From Fermions to Qubits: A ZX-Calculus Perspective

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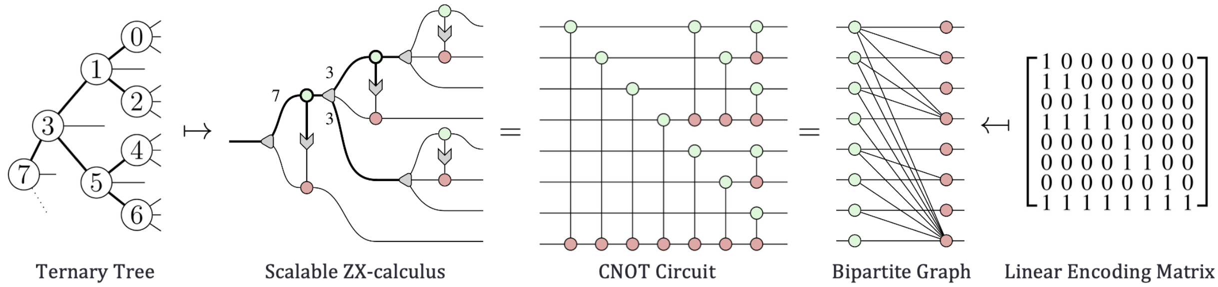


Figure 1: Different ways of representing the same fermion-to-qubit mapping; in this case, the Bravyi-Kitaev mapping for 8 fermionic modes.

Simulating quantum systems, such as molecules in quantum chemistry or condensed matter physics, is one of the most promising applications of quantum computing. These quantum systems are fermionic in nature and are described by states in a Fock space. Thus, choosing a way to compile a fermionic system down to the qubits of a quantum device is often the first step for solving such problems. This allows us to map fermionic states to qubit states, and operations on fermionic states to operations on qubits, before implementing these operations on quantum hardware. This is called a *fermion-to-qubit mapping*.

Over the years, fermion-to-qubit mappings have been developed from distinct viewpoints, including binary-matrix linear encodings [2, 5], ternary-tree constructions [8, 12], and stabilizer-based local encodings [9, 11, 13]. Moreover, these mappings are often presented in different mathematical languages (e.g. encoded Fock states, Majorana operators, encoder circuits, or stabilizers), which makes direct comparison difficult and obscures when distinct constructions are equivalent [3]. As a result, a unified and intuitive framework is needed to compare mappings across representations, transfer methods between them, and clarify when different descriptions coincide.

To address this, we use the ZX-calculus as a common intermediate language connecting three major representation families: linear encodings, ternary trees, and local encodings. Within this framework, we derive fermionic creation and annihilation operators for arbitrary linear encodings using scalable ZX rewrites. We prove (Theorem 1) that every ternary-tree mapping defines a linear encoding, and we give an explicit algorithm to compute its binary matrix. We extend the same perspective to *local* encodings, where ancilla qubits and stabilizers are introduced to mitigate the non-locality of fermionic systems.

Background

In second quantization, a system of n fermionic modes is characterized in terms of a creation operator $a_i^\dagger$ and an annihilation operator a_i for each mode. This defines a basis of all possible occupation numbers $k_i \in \{0,1\}$ called the Fock basis: $|k_0 k_1 \ldots k_{n-1}) := \prod_{i=0}^{n-1} \left(a_i^\dagger\right)^{k_i} |\mathsf{vac})$, where $|\mathsf{vac})$ is the vacuum state containing no fermions. In other words, the fermionic Fock space is spanned by the basis $\{|\mathbf{f}) \mid \mathbf{f} \in \mathbb{F}_2^n\}$, where $\mathbb{F}_2^n$ is the vector space of n-dimensional binary vectors.

