Improving Hamiltonian encodings with the Gray code

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Due to the limitations of present-day quantum hardware, it is especially critical to design algorithms that make the best possible use of available resources. When simulating quantum many-body systems on a quantum computer, many of the encodings that transform Fermionic Hamiltonians into qubit Hamiltonians use $N$ of the available basis states of an $N$-qubit system, whereas $2^N$ are in theory available. We explore an efficient encoding that uses the entire set of basis states, where creation and annihilation operators are mapped to qubit operators with a Hamiltonian that acts on the basis states in Gray code order. This encoding is applied to the commonly-studied problem of finding the ground state energy of a deuteron with a simulated variational quantum eigensolver (VQE), and various trade-offs that arise are analyzed. The energy distribution of VQE solutions can be represented in terms of as few as $N$ qubits, and a shorter-deep variational ansatz also enables the encoding of larger problems on current-generation machines. This encoding also shows promise for simulating the time evolution of the same system, producing circuits for the evolution operators with roughly half as many single- and two-qubit gates than a Jordan-Wigner encoding.

I. INTRODUCTION

The simulation of quantum many-body systems remains a complex and computationally challenging problem in physics and quantum chemistry. Direct solutions are often limited by the rapid growth of the problem as the number of particles and relevant degrees of freedom increases. Quantum computers may play a key role in overcoming these computational challenges \cite{1, 2}, however it is only with recent advances in qubit technology \cite{3, 5} that such a use of quantum computers has begun to be feasible \cite{9, 14}.

Quantum many-body problems which are typically solved in a configuration interaction (CI) framework \cite{15, 19} may be well suited for quantum computers. In a CI framework, the wavefunction is expanded in terms of an occupation basis, where each basis state corresponds to a distribution of the particles over the different possible single particle substates. In nuclear physics applications, these substates are typically taken to be harmonic oscillator orbitals. The operators are then expressed in terms of second quantization creation $a_i^\dagger$ and annihilation $a_i$ operators which, respectively, create or annihilate a particle in the $i$th substate.

Calculations in a CI framework are inhibited by the rapid growth in the many-body basis. If the basis consists of particles distributed over $N$ possible substates, then the basis dimension is $2^N$. However, on a quantum computer those $2^N$ states can be represented in terms of as few as $N$ qubits in the most general case. The challenge, now, is to map the basis and operators in the CI framework onto qubits and operators in an efficient manner.

There are several widely used methods for mapping a CI framework onto a quantum system \cite{20}. The most common is the Jordan-Wigner encoding \cite{21, 23}, which directly maps the annihilation and creation operators of $N$ substates to $N$ qubit Pauli operators. Alternative encodings include the parity basis encoding \cite{20} and the Bravyi-Kitaev encoding \cite{24, 26}. For comparisons of these encodings, see \cite{27}. While in the general case these encodings use $N$ qubits to encode $N$ states, there are often symmetries associated with e.g., particle number, parity, or spin polarization, present in the problem which can reduce the number of qubits \cite{28, 29}. An encoding using $\lceil \log_2 N \rceil$ qubits to represent $N$ states, different than that considered here, has also been explored for the multi-particle case \cite{28}.

This work presents an encoding based on a Gray code that makes use of all the available basis states of a multi-qubit system. This encoding has been adapted from a similar encoding used in a quantum simulation of a lattice gauge theory \cite{20}. With this encoding, a many-body basis with $N$ single particle states can be represented in terms of $\lceil \log_2 N \rceil$ qubits. Although a number of trade-offs arise when using this Gray code encoding as compared to the Jordan-Wigner encoding, the reduction in both the number of qubits and the number of CNOT gates in circuits for various applications has important consequences in the noisy intermediate-scale quantum (NISQ) computing era \cite{31}.

As illustration, the Gray code encoding is applied to the problem of finding the ground state energy of a deuteron, one of the simplest nuclei, consisting of only one proton and one neutron. The low coherence times and high gate error rates of current quantum computers make direct solution of the deuteron eigenproblem on a quantum computer infeasible. However, a number of hybrid quantum-classical algorithms have emerged over the past decade, where an optimization problem run on a classical computer is assisted by a quantum computer that can compute its cost function more efficiently. One such hybrid classical-quantum algorithm is the variational quantum eigensolver (VQE) \cite{7, 32, 33}.
which can be used to find the ground state energy of a Hamiltonian \([7]\). Here a simulated VQE is used to obtain the
ground state energy of the deuteron. Results are obtained for both the Gray code encoding and the Jordan-Wigner
encoding and compared. As we will show, the variance in distribution of energies found from the VQE is significantly
smaller for the Gray code encoding, most notably in cases with simulated hardware noise.

Looking beyond the NISQ era, the problem of finding the ground state energy can also be addressed using quantum
phase estimation. Phase estimation circuits have depth beyond what is feasible for a NISQ machine, and require the
implementation of a unitary simulating the time evolution of the system, often termed Hamiltonian simulation \([2]\).
This work presents an initial analysis of applying the Gray code encoding to Hamiltonian simulation, and shows
reduced circuit depth and gate count of the unitary evolution operators when compared to those obtained using the
Jordan-Wigner encoding.

Section II provides an overview of how many-body problems are mapped to quantum computers, beginning with
the presentation of the deuteron Hamiltonian and the resultant qubit Hamiltonian under the Jordan-Wigner encod-
ing. The Gray code encoding is introduced and applied to the deuteron in Section III, followed by analysis of its
structure in a more general setting. Section IV details the implementation of the variational quantum eigensolver and
simulation results of computational experiments with shot noise, and simulated hardware noise. Section V presents
looking beyond the NISQ era, the problem of finding the ground state energy can also be addressed using quantum

II. ENCODING QUANTUM MANY-BODY PROBLEMS ON A QUANTUM COMPUTER

A. A Hamiltonian for the deuteron

Many-body operators, like the Hamiltonian of the system, are expressed in terms of creation \(a_i^\dagger\) and annihilation

\(a_i\) operators acting on the Fock space. The basis of the Fock space for an \(A\)-particle system is spanned by the set of
states in occupation number representation \(|n_0 \cdots n_{N-1}\rangle\) where \(n_i = 0\) or \(1\) if the \(i\)th state is unoccupied or occupied,
respectively, and \(N\) is the number of states that the \(A\) particles can occupy. The creation operator \(a_i^\dagger\) creates a
particle in the \(i\)th state while the annihilation operator \(a_i\) annihilates a particle in the \(i\)th state. In terms of these
operators the Hamiltonian is typically written as

\[ H = \sum_{i} H_{ii} a_i^\dagger a_i + \sum_{ij} H_{ij} a_i^\dagger a_j a_i a_j + \ldots \]  

In the special case of the deuteron, the complexity of the problem can be reduced by working in the deuteron’s
comoving inertial reference frame in which only the relative motion is relevant. To leading order in pionless effective
field theory \([34, 35]\), the constituent proton and neutron interact via a short-ranged contact interaction in the \(^3S_1\)
partial wave \((L = 0\) and \(S = 1, J = 1\)). Using a discrete variable representation in the harmonic oscillator basis, the
deuteron Hamiltonian can be given by \([10]\)

\[ H_N = \sum_{n,n'=0}^{N-1} \langle n'|T + V|n\rangle b_n^\dagger b_n, \]

where

\[ \langle n'|T|n\rangle = \frac{\hbar \omega}{2} \left( (2n + 3/2)\delta_{n'}^n - \sqrt{n(n+1/2)}\delta_{n-1}^{n'} - \sqrt{(n+1)(n+3/2)}\delta_{n+1}^{n'} \right), \]

\[ \langle n'|V|n\rangle = V_0 \delta_{n}^{n'}, \]

and \(n = 0, 1, \ldots, N - 1\) is the relative harmonic oscillator radial node number. The operators \(b_n^\dagger\) and \(b_n\) represent
creation and annihilation of the deuteron with relative motion described by radial harmonic oscillator node number
\(n\). For the calculations used in this paper, the harmonic oscillator basis parameter is chosen to be \(\hbar \omega = 7\) MeV and
thus \(V_0 = -5.68658111\) MeV following Ref \([10]\).

