Second-quantized fermionic Hamiltonians for quantum simulation with polylogarithmic qubit and gate complexity

William Kirby,1,2∗ Bryce Fuller,2 Charles Hadfield, and Antonio Mezzacapo2
1Department of Physics and Astronomy, Tufts University, Medford, MA 02155, USA
2IBM Quantum, T. J. Watson Research Center, Yorktown Heights, NY 10598, USA

We present a method for encoding second-quantized fermionic systems in qubits when the number of fermions is conserved, as in the electronic structure problem. When the number \( F \) of fermions is much smaller than the number \( M \) of modes, this symmetry reduces the number of information-theoretically required qubits from \( \Theta(M) \) to \( O(F \log M) \). In this limit, our encoding requires \( O(F^2 \log^4 M) \) qubits, while encoded fermionic creation and annihilation operators have cost \( O(F^2 \log^5 M) \) in two-qubit gates. This is the first second-quantized encoding of fermions in qubits whose costs in qubits and gates are both polylogarithmic in \( M \), which will permit studying fermionic systems in the high-precision regime of many modes.

I. INTRODUCTION

Simulating systems of many interacting fermions is one of the most promising applications for quantum computers and a prime candidate for practical quantum advantage. Many physical systems like molecules, whose accurate simulation would have great practical value, fall into this category. Classically approximating the ground state energy or simulating time evolution under a many-fermion Hamiltonian is believed to require resources growing exponentially with the system size. A quantum computer, on the other hand, can simulate time evolution efficiently \([1]\). Although ground state problems of interacting Hamiltonians are QMA-complete \([2]\), quantum computers do have an exponential memory advantage in representing ground states of interacting many-body systems, compared to classical methods. Finding efficient ways of simulating time evolution and investigating ground state properties of these systems are active research areas \([3]\).

Simulating a fermionic system on a quantum computer requires mapping fermionic states and operations to qubit states and operations. The most well-known methods for accomplishing this are the Jordan-Wigner \([4]\) and Bravyi-Kitaev \([5, 6]\) mappings, which both use one qubit per fermionic mode. However, the electronic structure Hamiltonian conserves particle number, so one would like to simulate it in the subspace whose number of fermions matches that of the molecule under consideration. For \( F \) fermions in \( M \) modes, the theoretical minimum number of qubits required for this is

\[
Q^* = \log_2 \left( \frac{M}{F} \right),
\]

the log of the dimension of the \( F \)-fermion subspace.

In the \( M \gg F \) limit, the minimum above approaches

\[
Q^* \approx F \log_2 M,
\]

which is exponentially smaller in dependence on \( M \) than the \( Q = M \) of Jordan-Wigner and Bravyi-Kitaev, where \( Q \) is number of qubits. This \( M \gg F \) limit is an important case in the electronic structure problem since it corresponds to studying a molecule at high precision by including many orbitals.

Qubit encodings related to the configuration-interaction matrix can asymptotically achieve the optimal scaling \([2]\) of qubit count in the \( M \gg F \) limit \([7–10]\) (referring to the “binary addressing code” in \([8, 9]\)), at the expense of operations whose cost scales at best linearly with \( M \). While these encodings are technically second-quantized because fermion antisymmetrization is enforced at the operator level, individual modes are not encoded in specific qubit registers, which leads to the higher operation cost. The best prior second-quantized encodings that do associate a specific qubit register to each mode obtain subleading improvements over \( Q = M \) \([8, 9]\).

In this paper, we show that it is possible to reduce qubit scaling to polylogarithmic in \( M \) in the \( M \gg F \) limit via a second-quantized encoding that does encode each mode in a specific subset of qubits. Because of this, the costs in two-qubit gates of our encoded fermionic operations are also polylogarithmic in \( M \). This is the first second-quantized fermion-to-qubit mapping whose cost in both qubits and operations is polylogarithmic in \( M \).

More specifically, for an integer parameter \( D \) called the “degree,” our encoding requires

\[
Q = M^{\frac{1-D}{2}} (2DF \log_2 M) + 1 + O(F \log^2 M)
\]

qubits, which yields

\[
Q = O(F^2 \log^4 M)
\]
when $D$ is chosen to be optimal in the $M \gg F$ limit. The cost in two-qubit gates (all controlled-phases) of an encoded fermionic operator is

$$O(D^2 F^2 \log^3 M)$$

for the degree-$D$ code, which becomes

$$O(F^2 \log^5 M)$$

for the optimal-degree code in the $M \gg F$ limit. For comparison, the cost of an oracle query in \cite{7} is $\Theta(M)$ (which is better than the cost in \cite{10}; the operation cost for the binary addressing code in \cite{8,9} is not analyzed.) Table \ref{tab:comparison} summarizes the comparison of our encoding to prior work.

This paper focuses on encodings of second-quantized fermionic systems, but first-quantized fermion-to-qubit mappings also exist. While some of these can achieve asymptotically better scalings than our encoding, they are only polynomially better, and they require operating within the antisymmetrized subspace as well as specific bases (such as the plane-wave basis; see \cite{12} for a review of such methods). Our second-quantized encoding avoids both of these constraints and demonstrates that second-quantized fermion-to-qubit mappings can be competitive with first-quantized simulation methods even in the limit of many modes.

### A. Preliminaries

We begin with a second-quantized particle-number conserving fermionic Hamiltonian $H$ acting on $M$ modes, i.e., a linear combination of products of creation and annihilation operators $\hat{a}_i^\dagger$ and $\hat{a}_i$. Although creation and annihilation operators are neither unitary nor Hermitian, the conjugate pairs

$$\hat{a}_i^\dagger + \hat{a}_i \text{ and } i(\hat{a}_i^\dagger - \hat{a}_i)$$

(i.e., Majorana operators) are both, and the Hamiltonian may be rewritten as a linear combination of products of these $\hat{a}_i^\dagger$. The Bravyi-Kitaev (BK) transformation \cite{5,6} maps fermionic operators and states to qubit operators and states, and has the property that conjugate pairs as in (7) are mapped to single Pauli operators that contain $O(\log M)$ nonidentity single qubit Pauli matrices (see \cite{6,eq. (39-40)}). Hence, under the BK mapping the Hamiltonian becomes a linear combination of Pauli operators:

$$H = \sum_{P \in P^\otimes M} h_P P,$$

where $P = \{I, X, Y, Z\}$ is the set of single-qubit Pauli matrices including the identity $I$, and the $h_P$ are real coefficients.

We want to study this Hamiltonian within the $F$-fermion subspace. In the BK mapping, each fermionic occupation number state is represented as a bitstring $b$ whose entries correspond to parities of subsets of the fermionic modes. We will refer to these as BK bitstrings. For a single-fermion state (i.e., an occupation number state in which a single mode is occupied), the corresponding BK bitstring contains at most $\lfloor \log M \rfloor$ 1s. The BK mapping is linear, so the BK bitstring corresponding to a multi-fermion state is the bitwise sum of the single-fermion BK bitstrings corresponding to occupied modes. Hence, a BK bitstring $b$ corresponding

\[
\begin{array}{|c|c|c|c|}
\hline
\text{Citation} & \text{Encoding} & \text{Qubits} & \text{Gates} \\
\hline
\text{Jordan-Wigner} \cite{4} & \text{Jordan-Wigner} & M & O(M) \\
\text{Bravyi-Kitaev} \cite{5,6} & \text{Bravyi-Kitaev} & M & O(\log M) \\
\text{Bravyi et al.} \cite{11} & \text{Z}_{2}\text{-symmetries} & M - O(1) & O(M) \\
\text{Bravyi et al.} \cite{11} & \text{LDPC} & M - \frac{M}{F} & O(M^2) \\
\text{Steudtner-Wehner} \cite{8,9} & \text{segment} & M - \frac{M}{F} & O(F^2) \\
\text{Babbushe et al.} \cite{7} & \text{Cl-matrix} & O(F \log M) & O(M) \\
\text{this work} & \text{degree-D} & O(M \frac{M}{F} DF \log M) & O(D^2 F^2 \log^3 M) \\
\text{this work} & \text{optimal-degree} & O(F^2 \log^4 M) & O(F^2 \log^5 M) \\
\hline
\end{array}
\]

\textbf{TABLE I. Comparison of this work to prior work on encoding second-quantized fermionic Hamiltonians in qubits.} “Gates” refers to the number of one- and two-qubit gates required to implement the encoding of a conjugate pair of fermionic creation and annihilation operators. The exception is the CI-matrix encoding in \cite{7}, where the number of operations listed is the cost of the sparse oracle in this sparsity-based approach. We refer to the codes presented in this work as degree-$D$ codes, for a positive integer $D$ that we can choose (subject to certain constraints) and that determines the properties of the code as shown. Choosing $D$ to optimize the qubits-to-modes ratio in the $M \gg F$ limit yields the optimal-degree code. For the “segment code” of \cite{8,9}, fermionic operations can be implemented using our method via quantum signal processing for a cost of $O(F^2)$, as described in Appendix C.
to an occupation number state of \( F \) fermions has Hamming weight at most \( F \lfloor \log_2 M \rfloor \), which we denote

\[
|b| \leq F \lfloor \log_2 M \rfloor \equiv G, \tag{9}
\]
i.e., \( b \) contains at most \( G = F \lfloor \log_2 M \rfloor \) 1s. Although the BK mapping is typically used to map a fermionic Hamiltonian to a qubit Hamiltonian, we will think of \( H \) in (8) as the unencoded Hamiltonian that will be the starting point for our encoding.

