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Reducing Qubit Requirements for Quantum Simulations Using Molecular Point Group Symmetries

Kanav Setia,* Richard Chen, Julia E. Rice, Antonio Mezzacapo, Marco Pistoia, and James D. Whitfield

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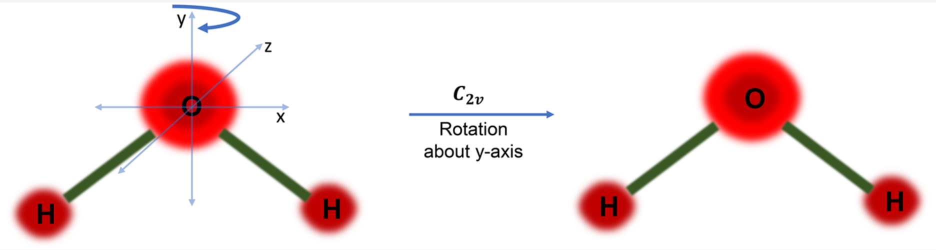

ABSTRACT: Simulating molecules is believed to be one of the early stage applications for quantum computers. Current state-of-the-art quantum computers are limited in size and coherence; therefore, optimizing resources to execute quantum algorithms is crucial. In this work, we develop the second quantization representation of spatial symmetries, which are then transformed to their qubit operator representation. These qubit operator representations are used to reduce the number of qubits required for simulating molecules. We present our results for various molecules and elucidate a formal connection of this work with a previous technique that analyzed generic Z_2 Pauli symmetries.

■ INTRODUCTION

Quantum simulation of chemistry is one of the most promising applications for near-term quantum computers. The interest in the field has grown exceptionally, resulting in many algorithms for quantum simulation on quantum computers. Of particular interest have been the improvements in algorithms for near-term noisy intermediate-scale quantum (NISQ) devices.[1]

There has been constant improvement in the resources required for quantum simulation. A prohibitively large number of gates required for the evolution of wave functions[2] in the case of phase estimation algorithms led to the development of hybrid algorithms such as the variational quantum eigensolver.[3]

At the same time, multiple error mitigation techniques for NISQ devices have been proposed.[4,5] Some of these techniques involve extrapolating errors[6] and make use of the symmetries present in the Hamiltonian[4,7] to partially correct errors. There has been some recent work that involved using different fermionic encodings[8] to reduce the number of gates and yield some error mitigation. The number of qubits required for such encodings is greater than the number of fermionic modes in the system. We refer readers to refs 9 and 10 for a review of the various techniques for quantum chemistry on quantum computers.

These developments have contributed toward the simulation of molecules such as beryllium hydride on quantum computers.[11] Further, there has been a lot of development of quantum computer architectures beyond superconducting qubits, e.g., trapped ion quantum devices.[12]

Even with all these exciting developments, we are still some time away from fault-tolerant quantum computers. The qubits remain precious resources for NISQ devices, and it is important to continue minimizing the number of qubits required for simulating a particular system. In this work, we present techniques where symmetries present in the molecules are used to reduce the number of qubits required for the simulation.

In ref 13, a procedure for tapering off qubits based on Z_2 symmetries was developed. The idea involved finding a Pauli string that commutes with the Hamiltonian. An efficient algorithm was presented to find Pauli strings that commute with the Hamiltonian. Such Pauli strings/operators are called the symmetries of the Hamiltonian. On the basis of these Pauli strings, a unitary operator could be found that transforms the Hamiltonian in such a way that the Hamiltonian acts trivially or at most with σ_x on a set of qubits. The qubits on which the Hamiltonian acts trivially or with σ_x can then be left out of the

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simulation. Effectively, the Hamiltonian has been projected into symmetry subspaces, all of which can be simulated using a lesser number of qubits. On the basis of the results in a previous paper,[13] it is natural to ask the physical meaning of the obtained symmetries. For a few of the Pauli strings (symmetries), it is easy to determine the physical meaning, e.g., if a Jordan−Wigner transform was used then the string $Z^{\otimes N}$ corresponds to the parity of the fermions. For many other Pauli strings, the correspondence to a physical symmetry was not obvious.