The Hamiltonian given in \((2)\) is truncated to include only states with \(n < N\). As the size of the harmonic oscillator
basis increases with \(N\), the eigenvalues of each Hamiltonian \(H_N\) converge towards the true ground state energy. With
the selected model parameters \([10]\), in the limit \(N \to \infty\), the ground state energy of the deuteron fits its experimental
value: $-2.224$ MeV.

B. Mapping using the Jordan-Wigner encoding

To solve a Hamiltonian eigenproblem using a quantum computer, the many-body basis and relevant operators must be re-expressed in the language of qubits. Specifically, we rewrite the Hamiltonian over the $N$-qubit Pauli group $P_N$. The Pauli operators are expressed here using the notation $\{X_i, Y_i, Z_i\}$, where $X_i$, $Y_i$, and $Z_i$ represent the application of the associated Pauli on qubit $i$, and identity on all unspecified qubits.

For a quantum many-body system, the most commonly applied encoding is the Jordan-Wigner encoding. Under this encoding, the $ith$ state is mapped to the $ith$ qubit. In the deuteron example, this corresponds to mapping the $N$ relative states to $N$ qubits. For example, if $N = 4$ the Jordan-Wigner encoding effects the mapping

$$
|0\rangle \rightarrow |000\rangle, \quad |1\rangle \rightarrow |010\rangle, \quad |2\rangle \rightarrow |011\rangle, \quad |3\rangle \rightarrow |001\rangle.
$$

The creation and annihilation operators are mapped directly onto quantum gates via the standard Jordan-Wigner encoding $[22]$. Under this transformation, the Hamiltonian (2) becomes

$$
H_N = \frac{1}{2} \sum_{n=0}^{N-1} \langle n|H|n \rangle (1 - Z_n) - \frac{1}{2} \sum_{n=0}^{N-2} \langle n + 1|H|n \rangle (X_nX_{n+1} + Y_nY_{n+1}),
$$

where $1$ simply represents the identity on all qubits. For $N = 2, 3$ the Hamiltonian is that given by $[10]$ and later $[12]$. For $N = 4$, the Hamiltonian is

$$
H_4 = 28.657 \cdot 1 + 0.218 \cdot Z_0 - 6.125 \cdot Z_1 - 9.625 \cdot Z_2 - 13.125 \cdot Z_3 - 2.143 \cdot X_0X_1
- 3.913 \cdot X_1X_2 - 5.671 \cdot X_2X_3 - 2.143 \cdot Y_0Y_1 - 3.913 \cdot Y_1Y_2 - 5.671 \cdot Y_2Y_3.
$$

III. MAPPING USING A GRAY CODE BASIS ORDERING

The Jordan-Wigner encoding, though simple in implementation, fails to make full use of the qubit states available. Under the Jordan-Wigner encoding, the entire $2^N$ dimensional Fock space is mapped onto the $2^N$-dimensional Hilbert space of an $N$ qubit system. However, for particle conserving operators, like the Hamiltonian, the full set of basis states is not required. For the deuteron example considered here, only $N$ of those states are relevant, and so it can be represented by a system of fewer than $N$ qubits.

The motivation of the Gray code encoding is to perform such a mapping, from an $N$ qubit system using only $N$ of its basis states, down to a $[\log_2 N]$-qubit system using all its basis states. In principle, a simple mapping between the states and their binary equivalent will suffice - this case and its disadvantages for this particular problem are discussed in Appendix $\Box$. In this section, it is shown how utilizing a Gray code ordering of the basis states not only uses fewer qubits than Jordan-Wigner, but also simplifies the measurement process in the VQE.

A. The Gray code

A Gray code is an ordering of binary values where any two adjacent entries differ by only a single bit. For example,

$$
000 \rightarrow 100 \rightarrow 110 \rightarrow 010 \rightarrow 011 \rightarrow 111 \rightarrow 101 \rightarrow 001 \rightarrow 000.
$$
Gray codes rose to fame in the mid-20th century when they were used for signal conversion in early vacuum-tube
television. They have since found numerous other applications in mathematics, computing, and engineering,
such as error correction, Boolean circuit optimization [37], and even quantum circuit synthesis [38].

More formally a Gray code with \( \eta \) bits, denoted \( G_\eta \), is given by
\[
G_\eta = (g_0, g_1, \ldots, g_{2^\eta-1}),
\]
where each \( g_\alpha \) can be expanded as a sequence of \( \eta \) bits \( g_\alpha = g_{\alpha,0}, g_{\alpha,1}, \ldots g_{\alpha,\eta-1} \). For example, a Gray code with three bits is
\[
G_3 = (000, 100, 110, 010, 011, 111, 101, 001).
\]

In addition to the representation as bits, a Gray code \( G_\eta \) can be expressed as a sequence indicating the bit that changes between each step, i.e.
\[
S_{G_\eta} = (s_0, s_1, \ldots, s_{2^\eta-1}), \quad s_i \in \{0, 0, \ldots, \eta - 1\} \quad \forall \ i \in 0, \ldots, 2^\eta - 1.
\]
Explicitly, \( s_\alpha = k \) indicates that the \( k \)th bit is flipped when transitioning from \( g_\alpha \) to \( g_{\alpha+1} \), with addition in the subscript taken modulo \( 2^\eta \) as Gray codes are cyclic. For example, the Gray code in (10) can be expressed as
\[
S_{G_3} = (0, 1, 0, 2, 0, 1, 0, 2).
\]

This work makes use of a Gray code construction known as a binary reflective code [39]. For a Gray code \( G_\eta \), let \( \overline{G_\eta} \) represent a Gray code where the \( g_\alpha \) appear in the same order but with their bits reversed, i.e. \( \overline{g_\alpha} = g_{\eta,\eta-1}, g_{\eta,\eta-2}, \ldots g_{\eta,0} \). Binary reflective Gray codes are constructed recursively,
\[
G_\eta = (G_{\eta-1} \cdot 0, \overline{G_{\eta-1}} \cdot 1),
\]
where \( \cdot \) indicates concatenation.

### B. Gray code basis ordering

The essence of the Gray code mapping for Hamiltonians is that a basis state \( |n\rangle \) in an \( N \)-dimensional space is mapped to the multi-qubit state \( |g_n\rangle \), \( g_n \in G_\eta \), where \( \eta = \lceil \log_2 N \rceil \) is the minimum number of qubits required to represent a system with \( N \) states. In what follows, \( N \) is used to refer to the number of basis states (equivalent to the number of qubits used in the Jordan-Wigner encoding), while \( \eta \) refers to the number of qubits in the Gray code encoding.

For example, if \( N = 8 \) then an example mapping with \( \eta = 3 \) qubits is
\[
|0\rangle \rightarrow |000\rangle, \quad |1\rangle \rightarrow |100\rangle, \quad |2\rangle \rightarrow |110\rangle, \quad |3\rangle \rightarrow |010\rangle,
|4\rangle \rightarrow |011\rangle, \quad |5\rangle \rightarrow |111\rangle, \quad |6\rangle \rightarrow |101\rangle, \quad |7\rangle \rightarrow |001\rangle.
\]

A new qubit Hamiltonian must now be constructed such that it performs the same action on the qubit states as the Hamiltonian did on the occupation basis states. The terms in the deuteron Hamiltonian [2] can be organized into number-operator-like terms, which act on a basis state as \( b_n^* b_n |m\rangle \propto |m\rangle \delta_{m,n} \) or as ladder operators \( b_n^\dagger b_n \), which ladder between states as \( b_n^\dagger b_n |m\rangle \propto |m + 1\rangle \delta_{n,m} \). The corresponding qubit operators can be constructed using a sequence of Pauli \( Z \), and Pauli \( X \) operators. Recall that
\[
Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad Z |0\rangle = |0\rangle, \quad Z |1\rangle = -|1\rangle,
\]
\[
X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad X |0\rangle = |1\rangle, \quad X |1\rangle = |0\rangle.
\]
A projection operator, which acts as the number operator on a single qubit state, \( P^{(\alpha)} |\beta\rangle = \delta_{\alpha\beta} |\beta\rangle \), for \( \alpha, \beta = 0, 1 \) can be expressed in terms of a \( Z \) operator as
\[
P^{(0)} = \frac{1}{2} (1 + Z) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad P^{(1)} = \frac{1}{2} (1 - Z) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.
\]
The number operator on a multi-qubit state is obtained by taking products of these single qubit projection operators. For the Gray code $G_\eta$ given in [9] the $\eta$-qubit number operators are defined as

$$B_\alpha = \bigotimes_{\beta=0}^{\eta-1} P^{(g_{\alpha,\beta})}, \quad g_{\alpha} \in G_\eta \quad \forall \alpha = 0, \ldots, 2^n - 1,$$

such that $B_\alpha |g_\alpha\rangle = |g_\alpha\rangle$.