## II. ENCODING STATES

We will encode the Hamiltonian \( H \) in (8) in a qubit Hamiltonian that acts on \( Q < M \) qubits. The encoding \( \mathcal{E} \) will satisfy several properties:

1. \( \mathcal{E} \) maps fermionic occupation number states containing up to \( F \) fermions, i.e., BK bitstrings of Hamming weight up to \( G \), to qubit computational basis states.

2. \( \mathcal{E} \) is linear on bitwise addition \( \oplus \) of bitstrings (bitwise XOR), i.e.,

\[
\mathcal{E}(a \oplus b) = \mathcal{E}(a) \oplus \mathcal{E}(b) \tag{10}
\]

for two BK bitstrings \( a, b \).

3. The \( i \)th bit in \( b \) (\( b_i \), for any \( i \in [M] \)) is associated to some set \( S_i \) of qubits such that in the encoding of an up to \( F \)-fermion state, \( b_i = 1 \) if and only if more than half of the qubits in \( S_i \) are 1.

4. \( \mathcal{E} \) is invertible for fermionic occupation number states containing up to \( F \) fermions, i.e., BK bitstrings \( b \) with \( |b| \leq G \). (This follows from property 3.)

Since the occupation number states form a basis for the fermionic Hilbert space, properties 1, 2, and 4 above imply that the map \( \mathcal{E} \) extends to an invertible linear transformation sending the space of \( F \)-fermion wavefunctions into a subspace of the \( Q \)-qubit Hilbert space. We will call \( \mathcal{E}(b) \) the codeword for \( b \), where \( b \) is a fermionic occupation number state. The span of the codewords will be called the codespace, and not every qubit computational basis state must be a codeword, so the codespace is not necessarily the entire \( Q \)-qubit Hilbert space.

In Section III, we will use the third property above to construct efficient implementations of the encoded fermionic operators. The first two properties above imply that we can specify the encoding by specifying its action on BK bitstrings with Hamming weight one. We will refer to these as the elementary bitstrings. By linearity, if we specify the encodings of these, then the encoding of any higher-weight BK bitstring is the bitwise sum of the elementary bitstrings it is composed of. Hence, the fourth property (invertibility) will hold if and only if bitwise sums of up to \( G \) of the encoded elementary bitstrings are unique.

To guarantee that properties three and four above hold, the encoding we construct will satisfy the following: if \( \alpha = \mathcal{E}(a) \) and \( \beta = \mathcal{E}(b) \) are codewords encoding different elementary bitstrings \( a \) and \( b \), then

\[
\begin{align*}
\text{len}(\alpha) &= \text{len}(\beta) = Q, \\
|\alpha| &= |\beta| = L, \\
\alpha \cdot \beta &= \sum_{i=0}^{Q-1} \alpha_i \beta_i \leq D < \frac{L}{2G},
\end{align*}
\]

where \( D \) is some maximum allowed overlap of the codewords. If \( b \) is the elementary bitstring in which (only) bit \( b_i = 1 \), the \( L \) 1s in \( \mathcal{E}(b) \) are exactly the qubits in \( S_i \). Sets that satisfy (11) also satisfy properties three and four of \( \mathcal{E} \), above, which we prove as Lemma A.1 in Appendix A.

Having established the properties that \( \mathcal{E} \) must satisfy, we can now specify \( \mathcal{E} \) by constructing the elementary codewords, i.e., the encodings of the elementary bitstrings. For fixed \( G = F \lfloor \log_2 M \rfloor \), \( \mathcal{E} \) is parametrized by positive integers \( L \) and \( D \) satisfying (11). For a given \( D \), we will later want \( L \) to be as small as possible, so we will choose

\[
L = 2DG + 1. \tag{12}
\]

Let the range of \( \mathcal{E} \) be the computational basis states of \( Q = L'L \) qubits, which are partitioned into \( L \) blocks of \( L' \) qubits where \( L' \) is a prime number lower bounded by \( L \). In each block, one of the qubits will be 1 and the others will be 0, so \( L \) qubits in total are 1, i.e., the elementary codewords have Hamming weight \( L \), as required by (11). Each elementary codeword is thus equivalent to a vector of \( L \) numbers in \( \mathbb{Z}_{L'} \) (the integers modulo \( L' \)), where the \( x \)th number gives the location of the 1 in the \( x \)th block of qubits. Alternatively, we may represent the elementary codeword as a function \( y : \mathbb{Z}_L \rightarrow \mathbb{Z}_{L'} \), which maps the index \( x \) of a block to the position of the 1 in that block. Examples of this mapping are given in Fig. [1] and [2].

We want \( D \) to be an upper bound on the overlaps of the elementary codewords, as in (11). Since for any pair \( \alpha, \beta \) of elementary codewords, each contains a single 1 in each block of qubits and the corresponding functions \( y_\alpha \) and \( y_\beta \) give the locations of the 1s, this is equivalent to \( D \) being an upper bound on the number of intersections of \( y_\alpha \) and \( y_\beta \). Therefore, let \( y_\alpha \) and \( y_\beta \) be distinct degree-\( D \) polynomials
(functions) over \( \mathbb{Z}_{L'} \), with their domains restricted to \( \mathbb{Z}_L \subseteq \mathbb{Z}_{L'} \). In this case, their difference is also a polynomial of degree at most \( D \), so it can have at most \( D \) roots. Hence \( y_\alpha \) and \( y_\beta \) can intersect in at most \( D \) points, and thus the corresponding codewords can overlap in at most \( D \) bits, as desired. Note that technically, \( y_\alpha \) and \( y_\beta \) are polynomial functions (as opposed to formal algebraic polynomials), but here we refer to them as polynomials for simplicity; see Appendix \([D]\) for details and a review of the properties of polynomials over finite fields.

It follows that if each of our elementary codewords corresponds to a distinct degree-\( D \) polynomial over \( \mathbb{Z}_{L'} \) as described above, its overlap with any other elementary codeword is upper bounded by \( D \). There are \( (L')^{D+1} \) distinct degree-\( D \) polynomials over \( \mathbb{Z}_{L'} \), since each polynomial is uniquely specified by its coefficients, and each of the \( D + 1 \) coefficients of \( x^0, x^1, ..., x^D \) is one of the \( L' \) elements of \( \mathbb{Z}_{L'} \) (this relies on the fact that \( \mathbb{Z}_{L'} \) has prime order and that \( D < L' \); see Appendix \([D]\)). We encode one Bravyi-Kitaev bit in each of the corresponding codewords, and the number of modes is equal to the number of Bravyi-Kitaev bits, so we encode \( (L')^{D+1} \) modes in \( L' \) qubits. Hence as long as \( D \geq 2 \), or \( L' > L \) and \( D \geq 1 \), this encoding permits \( Q < M \). Also note that the \( D = 0 \) case reduces to the Bravyi-Kitaev encoding: by \([12]\), the elementary codewords have Hamming weight \( L = 1 \), so there is a single block of \( L' \) qubits, and the \( L' \) degree-0 polynomials (constants) simply give the possible locations of the single 1.

For generic values of \( L, L', M, \) and \( D \), we could partition our qubits into subsets of size \( L' \), and use each subset to encode \( (L')^{D+1} \) modes as described above: this would require

\[
Q = \left\lceil \frac{M}{(L')^{D+1}} \right\rceil L' L
\]

qubits. Thus for fixed \( D \) (and \( L \)), it is in fact best to choose \( L' \) to be the least prime such that

\[
(L')^{D+1} \geq M
\]

(provided \( L' \geq L \)). This is the minimum value of \( L' \) such that all of the modes are encoded in a single set of \( L' \) qubits, so choosing \( L' \) larger than this would be disadvantageous. This value of \( L' \) yields the number of qubits required to encode \( F \) fermions in \( M \) modes via the degree-\( D \) code: by \([12]\) and \([14]\),

\[
Q = L' L = M \frac{1}{\pi^{D+1}} (2DF \lceil \log_2 M \rceil + 1) + O \left( F \log^2 M \right)
\]

on average, since by the prime number theorem, the least prime greater than \( M \frac{1}{\pi^{D+1}} \) exceeds it by \( O \left( \log M \frac{1}{\pi^{D+1}} \right) = O \left( \frac{\log M}{D} \right) \) on average.

We can optimize the number of qubits required for given \( F \) and \( M \) in the \( M \gg F \) limit, which is the case where we expect the greatest savings in number of qubits. This is also an important case in many practical quantum algorithms; for example, for a molecular electronic structure problem, the \( M \gg F \) limit corresponds to simulating many orbitals for a
fixed molecule.

**Theorem 1.** In the $M \gg F$ limit, our code satisfies

$$Q = O\left(F^2 \log^4 M\right),$$

with $D$ satisfying $D = O(\log M)$.

The proof can be found in Appendix A.