In our current work, we have developed a collection of new techniques. These enable us to write down the second quantization representation of the point group symmetries. This second quantization representation could then be transformed to qubit operator representation. In general, this qubit operator representation is a summation of the Pauli strings. We then introduce a technique to turn the summation of the Pauli strings representation of a subset of these symmetries to a single Pauli string. Some of the symmetries obtained are the same as the ones found in ref 13. Therefore, our work also provides the physical meaning for the symmetries found in the previous work. The commuting set of symmetries that are represented by single Pauli strings can be used to reduce the qubit count using the tapering off qubit procedure (Qubit Tapering). We also present a way to pick out the correct eigensector of the Hamiltonian. Knowing the correct eigensector beforehand reduces the number of experiments to be run compared to the previous work. This improvement is exponential in the number of qubits tapered, e.g., if five qubits are tapered then instead of running the experiment 32 times (because we do not know which eigensector contains the ground state) we just need to run it once.[14]

An outline of the paper is as follows: in Qubit Tapering, we review a result on qubit tapering of second-quantized Hamiltonians presented in ref 13. Building on that, in Point Group Symmetries and Point Group Symmetries in Second Quantization we discuss point group symmetries and formalize a second quantization representation of point group symmetries in molecular systems. In Representing Point Group Symmetries as Pauli Operators, we present the procedure to diagonalize the matrix representation of the second quantization representation. These diagonal matrices transform to a single Pauli string. These Pauli operators can then be used to taper off qubits using results from ref 13. Finally, in Results, we present our results for different molecules belonging to different point groups.

QUBIT TAPERING BASED ON Z_2 SYMMETRIES

A system with M fermionic modes can be described by the following Hamiltonian:

$$\mathcal{H} = \sum_{ij}^{M} h_{ij} a_i^\dagger a_j + \frac{1}{2}\sum_{ijkl}^{M} h_{ijkl} a_i^\dagger a_j^\dagger a_k a_l \tag{1}$$

where h_{ij} and h_{ijkl} are the one-body and two-body integrals. For a given molecule, these can be obtained from various quantum chemistry software packages.[15,16] Additionally, $\{a_i^\dagger, a_j^\dagger, ...\}$ and $\{a_i, a_j, ...\}$ are the creation and annihilation operators, which obey the canonical commutation relations:

$$a_i a_j + a_j a_i = 0, \quad a_i a_j^\dagger + a_j^\dagger a_i = \delta_{i,j} I \tag{2}$$

To simulate eq 1 on a quantum computer, we need to map the Hamiltonian to qubit operators. This can be achieved with one of the many transformations available, e.g., the Jordan−Wigner transformation, parity, etc. The transformed fermionic Hamiltonian takes the following form:

$$H = \sum_{j}^{r} c_j \boldsymbol{\eta}_j \tag{3}$$

where r is the total number of terms, $\boldsymbol{\eta}_j \in \mathcal{P}_M$, and $\mathcal{P}_M$ is the Pauli group given by

$$\mathcal{P}_M = \pm\{I, \sigma_x, \sigma_y, \sigma_z\}^{\otimes M} \tag{4}$$

For the Jordan−Wigner, parity, and Bravyi−Kitaev[17] transformations (encoding), the length of the string is M, which is the same as the number of modes, but this could be different for mappings like superfast encoding (SE) and generalized superfast encoding (GSE).[8]

Consider a set of k qubits out of a total M, on which all the terms $\{\boldsymbol{\eta}_j\}$ in the Hamiltonian act trivially (with an identity operator). Then, it is easy to see that we do not need to include those k qubits in the simulation. Furthermore, the qubits can still be left out even if all the terms, $\boldsymbol{\eta}_j$, act on the k qubits with at most one Pauli gate, e.g., σ_x. In such a scenario, the single qubit Pauli gate appearing in various $\boldsymbol{\eta}_j$ terms can be replaced by their eigenvalues, ± 1, such that the jth qubit can be tapered off.