Fermion-to-qubit mappings simulate fermionic systems on qubit hardware by mapping a fermionic Hilbert space $\mathscr{H}_f$ to an M-qubit Hilbert space $(\mathbb{C}^2)^{\otimes M}$. As a reference point, we use the Jordan–Wigner (JW) transformation [5], which maps occupation-number basis states as $|n_0n_1...n_{N-1}) \mapsto |n_0n_1...n_{N-1}\rangle$. More generally, we describe a mapping $m : \mathscr{H}_f \to (\mathbb{C}^2)^{\otimes M}$ by a qubit isometry U_m acting on the Fock basis as:

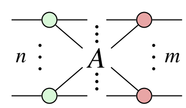
$$|\mathbf{f}) \xmapsto{\text{JW}} |\mathbf{f}\rangle \xmapsto{U_m} U_m|\mathbf{f}\rangle \tag{1}$$

Linear Encodings

We can represent any Fock basis vector $|\mathbf{f})$ by its corresponding bitstring $\mathbf{f}$ as a vector in $\mathbb{F}_2^n$. Given an invertible matrix $A \in \mathbb{F}_2^{n\times n}$, the induced map $|\mathbf{f}) \mapsto |A\mathbf{f}\rangle$ from the fermionic Fock space to the qubit space is known as a *linear encoding* of the Fock basis. For example, the Jordan-Wigner encoding corresponds to the identity matrix over $\mathbb{F}_2$.

Suppose $A \in \mathbb{F}_2^{m\times n}$. Then its matrix arrow is defined as

$$n \xrightarrow{A} m \quad :=$$



$$\xmapsto{[\![\cdot]\!]} \quad \sum_{\vec{x}\in\mathbb{F}_2^n} |A\vec{x}\rangle\langle\vec{x}| \tag{2}$$

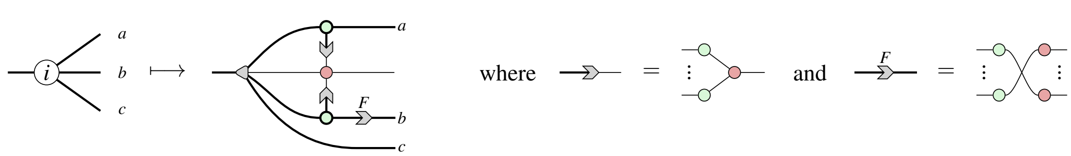
where, in the middle ZX diagram, A is the biadjacency matrix of the bipartite graph on input Z and output X spiders, i.e. $A_{ij} = 1$ if and only if the i'th Z spider is connected to the j'th X spider, and $|\vec{x}\rangle$, $\vec{x} \in \mathbb{F}_2^n$, is a computational basis state.

In the ZX-calculus, linear encodings correspond to unitary phase-free ZX diagrams. Any such diagram can be simplified to a normal form [1], which is a matrix arrow shown in Equation (2). Concretely, the linear encoding given by a matrix $A \in \mathbb{F}_2^{n\times n}$ corresponds to a matrix arrow labelled by A. These unitary phase-free ZX diagrams can also be rewritten to CNOT circuits [7], i.e. quantum circuits made out of only CNOT gates.

Ternary Tree Encodings

A ternary tree is a labelled ordered tree graph where each node has at most three children. We orient the tree from left to right, with the root at the leftmost node, to match the orientation of ZX-diagrams in this paper. The leftmost diagram in Figure 1 is an example of a ternary tree. To any ternary tree, we can associate a set of anti-commuting Pauli strings by listing each root-to-leaf path, where the X, Y, and Z (top, middle, and bottom) branches at node i correspond to the Pauli operators X_i, Y_i, and Z_i respectively.

We can translate a ternary tree mapping to a ZX diagram by replacing each node in the tree with the following diagram, while keeping the same connectivity as the ternary tree.



(3)

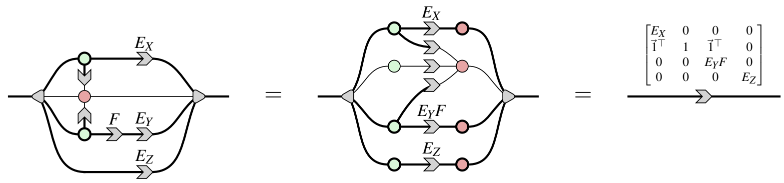
Here, a, b, and c are the numbers of descendants of i along its X, Y, and Z legs, respectively, and they also correspond to the thicknesses of the wires in the ZX diagram.