Finally, as discussed above, $D = 1$ is the least degree for which our encoding can be advantageous over Jordan-Wigner and Bravyi-Kitaev. In this case, $L'/L = \Theta\left(\sqrt{MF} \log M\right)$, so our code is advantageous when $F = O\left(M^{1/2-\epsilon}\right)$ for $\epsilon > 0$. The exact point at which the transition occurs is discussed in Appendix B. For smaller $M$, we recommend using the “segment code” of [8,9] (see Table I), for which operations can be implemented efficiently using the construction in the proof of Theorem 2. This is discussed in Appendix [C]. The segment code becomes advantageous over Jordan-Wigner when $F < \frac{M}{2} - 1$ and reduces the number of required qubits to approximately $(1 - \frac{1}{F}) M$, so it bridges the gap to the large-$M$ regime where our encoding becomes preferable.

**III. ENCODING OPERATIONS**

In the Bravyi-Kitaev mapping, a conjugate pair of fermionic operators as in (7) is mapped to a Pauli operator with nonidentity action on

$$O(\log M) \quad \tag{17}$$

qubits, i.e., bits in the BK bitstring $b$ [5,6]. Up to a phase $\pm 1$ or $\pm i$, each such Pauli operator can be expressed as a product of $O(\log M)$ single-qubit Pauli operators $X$ and $Z$. Let us denote these as $X_i^{(BK)}$ and $Z_i^{(BK)}$, where $i$ indexes the bit $b_i$ they act upon; operators on the codespace will be written with no superscript.

If we can implement the encodings of $X_i^{(BK)}$ and $Z_i^{(BK)}$ as unitaries on the codespace, we can implement any term in the Hamiltonian [8] as a unitary operator. This means that we can implement the Hamiltonian as a linear combination of unitaries [13] and simulate time-evolution [13-19], or we can estimate the expectation value of each term in the Hamiltonian via Hadamard tests and implement a variational quantum eigensolver (VQE) that searches for the Hamiltonian’s ground state energy [20]. In order to implement VQE, we also need to construct fermion number preserving ansatz circuits. In Appendix A we will prove the following lemma:

**Lemma 1.** Provided we can implement the actions of $X_i^{(BK)}$ and $Z_i^{(BK)}$ on the codespace for any $i$, we can implement an encoded hop gate, which is a universal fermion number preserving operator [21], using $O(\log M)$ singly-controlled applications of $X_i^{(BK)}$ and $Z_i^{(BK)}$, $O(1)$ additional single-qubit gates, and one ancilla qubit.

This means that we can implement any desired fermion number preserving ansatz circuit.

Each bit $i$ in the BK bitstring is associated to some set $S_i$ containing the indices of the $L$ qubits that are 1 in the corresponding elementary codeword. Because our encoding is linear [10], $X_i^{(BK)}$ is encoded as

$$\mathcal{E}(X_i^{(BK)}) = \prod_{j \in S_i} X_j, \quad \tag{18}$$

i.e., bitflips on all bits that are 1 in the elementary codeword corresponding to $i$ (we abuse the notation $\mathcal{E}$ to denote the encoding of operators in this section).

To compute the encoding of $Z_i^{(BK)}$, we use the fact that the unencoded bit $b_i = 1$ if and only if more than half of the code qubits in $S_i$ are 1 (property 3 in the list in Section II). Any computational basis state $|q\rangle$ of the code qubits is an eigenstate of the operator $\sum_{j \in S_i} Z_j$, and by the previous sentence, the eigenvalue is negative if and only if $b_i = 1$. In other words, for integer $z_i$ defined by

$$\sum_{j \in S_i} Z_j|q\rangle = z_i|q\rangle, \quad \tag{19}$$

we obtain

$$\mathcal{E}(Z_i^{(BK)})|q\rangle = \begin{cases} |q\rangle & \text{if } z_i \geq 0, \\ -|q\rangle & \text{if } z_i < 0. \end{cases} \quad \tag{20}$$

Hence, we can implement the encoding of a term that is a product of $X_i^{(BK)}$ s and $Z_i^{(BK)}$ s if we can implement the operation given by (20) for any set $S_i$ of $L$ qubits. The following theorem shows that we can do this efficiently:

**Theorem 2.** The operation $\mathcal{E}(Z_i^{(BK)})$ defined by (20) can be implemented using

$$L(2L - 1) = 8D^2 F^2 \log^2 M + 6DF \log^2 M + 1 = O(D^2 F^2 \log^2 M) \quad \tag{21}$$

two-qubit operators, all of which are controlled phases, $O(L)$ additional single-qubit operations, and one ancilla qubit.
The proof of this theorem is in Appendix A and relies on a conjecture that we have checked directly out to 251001 qubits. It follows that the cost in two-qubit gates of implementing an encoded conjugate pair of fermionic operators is $O \left(D^2F^2 \log^3 M \right)$ where the $M \gg F$ limit is obtained by substituting $D = O(\log M)$, per Theorem 1.

Theorem 2 assumes arbitrary connectivity. A fixed qubit architecture requires additional qubit swaps. In Appendix A we prove as Lemma A.4 that the number of swaps required to implement $E \left(Z_{\phi}^{(BK)} \right)$ on a linear qubit architecture is $O(\Lambda L)$, which is still polylogarithmic in $M$. This therefore also holds on any architecture such as planar architecture that includes linear connectivity as a subgraph. In other encodings this is not necessarily true: for example, the gate cost for Bravyi-Kitaev becomes linear in local qubit architectures, rather than logarithmic.

### IV. CONCLUSION

In this paper, we presented the first second-quantized fermion-to-qubit mapping that uses polylogarithmically-many qubits and quantum gates in the number of fermionic modes, to simulate fermionic creation and annihilation operators. This is an exponential improvement in the dependence on number of modes compared to prior second-quantized encodings, for either qubits, operations, or both. Polylogarithmic dependence on the number of modes will permit simulation of molecules in the high-precision limit of large bases, as well as many-body problems such as the Hubbard model. However, the optimal scaling of qubit count is still better than that of our encoding by several factors of $\log M$. We foresee that further improvements for second-quantized encodings could be found that approach the optimal scaling, while still having operation costs polylogarithmic in the number of modes.

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Appendix A: Proofs

**Lemma A.1.** Let \( \mathcal{B} \) be a set of length-\( Q \), Hamming-weight-\( L \) bitstrings whose overlaps are upper-bounded by \( D \), i.e., \( \alpha \cdot \beta \leq D \) for any distinct \( \alpha, \beta \in \mathcal{B} \). Let \( \gamma \) be a bitwise sum of \( n \leq G \) elements in \( \mathcal{B} \), for any \( G \) such that
\[
L > 2DG.
\]
Then both of the following are true:

1. \( \alpha \) appears in the sum that defines \( \gamma \) if and only if
   \[
   \alpha \cdot \gamma = \sum_{i=0}^{Q-1} \alpha_i \gamma_i > \frac{L}{2}.
   \]

2. all sums of up to \( F \) elements in \( \mathcal{B} \) are unique.

Note: in Lemma A.1, \( \mathcal{B} \) is the set of elementary codewords, i.e., the image of \( \mathcal{E} \) acting on the set of Hamming-weight-one bitstrings (elementary bitstrings); see Section II for definitions.

**Proof.** Let \( \alpha, \beta^{(1)}, ..., \beta^{(n)} \in \mathcal{B} \) for \( n \leq G \). By assumption, \( \alpha \cdot \beta^{(j)} \leq D \) for all \( j \). Hence if
\[
\gamma = \beta^{(1)} \oplus \cdots \oplus \beta^{(n)}
\]
where \( \oplus \) denotes bitwise sum, then
\[
\alpha \cdot \gamma = \alpha \cdot (\beta^{(1)} \oplus \cdots \oplus \beta^{(n)}) \leq \sum_{j=1}^{n} \alpha \cdot \beta^{(j)} \leq Dn \leq DG
\]
by the triangle inequality. In other words, when \( \alpha \) is not included in the sum that defines \( \gamma \),
\[
\alpha \cdot \gamma \leq DG < L/2.
\]

However, if
\[
\gamma = \alpha \oplus \beta^{(1)} \oplus \cdots \oplus \beta^{(n-1)},
\]
then
\[
\alpha \cdot \gamma = \alpha \cdot (\alpha \oplus \beta^{(1)} \oplus \cdots \oplus \beta^{(n-1)})
\]
\[
\geq \alpha \cdot \alpha - \sum_{j=1}^{n-1} \alpha \cdot \beta^{(j)} \geq \alpha \cdot \alpha - \sum_{j=1}^{n-1} \alpha \cdot \beta^{(j)} = \alpha \cdot \gamma \geq L - (n - 1)D
\]
\[
\geq L - (G - 1)D
\]
by the reverse triangle inequality. In other words, when \( \alpha \) is included in the sum that defines \( \gamma \),
\[
\alpha \cdot \gamma \geq L - (G - 1)D > L/2.
\]

This completes the proof of claim 1 in the lemma statement.

Claim 2 in the lemma statement follows from this because claim 1 provides a method for determining whether \( \alpha \) is in a sum of up to \( G \) elements of \( \mathcal{B} \), for each \( \alpha \in \mathcal{B} \). Hence, given the sum, we can identify which elements of \( \mathcal{B} \) formed it, which would be impossible if not all such sums were unique.

**Theorem** [1] In the \( M \gg F \) limit, our code satisfies
\[
Q = O\left(F^2 \log^4 M\right),
\]
with \( D \) satisfying \( D = O(\log M) \).