So, we are motivated to transform the Hamiltonian in such a way that it acts trivially or at most with one Pauli gate on a subset of qubits. For this, we make use of the symmetries present in the system. Consider an abelian group $\mathcal{S} \in \mathcal{P}_M$, such that $-I \notin \mathcal{S}$. Such a group is called the symmetry of the Hamiltonian if all the elements of $\mathcal{S}$ commute with each Pauli term of the Hamiltonian. We know that every group has a set of generators, $\{\boldsymbol{\tau}_1, ..., \boldsymbol{\tau}_k\}$, and from stabilizer theory,[18,19] we know:

$$U_i \boldsymbol{\tau}_i U_i^\dagger = \sigma_x^{q(i)}, \quad q = \{a, b, ...\} \tag{5}$$

where $U_i \in C_M$. The Clifford group,[20] C_M, on M qubit is defined as the set of unitary operators, U, such that

$$U\gamma U^\dagger \in \mathcal{P}_M, \quad \forall\, \gamma \in \mathcal{P}_M$$

If we could find the group of symmetries of the Hamiltonian then we could transform the generator set of the symmetries to single qubit Pauli operators using eq 5. For a given symmetry, if we transform the Hamiltonian using the unitary U_i in eq 5 then each Pauli term in the transformed Hamiltonian, $U_i H U_i^\dagger$, must commute with $\sigma_x^{q(i)}$. In other words

$$U_i H U_i^\dagger = \sum_j c_j \boldsymbol{\sigma}_j, \quad [\boldsymbol{\sigma}_j, \sigma_x^{q(i)}] = 0$$

where $\boldsymbol{\sigma}_j = U_i \boldsymbol{\eta}_j U_i^\dagger$. This would imply that the transformed Hamiltonian must be acting trivially or at most with σ_x on the $q(i)$th qubit. This would allow us to replace the σ_x on the $q(i)$th qubit by its eigenvalue and remove the qubits from the simulation.

We now describe two important subprocedures for the above technique to work. First, we describe how to find the symmetry group, and then, we will describe the procedure to find the unitary U to transform the generating set of the symmetries as well as the Hamiltonian.

Finding Symmetries. A Pauli string, $\boldsymbol{\eta}$, acting on N qubits can be parametrized by a binary string $(a_x|a_z)$ of length $2N$, where each component of vectors a_x and a_z are zero or one.[21] Qiskit uses the same representation for the Pauli class to represent a Pauli string. This way, each $\boldsymbol{\eta}(a_x|a_z)$ can be represented as

$$\boldsymbol{\eta}(a_x|a_z) = \prod_{i \in a_x} \sigma_x^{\,i} \cdot \prod_{j \in a_z} \sigma_z^{\,j}$$

This parametrization is very effective when we need to multiply two Pauli strings or if we want to check whether the terms commute.

$$\boldsymbol{\eta}(a_x|a_z)\boldsymbol{\eta}(b_x|b_z) = (-1)^{a_x b_z + a_z b_x}\boldsymbol{\eta}(b_x|b_z)\boldsymbol{\eta}(a_x|a_z)$$

In order for the terms to commute, $a_x b_z + a_z b_x = 0 \bmod 2$. We can represent all the Pauli strings appearing in the Hamiltonian by a binary matrix:

$$G(H) = \begin{bmatrix} G_x \\ G_z \end{bmatrix} \tag{6}$$

where the jth column of G is a binary matrix corresponding to $(a_x|a_z)$ representing $\boldsymbol{\eta}_j$. It can be seen that the size of the G matrix will be $2M \times r$, where r is the total number of terms in the Hamiltonian. From the G matrix, we can construct another check matrix, E:

$$E = [(G_z)^{\mathrm{T}} \;\; (G_x)^{\mathrm{T}}] \tag{7}$$

It can be observed that the kernel of the check matrix of E, Ker(E), gives the elements of the symmetry group. Using Ker(E), one can obtain the generators, $\boldsymbol{\tau}_i$, of the group by using the Gram−Schmidt orthogonalization procedure over the binary field, Z_2.

