# The Bravyi–Kitaev Transformation: Properties and Applications

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Quantum chemistry is an important area of application for quantum computation. In particular, quantum algorithms applied to the electronic structure problem promise exact, efficient methods for determination of the electronic energy of atoms and molecules. The Bravyi–Kitaev transformation is a method of mapping the occupation state of a fermionic system onto qubits. This transformation maps the Hamiltonian of $n$ interacting fermions to an $O(\log n)$-local Hamiltonian of $n$ qubits. This is an improvement in locality over the Jordan–Wigner transformation, which results in an $O(n)$-local qubit Hamiltonian. We present the Bravyi–Kitaev transformation in detail, introducing the sets of qubits which must be acted on to change occupancy and parity of states in the occupation number basis. We give recursive definitions of these sets and of the transformation and inverse transformation matrices, which relate the occupation number basis and the Bravyi–Kitaev basis. We then compare the use of the Jordan–Wigner and Bravyi–Kitaev Hamiltonians for the quantum simulation of methane using the STO-6G basis. © 2015 Wiley Periodicals, Inc.

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## Introduction

Quantum simulation was first proposed by Feynman[1] and allows for an exponential speedup over classical simulation of some quantum mechanical systems.[2–6] In the context of quantum chemistry, efficient algorithms have been developed for the calculation of energy spectra,[7] reaction rates,[8,9] and reaction details.[10] Quantum computational schemes have been extended into the study of relativistic quantum chemistry.[11] Crucially for this project, the quantum-phase estimation algorithm[12] allows for efficient calculation of molecular energies at an accuracy equivalent to that of classical full configuration interaction calculations. There are three basic approaches to the quantum simulation of chemical systems.

One approach—the so called "first quantization" approach—has been studied in the context of chemical reactive scattering.[10] Here, physical position space is discretized. The electronic wavefunction is then represented in the position representation by the state of the qubits. The chemical Hamiltonian is:

$$\hat{H} = \sum_i \frac{p_i^2}{2M_i} + \sum_{i \leq j} \frac{q_i q_j}{r_{ij}} \tag{1}$$

where sums are over nuclei and electrons, $p_i$ is the momentum of the $i$th particle, $M_i$ is the mass of the $i$th particle, $q_i$ is the charge of the $i$th particle, and $r_{ij}$ is the distance between particles $i$ and $j$ in atomic units. We can simulate the effect of this Hamiltonian by unitarily evolving the qubits through the propagator corresponding to the molecular Hamiltonian, approximated using the quantum split operator method of Zalka[4] or by quantum lattice gas methods.[5,6]

An alternative to grid-based first-quantized approaches is the use of a second-quantized formalism. Here, the molecular Hamiltonian is expressed in terms of creation and annihilation operators acting on some basis of molecular orbitals. This method is the main topic of this article and so discussed in

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greater detail below. While this technique scales less efficiently than the prior method in the asymptotic limit, smaller scale simulations require substantially fewer resources. The reason is that a molecular orbital basis is more efficient for the representation of localized chemical wavefunctions than a Cartesian grid, and hence the first-quantized methods lead to wider, but shallower circuits. Details of resource requirements for such first-quantized simulations for chemistry are given in [10].

One of the differences between the first- and second-quantized approaches lies in whether the antisymmetric nature of the wavefunction is represented through properties of the state (first quantized) or the operators (second quantized). An alternative to grid-based methods in which the dynamics preserves an initially antisymmetric wavefunction is the use of a basis of Slater determinants. In this case, the challenge for quantum algorithms is the evolution under the CI matrix representation of the Hamiltonian. Unlike the second-quantized case, this matrix has no natural expression as a sum of local terms, and no tensor product structure. However, the CI matrix is sparse, and hence quantum simulation techniques for sparse matrices may be applied to this problem. This yields methods that both use an efficient molecular orbital representation of the wavefunction and have optimal asymptotic scaling. This also enables the use of sparse methods, which scale logarithmically with the error. The penalty is that the molecular integrals must be computed on the fly during the quantum computation.[13–15]

The calculation of the energies of molecular Hydrogen and Helium-Hydride using minimal basis sets have been experimentally achieved using linear optical quantum, NMR, and Nitrogen vacancy in diamond quantum computers.[16–19] The first digital fermionic quantum simulation was recently achieved of a four-site Hubbard model in superconducting hardware.[20] These proofs of principle demonstrations are comparable to early quantum chemical calculations carried out in the twentieth century.[21]

The development and optimization of quantum algorithms for chemistry is ongoing. This work is driven by two goals. First is the desire to determine the true optimal asymptotic scaling of these algorithms for large quantum computers. The second is to reduce the resource requirements of small examples to the point that they can be realized experimentally in the near future. Recently, the possibility of using a small quantum computer of around a hundred qubits for the purposes of quantum chemistry has been investigated in detail. Initial upper bounds on the cost indicated that large polynomial scaling would be impractical for such problems.[22] Further analysis developing circuit improvements, tighter upper bounds, and numerical investigation of errors restricted to the chemical ground state resulted in tight and efficiently computable upper bounds on the resources required.[23–25] One may also improve these algorithms by exploiting locality.[26]

The topic of this article is the Bravyi–Kitaev transformation, an alternative to the use of the Jordan–Wigner transformation to map fermions to spins.[27–29] This transformation was defined in [28] in the context of using fermions to perform quantum computations. Its use for the simulation of fermions

by quantum computers, and in particular, its use for the quantum simulation of quantum chemistry, was introduced in [29]. We describe the transformation in detail, and derive some new properties of the transformation that are relevant to the specific case of second-quantized Hamiltonians defined in a basis of spin–orbitals. We give a new recursive definition for the inverse Bravyi–Kitaev transformation matrix, as well as recursive relationships for the update, parity, and flip sets (defined below) which facilitate the computation of these sets. We analyze the efficiency of the Bravyi–Kitaev method for the simulation of the methane molecule. We find that the Bravyi–Kitaev mapping leads to a small improvement, particularly in the number of nonlocal gates required for accurate simulation.

## The Second-Quantized Hamiltonian

As in classical quantum chemistry, we invoke the Born-Oppenheimer approximation, fixing the nuclear coordinates, and calculating the electronic energy at a given geometry. In the second-quantized formalism previously mentioned, the electronic Hamiltonian is given by:

$$\hat{H} = \sum_{i,j} h_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l} h_{ijkl} a_i^\dagger a_j^\dagger a_k a_l \qquad (2)$$

where $h_{ij}$ and $h_{ijkl}$ are integrals, which can be efficiently classically precomputed.

The $a^\dagger$ and $a$ operators in the Hamiltonian are creation and annihilation operators on a basis set of molecular orbitals, as discussed below. Note that here, the two-operator terms effectively correspond to single-electron terms, and the four-operator terms effectively correspond to electron–electron interaction terms.