Similarly the ladder operators can be mapped to products of $P^{(g)}$ and $X$ operators. The form of the ladder operator can be written compactly using the sequence representation of the Gray code, $S_{G_\eta}$ given in [12] Define the ladder operators

$$C_\alpha = \left( \bigotimes_{\beta=0}^{s_\alpha-1} P^{(g_{\alpha,\beta})} \right) \otimes X \otimes \left( \bigotimes_{\beta=s_\alpha + 1}^{\eta-1} P^{(g_{\alpha,\beta})} \right), \quad s_\alpha \in S_{G_\eta},$$

such that $C_\alpha |g_\alpha\rangle = |g_{\alpha+1}\rangle$. Intuitively, this applies an $X$ on the qubit $s_\alpha$ that indicates the flipped bit in the Gray code between $g_\alpha$ and $g_{\alpha+1}$; the remaining qubits are kept in their present state using the associated projectors.

By replacing the operators in [2] by those of [18] and [19] the full qubit Hamiltonian for the deuteron under the Gray code encoding is

$$H_N = \sum_{\alpha=0}^{2^n-1} \langle g_\alpha | H | g_\alpha \rangle B_\alpha + \sum_{\alpha=0}^{2^n-1} \langle g_{\alpha+1} | H | g_\alpha \rangle C_\alpha,$$

where $\eta = \lceil \log_2 N \rceil$ and $g_\alpha \in G_\eta$. Under the mapping of $|n\rangle \rightarrow |g_n\rangle$, the matrix elements $\langle g_{n+1} | H | g_n \rangle = \langle n+1 | H | n \rangle = \langle n | H | n + 1 \rangle$ for $n = 0, \ldots, N - 1$, which are given in [3].

### C. Examples

Unlike the Jordan-Wigner encoding which mapped the Hamiltonian with $N = 4$ to four qubits in [2], the Gray code encoding can map this same Hamiltonian onto only two qubits, for example

$$|0\rangle \rightarrow |00\rangle, \quad |1\rangle \rightarrow |10\rangle, \quad |2\rangle \rightarrow |11\rangle, \quad |3\rangle \rightarrow |01\rangle.$$

The corresponding Hamiltonian is then given by [20] for a two-qubit system. The specific number and ladder operators for this mapping are summarized in Table V in Appendix [3]. The resulting Hamiltonian is given by

$$H_4 = \frac{1}{4} \left[ |0\rangle H |0\rangle + |1\rangle H |1\rangle + |2\rangle H |2\rangle + |3\rangle H |3\rangle \right] \cdot \mathbb{I} + \frac{1}{2} \left[ |0\rangle H |1\rangle - |1\rangle H |0\rangle - |2\rangle H |2\rangle + |3\rangle H |3\rangle \right] \cdot X_0 + \frac{1}{2} \left[ |0\rangle H |0\rangle + |1\rangle H |1\rangle - |2\rangle H |2\rangle + |3\rangle H |3\rangle \right] \cdot Z_0 + \frac{1}{4} \left[ |0\rangle H |0\rangle + |1\rangle H |1\rangle - |2\rangle H |2\rangle - |3\rangle H |3\rangle \right] \cdot Z_0 X_1 + \frac{1}{4} \left[ |0\rangle H |0\rangle + |1\rangle H |1\rangle + |2\rangle H |2\rangle - |3\rangle H |3\rangle \right] \cdot Z_0 Z_1,$$

where the matrix elements are as expressed in [3]. Evaluating these elements with the selected parameter values gives

$$H_4 = 14.328 \cdot \mathbb{I} - 7.814 \cdot X_0 - 3.913 \cdot X_1 - 1.422 \cdot Z_0 - 8.422 \cdot Z_1 + 3.527 \cdot Z_0 Z_1 + 3.913 \cdot Z_0 X_1 - 4.922 \cdot Z_0 Z_1.$$

As the Gray code encoding for two qubits is particularly simple, it is instructive to consider an example with more qubits. As shown in [14] the eight states that make up the $N = 8$ basis can be mapped onto only three qubits. Evaluating [20] for this case yields
\[ H_8 = 29.039 \cdot \mathbb{1} - 0.711 \cdot Z_0 - 0.711 \cdot Z_1 - 14.711 \cdot Z_2 \\
- 0.711 \cdot Z_0 Z_1 - 0.711 \cdot Z_0 Z_2 - 7.711 \cdot Z_1 Z_2 - 4.211 \cdot Z_0 Z_1 Z_2 \\
- 14.835 \cdot X_0 + 0.012 \cdot X_0 Z_1 + 7.022 \cdot X_0 Z_2 + 3.515 \cdot X_0 Z_1 Z_2 \\
- 7.421 \cdot X_1 + 7.421 \cdot Z_0 X_1 + 3.508 \cdot X_1 Z_2 - 3.508 \cdot Z_0 X_1 Z_2 \\
- 3.712 \cdot X_2 - 3.712 \cdot Z_0 X_2 + 3.712 \cdot Z_1 X_2 + 3.712 \cdot Z_0 Z_1 X_2. \]

(24)

The specific form of the number and ladder operators in the Gray code ordering used to obtain the Hamiltonian above from the general expression \([20]\) for \(N = 8\) are summarized in Table VI of Appendix B.

D. Pauli structure of the Hamiltonians

An important consideration for both the VQE and simulating time evolution is the way in which the constituent Paulis of a Hamiltonian can be partitioned into commuting sets. In the VQE, this partitioning reduces the number of measurements that need to be taken, since expectation values of commuting Paulis can be measured simultaneously. For simulating time evolution, the structure of the commuting sets and the order in which Paulis are written affects the accuracy of the simulation. These aspects will be discussed further in Section IV A and Section V respectively.

A key feature of the Jordan-Wigner encoding is that Pauli terms in the Hamiltonian partition into the three commuting sets shown in Table I. Note that the weight of the Pauli strings is at most 2. In addition, within each set, measurements on all qubits take place in the same basis so there is no need to perform a rotation to a common eigenbasis when measuring the expectation values of these Pauli operators; we need only apply a Hadamard \(H\) to all qubits for the set with \(X\), or \(HS^\dagger\) for the set with \(Y\), where

\[
H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}.
\]

(25)

| 0 | \(Z_0, Z_1, \ldots, Z_{N-1}\) |
| 1 | \(Y_0 Y_1, Y_1 Y_2, \ldots, Y_{N-2} Y_{N-1}\) |
| 2 | \(X_0 X_1, X_1 X_2, \ldots, X_{N-2} X_{N-1}\) |

TABLE I: Structure of the sets of commuting operators for the deuteron Hamiltonian using the Jordan-Wigner encoding.