Finding the Unitaries. Once we have the generators of the symmetries $\{\boldsymbol{\tau}_i \in \mathcal{P}\}$ of the Hamiltonian then, as discussed above, each of these symmetries can be turned into a Pauli X operator on a single qubit using eq 5. To find the unitary U, we try to find the σ_x value on a qubit such that it anticommutes with one of the symmetries and commutes with all of the other symmetries. Then

$$U_i = \frac{1}{\sqrt{2}}(\tau_i + \sigma^x_{q(i)})$$

Furthermore, we can use the permutation operators to bring qubits belonging to set q to the end. These U_i's, along with permutation operators W_i's, can then be used to transform the Hamiltonian.

$$(U_1W_1U_2W_2 \ldots U_kW_k)H(W_k^{\dagger}U_k^{\dagger} \ldots W_1^{\dagger}U_1^{\dagger}) = \sum_j c_j \boldsymbol{\sigma}_j$$

where W_i's are the permutation matrices. The transformed Hamiltonian now commutes with $\sigma_x^{\,q(i)}$. This implies that all the terms in the Hamiltonian must act trivially on the last k qubits or with just the σ_x's. In case of the variational quantum eigensolver algorithm, we can therefore remove the last k qubits, and the σ_x operators are replaced with their eigenvalues ±1.

This tapering off qubit procedure was shown to find many symmetries of molecular systems.[13] Bravyi et al. used the procedure on Hamiltonians of many molecules such as H_2O, LiH, BeH_2, etc. For all the molecules, a standard geometry and the STO-3G basis set were used. Furthermore, many different fermionic encodings, such as the Jordan−Wigner, Bravyi−Kitaev, and parity transformations, were explored to transform the fermionic Hamiltonian. The different encodings did not affect the total number of qubits tapered. For LiH, H_2O, and BeH_2, 4, 4, and 3 qubits were tapered off, respectively.

The following question, which is also the inspiration for the present work, was left unanswered: "what is the physical significance of the symmetries obtained using the tapered off qubit procedure?" Furthermore, we are also interested in exploring their connection to the point group symmetries of the molecules.

■ POINT GROUP SYMMETRIES

For describing point group symmetries in molecules, only four types of nontrivial point group symmetry operations are required.[22] These are the following:

1. Proper rotation (C_n) is a rotation by $360/n$ degrees.
2. Plane-reflection (σ) is a reflection in a given plane.
3. Improper axis rotation (S_n) is a rotation by $360/n$ degrees followed by reflection in a plane perpendicular to the rotation axis.
4. Center of inversion (i) is the inversion ($\vec{x} \rightarrow -\vec{x}$) of all atomic coordinates about the center.

It can be shown that center of inversion (i) is actually the same as S_2.

Furthermore, if we consider all the symmetry elements of a given molecule, then it can be proven that they satisfy the axioms of a group. All four symmetries leave at least one point unchanged in space; hence the name "point group symmetry".

Molecules belong to different point groups based on the different symmetry elements that leave the molecule unchanged. For example, water (H_2O) belongs to the C_{2v} group because it has a vertical proper rotation axis (C_2) and a plane of reflection in the symmetry group, and ammonia (NH_3) belongs to the C_{3v} group because it has a vertical proper rotation axis C_3 and a vertical plane of reflection. The groups are represented using character tables, e.g., the character table for the C_{3v} group is given in Table 1.

Table 1. Character Table for the C_{3v} Group

C_{3v}	E	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	−1
E	2	−1	0

The entries of the table are the characters of symmetry operations within different irreducible representations. For each irreducible representation, the trace of the matrix representation is called the character. The labels for each row correspond to different irreducible representations, and the symmetry elements are grouped into classes matching each column.[22]

There are many other valid representations of the group. One of the ways to build a representation is to consider a vector representation of a point in space and build matrices that transform the vector according to the group action. Another way, which is used to build symmetry adapted linear combinations (SLACs), is to consider a vector representation of atomic orbital functions or molecular orbital functions and build matrices that transform the vector according to the group action. Traditionally, such a procedure is used to build symmetry adapted molecular orbitals from the atomic orbitals. We show that such a representation could also be used to taper off qubits.