Because electrons are fermions, we require antisymmetry on exchange of particle index. This is enforced through the use of anticommutator restrictions on the creation and annihilation operators:

$$\{a_j, a_k\} = \{a_j^\dagger, a_k^\dagger\} = 0$$

$$\{a_j, a_k^\dagger\} = \delta_{jk} I \qquad (3)$$

Our task, therefore, is effectively to find the lowest eigenvalue of this Hamiltonian. As the dimension of the Fock space grows exponentially with the number of basis orbitals, this is classically intractable for systems of any reasonable size. However, a quantum computer could remove this problem using quantum-phase estimation.[7]

To achieve this, three steps must be taken. First, a mapping between the physical electronic states and qubit states in a quantum computer must be established. Second, a well-defined evolution operator equivalent to that of the molecular Hamiltonian must be determined for the qubit basis. This necessitates the derivation of qubit representations of the electronic creation and annihilation operators. Finally, the phase estimation algorithm requires the preparation of a *guiding state*. A guiding state is an input state to the algorithm,

which has an overlap with the true ground state, which decays at worst as an inverse polynomial in the system size.

In the worst case, Hamiltonians are known for which the problem of finding the ground state is QMA-complete (the quantum equivalent of NP-complete).[30,31] Quantum computers are not believed to be capable of efficiently solving QMA-complete problems in the worst case, just as classical computers are not believed to be capable of efficiently solving NP-complete problems in the worst case. Assuming this is true, there exist Hamiltonians for which no efficiently preparable guiding state is likely to be available, and for which, the phase estimation algorithm is, therefore, incapable of finding the ground state.

However, these worst case Hamiltonians rely on clock constructions so that their ground states are superpositions of quantum states corresponding to time slices of an arbitrary quantum circuit of depth polynomial in the number of qubits.[30] Even constructions that show the QMA-completeness of specific physical models rely on geometrically complex interactions.[32] It is, therefore, a widely believed conjecture that typical physical Hamiltonians do not correspond to worst case instances, and therefore, have efficiently preparable ground states. Specific algorithms for state preparation are considered in [7,33–36].

One may also ask whether the requirement to prepare guiding states may rely on features of physical Hamiltonians, which can also be exploited for the development of classical algorithms. The requirement on a guiding state for a quantum computation of an energy eigenvalue is only that its overlap with the true ground state is bounded by an inverse polynomial in the system size. Recent consideration of Quantum Monte Carlo methods (which simulate quantum systems using conventional computers) showed that a much stronger guiding state was required to make these methods efficient, even in the case of so-called stoquastic Hamiltonians where there is no fermion sign problem.[37]

## Qubit creation and annihilation operators

In this section, we describe three mappings of fermionic states and operators to qubit states and operators. In each case, we map the occupation number basis to the qubit basis. The occupation number configuration basis states are given by specifying the occupation $f_i \in \{0, 1\}$ of every orbital. The fermionic creation and annihilation operators, when acting on a system of $n$ orbitals with occupation state vector, $|f_{n-1}f_{n-2}...f_1f_0\rangle$ yield:

$$a_j^\dagger |f_{n-1}...f_{j+1}0f_{j-1}...f_1f_0\rangle = (-1)^{\sum_{s=0}^{j-1} f_s} |f_{n-1}...f_{j+1}1f_{j-1}...f_1f_0\rangle \quad (4)$$

$$a_j^\dagger |f_{n-1}...f_{j+1}1f_{j-1}...f_1f_0\rangle = 0 \quad (5)$$

$$a_j |f_{n-1}...f_{j+1}1f_{j-1}...f_1f_0\rangle = (-1)^{\sum_{s=0}^{j-1} f_s} |f_{n-1}...f_{j+1}0f_{j-1}...f_1f_0\rangle \quad (6)$$

$$a_j |f_{n-1}...f_{j+1}0f_{j-1}...f_1f_0\rangle = 0 \quad (7)$$

We note that one is free to choose the ordering of the orbitals here. We have chosen an ordering in which the orbitals $f_s$ with $s < j$ determine the parity, but the choice $s > j$ is equally valid from the point of view of realizing the anticommutation relations, and is more common in the chemical literature.

As can be seen in Eqs. (4) through (7), these operators depend on both the occupation of orbital $j$ as well as its parity $p_j = \sum_{s=0}^{j-1} f_s$, as the phase shift in Eqs. (4) and (6) can be written in terms of the parity as $(-1)^{p_j}$. If the parity is odd, the state is multiplied by a factor of $-1$, and if it is even, there is no phase shift. Since the fermionic creation and annihilation operators change both occupation and parity, their qubit analogues also need to do so. Therefore, both the occupation and parity of each orbital must be stored when mapping from the occupation basis state onto a qubit basis state.

We consider three mappings where sums of fermionic occupations are stored in the qubit state. These are the Jordan–Wigner basis, the parity basis and the Bravyi–Kitaev basis. In all cases, it is helpful to define several subsets of the qubits, which contain the information needed to apply fermionic operators to the state. These sets are defined below, and we use $\bar{f}_i$ to indicate Boolean negation $\bar{0} = 1$, $\bar{1} = 0$.

1. The update set, $U(i)$. This is the set of qubits, apart from $i$ that must be updated, when the occupancy $f_i$ changes.
2. The parity set $P(i)$. This is the set of qubits that determines the parity $p_i = \sum_{j<i} f_j$. Note that the occupancy $f_i$ is not included in this sum.
3. The flip set $F(i)$. This is the set of qubits that determines whether the qubit value is equal to the occupancy $f_i$ or its negation $\bar{f}_i$
4. The remainder set $R(i)$. The flip set is a subset of the parity set, and so it is convenient to define the complement of the flip set in the parity set—$R(i) = P(i) \backslash F(i)$.

Note that all of the sets $U(i)$, $P(i)$, $F(i)$ and $R(i)$ are defined such that the reference qubit $i$ is never a member of them.

Our task is then to represent the electronic creation and annihilation operators as operators on the qubit space. Qubit creation and annihilation operators can be defined in terms of Pauli operators as follows:

$$\hat{Q}^+ = |1\rangle\langle 0| = \frac{1}{2}(X - iY)$$

$$\hat{Q}^- = |0\rangle\langle 1| = \frac{1}{2}(X + iY) \quad (8)$$

These operators contain only Pauli operators acting on the qubit being created or annihilated. They, therefore, commute for different qubits, and so clearly do not fulfil the anticommutation relations required. We must combine these operators with actions on the sets defined above to obtain qubit creation and annihilation operators that satisfy the canonical fermionic commutation relations.

### The Jordan–Wigner transformation

In the Jordan–Wigner transformation, we use the state of a qubit to denote whether or not a particular basis orbital is occupied—clearly, as electrons are fermionic, occupation numbers which are not zero or one are impossible. The qubits directly store the

*occupation basis.*[38] In this case, the update set is empty (recall that qubit $i$ is not a member of the update set).