**Proof.** For given \( D, M, \) and \( L = 2DF\lceil \log_2 M \rceil + 1 \), we encode the \( M \) modes in \( L' \) qubits, where \( L' \) is the least prime such that
\[
(L')^{D+1} \geq M \quad \text{and} \quad L' \geq L.
\]

Hence, for fixed \( D \) the total number of qubits required in the large-\( M \) limit is \([5]\), which we reproduce here for convenience:
\[
Q = M \frac{1}{\log M} (2DF\lceil \log_2 M \rceil + 1) + O(F \log^2 M),
\]
for which the corresponding \( L' \) is
\[
L' = M \frac{1}{\log M} + O\left(\frac{\log M}{D+1}\right),
\]
since \( L' \) is the least prime greater than or equal to \( M \frac{1}{\log M} \), and by the prime number theorem, the least prime greater than \( M \frac{1}{\log M} \) exceeds it by \( O\left(\frac{\log M}{\log M}\right) \) on average.

However, in order to find the optimal value of \( D \), we want to allow \( D \) to be a function of \( M \), in which case the constraint \( L' \geq L \) means that we should modify [1] to
\[
L' \approx \max \left\{ M \frac{1}{\log M}, 2DF\lceil \log_2 M \rceil + 1 \right\},
\]
and [11] correspondingly becomes
\[
Q \approx \max \left\{ M \frac{1}{\log M}, 2DF\lceil \log_2 M \rceil + 1 \right\} (2DF\lceil \log_2 M \rceil),
\]
where \( \approx \) indicates that subleading terms are suppressed. Therefore, in the large-\( M \) limit the best
choice of \( D \) is whatever value minimizes (A14). Equivalently, we want to minimize the cost function

\[
\max \left\{ D M \frac{\pi}{\sqrt{2}}, 2D^2 F \lceil \log_2 M \rceil + 1 \right\} \quad \text{(A15)}
\]

over \( D \).

First, take a derivative of \( D M \frac{\pi}{\sqrt{2}} \) (the first argument of the max above) with respect to \( D \), set equal to zero, and solve, which results in

\[
D = D^* = \frac{\log(M) - 2 \pm \sqrt{\log^2(M) - 4 \log(M)}}{2} \quad \text{(A16)}
\]

Note that when we use \( \log \) without an explicit base, we mean natural logarithm. Both solutions are positive, and one can verify that the smaller value of \( D^* \) corresponds to a local maximum of \( D M \frac{\pi}{\sqrt{2}} \) and the larger corresponds to a local minimum. Hence, \( D M \frac{\pi}{\sqrt{2}} \) decreases monotonically between the two values of \( D^* \) given in (A16).

However, it turns out that the minimum of \( D M \frac{\pi}{\sqrt{2}} \) (at the larger value of \( D^* \)) is smaller than the second argument of the max in (A15) evaluated at the same point. To see this, note that for \( D^{**} \) defined by

\[
D^{**} = \frac{1}{2} \log(M) - 1, \quad \text{(A17)}
\]

\( D^{**} \) is smaller than the larger value of \( D^* \) in (A16). Evaluating each argument of the max in (A15) at \( D^{**} \) yields

\[
D^{**} M \frac{\pi}{\sqrt{2}} = D^{**} e^2 = \Theta(\log M), \\
2(D^{**})^2 F \lceil \log_2 M \rceil + 1 = \Theta(F \log^3 M), \quad \text{(A18)}
\]

so since \( 2D^2 F \lceil \log_2 M \rceil + 1 \) grows with \( D \) and \( D M \frac{\pi}{\sqrt{2}} \) decreases between \( D^* \) and its actual minimum at \( D^* > D^{**} \), the two arguments of the max in (A15) cross between the two values of \( D^* \). Therefore, the minimum of (A15) is the point where the two arguments of the max are equal, which gives

\[
M \frac{\pi}{\sqrt{2}} = 2DF \lceil \log_2 M \rceil + 1. \quad \text{(A19)}
\]

At this point, (A11) becomes

\[
Q = (2DF \lceil \log_2 M \rceil + 1)^2 + O(F \log^2 M). \quad \text{(A20)}
\]

We can evaluate \( D \) by taking the log of (A19) and rearranging to obtain

\[
D = \frac{\log M}{\log (2DF \lceil \log_2 M \rceil + 1)} - 1. \quad \text{(A21)}
\]

We could apply this formula recursively to obtain arbitrarily good approximations of \( D \), but for the purpose of this proof, we instead simply observe that it is upper bounded by

\[
D \leq \log M, \quad \text{(A22)}
\]

which when inserted in (A20) yields our final expression,

\[
Q = (2F \lceil \log_2 M \rceil \log M + 1)^2 + O(F \log^2 M) = O \left( F^2 \log^4 M \right). \quad \text{(A23)}
\]

\[\square\]

**Lemma 1.** Provided we can implement the actions of \( X_i^{(BK)} \) and \( Z_i^{(BK)} \) on the codespace for any \( i \), we can implement an encoded hop gate, which is a universal fermion number preserving operator \( \hat{O} \), using \( O(\log M) \) singly-controlled applications of \( X_i^{(BK)} \) and \( Z_i^{(BK)} \), \( O(1) \) additional single-qubit gates, and one ancilla qubit.\n
**Proof.** The hop gate is a gate that acts on two fermionic modes as

\[
h(\varphi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\
0 & \cos \varphi & -\sin \varphi & 0 \\
0 & \sin \varphi & \cos \varphi & 0 \\
0 & 0 & 0 & -1 \end{pmatrix}, \quad \text{(A24)}
\]

which we can decompose as

\[
h(\varphi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\
0 & \cos \varphi & -\sin \varphi & 0 \\
0 & \sin \varphi & \cos \varphi & 0 \\
0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & -1 \end{pmatrix}. \quad \text{(A25)}
\]

In other words, we can think of the hop gate as first applying a controlled phase, and then rotating occupation between the two modes.

It will be useful to first decompose the hop gate into fermionic Pauli operators \( X^{(i)}, Y^{(i)}, \) and \( Z^{(i)} \), meaning Pauli operators applied directly as unitaries acting on fermionic modes. In terms of these, the controlled phase in (A25) can be implemented as follows. Introduce an ancilla qubit initially in state \( \lvert 0 \rangle_h \), distinct from the ancilla \( \lvert \gamma \rangle_a \) used for quantum signal processing as described in Section III. Let \( \lvert z \rangle \) denote an encoded occupation number state, i.e., an eigenstate of \( Z^{(i)} \) acting on every fermionic mode. Such states are a basis for the fermionic Hilbert space, so if we can implement the controlled phase for an arbitrary \( \lvert z \rangle \), then the same implementation will apply it to an arbitrary fermionic state.
If the two modes to which the controlled phase is to be applied are \(i\) and \(j\), implement
\[
|0\rangle_b \otimes |z\rangle \xrightarrow{H \otimes I} \frac{1}{\sqrt{2}}\left(|0\rangle_b + |1\rangle_b\right) \otimes |z\rangle
\]
\[
\xrightarrow{\text{ctrl-}Z_i^{(f)}} \frac{1}{\sqrt{2}}\left(|0\rangle_b \otimes |z\rangle + |1\rangle_b \otimes Z_i^{(f)}|z\rangle\right)
\]
\[
\xrightarrow{H \otimes I} \begin{cases} 
|0\rangle_b \otimes |z\rangle & \text{if } Z_i^{(f)}|z\rangle = |z\rangle, \\
|1\rangle_b \otimes |z\rangle & \text{if } Z_i^{(f)}|z\rangle = -|z\rangle
\end{cases}
\]
\[
\xrightarrow{\text{ctrl-}Z_i^{(f)}} \begin{cases} 
|0\rangle_b \otimes |z\rangle & \text{if } Z_i^{(f)}|z\rangle = |z\rangle, \\
|1\rangle_b \otimes |\zeta z\rangle & \text{if } Z_i^{(f)}|z\rangle = -|z\rangle
\end{cases}
\]
\[
\text{(A26)}
\]
where \(\zeta = -1\) if \(Z_i^{(f)}|z\rangle = -|z\rangle\) and \(Z_i^{(f)}|z\rangle = |z\rangle\), and \(\zeta = 1\) otherwise, i.e., \(\zeta\) is the desired phase due to the controlled phase operation. All that remains is to uncompute the ancilla which we can do by reversing the first three operations above. Thus we implement the controlled phase via three controlled applications of \(Z_i^{(f)}\) operators, together with four single-quet gates.

