A Compact Fermion-to-Qubit Mapping

arXiv:2003.06939 and arXiv:2101.10735

April 8, 2021

Motivation

- Simulation of fermionic quantum systems (e.g., for quantum chemistry applications) on a quantum computer — Hamiltonians of the form

$$H = \sum_{i,j} h_{i,j} a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,\ell} h_{i,j,k,\ell} a_i^\dagger a_j^\dagger a_k a_\ell .$$

- Need a translation from fermionic language to qubit language.
- The choice of transformation has consequences, esp. for near-term devices. (e.g., transformations should minimize number of qubits, circuit depth.)

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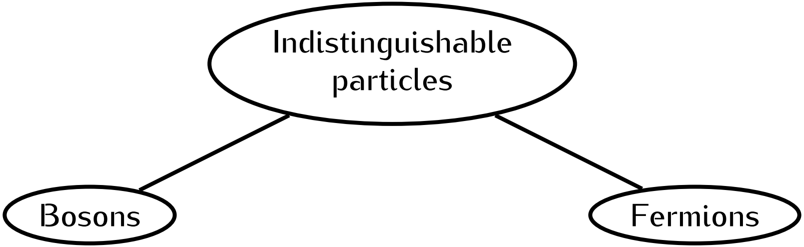
Summary of work

- Fermion-to-qubit mapping with < 1.5 qubits per mode on a square lattice — less than all prior work.
- Mapping is essentially a stabilizer code: observables are local, but basis states are highly entangled.
- Other lattice geometries considered as well.
- General theory of fermion-to-qubit mappings.

Mapping	[13]	[10, 11]	[15]	[12]	[14]	even face number	majority even faces	majority odd faces
Qubit Number	$2L(L-1)$	$2L^2$	$2L(L-1)$	$2L^2-L$	$3L^2$	$1.5L^2-L$	$1.5L^2-L-1$	$1.5L^2-L+1$
Qubit to Mode Ratio	$2-\frac{2}{L}$	2	$2-\frac{2}{L}$	$2-\frac{1}{L}$	3	$1.5-\frac{2}{L}$	$1.5-\frac{2}{L}-\frac{1}{2L^2}$	$1.5-\frac{2}{L}+\frac{1}{2L^2}$
Max Weight Hopping	6	4	4	5	4	3	3	3
Max Weight Coulomb	8	2	6	6	6	2	2	2
Encoded Fermionic Space	Even	Full	Even	Full	Even	Full	Even	Full Plus Qubit
Graph Geometry	General	General	Square Lattice	Square Lattice	General	Square Lattice	Square Lattice	Square Lattice

TABLE I. A comparison of existing local fermion to qubit mappings on an $L \times L$ lattice of fermionic modes. The mapping presented in this work is given in the three rightmost columns. Max weight Coulomb and max weight hopping denote the maximum Pauli weights of the mapped Coulomb ($a_i^\dagger a_i a_j^\dagger a_j$) and nearest neighbour hopping ($a_i^\dagger a_j + a_j^\dagger a_i$) terms respectively. Encoded fermionic space denotes whether the full or even fermionic fock space is represented. Graph geometry denotes the hopping interaction geometry which the mapping is tailored to.



Bosons

- e.g., photons
- Symmetric wavefunction: $\Psi(x_1, x_2) = \Psi(x_2, x_1)$
- Unlimited occupation of energy levels/“modes”

Fermions

- e.g., electrons
- Anti-symmetric wavefunction: $\Psi(x_1, x_2) = -\Psi(x_2, x_1)$
- At most one fermion can occupy an energy level/“mode”

Hilbert space of indistinguishable particles

For n distinguishable particles: $\mathcal{H}^{\otimes n}$ ($\mathcal{H} = \mathbb{C}^m \Rightarrow m$ modes)

For n indistinguishable particles

Bosons

Symmetric subspace of $\mathcal{H}^{\otimes n}$:

$$\begin{aligned} &\mathrm{Sym}_n(\mathcal{H}) \\ &:= \mathrm{span}\left\{|\psi\rangle \in \mathcal{H}^{\otimes n} : W^{\pi}|\psi\rangle = |\psi\rangle \quad \forall \ \in \mathcal{S}_n\right\}. \end{aligned}$$

Bosonic Fock space for m modes:

$$\mathcal{F}_{\mathrm{B}}(\mathcal{H}) := \bigoplus_{n=0}^{\infty} \mathrm{Sym}_n(\mathcal{H})$$

Fermions

Anti-symmetric subspace of $\mathcal{H}^{\otimes n}$:

$$\begin{aligned} &\mathrm{ASym}_n(\mathcal{H}) \\ &:= \mathrm{span}\left\{|\psi\rangle \in \mathcal{H}^{\otimes n} : W^{\pi}|\psi\rangle = \mathrm{sgn}(\pi)|\psi\rangle \quad \forall\ \pi \in \mathcal{S}_n\right\}. \end{aligned}$$

Fermionic Fock space for m modes:

$$\mathcal{F}_{\mathrm{F}}(\mathcal{H}) := \bigoplus_{n=0}^{m} \mathrm{ASym}_n(\mathcal{H}). \quad (\text{dimension } 2^m)$$

Creation and annihilation operators

Bosons

$$|n_1, \ldots, n_m\rangle = \frac{(a_1^\dagger)^{n_1}}{\sqrt{n_1!}} \cdots \frac{(a_m^\dagger)^{n_m}}{\sqrt{n_m!}} |0, \ldots, 0\rangle.$$

$$a_j^\dagger |\ldots, n_j, \ldots\rangle = \sqrt{n_j + 1} |\ldots, n_j + 1, \ldots\rangle,$$

$$a_j |\ldots, n_j, \ldots\rangle = (1 - \delta_{n_j,0}) \sqrt{n_j} |\ldots, n_j - 1, \ldots\rangle.$$

$$[a_j, a_j^\dagger] = \delta_{j,k} \mathbb{1}, \quad [a_j, a_k] = [a_j^\dagger, a_k^\dagger] = 0.$$

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Fermionic modes have non-local structure!