■ POINT GROUP SYMMETRIES IN SECOND QUANTIZATION

Our aim is to explore the relation of point group symmetries to the symmetries found using the tapering off qubit procedure. For this, we first develop the second quantization representation of the point group symmetries. We start by considering a finite set of the single particle wave functions given by

$$\{\phi_i(x), \quad i \in [1, M]\} \tag{8}$$

These functions form a basis set which becomes complete as $M \to \infty$. As it is computationally very expensive to deal with large basis sets, truncated basis sets are used. Now, assume the system under consideration has some point group symmetry. If $\boldsymbol{R}$ is the operator that defines the symmetry operation then we get

$$\phi_i'(x) = \boldsymbol{R}(\phi_i(x))$$

It is possible to pick the truncated basis set in such a way that $\boldsymbol{R}$ ends up being a linear transformation, R, which gives us

$$\phi_i'(x) = \sum R_{ji}\phi_j(x)$$

Furthermore, we require that R be a unitary matrix such that the transformed second quantization operators still satisfy the canonical commutation relations (eq 2). In the second quantization formalism, the R matrix is given by

$$b_i = \sum_{j=1}^{M} R_{ji}a_j \tag{9}$$

where b_i and a_j are the second quantization operators associated with $\phi'_i(x)$ and $\phi_j(x)$, respectively. For a given molecule, we can find an $M \times M$ matrix representation for each symmetry operation, R. The matrices will then follow the multiplication table of the symmetry group.

The one-body integrals, $\{h_{ij}\}$, can be represented by an $M \times M$ matrix, and the two-body integrals, $\{h_{ijkl}\}$, can be represented by an $M \times M \times M \times M$ tensor. We can use the unitary matrix R to transform the one-body and two-body tensors and check whether the Hamiltonian remains the same. This is the same as checking the commutator of the Hamiltonian by symmetry. The commutation of the R matrix with the Hamiltonian verifies that it is a symmetry.

It is important to note that we are able to check the commutation of the R matrix with the Hamiltonian without going to the $2^M \times 2^M$ representation of the Hamiltonian. Given the matrix for the unitary R, it is not trivial to get its second quantization representation. However, if we restrict the unitary to be signed permutation matrices then the second quantization representation could be constructed easily. For example, the second quantization representation for swapping mode p and mode q is given by

$$\mathcal{R}_{pq} = I - a_p^\dagger a_p - a_q^\dagger a_q + a_p^\dagger a_q + a_q^\dagger a_p \tag{10}$$

It can be shown that any permutation can be decomposed into a series of transpositions each by swapping two elements at a time. The second quantization operator that gets us the (-1) phase is given by $1 - 2a_p^\dagger a_p$. This operator, along with the second quantization operator for the permutation matrix, lets us generate second quantization representation of any signed permutation matrix.

It can be seen that the R matrices can be constructed using just the signed permutation matrices if the basis sets chosen are atom-centered basis sets. This, in fact, is a common choice while performing molecular calculations.

With the second quantization representation available for the symmetries, we can use any fermion−qubit transformation to get a qubit operator representation of the R matrix. In general, the qubit representation of R ends up being a summation of Pauli strings. The procedure presented in Representing Point Group Symmetries as Pauli Operators can be used if the symmetry is a single Pauli string. In the following section, we present the conditions under which this could be achieved as well as the procedure to do so.

■ REPRESENTING POINT GROUP SYMMETRIES AS PAULI OPERATORS

Consider the Hamiltonian in eq 1. In the following, we consider the symmetries of the Hamiltonian represented by the signed permutation matrix. Suppose $\boldsymbol{\pi}$ is a permutation under which the Hamiltonian is invariant. We show below that in such a case we can remove a qubit.