Next, we implement the rotation in (A25), which may be rewritten as
\[
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \cos \varphi & -\sin \varphi & 0 \\
0 & \sin \varphi & \cos \varphi & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
= e^{i\varphi(X^{(f)}Y^{(f)} - Y^{(f)}X^{(f)})/2}
= e^{i\varphi X^{(f)}Y^{(f)}} e^{-i\varphi Y^{(f)}X^{(f)}}
= e^{i\varphi X^{(f)}Y^{(f)}} e^{-i\varphi Y^{(f)}X^{(f)}}
\cdot e^{i\varphi Y^{(f)}X^{(f)}} e^{-i\varphi X^{(f)}Y^{(f)}} \cdot e^{i\varphi X^{(f)}Y^{(f)}} e^{-i\varphi Y^{(f)}X^{(f)}}
\]
\[
\text{(A27)}
\]
where tensor product symbols are suppressed, e.g., \(X^{(f)}X^{(f)} = X^{(f)} \otimes X^{(f)}\). Let \(|x\rangle\) denote a common eigenstate of the \(X^{(f)}\)'s acting on every mode. As above, such states form a basis for the fermionic Hilbert space, so operations that have the correct action on an arbitrary \(|x\rangle\) will have the correct action on arbitrary fermionic states. Perform the following operations:
\[
|0\rangle_b \otimes |x\rangle \xrightarrow{H \otimes I} \frac{1}{\sqrt{2}}\left(|0\rangle_b + |1\rangle_b\right) \otimes |x\rangle
\]
\[
\xrightarrow{\text{ctrl-}X_i^{(f)}X_j^{(f)}} \frac{1}{\sqrt{2}}\left(|0\rangle_b \otimes |x\rangle + |1\rangle_b \otimes (-1)^x|x\rangle\right)
\]
\[
= \frac{1}{\sqrt{2}}\left(|0\rangle_b + (-1)^x|1\rangle_b\right) \otimes |x\rangle,
\]
\[
\text{(A28)}
\]
where \((-1)^x\) for \(x \in \{0, 1\}\) is the eigenvalue of \(X_i^{(f)}X_j^{(f)}\) for the state \(|x\rangle\). Continuing from where we left off...
\[
\cdot \frac{1}{\sqrt{2}}\left(|0\rangle_b + (-1)^x|1\rangle_b\right) \otimes |x\rangle
\]
\[
\xrightarrow{H \otimes I} \begin{cases} 
|0\rangle_b \otimes |x\rangle & \text{if } \chi = 0, \\
|1\rangle_b \otimes |x\rangle & \text{if } \chi = 1
\end{cases}
\]
\[
R_{-2\phi} \xrightarrow{\text{ctrl-}X_i^{(f)}X_j^{(f)}} \frac{e^{2i\phi} |1\rangle_b \otimes |x\rangle}{\sqrt{2}}
\]
\[
\text{(A29)}
\]
Thus, we have implemented the desired operation up to an overall phase.

The remaining operations in (A27) are rotations around single \(Z_i^{(f)}\) operators. In particular, we want to implement \(e^{i\pi Z_i^{(f)}/4}\). This can be done using the same method as for the \(X_i^{(f)}X_j^{(f)}\) rotations, above, with the following changes:

1. replace the initial state \(|x\rangle\) with an occupation number state \(|z\rangle\);

2. replace the rotation angle \(\phi\) in (A29) with \(\pi/4\);

3. replace the controlled-\(X_i^{(f)}X_j^{(f)}\) operations in (A28) and (A29) with controlled-\(Z_i^{(f)}\) operations.

Hence, we can implement the entire hop gate using \(O(1)\) singly-controlled applications of \(X_i^{(f)}X_j^{(f)}\) and \(Z_i^{(f)}\), as well as \(O(1)\) single-quet gates. Under the Bravyi-Kitaev mapping, each \(X_i^{(f)}\) becomes a product of \(O(\log M)\) \(X^{(BK)}\) operators, so \(X_i^{(f)}X_j^{(f)}\) also becomes a product of \(O(\log M)\) \(X^{(BK)}\) operators. Similarly, each \(Z_i^{(f)}\) becomes a product of \(O(\log M)\) \(Z^{(BK)}\) operators. This completes the construction.

\[\square\]

**Theorem 2.** The operation \(\mathcal{E}(Z_i^{(BK)})\) defined by (20) can be implemented using
\[
L(2L - 1) = 8D^2F^2[\log_2 M]^2 + 6DF[\log_2 M] + 1 = O(D^2F^2 \log_2 M)
\]
\[\text{(A30)}\]
two-qubit operators, all of which are controlled phases, \( O(L) \) additional single-qubit operations, and one ancilla qubit.

**Proof.** We want to implement the encoded parity operator \( E \left( Z^{(BK)}_i \right) \) whose action on qubits is given by (20), which we reproduce as (A32) below for convenience: for integer \( z_i \) defined by

\[
\sum_{j \in S_i} Z_j |q\rangle = z_i |q\rangle,
\]

we obtain

\[
E \left( Z^{(BK)}_i \right) |q\rangle = \begin{cases} |q\rangle & \text{if } z_i \geq 0, \\ -|q\rangle & \text{if } z_i < 0. \end{cases}
\]

(A32)

To do this, we can use quantum signal processing [16, 18, 22]. First, define a Hamiltonian

\[
\mathcal{H}_i \equiv \cos \mathcal{G}_i \equiv \cos \left( \frac{\pi}{2} \left( 1 - \frac{1}{L} \sum_{j \in S_i} Z_j \right) \right),
\]

(A33)

for

\[
\mathcal{G}_i \equiv \frac{\pi}{2} \left( 1 - \frac{1}{L} \sum_{j \in S_i} Z_j \right).
\]

(A34)

By definition, \( \mathcal{H}_i \) has eigenvalues

\[
\{ \cos \left( \frac{m \pi}{L} \right) | m = 0, 1, 2, ..., L \}. \quad (A35)
\]

Any computational basis state \( |q\rangle \) is an eigenvector of \( \mathcal{H}_i \), so if we let

\[
\mathcal{H}_i |q\rangle = \lambda_q |q\rangle,
\]

(A36)

then by the definition of \( \mathcal{H}_i \),

\[
E \left( Z^{(BK)}_i \right) |q\rangle = \begin{cases} \lambda_q |q\rangle & \text{if } \lambda_q \geq 0, \\ -\lambda_q |q\rangle & \text{if } \lambda_q < 0. \end{cases}
\]

(A37)

Next, we define a block-encoding \( W_\phi \) of \( \mathcal{H}_i \) \( (W_\phi \) is the **phased iterate** of [18]):

\[
W_\phi \equiv \begin{pmatrix} \mathcal{H}_i & -ie^{-i\phi} \sqrt{1 - \mathcal{H}_i^2} \\ -ie^{i\phi} \sqrt{1 - \mathcal{H}_i^2} & \mathcal{H}_i \end{pmatrix},
\]

(A38)

which acts on the codespace and one additional ancilla qubit whose states \( |\phi\rangle \) define the blocks in (A38). Using quantum signal processing, via \( N \) queries to \( W_\phi \) we can implement

\[
\begin{pmatrix} A(\mathcal{H}_i) \cdot \\ . \end{pmatrix}
\]

(A39)

for any degree-\( N \) real polynomial \( A \) such that

\[
\begin{align*}
|A(\lambda)| &\leq 1 \quad \forall \lambda \in [-1, 1], \\
|A(\lambda)| &\geq 1 \quad \forall \lambda \not\in (-1, 1),
\end{align*}
\]

(A40)

by [18, Lemma 12] (for us, \( N \) will always be odd, so the final condition in [18, Lemma 12] is irrelevant). Hence, we just want to find a polynomial \( A \) that satisfies the above properties and passes through the points

\[
\{ \cos \left( \frac{m \pi}{L} \right), 1 \} \mid m = 0, 1, 2, ..., \left\lfloor \frac{L}{2} \right\rfloor \}
\]

\[
\cup \{ \cos \left( \frac{m \pi}{L} \right), -1 \} \mid m = \left\lfloor \frac{L}{2} \right\rfloor + 1, ..., L, \}
\]

(A41)

since this will give

\[
E \left( Z^{(BK)}_i \right) |q\rangle = A(\mathcal{H}_i) |q\rangle
\]

(A42)

for any computational basis state \( |q\rangle \) by (A37), and thus for all qubit states, including the codespace. Note that (A41) finally justifies why we require \( L \) to be odd: this guarantees that the numbers of points with value \(+1\) and points with value \(-1\) are the same.

We can find such a polynomial by Hermite interpolation of the points (A41) together with the constraints that the first derivative be zero at each non-edge point (i.e., all points except for \((1,1)\) and \((-1,-1)\), the leftmost and rightmost points). See Fig. 3 for an example, and see Appendix E for a review of Hermite interpolation. We can prove (see Lemma A.3 in Appendix A) that this polynomial satisfies the constraints (A40) except for

\[
\begin{align*}
A(\lambda) &\geq -1 \quad \forall \lambda \in [0, 1], \\
A(\lambda) &\leq 1 \quad \forall \lambda \in [-1, 0].
\end{align*}
\]

(A43)
Confirming these for general $L$ proved difficult because of the high degree of the polynomial. However, we checked (A43) for all odd $L$ up to 501, and found that for all such $L$, the least local minimum in the $\lambda > 0$ region is greater than 0.8 and increases slightly with $L$. Correspondingly, the greatest local maximum in the $\lambda < 0$ region is less than −0.8 and decreases slightly with $L$. Since $L = 501$ corresponds to at least $L^2 = 251001$ qubits, we consider this result to be adequate for near-future applications, and we conjecture that (A43) holds for all odd $L$.

Since $E(Z_i^{(BK)})$ is unitary and its block-encoding via $A(H_i)$ as in (A39) must also be unitary, the resulting block encoding must be

$$
(A(H_i) \ 0) = E(Z_i^{(BK)}) \ 0,
$$

i.e., there is no leakage out of the upper left block. Hence if we start with a state $|0\rangle_a \otimes |q\rangle$, the quantum signal processing algorithm will map this to

$$
|0\rangle_a \otimes E(Z_i^{(BK)}) |q\rangle
$$

as desired. Hermite interpolation of $L+1$ points and $L-1$ first derivatives results in a degree

$$
N = 2L - 1
$$

polynomial, so this algorithm requires $2L-1$ queries to $W_\phi$.