From the examples in Section III C one observes that a consequence of the Gray code encoding is that each \(\eta\)-qubit Pauli term contains at most a single \(X\). This naturally partitions the operators into \(\eta + 1\) commuting sets: one containing all combinations of \(\mathbb{1}\) and \(Z\), and the rest containing an \(X\) on a given qubit, and then all combinations of \(\mathbb{1}\) and \(Z\) on the rest. For the \(\eta = 3\) case, there are four sets:

\[
\begin{align*}
S_Z &= \{Z_0, Z_1, Z_2, Z_0 Z_1, Z_1 Z_2, Z_0 Z_2, Z_0 Z_1 Z_2\}, \\
S_{X0} &= \{X_0, X_0 Z_1, X_0 Z_2, X_0 Z_1 Z_2\}, \\
S_{X1} &= \{X_1, Z_0 X_1, Z_1 Z_2, Z_0 X_1 Z_2\}, \\
S_{X2} &= \{X_2, Z_0 X_2, Z_1 X_2, Z_0 Z_1 X_2\}.
\end{align*}
\]

(26)

Thus, for each commuting set, only one qubit ever needs to be rotated back to the computational basis. This reduces the number of such rotations over measurement of all sets to \(\eta\), down from 3\(N\) in the Jordan-Wigner encoding.

It is straightforward to generalize the structure of the Hamiltonians to arbitrary \(N\). When \(N\) is not a power of 2, a truncated Gray code can be used, but will still require \(\eta = \lceil \log_2 N \rceil\) qubits. Table II compares key properties of the Hamiltonians of the two encodings for an \(N\)-state problem.

The structure of the Hamiltonians reveals an interesting trade-off. For the same number of states, the Gray code Hamiltonian has more terms, and higher weight of the Pauli strings per term. Furthermore, the number of commuting sets is no longer constant, which may have consequences while running the VQE as more measurements must be made. However, the number of qubits is exponentially smaller, so it is necessary to explore whether the tradeoff of using fewer qubits is beneficial, especially in a noisy hardware setting.
IV. FINDING THE GROUND STATE ENERGY WITH THE VARIATIONAL QUANTUM EIGENSOLVER

A. Variational quantum eigensolver

The VQE [7] is based on the variational principle: given a Hamiltonian \( H \) with ground state \( |\psi_g\rangle \) and energy \( E_g \), the expectation value for any other state will always be greater,

\[
\langle \psi | H | \psi \rangle \geq \langle \psi_g | H | \psi_g \rangle = E_g.
\]

The VQE parameterizes the state \( |\psi\rangle \) as \( |\psi(\theta)\rangle \), and uses classical optimization to search for a set of suitable parameters \( \theta \) such that

\[
\langle \psi(\theta) | H | \psi(\theta) \rangle = E_g.
\]

In practice, the state \( |\psi(\theta)\rangle \) is expressed as the action of a variational ansatz circuit acting on an initial state, typically \( |0\rangle \): \( |\psi(\theta)\rangle = U(\theta) |0\rangle \). The goal is then to find a suitable ansatz \( U(\theta) \) and its parameters such that the resultant expectation value is as close as possible to the true ground state of the system. A Hamiltonian on \( N \) qubits, being a Hermitian matrix, can be expressed as a linear combination of the \( N \)-qubit Pauli operators,

\[
H = \sum_{i=0}^{4^{N-1}-1} q_i Q_i, \quad Q_i \in \mathcal{P}_N,
\]

for expansion coefficients \( q_i \in \mathbb{R} \). The expectation value of the Hamiltonian can be computed as a linear combination of the expectation values of the individual terms,

\[
\langle H \rangle = \sum_{i=0}^{4^{N-1}-1} q_i \langle Q_i \rangle, \quad Q_i \in \mathcal{P}_N.
\]

The role of the quantum computer is to apply \( U(\theta) \) and take measurements to obtain these expectation values, which are then processed on a classical computer during an optimization routine. Based on the results, a new value of \( \theta \) is chosen and the process is repeated again. To reduce the number of measurements, one typically takes advantage of the fact that expectation values of sets of Paulis that commute can be measured simultaneously. Algorithms for creating and analyzing such sets are under active development [40–43]; the upper bound for an \( \eta \)-qubit system is \( 2^{\eta} + 1 \), which corresponds to measuring in a complete set of mutually unbiased bases.

B. Choosing a variational ansatz

The choice of variational ansatz for the VQE depends on which encoding is used. To run the VQE in the Jordan-Wigner encoding requires a variational ansatz capable of producing general linear combinations over the occupation basis states. Since there are no imaginary components in the Hamiltonian, a variational form where all coefficients are real numbers may be used. A suitable choice is the generalized spherical coordinates. For \( N \) states this requires \( N \) qubits and \( N-1 \) parameters. As an example, for the 4-state case

\[
|\psi\rangle = \cos \theta_1 |0001\rangle + \sin \theta_1 \cos \theta_2 |0010\rangle + \sin \theta_1 \sin \theta_2 \cos \theta_3 |0100\rangle + \sin \theta_1 \sin \theta_2 \sin \theta_3 |1000\rangle.
\]
Such states can be constructed recursively using a cascade of controlled rotations and CNOTs \[12\]. The circuit for the 4-qubit case is shown in Fig. 1(left). Note that the ordering of the qubits here is reversed from that of \[12\], so that the basis state with the largest contribution to the ground state depends on all parameters. This re-ordering was found to provide improved stability during the optimization procedure when using the statevector simulator.

The gates indicated by \( \theta_i \) are Pauli \( Y \) rotations.

The Gray code encoding, since it incorporates all available states, enables the use of hardware-efficient variational ansatze consisting of layers of parameterized \( Y \)-rotations separated by layers of entangling gates \[9\]. The right panel of Fig. 1 presents such an ansatz for the \( N = 4 \) case using only two qubits; a further example with \( N = 8 \) is shown in Fig. 2. The wavefunction for the \( N = 4 \) case can be evaluated as

\[
|\psi\rangle = \cos \theta_1 \cos(\theta_2 + \theta_3) |00\rangle + \sin \theta_1 \sin(\theta_2 - \theta_3) |10\rangle + \\
\sin \theta_1 \cos(\theta_2 - \theta_3) |11\rangle + \cos \theta_1 \sin(\theta_2 + \theta_3) |01\rangle. \tag{32}
\]

In contrast to the wavefunction of (31), the coefficient for each basis state in the wavefunction above depends on every variational parameter.

The structure of the variational ansatz has a significant effect on the success of the VQE, especially in a noisy hardware environment. The number of gates, circuit depth, and in particular number of two-qubit gates are all important points of comparison. In what follows, the resources required to run the VQE ansatz of an \( N \)-state problem are computed, with results summarized in Table III.

To estimate the resource requirements for the Jordan-Wigner encoding ansatz of Fig. 1, the controlled rotations are first decomposed into two single-qubit rotations and two CNOTs. Thus, an \( N \)-qubit version of this circuit uses \( 3N - 5 \) two-qubit gates and \( 2N - 2 \) single-qubit gates, and runs in depth \( 4N - 6 \). Additional single-qubit rotations must also be performed to rotate back to the computational basis when measuring the commuting Pauli sets with \( X \) and \( Y \) (as was described in Section III D). These require \( N \) and \( 2N \) additional rotations respectively. Considering the execution of circuits for all three commuting sets of Paulis, the total number of gates is \( 18N - 21 \).

For the Gray code encoding ansatz, since there are no controlled rotations to decompose, the number of single-qubit gates depends on the number of qubits \( \eta = \lceil \log_2 N \rceil \). There are \( 2^\eta - 1 \) single qubit gates, and \( 2^\eta - 1 - \eta \) two qubit gates. This can be seen from the structure of the circuit as alternating layers of single qubit gates and CNOTs - each single-qubit gate is paired with a CNOT to its left, save for the first layer. Calculation of the depth is slightly more involved, but is shown in Table III. Finally, the structure of the commuting Pauli sets leads to a simple measurement procedure. To measure the set \( S_{X_i} \), one simply performs a Hadamard on qubit \( i \) before measurement to rotate it back to the computational basis. Across all sets this yields only \( \eta \) extra single-qubit gates, as opposed to \( 3N \).