As shown in Figure 1, we can derive a ZX diagram from a ternary tree simply by replacing each node of the tree with the ZX diagram in (3). This leads to the following theorem.

Theorem 1. *Ternary tree mappings are linear encodings. The encoder diagram for the ternary tree mapping can be reduced to phase-free ZX normal form.*

Proof. We prove this by induction on the height of the ternary tree. Assume the theorem holds for ternary trees of height at most h. Then for a tree of height $h+1$, let E_X, E_Y, and E_Z be the encoding matrices for the

X, Y, and Z subtrees respectively. Adding the diagram in (3) at the root node and simplifying, we arrive at the result:



(4)

□

This proof provides a recursive algorithm to translate any ternary tree into its linear encoding matrix.

Local Encodings

For many target Hamiltonians, the physically relevant couplings are *local* on an interaction graph: vertices represent fermionic modes and edges represent terms that couple nearby modes. A central example is a *hopping term*, which moves a fermion between neighboring sites and has the form $a_i^\dagger a_j + a_j^\dagger a_i$. Although this term is local in the fermionic model (it only involves sites i and j), standard fermion-to-qubit mappings can make it non-local on qubits.

The obstruction is the fermionic anti-commutation structure: in mappings such as Jordan–Wigner, creation and annihilation operators carry parity strings. For example, for $p < q$, a hopping term maps as $a_p^\dagger a_q \mapsto A_p^\dagger \otimes \left(\bigotimes_{i=p+1}^{q-1} Z_i\right) \otimes A_q$, where $A_r = (X_r + iY_r)/2$. Even nearest-neighbour fermionic couplings can therefore become long Pauli strings on qubits. In higher-dimensional geometries, this increases operator weight and circuit depth.

Local encodings address this by adding ancilla qubits together with commuting stabilizers that cancel or shorten these parity strings, so local fermionic couplings map to local qubit operators [9, 11, 13]. In our framework, we represent these encodings diagrammatically as isometries in the stabilizer fragment of ZX, rather than as phase-free unitaries. This lets us express stabilizers and encoder structure in one language and preserve the geometry of the interaction graph in the encoder diagram. Conceptually, this places local fermion-to-qubit encodings closer to ZX methods used in quantum error correction [4, 6]: the stabilizer ZX-calculus machinery is the same, but the objective differs, since we optimize locality of encoded fermionic operators rather than code distance.

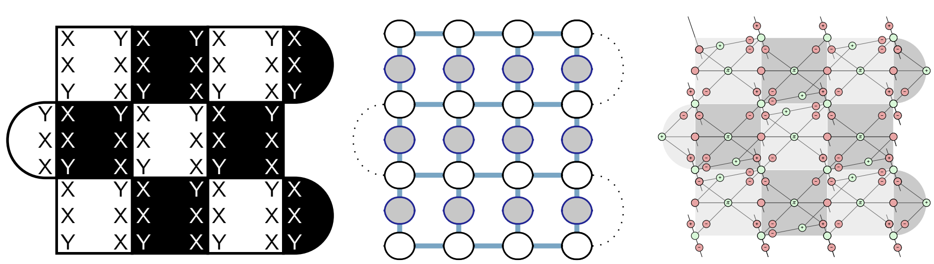


Figure 2: Left: Tiling of each plaquette stabilizer for the 4 by 4 square lattice AQM from Ref. [10]. Middle: Its connectivity graph. Right: Its encoder ZX-diagram. The $\pm$ labels are shorthand for $\pm\frac{\pi}{2}$.

As a concrete illustration of this stabilizer-ZX perspective, we give an encoder diagram for the square-lattice AQM of Ref. [10]. In this construction, rows of fermionic modes are interleaved with ancilla rows, and locality is enforced by commuting plaquette stabilizers acting on four data qubits together with two adjacent ancillas. The resulting encoder diagram (Figure 2) makes the connectivity explicit. By pushing hopping terms through the encoder, we can see that their encoded weight tracks Manhattan distance on the lattice, including boundary terms where the Jordan–Wigner chain wraps, making locality trade-offs visually analyzable.

The full paper is available at https://arxiv.org/abs/2505.06212.

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