It remains to show how to implement $W_\phi$. Lemma A.2 below, shows how this can be done. Hence, implementing $W_\phi$ requires $L$ two-qubit operations, the controlled-$Z$-rotations in (A50). Since the algorithm requires $2L-1$ queries to $W_\phi$, the total number of two-qubit operations required to implement a $Z_i^{(BK)}$, an encoded fermionic parity operation, is

$$
L(2L-1) = 8D^2 F^2 |\log_2 M|^2 + 6DF |\log_2 M| + 1.
$$

(A48)

The number of additional single-qubit operations required is only linear in $L$, by (A50).

**Lemma A.2.** For

$$
R_\phi \equiv \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}_a \otimes 1,
$$

(A49)

$W_\phi$ is given by the following sequence of operations:

$$
W_\phi = R_\phi (H \otimes 1) R_\pi \left( \prod_{i \in S_m} \text{ctrl-} e^{-i \pi Z_i} \right) (H \otimes 1) R_\pi^\dagger,
$$

(A50)

where $H$ is the Hadamard gate, $Z_i$ is a single-qubit Pauli-$Z$ acting on computational qubit $i$, and the controls are on the ancilla qubit.

**Proof.** The space that $W_\phi$ acts upon is the tensor product of a single ancilla $|\gamma\rangle_a$ and the computational space (with computational basis states $|q\rangle$) that we want $Z_i^{(f)}$ to act upon. We implement $W_\phi$ as follows, for $H_i$ and $G_i$ defined by (A33) and (A34), respectively:

$$
\begin{align*}
\left( \begin{array}{c} |0\rangle_a \\
|1\rangle_a 
\end{array} \right) \otimes |x\rangle & \xrightarrow{H \otimes 1} \frac{1}{\sqrt{2}} \left( |0\rangle \pm |1\rangle \right) \otimes e^{2ig_i} |x\rangle \\
& \xrightarrow{\text{ctrl-phase}} \frac{1}{\sqrt{2}} \left( |0\rangle \otimes |x\rangle \pm |1\rangle \otimes e^{2ig_i} |x\rangle \right) \\
& \xrightarrow{H \otimes 1} \frac{1}{2} \left( |0\rangle + |1\rangle \right) \otimes e^{2ig_i} |x\rangle \\
& \xrightarrow{\text{Hermite}} \left( \begin{array}{c} \cos G_i \\
- i \sin G_i \\
\end{array} \right) \left( \begin{array}{c} |0\rangle_a \\
|1\rangle_a 
\end{array} \right) \otimes |x\rangle \\
& \xrightarrow{\text{Hermite}} \left( \begin{array}{c} \frac{1}{2} \sqrt{1 - H_i^2} \\
- i \sqrt{1 - H_i^2} \\
\end{array} \right) \left( \begin{array}{c} |0\rangle_a \\
|1\rangle_a 
\end{array} \right) \otimes |x\rangle,
\end{align*}
$$

(A51)

where the upper (lower) entries in the vector expressions correspond to the upper (lower) values of the $\pm$s and $\mp$s. Hence

$$
W_{\phi=0} = (H \otimes 1) (\text{ctrl-} e^{2ig_i}) (H \otimes 1).
$$

(A52)

To obtain $W_{\phi}$ for $\phi \neq 0$, we conjugate this by the phases on the ancilla qubit [18], denoted by $R_\phi$ as defined in (A49):

$$
W_\phi = R_\phi W_0 R_\phi^\dagger = R_\phi (H \otimes 1)(\text{ctrl-} e^{2ig_i})(H \otimes 1) R_\phi^\dagger.
$$

(A53)

Finally, since $G_i$ is defined by (A34),

$$
e^{2ig_i} = \exp \left( i \pi \left( 1 - \frac{1}{L} \sum_{j \in S_i} Z_j \right) \right)
$$

(A54)

$$
= - \exp \left( - i \pi \frac{1}{L} \sum_{j \in S_i} Z_j \right)
$$

(A54)

$$
= \prod_{j \in S_i} e^{-i \pi Z_j/L},
$$

(A54)

so

$$
\text{ctrl-} e^{2ig_i} = R_\phi \prod_{j \in S_i} \text{ctrl-} e^{-i \pi Z_j/L},
$$

(A55)

i.e., $\text{ctrl-} e^{2ig_i}$ decomposes into a product of single-qubit phases controlled by the ancilla qubit. Thus
our final decomposition of $W_\phi$ is

$$W_\phi = R_\phi(H \otimes 1)R_\pi \left( \prod_{j \in S_i} \text{ctrl} e^{-i\pi Z_j/L} \right) (H \otimes 1)R_\phi^\dagger. \quad (A56)$$

**Lemma A.3.** For odd $L$, the polynomial $A$ obtained by Hermite interpolation of the points \([A41]\), together with the constraints that its first derivative be zero at all non-edge points, satisfies:

$$\begin{align*}
A(\lambda) &\leq 1 \quad \forall \lambda \in [0, 1], \\
A(\lambda) &\geq -1 \quad \forall \lambda \in [-1, 0], \\
|A(\lambda)| &\geq 1 \quad \forall \lambda \notin (-1, 1).
\end{align*} \quad (A57)$$

The $x$-coordinates of the non-edge points are

$$\{ \cos \left( \frac{m\pi}{L} \right) \mid m = 1, 2, \ldots, L - 2, L - 1 \}. \quad (A58)$$

**Proof.** By definition, $A$ is the least-degree polynomial that satisfies the given constraints, which implies that it has degree $2L - 1$ because there are $2L$ constraints. Hence, its derivative $A'$ has degree $2L - 2$, so $A$ has at most $2L - 2$ local extrema. By construction, one extremum is located at each non-edge point, of which there are $L - 1$. The remaining $L - 1$ extrema must therefore be located between all pairs of adjacent points for which the values of the polynomial are the same (i.e., all adjacent pairs except for the middle pair), since there are $L - 1$ such pairs. This follows because for any pair of adjacent points, the polynomial has zero slope at at least one of the points, and it cannot be a straight line between the points, so in order to pass through the other point it must have an extremum between the points. For a visual aid, see Fig. [4]. Therefore, all extrema of the polynomial are either located at interpolated points, or between interpolated points with the same values.

Hence, there is no extremum between the middle pair of points

$$\left( \cos \left( \frac{\pi}{L} \left[ \frac{L}{2} \right] \right), -1 \right) \quad \text{and} \quad \left( \cos \left( \frac{\pi}{L} \left[ \frac{L}{2} \right] \right), 1 \right), \quad (A59)$$

where the values switch from negative to positive. This implies that the slope of the polynomial must be positive between these points, i.e., it must approach the point $p^+ = \left( \cos \left( \frac{\pi}{L} \left[ \frac{L}{2} \right] \right), 1 \right)$ from below, and the point $p^- = \left( \cos \left( \frac{\pi}{L} \left[ \frac{L}{2} \right] \right), -1 \right)$ from above.

We established above that the derivative $A'$ has its $2L - 2$ roots at each interpolation point as well as between all interpolation points with the same values. This means that $A'$ must have extrema between each of its roots, which accounts for $2L - 3$ extrema. However, since these correspond to roots of the second-derivative $A''$, which has degree $2L - 3$, they must account for all of its roots, i.e., $A$ has zero curvature only between its extrema. Together with the fact that $p^+$ is an extremum of $A$ and $A$ approaches $p^+$ from below, this implies that $A$ must have negative curvature at $p^+$. Hence, $A$'s next extremum to the right of $p^+$ must be below $p^+$, $A$ must approach the next interpolation point to the right of $p^+$ from below, and so forth. This means that the first line in (A57) holds with equality only at the interpolation points. A similar argument implies that the second line in (A57) holds with equality only at the interpolation points.

Also, the above argument implies that $A$ must approach the rightmost point $(1, 1)$ from below. We also established that $A$ cannot have an extremum either at or to the right of $(1, 1)$, which means that $A(\lambda)$ must continue to grow for $\lambda \geq 1$, i.e., $A(\lambda) \geq 1$ for $\lambda \geq 1$. Similarly, we find that $A(\lambda) \leq -1$ for $\lambda \leq -1$. This proves the third line in (A57).

**Lemma A.4.** On a linear qubit architecture, where two-qubit operations can only be performed on adjacent qubits in the line, the number of qubit swaps required to implement $Z_i^{(BK)}$ as defined by (20) is $O(QL)$, where $Q$ is the number of qubits and $L$ is given by (12).

**Proof.** As shown in the proof of Theorem 2, $Z_i^{(BK)}$ is implemented via $2L - 1$ applications of the quantum signal processing iterate $W_\phi$. $W_\phi$ is implemented as in (A50), so the only two-qubit operations in the implementation of $Z_i^{(BK)}$ are the controlled phases
in (A50):\
\[
\prod_{j \in S_i} \text{ctrl-} e^{-i\pi Z_j/L}.
\] (A60)

These \(L\) controlled phases are all controlled on the same qubit, the quantum signal processing ancilla \(|\psi\rangle_s\).