Parity information needed to correctly apply the creation and annihilation operators for orbital $i$ is contained in all qubits $j < i$. Hence the parity set is defined by $P(i) = \{j | j < i\}$. This is the Jordan–Wigner transformation.[27] We consequentially have the qubit operators:

$$a_i^\dagger = \frac{1}{2}(X_i - iY_i) \bigotimes_{j<i} Z_i = Q_i^+ \otimes Z_{P(i)}$$

$$a_i = \frac{1}{2}(X_i + iY_i) \bigotimes_{j<i} Z_i = Q_i^- \otimes Z_{P(i)} \quad (9)$$

where $Z_{P(i)}$ means a Pauli $Z$ operator acting on all qubits in the set $P(i)$. The fact that these operators obey the fermionic anticommutation relations follows from the fact that $\{Z, Q^\pm\} = 0$ and $\{Q^+, Q_-\} = \mathbb{I}$.

### Parity basis

The Jordan–Wigner transformation stored occupancy locally, and parity is nonlocal. The parity basis stores the parity locally,[28] and the occupancy is nonlocal. The parity information of each orbital $j$ is stored in the corresponding qubit $j$,

$$q_j = p_j + f_j = \sum_{s=0}^{j} f_s. \quad (10)$$

Evidently, $P(j) = \{j-1\}$ in the parity basis. Whether qubit $j$ stores $f_j$ or $\bar{f}_j$ is determined by qubit $j-1$ in the parity basis. Hence, the flip set in this basis is equal to the parity set: $F(j) = P(j)$, and so the remainder set $R(j) = \varnothing$. The update set $U(j)$ is the set of qubits that must be updated when occupancy $f_j$ changes. Now $f_j$ appears in every $q_i$ such that $i > j$, and so when $f_j$ changes every qubit $i > j$ must be updated. Hence, $U(j) = \{i | i > j\}$ for the parity basis. Given the definitions of these sets, we can now write the qubit creation and annihilation operators.

$$a_j^\dagger = (\bigotimes_{i>j} X_i) \otimes (\Pi_{F(j)}^0 \otimes Q_j^- + \Pi_{F(j)}^1 \otimes Q_j^+) \otimes Z_{P(j)}$$

$$a_j = (\bigotimes_{i>j} X_i) \otimes (\Pi_{F(j)}^0 \otimes Q_j^+ + \Pi_{F(j)}^1 \otimes Q_j^-) \otimes Z_{P(j)} \quad (11)$$

where $\Pi^b = |b\rangle\langle b|$. Now, because $P(j) = F(j)$ and because $\Pi^x Z = (-1)^x \Pi^x$ we can write:

$$a_j^\dagger = (\bigotimes_{i>j} X_i) \otimes (\Pi_{F(j)}^0 \otimes Q_j^- - \Pi_{F(j)}^1 \otimes Q_j^+) = \frac{1}{2}(\bigotimes_{i>j} X_i)(Z_j \otimes Z_{j-1} - iY_j)$$

$$a_j = (\bigotimes_{i>j} X_i) \otimes (\Pi_{F(j)}^0 \otimes Q_j^+ - \Pi_{F(j)}^1 \otimes Q_j^-) = \frac{1}{2}(\bigotimes_{i>j} X_i)(Z_j \otimes Z_{j-1} + iY_j) \quad (12)$$

The number of nontrivial Pauli factors in these operators scales as $O(n)$, just as for Jordan–Wigner. In this case, it is the update set whose size scales linearly with the number of qubits.

### Bravyi–Kitaev transformation

The Bravyi–Kitaev transformation stores both occupation and parity nonlocally, rather than storing the occupation state locally and

parity nonlocally or vice versa, as is the case for the Jordan–Wigner and parity bases. In the Bravyi–Kitaev basis, for any index $j$, if $j$ is even, qubit $j$ holds only the occupation state of orbital $j$, and if $j$ is odd, qubit $j$ holds a partial sum of the occupation state of a set of orbitals of index less than $j$. The Bravyi–Kitaev transformation that maps the fermionic occupation state vector to the qubit state, denoted $\beta_n$ for $n$ orbitals such that $\beta_n \vec{f}_n = \vec{b}_n$, is given by:

$$\beta_{2^x} = \left(\begin{array}{c|c} \beta_{2^{x-1}} & 0 \\ \hline 0 & \\ \leftarrow 1 \rightarrow & \beta_{2^{x-1}} \end{array}\right) \text{ where } \beta_1 = \left(\ 1\ \right), \quad (13)$$

where $\leftarrow 1 \rightarrow$ indicates a row of ones in the bottom row.

For example, for eight qubits, the fermion occupation state vector is mapped to the qubit basis state as shown in Eq. (14) (all sums in mod(2)):

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \end{pmatrix} = \begin{pmatrix} f_0 \\ f_1 + f_0 \\ f_2 \\ f_3 + f_2 + f_1 + f_0 \\ f_4 \\ f_5 + f_4 \\ f_6 \\ f_7 + f_6 + f_5 + f_4 + f_3 + f_2 + f_1 + f_0 \end{pmatrix}$$

$$(14)$$

From this definition, we proceed to obtain the update, parity, flip, and remainder sets.

The update set, $U(j)$, is the set of qubits that must be updated when the occupation of some orbital $j$ is changed. This is the set of qubits that hold partial sums that depend on the occupation of orbital $j$. Because the transformation matrix $\beta_n$ is lower diagonal, only qubits with $i > j$ will be contained in $U(j)$. We abuse notation to write $U(j) > j$ to indicate this. Since qubits of even $j$ hold only the occupation state of orbital $j$, the update set will only contain odd qubit indices, as only qubits with odd $j$ hold partial sums. From the Bravyi–Kitaev transformation matrix, given that any column $j$ contains the vector that acts on occupation state vector entry $j$, the update set for changing the occupation of orbital $j$ is simply the set of qubits with index greater than $j$ and equal to the indices of the nonzero entries in column $j$.[29] The update sets for each orbital for systems of 1–8 orbitals are given in Table 1.

The parity set, $P(j)$, is the set of qubits needed to determine the parity of the set of orbitals with index $<j$. The parities are determined from the occupation number vector by the action of a matrix $\pi$, which is defined by

$$[\pi_n]_{ij} = \begin{cases} 1 & \text{if } i < j \\ 0 & \text{otherwise} \end{cases} \quad (15)$$

Note this is not the transformation matrix, which gives the parity basis, as $\pi_n$ has a zero diagonal, given that, it computes the parity of all orbitals strictly less than $i$. For four orbitals, this matrix is given by:

**Table 1.** Indices of qubits in the update set, $U(j)$, which is the set of all qubits whose state must be updated when the occupation state of an orbital $j$ is changed, for systems of 1–8 orbitals.

| # Qubits | # Orbitals | U(0) | U(1) | U(2) | U(3) | U(4) | U(5) | U(6) | U(7) |
|---|---|---|---|---|---|---|---|---|---|
| 2 | 1 | {1} | – | – | – | – | – | – | – |
| 2 | 2 | {1} | ∅ | – | – | – | – | – | – |
| 4 | 3 | {1, 3} | {3} | {3} | – | – | – | – | – |
| 4 | 4 | {1, 3} | {3} | {3} | ∅ | – | – | – | – |
| 8 | 5 | {1, 3, 7} | {3, 7} | {3, 7} | {7} | {5, 7} | – | – | – |
| 8 | 6 | {1, 3,7} | {3, 7} | {3, 7} | {7} | {5, 7} | {7} | – | – |
| 8 | 7 | {1, 3,7} | {3, 7} | {3, 7} | {7} | {5, 7} | {7} | {7} | – |
| 8 | 8 | {1, 3,7} | {3, 7} | {3, 7} | {7} | {5, 7} | {7} | {7} | ∅ |

$$\pi_4 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \end{pmatrix} \qquad (16)$$

and addition is taken modulo two in the matrix multiplication.