Table III shows that the depth of the Gray code ansatz is consistently better than the Jordan Wigner ansatz. One interesting point, however, is that the number of two-qubit (and total) gates in the Gray code ansatz always surpasses that of the ansatz in \[12\] starting at \( N = 256 \) (for lower \( N \), the Gray code gate counts are lower for \( N \) that are powers of 2). However one can surely argue that if one has access to that many qubits, we are no longer in the NISQ era and there are better methods available than the VQE.
TABLE III: Comparison of variational ansatz circuits for a Hamiltonian with \( N \) states for the two encodings. Numbers shown are the gate counts for a single evaluation of the expectation value using VQE, i.e. measuring all commuting sets of Paulis. The depth is given for the circuit without any additional basis rotations.

| Encoding          | Jordan-Wigner | Gray code |
|-------------------|---------------|-----------|
| Qubits            | \( N \)       | \( \lceil \log_2 N \rceil = \eta \) |
| Single-qubit gates| \( 3(2N - 2) \) | \( (\eta + 1)(2^\eta - 1) \) |
| Additional basis rotations | \( 3N \) | \( \eta \) |
| Two-qubit gates   | \( 3(3N - 5) \) | \( (\eta + 1)(2^\eta - \eta - 1) \) |
| Total gates for VQE | \( 18N - 21 \) | \( 2(\eta + 1)(2^\eta - 1) - \eta^2 \) |
| Individual circuit depth | \( 4N - 6 \) | \( \frac{2^\eta - 1}{\eta^2} (\eta + 1) - 2\eta + (2^\eta - 1) \mod \eta \) |

FIG. 3: Comparison of the average energy obtained over 100 independent executions of the VQE using the Qiskit QASM simulator with 10000 shots. Error bars in the left panel show the standard deviation, and values are offset for clarity. There is significantly more variance in the energies obtained for the Jordan-Wigner encoding. This is interesting as it shows that, despite having more Pauli terms and more commuting sets to measure in the Gray code case, the results are consistently closer to the true value in the presence of shot noise.

C. VQE simulation results

The quantum computing component of the implementation was simulated using Qiskit \cite{Qiskit} and OpenFermion \cite{OpenFermion}. The simultaneous perturbation stochastic approximation (SPSA) algorithm \cite{SPSA} was chosen as the classical optimization routine, using the implementation provided in the noisyopt Python package \cite{noisyopt}. SPSA was run using step parameters \( a = 0.628, c = 0.1 \). Initial values for the variational parameters were chosen uniformly at random from the range \( (-\pi/2, \pi/2) \). The number of iterations used was 2000 for \( N = 2 \), 4000 for \( N = 3 \), 5000 for \( N = 4 \), ..., 8 and 8000 for \( N = 16 \). Simulations for \( N = 16 \) were performed only with the Gray code encoding, due to the computational intensity of simulating thousands of VQE steps for a 16-qubit system. The implementation, as well as the data files and initial parameters, are available at \cite{VQE_code}.

The encoding was first analyzed using Qiskit’s statevector simulator to verify correctness. This was followed by testing with the QASM (quantum assembly language) simulator, which simulates the probabilistic behaviour of quantum computers and returns counts of the different measurement outcomes rather than an analytical solution. These simulations were run with 10000 trials (“shots”) per circuit. For each \( N \), 100 independent trials of the full VQE were performed. Since the number of iterations of SPSA is fixed, the quantity of interest is the solution quality and variance as compared to the true value obtained from diagonalization.

Results for the QASM simulations are plotted in Fig. 3. The variance of solutions is observed to be significantly higher for the JW encoding. It is of course possible in principle to get more accurate results with this encoding were we to increase the number of shots. However this demonstrates that, using the same computational resources (save for number of qubits), the Gray code encoding gives a more reliable solution.

The difference between the two methods is even more visible in Fig. 4 the density plots of the energy distribution...
FIG. 4: The data from Fig. 3 as a density plot. Each curve presents data over 100 independent VQE simulations. There is significantly more spread of values for the Jordan-Wigner encoding (see right panel of Fig. 3 for the explicit variances).

for the QASM simulations. The Gray code energies have significantly less variance, and the difference is amplified as \( N \) increases.

D. Resilience in the presence of simulated hardware noise

Given that the Gray code encoding uses fewer qubits and has circuits of shorter depth with fewer two-qubit gates, it is reasonable to expect its performance may improve over that of the Jordan-Wigner encoding when there is hardware noise present. To investigate this, a noise model from the IBM Q device Vigo \cite{vigo} was applied, and simulations for both encodings are compared in the \( N = 4 \) case. Results from an additional simulated IBM device are shown in Appendix C. The hardware graph and error rates for the simulated device are shown in Fig. 5. The noise model approximates the physical device by implementing single-qubit and two-qubit gate errors as well as measurement readout errors. Data for the particular noise models used is provided in the code \cite{code}. The results of the simulations are shown in Fig. 6.

Unsurprisingly, the Jordan-Wigner version suffers far more from the additional noise than the Gray code version. Even after performing measurement error mitigation i.e correcting for expected errors based on calibration circuits (carried out using Qiskit’s Ignis library), the obtained results are displaced from the exact answer, which is calculable on classical computers. The Gray code is much closer, both before and after mitigation, with some overlap of the distribution with the exact value. These findings suggest that in the near term, it may be beneficial to use an encoding with fewer qubits and shorter circuits despite the trade-offs in the structure of the Hamiltonian, i.e. making far more measurements.

To obtain results on noisy hardware that are comparable to those from the clean simulations, extrapolation to the noise-less limit can be performed using a technique called zero-noise extrapolation \cite{zero_noise1, zero_noise2}. Let \( E(\varepsilon) \) be an expectation value depending on a noise parameter \( \varepsilon \). The noise-less result is \( E(\varepsilon = 0) \) and the simulation result is \( E(\varepsilon = \varepsilon_0) \), where \( \varepsilon_0 \) is the noise parameter of a NISQ device. The value of \( E(\varepsilon = 0) \) can be estimated by simulating \( E(\varepsilon) \) at \( \varepsilon > \varepsilon_0 \) and extrapolating to \( \varepsilon = 0 \). Several discussions have been made to calculate \( E(\varepsilon) \) at \( \varepsilon \) other than \( \varepsilon_0 \) \cite{other_cases}.
FIG. 5: Hardware graph for the IBM Q machine Vigo. Each node of the graph corresponds to a physical qubit. Calibration data were retrieved from the IBM Q Experience portal on July 8, 2020. The pair of values in the node label corresponds to the single-qubit gate error rate (left) and measurement error rate (right) that were used for the simulations. The edge label corresponds to the two-qubit gate error rate. Lighter colour, larger node size and larger edge width correspond to higher error rates.

FIG. 6: Distribution of VQE energies in QASM simulations (10000 shots) with additional simulated hardware noise using the Vigo device noise model, noise with measurement error mitigation, and no simulated hardware noise. Each simulation is carried out using a particular layout of qubits on the hardware graph. The simulation using the Gray code maps the logical qubits \{0,1\} to the “physical” qubits \{2,1\} of the layout shown in Fig. 5. The Jordan-Wigner simulation maps logical qubits \{0,1,2,3\} to physical qubits \{2,1,3,4\}.

The method used in this work is to add redundant CNOT gate pairs to the original circuit to simulate $E(\varepsilon > \varepsilon_0)$ as done in the earlier deuteron simulations. Since the noise of a single-qubit gate is much smaller than that of two-qubit gates (CNOT gate), $E(\varepsilon)$ is mainly affected by the number of CNOT operations. This suggests that $\varepsilon$ can be scaled by the number of CNOTs in the circuit, e.g., $\varepsilon$ would be $2\varepsilon_0$ when the number of CNOTs is twice that of the original circuit. Given that $(\text{CNOT})^{2n} = 1$ is satisfied at the $\varepsilon_0 = 0$ limit (for $n = 0, 1, 2, \ldots$), $E(\varepsilon)$ at $\varepsilon = (2n + 1)\varepsilon_0$ can be calculated by replacing every CNOT gate in the original circuit with $(\text{CNOT})^{2n}\text{CNOT}$. 

