | - | - | - | 22.13 | 153 | 53 | 20.42 |
| \( \text{CO} \) | 18 | 4426 | 128 | 34.58 | 13.48 | - | - | - | - | 21.31 | 153 | 50 | 20.23 |
| \( \text{HCl} \) | 18 | 4538 | 123 | 36.89 | 13.87 | - | - | - | - | 10.36 | 153 | 49 | 20.35 |
| \( \text{NaH} \) | 18 | 5850 | 135 | 43.33 | 14.73 | - | - | - | - | 12.90 | 153 | 45 | 21.44 |
| \( \text{H}_2\text{S} \) | 20 | 6277 | 147 | 42.70 | 16.06 | - | - | - | - | 11.60 | 190 | 58 | 25.98 |
| \( \text{PH}_3 \) | 22 | 19746 | 304 | 64.95 | 18.77 | - | - | - | - | 13.05 | 231 | 67 | 28.02 |
| \( \text{SiH}_4 \) | 24 | 18713 | 304 | 61.56 | 20.98 | - | - | - | - | 13.94 | 276 | 77 | 36.03 |
| \( \text{NaF} \) | 26 | 16538 | 287 | 57.62 | 20.44 | - | - | - | - | 23.36 | 325 | 90 | 42.28 |
| \( \text{LiCl} \) | 26 | 17044 | 292 | 58.37 | 20.46 | - | - | - | - | 12.22 | 325 | 89 | 39.42 |
| \( \text{KH} \) | 26 | 24290 | 325 | 74.74 | 22.30 | - | - | - | - | 12.87 | 325 | 115 | 45.18 |
| \( \text{CO}_2 \) | 28 | 11429 | 216 | 52.91 | 21.02 | - | - | - | - | 38.47 | 378 | 104 | 44.51 |
| \( \text{F}_2\text{O} \) | 28 | 20541 | 317 | 64.80 | 22.83 | - | - | - | - | 36.82 | 378 | 105 | 46.12 |
| \( \text{NO}_2 \) | 28 | 20549 | 311 | 66.07 | 22.93 | - | - | - | - | 40.69 | 378 | 109 | 46.25 |
| \( \text{Cl}_2 \) | 34 | 34334 | 378 | 90.83 | 28.09 | - | - | - | - | 26.58 | 561 | 156 | 73.24 |
| \( \text{NaCl} \) | 34 | 42826 | 498 | 86.00 | 28.54 | - | - | - | - | 20.46 | 561 | 166 | 74.34 |
| \( \text{SF}_2 \) | 36 | 56025 | 567 | 98.81 | 31.96 | - | - | - | - | 30.65 | 630 | 180 | 78.67 |
| \( \text{HBr} \) | 36 | 62589 | 602 | 103.97 | 31.88 | - | - | - | - | 16.03 | 630 | 154 | 78.98 |
| \( \text{SO}_2 \) | 36 | 75315 | 691 | 108.99 | 33.21 | - | - | - | - | 29.75 | 630 | 187 | 66.90 |
| \( \text{NO}_3^- \) | 38 | 61132 | 622 | 92.28 | 31.23 | - | - | - | - | 65.01 | 703 | 182 | 86.40 |
| \( \text{H}_2\text{Se} \) | 38 | 69684 | 631 | 110.43 | 33.91 | - | - | - | - | 16.49 | 703 | 196 | 86.88 |

TABLE IV. The full set of results of the numerical simulations discussed in the main text, with molecules as listed. The molecular geometry is approximately that of the equilibrium configuration. For each molecule, we show a number of results related to the grouping of Hamiltonian terms, how the grouping reduces the number of measurements required, and the number of two-qubit gates in the resulting rotation circuits. In all cases, we used OpenFermion [57] and Psi4 [64] to obtain Hamiltonians in the STO-3G basis and under the symmetry conserving Bravyi-Kitaev transformation [17, 58]. Using the grouping method described in the text, SORTED INSERTION, the number of groups, \( N \), the average number of terms per group, \( m_i \), and the average rank of the groups, \( k_i \), are shown, for molecules with \( n \) qubits and \( t \) Pauli operators, excluding the identity, in the Hamiltonian sum. Given the groupings shown, for the smallest nine molecules, we calculated the ratio \( R \), as given in Eq. (19), for 100 randomly selected trial states, prepared by choosing random sets of parameters for a hardware efficient ansatz preparation circuit of depth 1. For each molecule, we show the mean, minimum and maximum values of \( R \) obtained from the 100 runs. We also show the value of \( \hat{R} \), obtained by Eq. (29), which we can see is close in value to the mean value of \( R \) where this has been calculated. A key result of interest is the maximum number of two-qubit gates required to obtain a measurement of all the operators in a given Hamiltonian. We show the theoretical maximum, given by the largest value of \( k_n - \frac{1}{2}k(k + 1) \) for any group, and the true largest value for any group once the rotation circuits have been found. The ratio of these two numbers is shown in Fig. 3(c), and we can see it has a value of approximately 3.5. We also show the mean number of two-qubit gates required in a rotation circuit, averaged across all groups for a given molecule.