Suppose R is a unitary matrix of size $n \times n$. Then there exists an n qubit unitary matrix $\hat{R}$ such that

$$\hat{R}a_p\hat{R}^\dagger = \sum_{q=1}^{n} \langle p|R|q\rangle a_q \tag{11}$$

for all $1 \le p \le n$.

We define a permutation matrix R of size $n \times n$ such that

$$R|p\rangle = |\boldsymbol{\pi}(p)\rangle \tag{12}$$

for all $1 \le p \le n$. By assumption

$$\hat{R}H\hat{R}^\dagger = H \tag{13}$$

Now, since R is unitary, it can be written as

$$R = \exp(iG)$$

for some hermitian matrix G of size $n \times n$. The n qubit unitaries for R and G are given by

$$\hat{R} = \exp(i\hat{G}), \qquad \hat{G} = \sum_{p,q=1}^{n} \langle p|G|q\rangle a_p^\dagger a_q \tag{14}$$

A unitary $n \times n$ matrix V that diagonalizes G is chosen such that

$$V^\dagger GV = \sum_{p=1}^{n} \lambda_p|p\rangle\langle p| \tag{15}$$

for some real eigenvalues λ_p. Let $\hat{V}$ be the n qubit unitary matrix constructed from V following eq 11. Next, we define a new symmetry operator

$$S \equiv \hat{V}\hat{R}\hat{V}^\dagger = \exp(\hat{V}\hat{G}\hat{V}^\dagger) = \prod_{p=1}^{n} \exp(i\lambda_p a_p^\dagger a_p) \tag{16}$$

Note that $SH'=H'S$, where $H'=\hat{V}H\hat{V}^\dagger$. In other words, S is a symmetry of H'. Let us now assume that $\boldsymbol{\pi}$ swaps some pairs of modes. Then $\boldsymbol{\pi}^2$ is the identity permutation. Thus, $R^2 = I$, which is possible only if G has eigenvalues $\lambda_p \in \{0, \pi\}$. Let M be the subset of modes p such that $\lambda_p = \pi$. Then

$$S = \prod_{p \in M} (-1)^{a_p^\dagger a_p}$$

If we use the Jordan−Wigner encoding of fermions into qubits then S becomes a Z-type Pauli operator. Thus, we can simulate H' using a system of $n - 1$ qubits by exploiting the Pauli symmetry S. Finally, if H includes only single-particle and two-particle operators then so does H'.

Further, it can be realized that we do not need to construct the G matrix, and in fact, we can diagonalize the R matrix directly to obtain the S matrix. Similar results were obtained in ref 23, where the qubit representation of symmetries was used to build projectors on target symmetry sectors. The qubit operator representing S is an operator that acts with σ_z on qubits, j, where $S(j, j) = -1$.

Another important thing to note is that in case of multiple symmetries, we will be required to simultaneously diagonalize them. Simultaneous diagonalization will only be possible when the symmetries commute. In the case of noncommuting symmetries, the maximal set of commuting symmetries will be used to taper off qubits. This will become more clear in our discussion on the NH_3 molecule.

For example, if for a 5 dimensional S matrix the -1 eigenvalues are in positions (2, 2) and (4, 4) then the Pauli Z symmetry will be Z_2Z_4.

The techniques presented in Point Group Symmetries and Point Group Symmetries in Second Quantization can be used to develop the following procedure for tapering off qubits.

Summary of Algorithm.

(1) For a given molecule with a fixed geometry, get the Hamiltonian in the atomic orbital basis.
(2) For a given geometry of a molecule, the point group symmetries can be found using one of many algorithms available.[24]
(3) Find the matrix form of the point group symmetries.
(4) Choose the largest abelian group of the symmetries.
(5) Find the single Pauli string representation of the symmetries using techniques in Point Group Symmetries and Point Group Symmetries in Second Quantization.
(6) Taper off qubit using the technique in Representing Point Group Symmetries as Pauli Operators.

As we have mentioned previously, the general qubit operator representation of the symmetries is not a single Pauli string. This implies that all the spatial symmetries must not have been found using the method in ref 13. We show that this indeed is the case by finding extra symmetries in the molecules.