Expanding \( E(\varepsilon) \) around \( \varepsilon = 0 \) and plugging in \( \varepsilon = (2n + 1)\varepsilon_0 \), \( E(\varepsilon) \) is
\[
E(\varepsilon) \sim E(0) + \varepsilon_0 \left. \frac{dE(\varepsilon)}{d\varepsilon} \right|_{\varepsilon=0} (2n + 1). \tag{33}
\]
Note that \( \varepsilon_0 \approx m \times 10^{-2} \), using the number of CNOT operators in the original circuit \( m \) (see Table II and Fig. 5 for practical cases), on currently available devices, and higher order terms in \( \varepsilon_0 \) should be negligible. Eq. (33) enables us to extrapolate to the zero-noise limit in terms of \((2n + 1)\) instead of \( \varepsilon \).

To examine Eq. (33), the extrapolations of the energies for both Gray code and Jordan-Wigner encodings are demonstrated in Fig. 7. To avoid considering uncertainties from the VQE process, the input energies with the IBM Q Vigo noise model (indicated by the solid symbols in the figure) are calculated with the optimal variational parameters, which are determined by classical calculations. Since the slope is proportional to \( \varepsilon_0 \) which would be also roughly proportional to the number of CNOT gates, it is reasonable that the slope for the Gray code encoding is smaller than that for the Jordan-Wigner encoding. Also, the linear extrapolation tends to worsen as \( \varepsilon_0 \) increases, i.e., the error of the linear fit in the Jordan-Wigner case is larger than that of the Gray code case. For the extrapolated energies, the Gray code energy seems slightly higher than the exact number, but still agrees within the error, while the Jordan-Wigner energy is clearly off from the exact answer. One might think the discrepancy is due to the single-qubit gate error rate. However, it was observed that there is no significant changes even if the single-qubit gate error is taken into account, using the unitary folding method discussed in [56]. Further studies about zero-noise extrapolation would be needed to obtain a better estimation.

As zero-noise extrapolation does not quite yield the energy of the noise-less simulation, we combine extrapolation with the VQE process to try and improve these results. To do this, the expectation value used at each VQE optimization step is evaluated by extrapolation using the CNOT pair insertion technique. Employing the IBM Q Vigo noise model, the deuteron ground-state energies with 100 independent runs with 10000 shots are \( E_{g.s.}^{(GC)} = -2.08 \pm 0.09 \) MeV and \( E_{g.s.}^{(JW)} = -1.89 \pm 0.14 \) MeV with the Gray code and Jordan-Wigner encodings, respectively. Note that the uncertainties are estimated as the standard deviation of the distribution of 100 run results.

Since the extrapolation at each optimization step is done with the energies evaluated with the single 10000 shots calculations, which would be within the standard deviation of the distribution, it would be more reasonable to assign the uncertainty as the standard deviation than the standard error of the 100 independent runs. Comparing to the exact energy \( E_{g.s.}^{(exact)} = -2.14 \) MeV, similarly to the energies evaluated at the optimal parameters (see Fig. 7), both...
encoding results provide higher energy than the exact, but the Gray code result agrees within the error. Thus, the Gray code encoding yields better performance and enables us to estimate more accurate noise-less results.

V. APPLICATION TO HAMILTONIAN SIMULATION

This section presents a first analysis of the Gray code encoding’s potential for simulating the time evolution of quantum systems. Simulating time evolution, or Hamiltonian simulation, is one of the key applications of future large-scale quantum computers, but the resource requirements for non-trivial systems are beyond the capabilities of today’s NISQ devices. Given a Hermitian Hamiltonian $H$, a unitary operation that performs evolution for time $t$ can be computed as

$$U(t) = e^{-itH}.$$  \hspace{1cm} (34)

The idea of Hamiltonian simulation using a quantum computer is to find (and then execute) a quantum circuit $\tilde{U}(t)$ expressed in terms of elementary gates that approximates $U(t)$ well, i.e. $\|\tilde{U}(t) - U(t)\| < \varepsilon$ where $\varepsilon$ is small and $\|\cdot\|$ is the spectral norm. Such a circuit is then typically used as a subroutine in a larger context, such as quantum phase estimation. A circuit can be found by first expressing $H$ as a linear combination of Paulis as in $[29]$, $[4]^2$.

$$U(t) = e^{-it\sum_j q_j Q_j} \approx \prod_j e^{-itq_j Q_j} + O(t^2).$$ \hspace{1cm} (35)

This expression is convenient because it involves sequential applications of unitaries of the form $e^{-itQ_j}$, which are straightforward to implement for a Pauli operator $Q_j$ $[58]$. However, an additional error operator term $O(t^2)$, the Trotter error, arises due to the fact that for Pauli operators $Q_1$ and $Q_2$ that do not commute, $e^{Q_1Q_2} \neq e^{Q_1}e^{Q_2}$.

The error can be decreased by Trotterization. Intuitively, rather than evolving each term for time $t$, this process is divided up into $T$ repeated steps of time $t/T$,

$$U(t) = \left(\prod_j e^{-itq_j Q_j} \frac{t}{T}\right)^T + O(t^2/T),$$ \hspace{1cm} (36)

$T$ is known as the Trotter number, or number of Trotter steps. There also exist higher-order versions of this formula $[59]$, though only the first-order expansion as written in $[36]$ is used in this initial investigation.

Trajectory of basis states evolving under N=4 Hamiltonian

FIG. 8: Output probability distribution for the basis states in the $N = 4$ deuteron problem. This plot shows how the system evolves over a period of time; in later figures the simulation at $t = 1$ is investigated in detail.
As a first point of comparison, the $N = 4$ case is explored. The evolution time $t$ is set arbitrarily to $t = 1$, and for each encoding the system is initialized in the uniform superposition of its relevant basis states (occupation basis for the Jordan-Wigner case, and full computational basis for the Gray code case). The evolution of the probability distribution of basis state measurement outcomes is shown in Fig. 8 for reference.

The evolution circuit is generated using the evolve functionality of Qiskit Aqua’s WeightedPauliOperator class. The number of Trotter steps was varied from 1 to 100, and the probability distribution of each basis state after evolution was estimated using the QASM simulator with 10000 shots. An example of this is plotted in Fig. 9, where it can be seen that the probability distributions approach the true values as the number of Trotter steps is increased.

![N=4 encoding comparison for Hamiltonian evolution time t = 1, QASM 10000 shots](image)

**FIG. 9:** Comparison of Hamiltonian simulation using the standard Trotter decomposition for Gray code (dots) and Jordan-Wigner (x’s) encodings. Evolution time is fixed at $t = 1$ using 10000 QASM shots at each step. Dotted lines show the true value, computed analytically from exponentiating the Hamiltonian and applying it to the uniform superposition.

To quantify the quality of the evolution circuit, the trace distance is taken between the output state after evolution and the ideal output state as computed directly from $e^{-iHt}|\psi\rangle$ for the uniform superposition $|\psi\rangle$. For two quantum states represented by density matrices $\rho$ and $\rho'$, the trace distance is defined as [60]

$$D(\rho, \rho') = \frac{1}{2} \text{Tr}|\rho - \rho'|,$$

(37)

where the norm $|A| = \sqrt{A^\dagger A}$ (thus smaller trace distance is better).

A density matrix for the output state from the QASM simulations is estimated using state tomography with Qiskit’s Ignis library. In Fig. 10a, the trace distances are plotted. It can be seen that while the Gray code version fares slightly better, the trace distances are comparable, and as expected both decrease as the number of Trotter steps increases.