Hence, on a line of qubits, we can successively swap this control qubit along the line so that it is adjacent to each qubit it needs to control, which are the qubits in \(S_i\) as in (A60). Since the controlled phases in (A60) all commute, the order in which they are applied is irrelevant. Therefore, given any initial location of the control qubit in the line, we can classically choose a path whose length is upper bounded by \(3Q/2\) that brings the control qubit adjacent to each qubit in \(S_i\). The worst case is when the control qubit is initially in the center of the line, and \(S_i\) contains the qubits at both ends of the line, in which case the shortest path is to first swap the control qubit to the end of the line it is closer to, and then swap it back along the whole line. Since this path brings the control qubit adjacent to all other qubits (not just those in \(S_i\)), there can be no worse case.

Therefore, each implementation of the sequence of controlled phases and hence each implementation of \(W_\phi\) requires at most \(3Q/2\) swaps. Since \(Z_i^{BK}\) requires \(2L - 1\) applications of \(W_\phi\), it requires
\[
\frac{3Q}{2}(2L - 1) = O(QL)
\] (A61)
swaps.

\[\square\]

Appendix B: Threshold for outperforming Jordan-Wigner and Bravyi-Kitaev

As discussed in the main text, the minimum number of modes for which our encoding is advantageous over Jordan-Wigner and Bravyi-Kitaev occurs when \(D = 1\). In this case, \(L = 2G + 1\) for \(G = F\lceil\log_2 M\rceil\), so for
\[
L' = \text{NextPrime}(2G + 1)
\] (B1)
the least prime greater than \(2G + 1\), the number \((L')^2\) of modes we can encode is greater than the number \(L'/L\) of qubits. This means that for
\[
L'L = (2G + 1)\text{NextPrime}(2G + 1)
< M
\] (B2)
\[
\leq (L')^2 = (\text{NextPrime}(2G + 1))^2
\]
our encoding is advantageous over Jordan-Wigner.

However, depending on the gaps between primes greater \(\text{NextPrime}(2G + 1)\), there may be one or more subsequent ranges of \(M\) in which the encoding reduces to Jordan-Wigner. Let
\[
\text{NextPrime}^k(2G + 1)
\] (B3)
de note the \(k\)th prime greater than \(2G + 1\). Then if for any \(k = 1, 2, ...,\)
\[
(\text{NextPrime}^k(2G + 1))^2
< (2G + 1)\text{NextPrime}^{k+1}(2G + 1),
\] (B4)
our encoding will reduce to Jordan-Wigner for any values of \(M\) contained in
\[
\left((\text{NextPrime}^k(2G + 1))^2, (2G + 1)\text{NextPrime}^{k+1}(2G + 1)\right],
\] (B5)
since \(M\) is larger than
\[
(\text{NextPrime}^k(2G + 1))^2
\] (B6)
the number of modes that can be encoded in
\[
(2G + 1)\text{NextPrime}^k(2G + 1)
\] (B7)
qubits, but smaller than the number of qubits
\[
(2G + 1)\text{NextPrime}^{k+1}(2G + 1)
\] (B8)
required for the next code size. However, since the gaps between primes are on average logarithmic in the sizes of the primes, for all but at most a few small values of \(k\), (B4) will not hold and thus the corresponding ranges will be empty, so our encoding will be advantageous. For \(L = 2G + 1\) up to 501 (corresponding to at least \(L^2 = 251001\) qubits), we directly checked the maximum values of \(k\) for which (B4) holds, and found that in this range \(k\) did not exceed four.

Appendix C: Application of quantum signal processing construction of fermion operators to segment code of \([8, 9]\)

The construction in Section III allows us to implement \(Z_i^{BK}\) as given by (20). In other words, given some set of \(L\) qubits for odd \(L\), we can implement a \(−1\) phase controlled on more than half of the qubits being in state \(|1\rangle\); i.e., on the Hamming weight of a computational basis state of the qubits being greater than \(L/2\). This requires \(O(L^2)\) one- and two-qubit gates, as in (21).

This operation is exactly that required to implement the “binary switch” used to implement the
“segment code” of [8,9]. The remainder of the segment code is linear, so the corresponding encoded operations are Pauli operators. Our L corresponds to \( n \) in [8,9], and in their code \( G = F[\log_2 M] \) is replaced by \( F \) (which is \( K \) in their notation). Since we require \( L \) to be odd, we set

\[
L = n = 2K + 1 = 2F + 1
\]

(C1)

instead of \( n = 2K \) as in [8,9] (i.e., we just use one extra qubit per segment).

Hence, one can implement encoded fermionic operators for the segment code using \( O(L^2) = O(F^2) \) one- and two-qubit operations, and the encoding maps each segment of \( L + 1 \) fermionic modes to \( L \) qubits. Therefore, the number of qubits required is

\[
Q = \left\lfloor \frac{M}{L+1} \right\rfloor L + \left( M - \left\lfloor \frac{M}{L+1} \right\rfloor (L+1) \right) < \frac{M}{L+1} L + L = \left( 1 - \frac{1}{L+1} + \frac{L}{M} \right) M.
\]

(C2)

For \( M \gg F \gg 1 \), this is approximately

\[
Q \approx \left( 1 - \frac{1}{2F} \right) M = \left( 1 - \frac{1}{2K} \right) M,
\]

(C3)

which is the value quoted from [8,9]. As noted in the main text, since this encoding begins to be advantageous over Jordan-Wigner as soon as \( M \geq L + 1 = 2F + 2 \), while our encoding does not become advantageous until \( M = \Omega(F^2) \) we recommend using the segment code to bridge this gap for in the small-\( M \) regime.

Appendix D: Polynomials over finite fields

Let \( \mathbb{Z}_n \) denote the ring of integers modulo \( n \), i.e.,

\[
\mathbb{Z}_n = \{0, 1, 2, ..., n-1\}
\]

(D1)

and addition and multiplication are carried out modulo \( n \). When \( n = L' \) for prime \( L' \), \( \mathbb{Z}_{L'} \) is a field as well as a ring, which roughly means that it also possesses a division operation that satisfies the same properties as the usual division over real or rational numbers. Furthermore, it is a field of characteristic \( L' \), which means that \( L' \) is the least number such that

\[
x + x + \cdots + x = 0 \quad \forall x \in \mathbb{Z}_{L'},
\]

(D2)

\( L' \) copies

which implies that there is no \( y \in \mathbb{Z}_{L'} \) such that \( yx = 0 \) for all \( x \in \mathbb{Z}_{L'} \). See [23] for a thorough introduction to rings and fields. All arithmetic operations in this appendix are assumed to be modulo the order of the ring or field presently under consideration.

For any \( D \in \mathbb{Z}_{L'} \), a degree-\( D \) polynomial over the finite field \( \mathbb{Z}_{L'} \) is a formal expression

\[
c_0 x^0 + c_1 x^1 + \cdots + c_D x^D,
\]

(D3)

where the \( c_i \) are coefficients in \( \mathbb{Z}_{L'} \), and \( x \) is the variable or indeterminate. For our purposes, we can think of a formal polynomial as simply being the list of its coefficients, so it is uniquely specified by these. A formal polynomial induces a function \( f : \mathbb{Z}_{L'} \rightarrow \mathbb{Z}_{L'} \), called the induced polynomial function, by replacing the variable \( x \) with a value in \( \mathbb{Z}_{L'} \) and evaluating the resulting expression modulo \( L' \).

In the main text, we simply referred to these functions themselves as polynomials, for simplicity, but here we will explicitly refer to them as (induced) polynomial functions.

Over general finite fields, distinct formal polynomials can induce the same polynomial function. However, over \( \mathbb{Z}_{L'} \) (for prime \( L' \)) all distinct formal polynomials of degree less than \( L' \) induce distinct polynomial functions. This follows from the well-known fact that every function over a finite field is a polynomial function. To see how our desired property follows, first note that there are \( (L')^{L'} \) distinct functions over \( \mathbb{Z}_{L'} \). Next, using Fermat’s Little Theorem, which states that \( x^{L'} = x \) modulo \( L' \) for any \( x \in \mathbb{Z}_{L'} \), we can reduce any arbitrary polynomial function to a polynomial function of degree less than \( L' \). Note that we cannot reduce away \( x^{L'-1} \) if its coefficient is nonzero, because Fermat’s Little Theorem only implies \( x^{L'-1} = 1 \) for nonzero \( x \in \mathbb{Z}_{L'} \).

Hence, the polynomial function induced by any arbitrary formal polynomial is identical to the polynomial function induced by a formal polynomial of degree less than \( L' \), so every function over \( \mathbb{Z}_{L'} \) is a polynomial function induced by a formal polynomial of degree less than \( L' \). A formal polynomial of degree less than \( L' \) over \( \mathbb{Z}_{L'} \) is uniquely characterized by its \( L' \) coefficients (of \( x^0, x^1, ..., x^{L'-1} \), allowing any of the coefficients to be zero), so there are \( (L')^{L'} \) formal polynomials of degree less than \( L' \) over \( \mathbb{Z}_{L'} \). Therefore, all of these must induce distinct polynomial functions, because if any pair of them induced the same polynomial function then there would not be enough of them to match all of the \( (L')^{L'} \) general functions.