This method stores the parity of orbital $j$ in partial sums held in several qubits of index less than or equal to $j$, where the

number of these qubits scales as $O(\log(j)) \leq O(\log(n))$.[28,29] Since the fermionic occupation state vector $\vec{f_n}$ is transformed into the Bravyi–Kitaev basis, $\vec{b_n}$ by $\beta_n \vec{f_n} = \vec{b_n}$, this transformation can be reversed to get back to the fermionic occupation basis by $\beta_n^{-1} \vec{b_n} = \vec{f_n}$. We find that the parity transformation for the Bravyi–Kitaev basis is $\pi_n \beta_n^{-1}$. For eight orbitals:

$$\vec{p_8} = \pi_8 \vec{f_8} = \pi_8 \beta_8^{-1} \vec{b_8} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \\ b_6 \\ b_7 \end{pmatrix} = \begin{pmatrix} 0 \\ b_0 \\ b_1 \\ b_2 + b_1 \\ b_3 \\ b_4 + b_3 \\ b_5 + b_3 \\ b_6 + b_5 + b_3 \end{pmatrix} \qquad (17)$$

Therefore, the parity set, $P(j)$, is the set of qubits with index equal to the nonzero entries of $\pi_n \beta_n^{-1}$ in row $j$ as these are the qubits whose sum gives the parity of orbital $j$.[29] The product $\pi_n \beta_n^{-1}$ is lower triangular because it is the product of two lower triangular matrices. Hence, the parity set $P(j)$ only contains indices $i < j$, so $P(j) < j$. This also implies that the intersection of parity and update sets is always empty. The parity sets for each orbital for systems of 1 through 8 orbitals are given in Table 2.

Lastly, the flip set, $F(j)$, is the set of qubits that determine whether qubit $j$ and orbital $j$ are equal or opposite. The flip set is the set of qubits that hold the parity of the occupation of the orbitals with index $<j$ included in the partial sum held in qubit $j$. Note that this definition implies that the flip set is a subset of the parity set, and because the qubits hold partial sums, it is usually a proper subset of the parity set. As for even $j$, qubit $j$ holds the occupation of orbital $j$, the flip set is empty for all even $j$. However, for odd $j$, we need to find which occupation states are included in each partial sum to trans-

form back to the fermionic occupation state. To do this, we can look at the inverse transformation. For eight qubits,

$$\beta_8^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 1 & 1 \end{pmatrix} \qquad (18)$$

As $\beta_n^{-1} \vec{b_n} = \vec{f_n}$, the set of qubits whose states sum to the occupation state of orbital $j$ are those with indices equal to the indices of nonzero entries in row $j$ of $\beta_n^{-1}$. Therefore, the flip set of orbital $j$ is the set of these qubits with indices $<j$, as this is the set of qubits that hold the sum of all occupation

**Table 2.** Indices of qubits in the parity set, $P(j)$, which is the set of qubits whose occupation is needed to determine the parity of the orbital $j$, for each orbital in systems of 1–8 orbitals.

| # Qubits | # Orbitals | P(0) | P(1) | P(2) | P(3) | P(4) | P(5) | P(6) | P(7) |
|---|---|---|---|---|---|---|---|---|---|
| 2 | 1 | ∅ | – | – | – | – | – | – | – |
| 2 | 2 | ∅ | {0} | – | – | – | – | – | – |
| 4 | 3 | ∅ | {0} | {1} | – | – | – | – | – |
| 4 | 4 | ∅ | {0} | {1} | {1, 2} | – | – | – | – |
| 8 | 5 | ∅ | {0} | {1} | {1, 2} | {3} | – | – | – |
| 8 | 6 | ∅ | {0} | {1} | {1, 2} | {3} | {3, 4} | – | – |
| 8 | 7 | ∅ | {0} | {1} | {1, 2} | {3} | {3, 4} | {3, 5} | – |
| 8 | 8 | ∅ | {0} | {1} | {1, 2} | {3} | {3, 4} | {3, 5} | {3, 5, 6} |

states of orbitals with index $<j$ held in qubit $j$. The flip sets for each orbital of systems of 1–8 orbitals are listed in Table 3.

One final property of these sets is worth remarking upon. The Jordan–Wigner transformation finds application in condensed matter physics to map one-dimensional spin systems to noninteracting spinless fermions, hence, enabling exact diagonalization of several systems of interest.[39] Here, we are using the Bravyi–Kitaev transformation to map fermions with spin to spin one-half systems. The fact that we are mapping spin-orbitals to qubits manifests itself in the pairing of spin-orbitals that correspond to the same spatial orbital, and in extra structure present in our second-quantized Hamiltonian. We assume that even-numbered spin-orbitals correspond to one spin function and odd to the other, such that adjacent spin-orbitals correspond to the same spatial function. The fact that Bravyi–Kiatev treats even and odd orbitals differently is convenient in this case. In particular, the fact that $U(j) > j$ and $P(j) < j$ gives rise to the intersections among even and odd parity and update sets shown in Table 4.

### Bravyi–Kitaev operators

Having defined the update, parity, and flip sets for the Bravyi–Kitaev transformation, we can define qubit creation and annihilation operators. For even indexed qubits, this is relatively simple. Even indexed qubits only store their corresponding occupation, performing operations requires only the actual creation or annihilation operation ($\hat{Q}^{\pm}$), updating the update set with a bit flip, and introducing a negative sign depending on the parity of the parity set. Hence, the creation and annihilation operator equivalents for even indexed qubits are:

$$a_j^{\dagger} = X_{U(j)} \otimes \hat{Q}_j^{+} \otimes Z_{P(j)} = \frac{1}{2}\left(X_{U(j)} \otimes X_j \otimes Z_{P(j)} - iX_{U(j)} \otimes Y_j \otimes Z_{P(j)}\right) \tag{19}$$

$$a_j = X_{U(j)} \otimes \hat{Q}_j^{-} \otimes Z_{P(j)} = \frac{1}{2}\left(X_{U(j)} \otimes X_j \otimes Z_{P(j)} + iX_{U(j)} \otimes Y_j \otimes Z_{P(j)}\right) \tag{20}$$

where we know that $U(j) > j$ and $P(j) < j$, so these operators act on disjoint sets of qubits.