As with the VQE, the situation of greater interest is when hardware noise is present. The same simulations were repeated using the Vigo device noise model (including measurement error mitigation), and the resultant trace distances are plotted in Fig. 10b. Here, the Jordan-Wigner encoding yielded a consistently high trace distance, whereas the Gray code improved with increasing amount of Trotter steps only up to a point, after which it plateaued. For both encodings, the value at the plateau corresponds roughly to the trace distance between the true expected output (computed analytically), and the maximally mixed state, indicating decoherence of the system.

To analyze the inflection point in the Gray code version, the gate operation times of the Vigo device model were used to estimate the run time of the circuit. Around the 12-13 Trotter step mark, the execution time of the circuit is about double the smallest coherence times of the individual qubits, so even though the number of Trotter steps
FIG. 10: Assessing quality of Hamiltonian simulation results using the trace distance. The output state was computed using state tomography on QASM runs with 10000 shots at each Trotter step, and compared to the state obtained analytically.

(a) Shot noise only. The trace distances are quite similar between the two encodings. As they quickly approaches 0 in both cases, the log$_{10}$ is plotted to emphasize differences.

(b) Simulated hardware noise using the Vigo device model with measurement error mitigation applied. The low trace distance is unsurprising given the size of the circuits, however the inflection point for the Gray code encoding is a unique feature. The value of the trace distances at the plateau correspond roughly to the trace distance of the expected output state with the maximally mixed state, indicating that the system has fully decohered.
begins to give a more accurate simulation, the circuit depth is too high and the system decoheres significantly.

For a fixed number of Trotter steps, the circuits for the Gray code version require fewer resources to implement. The gate counts are plotted in Fig. 11a, where it can be observed that the Gray code encoding circuits require roughly half the amount of CNOT gates and 44% of the single-qubit gates, and roughly 90% of the depth. Together these reductions suggest that Hamiltonian evolution could be performed with significantly fewer resources in the Gray code encoding, though we note that for both encodings the gate count and depth are far beyond what can be done with a NISQ-era machine, as is evidenced by Fig. 10b.

There are a number of additional aspects of Hamiltonian simulation for which the two encodings should be compared in future work. A key one is to quantify the Trotter error, and investigate the effect of the partitioning of the Paulis into commuting sets. For the deuteron Hamiltonian with $N$ states, recall that the Gray code encoding yields $N + 1$ sets of commuting Paulis, while Jordan-Wigner yields 3. Furthermore, the order in which to perform the product terms of (36) is a subject of active investigation [61]. Studying different Trotter decomposition formulae, or even different Hamiltonian simulation schemes such as qubitization [62] might also reveal interesting differences.

VI. CONCLUSIONS AND FUTURE WORK

A mapping that orders the computational basis states in a Gray code yields a number of advantages in the context of the VQE. It requires exponentially fewer qubits compared to the same problem solved using the Jordan-Wigner encoding, and can use smaller, hardware-efficient variational ansatze that require fewer CNOT gates for problems solvable on NISQ-era machines. It also suggests a natural partitioning into $N + 1$ sets of commuting operators where only one qubit's basis must be rotated during measurement. While the number of measurements is larger and also increases with system size, this method may nevertheless be beneficial in the near term due to the trade-off with number of qubits and gate counts, as the variance in energies produced by the VQE is reduced (most notably in the presence of simulated hardware noise).

In order to demonstrate any long-term advantages, the Gray code encoding must be extended and adapted to non-trivial situations. There are a number of future directions to be investigated. First, testing must be done on actual hardware to analyze how additional limitations affect the solution quality. The deuteron is fully solvable using present-day classical methods, and so an immediate next step is to extend and test the method in a multi-particle scenario. This could be done by simply concatenating a set of registers, one for each particle, with each expressed independently in a Gray code. However, care must be taken to ensure antisymmetrization of the basis is satisfied.

Another avenue is to extend the Gray code encoding to calculating the ground state of the deuteron using a full \textit{ab initio} chiral interaction [63–65]. The inclusion of higher order chiral terms in the interaction will result in more complicated ladder operators, which will likely remove the useful property of having only one $X$ per commuting Pauli set, making simultaneous measurement more complex. Especially in these more complex cases, the trade-offs with the Jordan-Wigner case must be studied.

The cyclic nature of the Gray code naturally suggests another application: working on a periodic lattice. Similar work that focuses on lattice methods indexes the lattice sites using qubits in binary order (for example [66]). This yields more complicated transformations when moving across the boundaries of the lattice, as one has to make the transition from $|1\cdots1\rangle$ back to $|0\cdots0\rangle$. Indexing using a Gray code, which can be done over both dimensions of a 2D lattice, will simplify these transitions.

Further analysis of time evolution is also necessary, in particular the effect of the encoding on the amount of Trotter error since there are more commuting sets of Paulis. Time evolution should also be extended to the multi-particle case, and investigated for different decompositions such as higher-order Trotter formulae, and Trotter-Suzuki decompositions. While the gate counts for this are far beyond the capabilities of NISQ hardware, it may still enable us to simulate larger systems sooner by making better use of available resources.

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FIG. 11: Resource estimation for Hamiltonian evolution circuits deuteron problem of Fig. 9.

(a) Gate counts computed by Qiskit for the Hamiltonian evolution in Fig. 9. The CNOT count of the Gray code encoding circuit is reduced to about 50% that of the Jordan-Wigner version. For single-qubit gates, the Gray code uses about 44% of the amount.

(b) Circuit depth computed by Qiskit for the Hamiltonian evolution in Fig. 9. The depth of the Gray code circuit is roughly 90% that of the equivalent Jordan-Wigner circuit.
official policy or position of IBM or the IBM Quantum team.

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Appendix A: Mapping using a standard basis ordering

As the Gray code is a re-ordering of the computational basis states, one might wonder what happens if the basis states were simply ordered in increasing binary value. While this can certainly be done, the Gray code encoding simplifies the measurement process in the VQE and thus reduces the number of gates that must be applied. As an example, consider the $N = 4$ case, whose operators are detailed in Table IV.

| HO operator | HO state | Qubit operator | Qubit state |
|-------------|----------|----------------|-------------|
| $b_0^1 b_0$ | $|0\rangle$ | $P_0^{(0)} P_0^{(0)}$ | $|00\rangle$ |
| $b_0^1 b_1$ | $|1\rangle$ | $P_0^{(0)} P_1^{(0)}$ | $|10\rangle$ |
| $b_0^1 b_2$ | $|2\rangle$ | $P_0^{(0)} P_1^{(1)}$ | $|01\rangle$ |
| $b_0^1 b_3$ | $|3\rangle$ | $P_1^{(1)} P_1^{(1)}$ | $|11\rangle$ |

(a) Number operator terms

| HO operator | HO state | Qubit operator | Qubit state |
|-------------|----------|----------------|-------------|
| $b_1^1 b_0$ | $|0\rangle \rightarrow |1\rangle$ | $X_0 P_1^{(0)}$ | $|00\rangle \rightarrow |10\rangle$ |
| $b_1^1 b_1$ | $|1\rangle \rightarrow |2\rangle$ | $X_0 X_1$ | $|10\rangle \rightarrow |01\rangle$ |
| $b_1^1 b_2$ | $|2\rangle \rightarrow |3\rangle$ | $X_0 P_1^{(1)}$ | $|01\rangle \rightarrow |11\rangle$ |

(b) Ladder operators terms.

TABLE IV: Mapping deuteron Hamiltonian (2) acting on the harmonic oscillator (HO) basis with $N = 4$ to a two-qubit system using the standard computational basis ordering.

The Paulis that will be present in the Hamiltonian are:

$$
1, \ Z_0, \ Z_1, \ Z_0 Z_1, \ X_0, \ X_0 Z_1, \ X_0 X_1 \tag{A1}
$$

These can be partitioned into 3 commuting sets, $S_Z = \{Z_0, Z_1, Z_0 Z_1\}$, $S_X = \{X_0, X_0 X_1\}$, and $S_{XZ} = \{X_0 Z_1\}$. Simultaneous measurements of $S_Z$ is done simply with the computational basis. For $S_X$ the basis of all qubits must be rotated by a Hadamard to perform the measurement. For $S_{XZ}$ only the basis of the first qubit must be rotated. Using this standard ordering on any $N$-qubit system will always produce a term in the Hamiltonian containing $X_0 \cdots X_{N-1}$, which will require rotation of all $N$ qubits prior to measurement (and similarly measurements that must rotate $N-1$ qubits, $N-2$, and so on). The total number of basis rotations for a full set of measurements is thus $N(N+1)/2 = O(N^2)$, which is higher than the $N$ required when using the Gray code encoding on the same system.