RESULTS

Table 2 presents our results for various molecules that we studied along with the number of qubits we were able to taper off. We have open-sourced our code and have made it available on github.[14] We now discuss three molecules from the table to illustrate three important points. We start with discussing the H_2 molecule to illustrate the procedure; then, we discuss the case of BeH_2 to demonstrate that the spatial symmetries could be used to reduce more qubits than what was possible in ref 13. Third, the NH_3 molecule is discussed to show that only the abelian subgroup of the symmetry point group could be used to taper off qubits.

Table 2. Molecules Tested with Our Technique and the Number of Qubits We Were Able to Taper off[a]

symmetry	molecule	qubits required	qubits tapered	qubits tapered (using ref 13)
C_{2v}	H_2O	14	4	3
C_{3v}	NH_3	16	3	2
D_{2h}	C_2H_4	28	5	3
D_{3h}	BF_3	40	5	3
$C_{\infty v}$	LiH	12	4	4
$D_{\infty h}$	CO_2	30	5	4
	C_2H_2	24	5	4
	BeH_2	14	5	4

[a] This includes the two qubit reduction due to the conservation of the spin up electrons and the spin down electrons. All the symmetries here form an abelian group. For all the molecules, an equilibrium geometry and the STO-3G basis set is used. The one-body and two-body terms are obtained on an atomic orbital (AO) basis by running PySCF python package.

H_2 (Symmetry Group: $D_{\infty h}$). As per the formalism presented in Point Group Symmetries in Second Quantization, we want to pick the basis set in such a way that the operation corresponding to the spatial symmetries ends up being a permutation matrix.

We consider the hydrogen molecule with a bond length of 0.7414 Å and choose the basis set to be STO-3G, where a single 1s orbital is placed on each of the hydrogen atoms. Therefore, both C_2 (rotation about z-axis by 180°) and $\sigma(yz)$ (reflection through the yz plane) will have the net effect of swapping the two hydrogen atoms. This corresponds to swapping the 1s orbitals, and hence, the rotation matrix, R, is a permutation matrix:

$$\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

It can be determined that the Hamiltonian does remain the same under this permutation of the fermionic modes. We can then diagonalize the G matrix corresponding to the R matrix and taper off the qubit.

BeH_2 (Symmetry Group: $D_{\infty h}$). For beryllium hydride, the total number of qubits that can be tapered off using point group symmetries is five. In contrast, the symmetries that one can find using the results from ref 13 (Point Group Symmetries) are only four. The geometry used is linear, where a bond length between beryllium and hydrogen atoms of 1.291 Å for both bonds and a STO-3G basis set are used.

Given this geometry, the symmetries that could be represented using a generalized permutation matrix are $\sigma(xy)$ (reflection in the xy plane), $\sigma(yz)$ (reflection in the yz plane), and $\sigma(xz)$ (reflection in the xz plane). The qubit operators for the R operator corresponding to $\sigma(xy)$ and $\sigma(xz)$ turn out to be single qubit operators. The final qubit operators for these symmetries match the symmetries found using ref 13. The unitary operator R for $\sigma(yz)$ symmetry is not diagonal, and the qubit operator representation is a sum of Pauli strings. For this reason, the symmetry is not observed using direct results from 13. However, the spatial symmetry can be used to taper off qubit using the procedure given in Representing Point Group Symmetries as Pauli Operators.

NH_3 (Symmetry Group: C_{3v}). Ammonia belongs to the symmetry group C_{3v}. In the symmetry group, there are two rotation operators and three reflection operators. The two rotation operators form a class and likewise the three reflection operators. If the symmetry group were abelian, we could reduced the qubit count by one for each class. Since the symmetry operators in two classes do not commute, we can reduce the qubit count by just one, corresponding to one of the symmetries. Furthermore, as per the formalism we developed, the unitary operator R must be square to the identity. This implies the only choice we have is the reflection operator. It should be noted that this symmetry did not appear by directly using the method presented in ref 13.