The qubit operators for qubits with odd index are more complicated. First, we note that where the flip set has nonzero parity, the occupation of the qubit in question is flipped from that of the electronic state. Consequentially, in this case, the creation operator must be applied to the qubit where the annihilation operator is applied to the electronic state, and vice versa. Therefore, defining projectors onto the even and odd states of a set, $S$, of qubits:

$$\hat{E}_S = \frac{1}{2}(I + Z_S)$$
$$\hat{O}_S = \frac{1}{2}(I - Z_S) \tag{21}$$

We then have new creation and annihilation operators to express this behavior:

$$\hat{\Pi}_j^{\pm} = \hat{Q}_j^{\pm} \otimes \hat{E}_{F(j)} - \hat{Q}_j^{\mp} \otimes \hat{O}_{F(j)} = \frac{1}{2}\left(X_j \otimes Z_{F(j)} \mp iY_j\right) \tag{22}$$

Here, we have already implicitly accounted for the phase of the qubits in $F(j)$. Thus, in determining whether a sign change must be implemented, we must only additionally determine the phase of the qubits in the parity set which are not in the

**Table 3.** Indices of qubits in the flip set, $F(j)$, which is the set of qubits that determine whether orbital $j$ and qubit $j$ have the same or flipped parity, for systems of 1–8 orbitals.

| # Qubits | # Orbitals | F(0) | F(1) | F(2) | F(3) | F(4) | F(5) | F(6) | F(7) |
|---|---|---|---|---|---|---|---|---|---|
| 2 | 1 | ∅ | – | – | – | – | – | – | – |
| 2 | 2 | ∅ | {0} | – | – | – | – | – | – |
| 4 | 3 | ∅ | {0} | ∅ | – | – | – | – | – |
| 4 | 4 | ∅ | {0} | ∅ | {1, 2} | – | – | – | – |
| 8 | 5 | ∅ | {0} | ∅ | {1, 2} | ∅ | – | – | – |
| 8 | 6 | ∅ | {0} | ∅ | {1, 2} | ∅ | {4} | – | – |
| 8 | 7 | ∅ | {0} | ∅ | {1, 2} | ∅ | {4} | ∅ | – |
| 8 | 8 | ∅ | {0} | ∅ | {1, 2} | ∅ | {4} | ∅ | {3, 5, 6} |

**Table 4.** Intersections between parity and update sets appearing in the Bravyi–Kitaev transformation for adjacent odd and even orbital indices.

|  | $U(2i)$ | $U(2i+1)$ | $P(2i)$ | $P(2i+1)$ |
|---|---|---|---|---|
| $U(2i)$ | $U(2i)$ | $\subset U(2i+1)$ | $\varnothing$ | $\varnothing$ |
| $U(2i+1)$ | $\subset U(2i+1)$ | $U(2i+1)$ | $\varnothing$ | $\varnothing$ |
| $P(2i)$ | $\varnothing$ | $\varnothing$ | $P(2i)$ | $\subset P(2i+1)$ |
| $P(2i+1)$ | $\varnothing$ | $\varnothing$ | $\subset P(2i)$ | $P(2i+1)$ |

flip set. To do this, we make use of the *remainder set*, defined above. This gives us the qubit representation of the electronic creation and annihilation operators for odd indexed orbitals:

$$a_j^\dagger = X_{U(j)} \otimes \hat{\Pi}_j^+ \otimes Z_{R(j)} = \frac{1}{2}\left(X_{U(j)} \otimes X_j \otimes Z_{P(j)} - iX_{U(j)} \otimes Y_j \otimes Z_{R(j)}\right) \tag{23}$$

$$a_j = X_{U(j)} \otimes \hat{\Pi}_j^- \otimes Z_{P(j)} = \frac{1}{2}\left(X_{U(j)} \otimes X_j \otimes Z_{P(j)} + iX_{U(j)} \otimes Y_j \otimes Z_{R(j)}\right) \tag{24}$$

The only difference between these operators and those of the even indexed qubits, is the application of $Z$ to the remainder set, rather than the parity set, in the second term. Thus, by defining a final set:

$$\rho(j) = \begin{cases} P(j), & j \text{ even} \\ R(j), & j \text{ odd} \end{cases} \tag{25}$$

We have a final expression for Bravyi–Kitaev representations of electronic creation and annihilation operators:

$$a_j^\dagger = \frac{1}{2}\left(X_{U(j)} \otimes X_j \otimes Z_{P(j)} - iX_{U(j)} \otimes Y_j \otimes Z_{\rho(j)}\right) \tag{26}$$

$$a_j = \frac{1}{2}\left(X_{U(j)} \otimes X_j \otimes Z_{P(j)} + iX_{U(j)} \otimes Y_j \otimes Z_{\rho(j)}\right) \tag{27}$$

These two expressions allow for general products—such as those observed in the molecular Hamiltonian—to be built up through simple multiplication.[29]

## Inverse Bravyi–Kitaev Transformation Matrix

We have constructive definitions for the Bravyi–Kitaev transformation matrix for any number of qubits that is a power of two, and for the parity transformation matrix in the occupation state basis. We do not have a constructive definition for the inverse Bravyi–Kitaev transformation matrix. The parity, update, and flip set are determined by these three matrices, so a constructive definition for $\beta_n^{-1}$ would greatly simplify the process of computing these sets. By inspection, we can see that the inverse matrix (again, in mod 2) can be defined recursively as follows:

$$\beta_{2^{x+1}}^{-1} = \left(\begin{array}{c|c} \beta_{2^x}^{-1} & 0 \\ \hline 0 & \beta_{2^x}^{-1} \\ \leftarrow 0\,1 \end{array}\right) \text{ where } \beta_1 = \begin{pmatrix} 1 \end{pmatrix} \tag{28}$$

where the top left and bottom right quadrants of $\beta_n^{-1}$ are given by $\beta_{\frac{n}{2}}^{-1}$, the top right quadrant is entirely zeroes, and the

bottom left quadrant is all zero except the bottom, right-most entry.