Appendix B: Gray code encoding tables

This appendix contains the tables of number and ladder operators of the Gray code encoding for $N = 4$ (Table V) and $N = 8$ (Table VI).

Appendix C: Additional Noise Models

The hardware errors experienced by NISQ-era physical quantum computers depend on parameters which can change over time. Noise models based on IBM devices are recalibrated daily, therefore the results obtained using these models cannot be expected to be replicated exactly. However, the improvement of VQE results achieved using the Gray code should be consistent. In this section, the same simulations as in Figure 6 are carried out on a second noise model of a different device (IBM Q Yorktown [67]) to verify the results of Section 4. Figure 12 compares the hardware graphs of Vigo and Yorktown, the latter has significantly higher error rates. Figure 13 compares the VQE results with different
The topology is significantly better than the line topology on Yorktown. The Vigo device cannot support a loop topology (connecting \{0,1\} and \{1,2\} or a loop (connecting \{0,2\} in addition). Executing the Gray code circuit for 8 states requires a CNOT gate on \{0,2\}. A line topology requires additional SWAP gates (each consisting of three CNOTs) and so experiences more noise. A simulated demonstration of this effect is shown in Figure 14. The loop topology is significantly better than the line topology on Yorktown. The Vigo device cannot support a loop topology encoding for both devices. The greater noise in Yorktown results in a shift of the energies relative to Vigo, but in both cases the Gray code encoding performs better than the Jordan-Wigner encoding.

| HO operator | HO state | Qubit operator | Qubit state |
|-------------|----------|----------------|-------------|
| $b_0^1 b_0$ | $|0\rangle$ | $P_0^{(0)} F_1^{(0)}$ | $|00\rangle$ |
| $b_0^1 b_1$ | $|1\rangle$ | $P_0^{(1)} F_1^{(1)}$ | $|10\rangle$ |
| $b_0^1 b_2$ | $|2\rangle$ | $P_0^{(2)} F_1^{(2)}$ | $|11\rangle$ |
| $b_0^1 b_3$ | $|3\rangle$ | $P_0^{(3)} F_1^{(3)}$ | $|01\rangle$ |

(a) Number operator terms.

| HO operator | HO state | Qubit operator | Qubit state |
|-------------|----------|----------------|-------------|
| $b_0^1 b_0$ | $|0\rangle \rightarrow |1\rangle$ | $X_0 P_0^{(0)}$ | $|00\rangle \rightarrow |10\rangle$ |
| $b_0^1 b_1$ | $|1\rangle \rightarrow |2\rangle$ | $P_0^{(1)} X_1 F_1^{(1)}$ | $|10\rangle \rightarrow |11\rangle$ |
| $b_0^1 b_2$ | $|2\rangle \rightarrow |3\rangle$ | $X_0 P_1^{(1)}$ | $|11\rangle \rightarrow |01\rangle$ |

(b) Ladder operator terms.

**TABLE V:** Mapping from operators of the deuteron Hamiltonian (2) acting on the harmonic oscillator (HO) basis with $N = 4$ to a two-qubit system using the Gray code encoding.

| HO operator | HO state | Qubit operator | Qubit state |
|-------------|----------|----------------|-------------|
| $b_0^1 b_0$ | $|0\rangle$ | $P_0^{(0)} F_1^{(0)} P_2^{(0)}$ | $|00\rangle$ |
| $b_0^1 b_1$ | $|1\rangle$ | $P_0^{(1)} F_1^{(1)} P_2^{(0)}$ | $|10\rangle$ |
| $b_0^1 b_2$ | $|2\rangle$ | $P_0^{(2)} F_1^{(2)} P_2^{(0)}$ | $|11\rangle$ |
| $b_0^1 b_3$ | $|3\rangle$ | $P_0^{(3)} F_1^{(3)} P_2^{(0)}$ | $|01\rangle$ |
| $b_0^1 b_4$ | $|4\rangle$ | $P_0^{(4)} F_1^{(4)} P_2^{(0)}$ | $|00\rangle$ |
| $b_0^1 b_5$ | $|5\rangle$ | $P_0^{(5)} F_1^{(5)} P_2^{(0)}$ | $|10\rangle$ |
| $b_0^1 b_6$ | $|6\rangle$ | $P_0^{(6)} F_1^{(6)} P_2^{(0)}$ | $|11\rangle$ |
| $b_0^1 b_7$ | $|7\rangle$ | $P_0^{(7)} F_1^{(7)} P_2^{(0)}$ | $|01\rangle$ |

(a) Number operator terms.

| HO operator | HO state | Qubit operator | Qubit state |
|-------------|----------|----------------|-------------|
| $b_0^1 b_0$ | $|0\rangle \rightarrow |1\rangle$ | $X_0 P_0^{(0)} F_1^{(1)} F_2^{(0)}$ | $|00\rangle \rightarrow |10\rangle$ |
| $b_0^1 b_1$ | $|1\rangle \rightarrow |2\rangle$ | $P_0^{(1)} X_1 F_1^{(1)} F_2^{(0)}$ | $|10\rangle \rightarrow |11\rangle$ |
| $b_0^1 b_2$ | $|2\rangle \rightarrow |3\rangle$ | $X_0 P_1^{(1)} F_2^{(1)}$ | $|11\rangle \rightarrow |01\rangle$ |
| $b_0^1 b_3$ | $|3\rangle \rightarrow |4\rangle$ | $P_0^{(3)} X_1 F_1^{(1)} F_2^{(1)}$ | $|00\rangle \rightarrow |01\rangle$ |
| $b_0^1 b_4$ | $|4\rangle \rightarrow |5\rangle$ | $X_0 P_1^{(1)} F_2^{(2)}$ | $|01\rangle \rightarrow |11\rangle$ |
| $b_0^1 b_5$ | $|5\rangle \rightarrow |6\rangle$ | $F_0^{(3)} X_1 F_1^{(1)} F_2^{(2)}$ | $|11\rangle \rightarrow |10\rangle$ |
| $b_0^1 b_6$ | $|6\rangle \rightarrow |7\rangle$ | $X_0 P_1^{(1)} F_2^{(3)}$ | $|01\rangle \rightarrow |00\rangle$ |

(b) Ladder operator terms.

**TABLE VI:** Mapping from operators of the deuteron Hamiltonian (2) acting on the harmonic oscillator (HO) basis with $N = 8$ to a three-qubit system using the Gray code encoding.
FIG. 12: The simulated hardware for IBM Q Vigo (left) and Yorktown (right). Each node of the graph corresponds to a physical qubit. The pair of values in the label correspond to the single-qubit gate error rate and measurement error rate respectively. The value on the edges corresponds to the two-qubit gate error rate. Lighter colour, larger node size and larger edge width correspond to higher error rates.

FIG. 13: Distribution of VQE energies in QASM simulations using the Vigo and Yorktown device noise models. In the legend, Vigo is denoted by (V) and Yorktown by (Y). The Vigo results are identical to those of Figure 6. For the Yorktown simulations, the Gray code maps the virtual qubits \{0,1\} to the “physical” qubits \{2,1\}, and the Jordan-Wigner simulation maps \{0,1,2,3\} to \{0,1,2,3\}. but due to its lower error rates a line topology is comparable to the loop topology on Yorktown.
FIG. 14: The distribution of VQE energies in QASM simulations using simulated qubits on the Vigo (V) and Yorktown (Y) devices using the Gray code encoding. The noisy results have measurement mitigation applied. The legend specifies the layout of qubits on the simulated device.