In the main text, we do not use all polynomial functions of degree less than the order of the field, but only those up to some fixed degree \( D \). However, this \( D \) is always less than the order of the field, so all such polynomial functions are distinct, which justifies our claim in the main text that there are \( (L')^{D+1} \) of them. That a degree-\( D \) polynomial function over \( \mathbb{Z}_{L'} \) can
have at most $D$ roots follows similarly to the argument over the real numbers. Polynomials over finite fields admit polynomial long division, so a polynomial function $f$ whose roots form a multiset $R \subseteq \mathbb{Z}_L$ (including multiple copies of roots with multiplicities greater than one) can be factored as

$$f(x) = g(x) \prod_{r \in R} (x - r) \quad (D4)$$

where $g(x)$ is some other polynomial over $\mathbb{Z}_L$. Thus since the product over $R$ is itself a polynomial of degree $|R|$, the number of roots, the degree of $f$ must be at least the number of roots. These are the main facts about polynomials over finite fields used in the main text.

**Appendix E: Hermite interpolation**

Hermite interpolation is a method for finding the least-degree polynomial (over the real numbers) that satisfies a certain set of constraints. A special case, Newton interpolation, applies when the constraints are specified, the least-degree polynomial that passes through the points has degree $n$: for example, any single point defines the constant polynomial whose value is the value at the point, any pair of points defines a line, and so forth.

Hermite interpolation generalizes this to cases where up to $m$th derivatives are also specified at each point. Different numbers of derivatives can be specified for different points. In this case, each derivative and each point is a constraint, and if there are $n$ constraints in total then the least-degree polynomial that satisfies the constraints has degree $n - 1$. For a thorough review of Hermite interpolation, see [24].

In this appendix, we will instead illustrate Hermite interpolation by showing how to implement it for the specific example in the main text. In that example, for some odd $L$, the points are \{\text{A41}\}, which we reproduce here for convenience

$$\{ \left( \cos \left( \frac{m\pi}{L} \right), 1 \right) \mid m = 0, 1, 2, \ldots, \left\lfloor \frac{L}{2} \right\rfloor \} \cup \{ \left( \cos \left( \frac{m\pi}{L} \right), -1 \right) \mid m = \left\lceil \frac{L}{2} \right\rceil + 1, \ldots, L \}. \quad (E1)$$

The derivative constraints are that the first derivatives be zero at all points except for the first and last ($m = 0$ and $m = L$).

Let us translate these constraints into a more general language: the value and derivatives at each point will be written as a list of numbers $(x_i, f_i, f'_i, f''_i, \ldots)$, which stands for the constraints

$$f(x_i) = f_i, \quad f'(x_i) = f'_i, \quad f''(x_i) = f''_i, \ldots \quad (E2)$$

where $f$ is the polynomial we are trying to construct. In this notation, the constraints we stated above may be rewritten

$$(x_0, f_0) = (1, 1), \quad (x_i, f_i, f'_i) = \left( \cos \left( \frac{i\pi}{L} \right), 1, 0 \right) \text{ for } i = 1, 2, \ldots, \left\lfloor \frac{L}{2} \right\rfloor, \quad (E3)$$

To implement Hermite interpolation, we construct a second list $\{z_i\}$. $\{z_i\}$ should be a list of the $x$'s, in order, but with each $x_i$ duplicated if its first derivative is specified: in other words,

$$z_0 = x_0, \quad z_1 = z_2 = x_1, \quad z_3 = z_4 = x_2, \quad \vdots \quad \quad (E4)$$

$$z_{2L-1} = z_{2L-2} = x_{L-1}, \quad z_{2L-1} = x_L.$$

Then the expression for the Hermite interpolating polynomial is

$$f(x) = \sum_{i=0}^{2L-1} f[z_i, z_{i-1}, \ldots, z_1, z_0] \prod_{j=0}^{i-1} (x - z_j), \quad (E5)$$

where the product $\prod_{j=0}^{i-1} (x - z_j) \equiv 1$, and $f[z_i, z_{i-1}, \ldots, z_1, z_0]$ is the divided difference of $f$, defined below. We can see that is a degree-$({2L - 1})$ polynomial, as we expect, since there are $L + 1$ value constraints and $L - 1$ first derivative constraints, for $2L$ constraints in total. We do not justify why \(E5\) is the correct expression, leaving that to one of the many texts on the subject, such as [24]. Instead we will conclude by defining the divided difference, which enables evaluation of the above expression.

The divided difference of $f$ is defined recursively as follows. First, to gain an intuition, if all of the $z_i$s were distinct then the divided difference would be defined by

$$f[z_i, z_{i-1}, \ldots, z_1, z_0] = \frac{f[z_i, z_{i-1}, \ldots, z_1] - f[z_{i-1}, \ldots, z_1, z_0]}{z_i - z_0} \quad (E6)$$

with the base case given by \( f[z_j] = f(z_j) \).
Hence, one can think of the divided difference \( f[z_i, z_{i-1}, \ldots, z_1, z_0] \) as analogous to an \( i \)th numerical derivative.

However, since in our case many adjacent pairs \( z_{i+1} \) and \( z_i \) are equal, the recursion above would become undefined when two arguments remain in the divided differences, e.g., \( f[z_2, z_1] = \frac{f(z_2) - f(z_1)}{z_2 - z_1} \) is undefined because \( z_2 = z_1 \). This is where the derivative constraints enter. In our case, we define the base case at the level of two arguments as follows:

\[
f[z_{i+1}, z_i] = \begin{cases} \frac{f(z_{i+1}) - f(z_i)}{z_{i+1} - z_i} & \text{if } z_{i+1} \neq z_i, \\ f'(z_i) & \text{if } z_{i+1} = z_i \end{cases} \quad \text{(E7)}
\]

In other words, since for example \( f[z_2, z_1] = \frac{f(z_2) - f(z_1)}{z_2 - z_1} \) is undefined because \( z_2 = z_1 \), we replace it with the specified derivative at that point. The recursion relation (E6) remains the same, but terminates at two arguments instead of one.

(E7) simplifies considerably. Note that in terms of the \( z_i \)s, the constraints (E3) become

\[
f(z_i) = f \left( x \left[ \frac{i+2}{2} \right] \right) = f \left[ \frac{i+2}{2} \right], \quad \text{(E8)}
\]

and for \( i = 1, 2, \ldots, 2L - 2, \)

\[
f'(z_i) = f' \left( x \left[ \frac{i+2}{2} \right] \right) = f' \left[ \frac{i+2}{2} \right] = 0. \quad \text{(E9)}
\]

Inserting these in (E7) yields

\[
f[z_{i+1}, z_i] = \begin{cases} \frac{f \left[ \frac{i+2}{2} \right] - f \left[ \frac{i+1}{2} \right]}{z_{i+1} - z_i} & \text{if } z_{i+1} \neq z_i, \\ 0 & \text{if } z_{i+1} = z_i \end{cases} \quad \text{(E10)}
\]

But most of the specified values are identical: we can see from (E3) that \( f \left[ \frac{i+2}{2} \right] - f \left[ \frac{i+1}{2} \right] = 0 \) unless

\[
\left\lfloor \frac{i + 2}{2} \right\rfloor = \left\lceil \frac{L}{2} \right\rceil \quad \text{and} \quad \left\lfloor \frac{i + 1}{2} \right\rfloor = \left\lceil \frac{L}{2} \right\rceil, \quad \text{(E11)}
\]

which simplifies to

\[
i = L - 1 \quad \text{(E12)}
\]

because \( L \) is odd. In this case, from (E3) we see that

\[
f \left[ \frac{i+2}{2} \right] - f \left[ \frac{i+1}{2} \right] = -2, \quad \text{so (E10) becomes}
\]

\[
f[z_{i+1}, z_i] = \begin{cases} \frac{\cos \left( \frac{\pi}{4} \right) - \cos \left( \frac{\pi}{4} \right)}{z_{i+1} - z_i} & \text{if } i = L - 1, \\ 0 & \text{otherwise.} \end{cases} \quad \text{(E13)}
\]

Combining this base case with the recursion (E6) yields all divided differences in the Hermite polynomial (E5).

Note that the recursion relation (E6) might lead to worry that evaluating the divided difference requires exponential time. In fact, it can be compute efficiently as follows. First, evaluate all of the two-argument divided differences as given by (E13), of which there are \( 2L - 1 \), since there is one for each consecutive pair \( z_{i+1}, z_i \) and there are \( 2L \) \( z_i \)s. Next, evaluate all of the three-argument divided differences, each of which is calculated by taking the difference of a consecutive pair of two-argument divided differences and dividing it by a difference between points, e.g.,

\[
f[z_{i+2}, z_{i+1}, z_i] = \frac{f[z_{i+2}, z_{i+1}] - f[z_{i+1}, z_i]}{z_{i+2} - z_i}. \quad \text{(E14)}
\]

Hence, the number of three-argument divided differences is one fewer than the number of two-argument divided differences. Then evaluate the four-argument divided differences using the three-argument divided differences in the same way, and so forth.

In this way, we build up a pyramid (called a divided differences table) of all of the divided differences, where moving up the pyramid corresponds to divided differences with more arguments. Since the base of the pyramid (the two-argument divided differences) has size \( 2L - 1 \), the total number of divided differences we need to evaluate to build up the whole pyramid is \( O(L^2) \).