We can verify this form for $\beta^{-1}$ directly. The equation for the inverse Bravyi–Kitaev transformation matrix satisfies the condition that $\beta_n \beta_n^{-1} = I$. From Eqs. (13) and (28), we obtain:

$$\beta_n \beta_n^{-1} = \left(\begin{array}{c|c} \beta_{\frac{n}{2}} & 0 \\ \hline 0 & \beta_{\frac{n}{2}} \\ \leftarrow 1 \rightarrow \end{array}\right) \left(\begin{array}{c|c} \beta_{2^x}^{-1} & 0 \\ \hline 0 & \beta_{2^x}^{-1} \\ \leftarrow 0\,1 \end{array}\right) \text{ where } \beta_1 = \begin{pmatrix} 1 \end{pmatrix}$$

$$= \left(\begin{array}{c|c} \beta_{\frac{n}{2}}\beta_{\frac{n}{2}}^{-1} & 0 \\ \hline \beta_{\frac{n}{2}}\begin{pmatrix} 0 \\ \leftarrow 0\,1 \end{pmatrix} + \begin{pmatrix} 0 \\ \leftarrow 1 \rightarrow \end{pmatrix}\beta_{\frac{n}{2}}^{-1} & \beta_{\frac{n}{2}}\beta_{\frac{n}{2}}^{-1} \end{array}\right)$$

because $\beta_{\frac{n}{2}}\beta_{\frac{n}{2}}^{-1} = I$, the condition that $\beta_n \beta_n^{-1} = I$ is:

$$\beta_{\frac{n}{2}}\begin{pmatrix} 0 \\ \leftarrow 0\,1 \end{pmatrix} + \begin{pmatrix} 0 \\ \leftarrow 1 \rightarrow \end{pmatrix}\beta_{\frac{n}{2}}^{-1} = 0 \tag{29}$$

By the definition of the Bravyi–Kitaev transformation, the upper triangle of any $\beta_n$ is entirely zeroes. Therefore, $\beta_{j,0} = 0$ for all $j > 0$, and so:

$$\beta_{\frac{n}{2}}\begin{pmatrix} 0 \\ \leftarrow 0\,1 \end{pmatrix} = \begin{pmatrix} 0 \\ \leftarrow 0\,1 \end{pmatrix}. \tag{30}$$

Now consider the second term in Eq. (29). For the multiplication of any two matrices, of the left-hand matrix, only the bottom row affects the bottom row of the product matrix. For example, if $A$ is matrix of all ones and $B$ is a matrix with ones in the bottom row and zeroes everywhere else, for any third matrix $C$, the bottom row of $AC$ is equivalent to the bottom row of $BC$ as the bottom rows of $A$ and $B$ are equal. By the definition of the Bravyi–Kitaev transformation, the bottom row of $\beta_n$ is all ones for all $n$. Therefore, the bottom row of $\beta_n \beta_n^{-1}$ is equivalent to the bottom row of the matrix product from Eq. (31). As we know that $\beta_n \beta_n^{-1} = I$, the bottom row of this product is $(0, 0, 0, \ldots, 0, 1)$.

$$\begin{pmatrix} 0 \\ \leftarrow 1 \rightarrow \end{pmatrix}\beta_{\frac{n}{2}}^{-1} = \begin{pmatrix} 0 \\ \leftarrow 0\,1 \end{pmatrix}. \tag{31}$$

Combining Eqs. (30) and (31), Eq. (29) becomes:

$$\beta_{\frac{n}{2}}\begin{pmatrix} 0 \\ \leftarrow 0\,1 \end{pmatrix} + \begin{pmatrix} 0 \\ \leftarrow 1 \rightarrow \end{pmatrix}\beta_{\frac{n}{2}}^{-1} = \begin{pmatrix} \vdots \ldots & 0 \\ 0\ldots & 2\bmod 2 \end{pmatrix} = 0 \tag{32}$$

as we are adding in modulo 2. Our definition for the inverse Bravyi–Kitaev transformation matrix in Eq. (28) is, therefore, correct for all $n$, as it trivially holds for $n = 1$. Now that we have a recursive definition for both the Bravyi–Kitaev transformation matrix and its inverse, in the next section, we use these definitions to obtain recursive expressions for the update, parity, and flip sets.

## Update, Parity, and Flip Set Formulae

The method of finding the parity, update, and flip sets needed for the Bravyi–Kitaev transformation described above in Bravyi–Kitaev Transformation section and in [29], while effective, is somewhat clumsy. Ideally, we want a formula that directly computes which qubits are in each of these sets. Given the recursive definition of the Bravyi–Kitaev transformation matrix and its inverse, we can define the update, parity, and flip sets recursively.

### Update set

As described above, the update set is given by the row-index of the nonzero entries of index greater than $j$ in column $j$ of the Bravyi–Kitaev transformation matrix.

The upper triangle of $\beta_{\frac{n}{2}}$ determines the update set for qubits $j < \frac{n}{2}$ for a system of $n$ qubits, and also determines the update sets for a system of $\frac{n}{2}$ qubits. Since $\beta_{\frac{n}{2}}$ is in the top left corner for this half of the matrix, all entries in $\beta_{\frac{n}{2}}$ maintain the same indices within $\beta_n$. Therefore, all elements in the update sets $U_{\frac{n}{2}}(j)$ are also elements in the update sets for $U_n(i)$ for $i < \frac{n}{2}$. For $\beta_n$, however, a row of 1s are added across the left half of the bottom row (row index $n-1$) of the matrix, and as these are nonzero entries in a row of index greater than $j$ for all qubits of index $j < \frac{n}{2}$, $n-1$ is in the update set for all qubits of index $j < \frac{n}{2}$ for a system of $n$ qubits in addition to the elements in the update sets for $\frac{n}{2}$ qubits.

If we inspect $\beta_n$, defined in Eq. (13), we see that the lower triangle of the matrix $\beta_{\frac{n}{2}}$ determines the update set for the $n$ qubit system when changing the occupation of orbital $\frac{n}{2} \leq j < n$. This is also the part of $\beta_{\frac{n}{2}}$ that determines the update sets for all qubits in a system of $\frac{n}{2}$ qubits. When the matrix $\beta_{\frac{n}{2}}$ is placed in the lower right quadrant of $\beta_n$, the row and column indices of all entries in that matrix are increased by $\frac{n}{2}$.

The recursive function for the elements in the update set of an $n$ qubits system when changing the occupation of orbital $j$ is:

$$U_n(j) = \begin{cases} \{U_{\frac{n}{2}}(j), (n-1)\} & \text{for} \quad j < \frac{n}{2} \\ \{U_{\frac{n}{2}}\left(j - \frac{n}{2}\right) + \frac{n}{2}\} & \text{for} \quad j \geq \frac{n}{2}. \end{cases} \quad (33)$$

This recursive definition clearly shows the logarithmic growth in locality of the operators in the Bravyi–Kitaev transformation, as the set is either the same size as the set for half the number of qubits, or increases by one. Having determined this recursive relation for the update set, we obtain a similar expression for the parity set in the following section.