Picking the Right Eigenvalues for the Symmetries. Once we are able to construct all the symmetries, S, of the Hamiltonian, we need to pick the right eigensector of the symmetry. This can be done using the relation between the σ_z qubit operator and the occupation number in the Jordan−Wigner transform:

$$\sigma_z^i = a_i^\dagger a_i - 1 \tag{17}$$

An occupied and unoccupied fermionic mode corresponds to the eigenvalues of −1 and +1 of the σ_z operator, respectively. This implies that a symmetry operator, S, which is a Pauli Z string on, for example, a set Q of qubits, is related to the parity operator of fermionic modes stored in those Q qubits. In our case, we started with atomic orbitals and then transformed them with a V matrix so as to get R into a diagonal form. Consequently, the occupation numbers of these transformed orbitals are stored in the qubits. Additionally, on the basis of whether the orbital is occupied or unoccupied in a given symmetry sector, it is possible to determine the correct eigensector corresponding to the symmetry.

For example, in the case of the BeH_2 molecule, there are 14 orbitals in total with six electrons. The symmetries corresponding to the conservation of spin up electrons and spin down electrons are $S_1=\sigma_z^1\sigma_z^2\sigma_z^3\sigma_z^4\sigma_z^5\sigma_z^6\sigma_z^7$ and $S_2=\sigma_z^8\sigma_z^9\sigma_z^{10}\sigma_z^{11}\sigma_z^{12}\sigma_z^{13}\sigma_z^{14}$, respectively. Since, there are six electrons in total, we know that each spin sector will have three electrons from the Hartree−Fock state. Thus, the correct sector for each of the symmetries, S_1 and S_2, is the one with a −1 eigenvalue.

Molecular Orbitals. Most of the quantum chemistry software recognizes symmetries from geometry and constructs the molecular orbitals for the Hartree−Fock procedure accordingly. This means that molecular orbitals are already symmetrized corresponding to different irreps and that the symmetry operators will be Z_2 symmetries. One way to construct Z_2 symmetries will be to start from R operators as presented in Point Group Symmetries in Second Quantization and then get the Pauli Z string corresponding to the symmetry operator. The R operator will require the knowledge of the molecular orbitals in terms of the atomic orbitals.

The other method to obtain the symmetries will be to just run the subroutine presented in ref 13 to find the Z_2 symmetries. This process is a little bit more efficient as it is automated, whereas currently, it is required to manually construct the R matrices in order to use the formalism presented in the present research. It may be possible to automate this, but we leave this for future works. One benefit of starting from R matrices is that one gets an intuitive understanding of the symmetries. The physical intuition allows us to tweak the details in order to have more symmetries in the system. It also serves as a verification procedure for debugging the software code as we already know the symmetries that we are expecting.

CONCLUSIONS

We have presented a formalism to exploit spatial symmetries present in molecular systems to reduce the number of qubits required for quantum simulations. Compared to one of the results presented in 13, we find that additional symmetries can be discovered, and more qubits can be spared in the mapping to a quantum computer. The results presented here are relevant for optimizing resources in the context of NISQ computing.[1]

AUTHOR INFORMATION

Corresponding Author

Kanav Setia − *Department of Physics and Astronomy, Dartmouth College, Hanover, New Hampshire 03755, United States;* orcid.org/0000-0003-2032-3993;
Email: kanav.setia.gr@dartmouth.edu

Authors

Richard Chen − *IBM T.J. Watson Research Center, Yorktown Heights, New York 10598, United States*
Julia E. Rice − *IBM Almaden Research Center, San Jose, California 95120, United States*
Antonio Mezzacapo − *IBM T.J. Watson Research Center, Yorktown Heights, New York 10598, United States*
Marco Pistoia − *JPMorgan Chase & Co., New York, New York 10172, United States*
James D. Whitfield − *Department of Physics and Astronomy, Dartmouth College, Hanover, New Hampshire 03755, United States;* orcid.org/0000-0003-2873-0622

Complete contact information is available at:
https://pubs.acs.org/10.1021/acs.jctc.0c00113

Notes

The authors declare no competing financial interest.

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