### Parity set

The parity set for a given orbital $j$ is given by the nonzero entries in row $j$ of the parity transformation matrix $p_n = \pi_n \beta_n^{-1}$ where $\pi_n$ is the parity transformation matrix in the occupation state basis, given by an upper triangular matrix with zeroes along the diagonal. From the definitions for $\pi_n$ and $\beta_n^{-1}$, we obtain:

$$p_n = \pi_n \beta_n^{-1} = \left( \begin{array}{c|c} \pi_{n/2} & 0 \\ \hline A_{n/2} & \pi_{n/2} \end{array} \right) \left( \begin{array}{c|c} \beta_{n/2}^{-1} & 0 \\ \hline T_{n/2} & \beta_{n/2}^{-1} \end{array} \right)$$

where we have defined

$$[A_{n/2}]_{ij} = 1 \ \forall i,j, \qquad [T_{n/2}]_{ij} = \delta_{i,n/2-1}\delta_{j,n/2-1} \quad (34)$$

which gives us:

$$p_n = \left( \begin{array}{c|c} \pi_{n/2}\beta_{n/2}^{-1} & 0 \\ \hline A_{n/2}\beta_{n/2}^{-1} & \pi_{n/2}\beta_{n/2}^{-1} \end{array} \right) = \left( \begin{array}{c|c} p_{n/2} & 0 \\ \hline A_{n/2}\beta_{n/2}^{-1} + \pi_{n/2}T_{n/2} & p_{n/2} \end{array} \right). \quad (35)$$

Now, $\pi_{n/2}T_{n/2} = 0$, because the last row and column of $\pi$ is zero, and only this row and column contributes to the product. To evaluate $A_{n/2}\beta_{n/2}^{-1}$, we first prove the following fact about $\beta_{n/2}^{-1}$: every column of $\beta_{n/2}^{-1}$ has two nonzero entries except the last column, which has one. We can proceed by induction. It is true that $\beta_2^{-1}$ has two nonzero entries in each column except the last, which has one. Following the recursive construction, if it is true of $\beta_{n/2}^{-1}$, it will be true of $\beta_n^{-1}$ by inspection, as the addition of the single additional nonzero entry adds one more nonzero entry to the last column of $\beta_{n/2}^{-1}$. Given this fact, it follows immediately that:

$$A_{n/2}\beta_{n/2}^{-1} = S_{n/2} \quad (36)$$

where we define:

$$[S_{n/2}]_{ij} = \delta_{j,n/2} \quad (37)$$

The parity transformation matrix in the Bravyi–Kitaev basis can, therefore, be defined as:

$$p_n = \left( \begin{array}{c|c} p_{\frac{n}{2}} & 0 \\ \hline \begin{array}{cc} \uparrow \\ 0 \quad 1 \\ \downarrow \end{array} & p_{\frac{n}{2}} \end{array} \right) \quad (38)$$

We can now define a recursive formula for the parity set as we did for the update set. For orbitals $j < \frac{n}{2}$, the parity is determined by the submatrix $p_{\frac{n}{2}}$ matrix. For $j \geq \frac{n}{2}$ the parity set contains the set $P(j)_{n/2}$ as the bottom quadrant is simply $p_{\frac{n}{2}}$. However, the column index of each element is increased by $\frac{n}{2}$ as it is shifted to the right side of the matrix. For rows $\frac{n}{2}$ through $(n-1)$, qubit $\frac{n}{2}-1$ is added to the parity set for qubits $\frac{n}{2}$ through $n-1$. We find that the parity set can be recursively expressed as:

$$P_n(j) = \begin{cases} P_{\frac{n}{2}}(j) & \text{for} \quad j < \frac{n}{2} \\ \{P_{\frac{n}{2}}\left(j - \frac{n}{2}\right) + \frac{n}{2}, \left(\frac{n}{2}-1\right)\} & \text{for} \quad j \geq \frac{n}{2} \end{cases} \quad (39)$$

Again, this recursive definition results in logarithmic growth in locality, as the set is again either the same size as the set

for half the number of qubits, or increases by one. We now have a recursive expression for both the update and parity sets, and in the next section, we will find a recursive relation for the flip set.

### Flip set

The elements of the flip set for a given orbital $j$ are defined by the indices of the nonzero entries in row $j$ with indices $<j$ of the matrix $\beta_n^{-1}$, as discussed above. By inspection, we see that the elements that determine the flip sets for a system of $\frac{n}{2}$ qubits also determine the flip sets of qubits with indices $j < n/2$ for a system of $n$ qubits. For the flip sets of orbitals of $\frac{n}{2} \leq j < n-1$, however, the row and column indices of the elements of the $\beta_{\frac{n}{2}}^{-1}$ are all increased by $\frac{n}{2}$ as they are in the lower right quadrant. The one nonzero entry in the lower right quadrant adds the qubit $\frac{n}{2}-1$ to the flip set of qubit $n-1$. The recursive expression for the flip set of an orbital $j$ in a system of $n$ qubits is given in Eq. (40):

$$F_n(j) = \begin{cases} F_{\frac{n}{2}}(j) & \text{for } j < \frac{n}{2} \\ \left\{ F_{\frac{n}{2}}\left(j-\frac{n}{2}\right) + \frac{n}{2} \right\} & \text{for } \frac{n}{2} \leq j < (n-1) \quad (40) \\ \left\{ F_{\frac{n}{2}}\left(j-\frac{n}{2}\right) + \frac{n}{2}, \frac{n}{2}-1 \right\} & \text{for } j = n-1 \end{cases}$$

Just as in the cases of parity and update sets, this exhibits the logarithmic growth in locality of the operators.

We now have a recursive expression for the update, parity, and flip sets given in Eqs. (33), (40), and (39). These allow each set to be computed directly, rather than through various steps of matrix manipulation, greatly simplifying the process of computing each set. This also connects the matrix definition of the Bravyi–Kitaev transformation given in [29] with the original definition given by Bravyi and Kitaev.[28]

## A Numerical Example: Methane in STO6G

While Trotterization and phase estimation for the quantum simulation of chemistry have been extensively studied and simulated, the sole example for Bravyi–Kitaev is given in [29]. In that work, the minimal basis representation of $H_2$ was studied. This is an example of considerable interest from the point of view of early experimental implementation of these algorithms, but is too small to exhibit all the properties of the Bravyi–Kitaev transformation. To examine characteristics of the mapping in a larger system than previously studied, we examined the performance of this technique for the determination of the ground-state energy of methane. The Hartree–Fock basis was used as our molecular orbital basis, and was determined through a Hartree–Fock calculation using GAMESS,[40,41] with a geometric $T_d$ symmetry, a CH bond length of 1.107902, and a STO-6G atomic orbital basis. Spatial molecular orbital integrals were also obtained from this calculation, and transformed into a spin-orbit basis in physicists' notation.

Python code was then used to generate Jordan–Wigner and Bravyi–Kitaev qubit Hamiltonians in terms of a symbolic sequence of strings of Pauli operations. This code automatically combines duplicate strings. Each Pauli string is represented by a sequence of $N$ numbers, where $N$ is the number of qubits (i.e., spin orbitals). Each number corresponds to the operation acting on its respective qubit—0 for the identity, 1 for Pauli $X$, 2 for Pauli $Y$, and 3 for Pauli $Z$. The numbers are ordered in reverse sequential order—the qubit with highest index is operated on by the leftmost operator, and the 0 indexed qubit is operated on by the right-most operator. Consequentially, each term is represented by a base-4 number. The terms are then ordered lexiographically—in ascending order of these base-4 numbers.

Having a symbolic expression of the Jordan–Wigner and Bravyi–Kitaev Hamiltonians, our code constructs CSC sparse matrix representations of these using SciPy's sparse matrix methods. It proceeds to diagonalize these Hamiltonians, providing both an exact ground-state eigenvalue (to compare against our Trotterized eigenvalue estimate) and a ground-state eigenvector, which is needed for the following stage of our calculation. Note that in an experimental realization on a quantum computer the ground-state eigenvector would be prepared by adiabatic-state preparation, or other methods.[7,33]

Using the eigenvector obtained as an input, our python code simulates the effect of applying a Trotterized unitary with specified Hamiltonian (as a sequence of strings of Pauli operations), Trotter-Suzuki approximation order, number of Trotter steps, and overall simulation time. Note that to reduce computational cost substantially, the whole unitary evolution matrix is not determined. Each Pauli string term in the Hamiltonian is instead exponentiated symbolically. Every Pauli operation in each exponentiated term is then directly implemented on the target state. With key functions compiled using Cython, this cuts computational resource requirements dramatically. Finally, our code uses the original ground-state vector and the post-Trotter vector to assess the phase gained through phase estimation, and thus, an eigenvalue estimate as a function of our parameters. The details of how a unitary given by the exponential of an arbitrary string of Pauli matrices is give in [29].

Our code also counts the gates associated with each Trotterization setting. We use the commonly used gate set consisting of controlled not gates and arbitrary single qubit gates. We note that this gate set is appropriate for small-scale experimental implementation without error correction. For fault tolerant implementations, a different gate set would be required, and these circuits could be obtained from those we developed with some overhead. Details of fault-tolerant implementations of these kinds of simulation algorithms are given in [42].

These gate counts do not include any cancellation within the gate structure, that is, between sequential CNOT strings. These results are shown in Figures 1 and 2, and demonstrate a small improvement associated with the Bravyi–Kitaev mapping. The number of CNOT gates to realize a single Trotter step, for either a first- or second-order Trotter scheme, is always less for the Bravyi–Kitaev mapping. This reflects the increased locality of the mapping. The number of single qubit gates for the Bravyi–Kitaev mapping is higher for a single Trotter step due to the changes of basis required by the more sophisticated
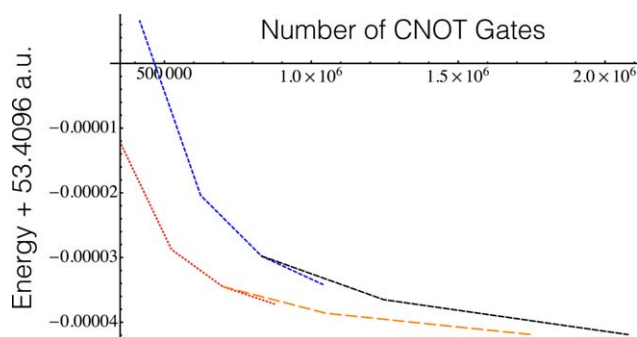
**Figure 1.** Energy as a function of number of total gates in the Trotterization. Blue-dashed line—Jordan–Wigner with first-order Trotterization. Red-dotted line—Bravyi–Kitaev with first-order Trotterization. Black-dashed line—Jordan–Wigner with second-order Trotterization. Orange-dashed line—Bravyi–Kitaev with second-order Trotterization. The energy is plotted as a difference from a reference energy of 53.4096 a.u.

form of the creation and annihilation operators. However, the accuracy of the Bravyi–Kitaev method for a given number of gates is better than for the Jordan–Wigner method, as shown in Figures 1 and 2.

These results compare gate sequences derived from both Bravyi–Kitaev and Jordan–Wigner transformations that are based on a lexicographic ordering of terms in the Hamiltonian. There is no reason to believe that this is optimal in either case, but it is reassuring that the simplest comparison of the two methods gives results which are slightly better for the Bravyi–Kitaev transformation. Naturally, the true costs of the two methods are only given by optimal Trotterizations. In the case of the Jordan–Wigner transformation such optimization has been performed recently.[23,24] However, such optimization of the Bravyi–Kitaev transformation is the subject of current research. In this case, simple circuit optimizations are made more complex by the more complex strings of Pauli operators that occur, but are also simpler due to the reduced locality of the transformation. The ordering of terms in the Trotterization also has a significant impact on the Trotter error, and new work on understanding the chemical basis of these Trotter errors should also act as a guide to future optimiza-
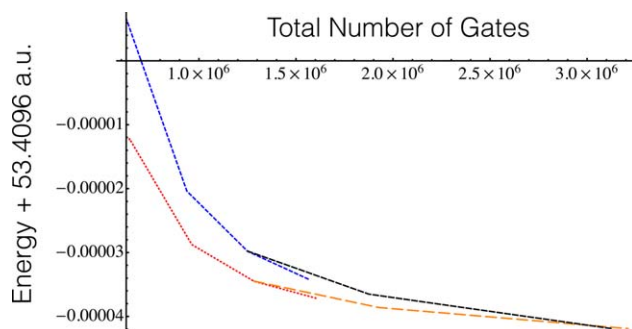
tions of the Trotter ordering for Bravyi–Kitaev.[25] Finally, the impact of the reduced locality of the operators will depend in detail on the architecture used.

## Conclusion

In exploring the Bravyi–Kitaev transformation, we found new, recursive equations for the update, flip, and parity set given in Eqs. (33), (40), and (39), allowing these sets to be computed directly rather than through various matrix operations. The recursive nature of these definitions underlies the logarithmic growth in locality of operators in the transformation. Such recursive approaches to algorithm development often provide such improvements, as in the examples of the Fast Fourier Transform and quicksort algorithms.

We presented a numerical example of the Bravyi–Kitaev mapping applied to the methane molecule, observing a small improvement over the traditional Jordan–Wigner mapping. The Bravyi–Kitaev mapping appears to result in a small decrease in the total amount of gates necessary to achieve an arbitrary precision approximation. However, a far more substantial drop is present for the amount of CNOT gates required. This emphasizes the increase in locality of the spin Hamiltonian realized under the Bravyi–Kitaev mapping.

The work presented here shows that the Bravyi–Kitaev method of quantum simulation of interacting fermionic systems can be systematically improved in ways that both clarify the method theoretically and bring experimental realization of these simulations closer.

**Figure 2.** Energy as a function of number of CNOT gates in the Trotterization. Blue-dashed line—Jordan–Wigner with first-order Trotterization. Red-dotted line—Bravyi–Kitaev with first-order Trotterization. Black-dashed line—Jordan–Wigner with second-order Trotterization. Orange-dashed line—Bravyi–Kitaev with second-order Trotterization. The energy is plotted as a difference from a reference energy of 53.4096 a.u.

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