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$|n_1, .$

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$a_j|\ldots,$

$[a_j,$

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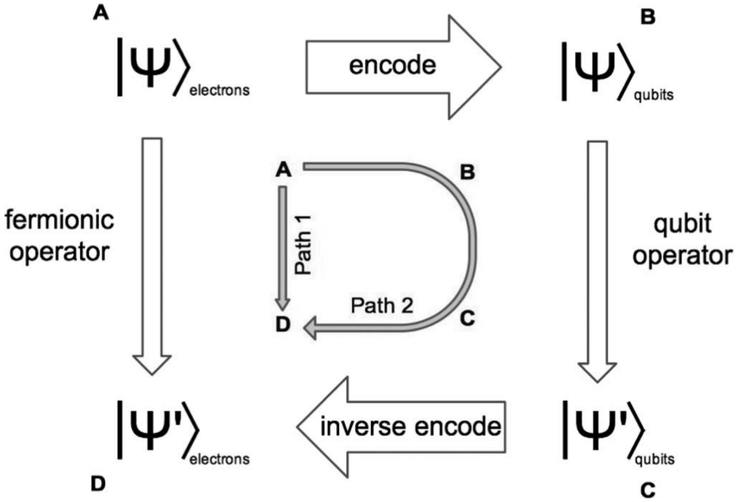
Fermionic modes have non-local structure!

Fermion-to-qubit mappings



Two parts to the mapping:

1. Map the occupation number basis states.
2. Map the creation and annihilation operators.

[J. Chem. Phys. **137**, 224109 (2012)

Jordan–Wigner transformation

$$|n_1, n_2, \ldots, n_m\rangle \longmapsto |n_1\rangle \otimes |n_2\rangle \otimes \cdots \otimes |n_m\rangle,$$

$$a_j^\dagger \longmapsto Z_1 \otimes \cdots \otimes Z_{j-1} \otimes \frac{1}{2}(X_j - \mathrm{i}\, Y_j) \otimes \mathbb{1}_{j+1} \otimes \cdots \otimes \mathbb{1}_m,$$

$$a_j \longmapsto Z_1 \otimes \cdots \otimes Z_{j-1} \otimes \frac{1}{2}(X_j + \mathrm{i}\, Y_j) \otimes \mathbb{1}_{j+1} \otimes \cdots \otimes \mathbb{1}_m.$$

⋆ Transformation of occupation basis states is local, but transformation of creation/annihilation operators is non-local!

Graphical formulation ["Fermionic Quantum Computation"; Annals of Physics 298, 210–226 (2002)]

Solution of Bravyi and Kitaev: increase number of qubits, and look only at mode interactions relevant to the problem; i.e., only those interactions appearing in the Hamiltonian.

Consider first the "Majorana operators":

$$\gamma_j := a_j + a_j^\dagger, \quad \overline{\gamma}_j := -\mathrm{i}(a_j - a_j^\dagger)$$

Then, define the following equivalent mode operators for edges and vertices of an undirected graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$:

$$E_{j,k} := -\mathrm{i}\gamma_j\gamma_k \quad \forall\ (j,k) \in \mathcal{E},$$

$$V_j := -\mathrm{i}\gamma_j\overline{\gamma}_j \quad \forall\ j \in \mathcal{V}.$$

It suffices for the fermion-to-qubit mapping to transform these operators to operators on qubits.

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Properties:

$$V_k = V_k^\dagger, \quad E_{j,k}^\dagger = E_{j,k}, \quad V_k^2 = \mathbb{1}, \quad E_{j,k}^2 = \mathbb{1}, \quad E_{k,j} = -E_{j,k},$$

$$V_k V_\ell = V_\ell V_k, \quad E_{j,k} B_\ell = (-1)^{\delta_{j,\ell}+\delta_{k,\ell}} V_\ell E_{j,k}, \quad E_{j,k} E_{\ell,s} = (-1)^{\delta_{j,\ell}+\delta_{j,s}+\delta_{k,\ell}+\delta_{k,s}} E_{\ell,s} E_{j,k},$$

$$\mathrm{i}^p E_{j_1,j_2} E_{j_2,j_3} \cdots E_{j_{p-1},j_p} E_{j_p,j_1} = \mathbb{1} \quad \text{for any closed path} \quad (j_1, j_2, \ldots, j_p).$$

Bravyi-Kitaev "superfast" transformation [Annals of Physics 298, 210–226 (2002)]

Procedure [J. Chem. Phys. **148**, 164104 (2018)]

1. **Associate every mode to the vertex of a graph.**
2. Given the Hamiltonian, get the number of edges required.
3. **Put the qubits on the edges.** # of qubits $= |\mathcal{E}| = \frac{1}{2}\sum_{v\in\mathcal{V}} \deg(v)$.
4. Define the following qubit operators for the edges and vertices:

$$\widetilde{E}_{j,k} = \epsilon_{j,k} X_{(j,k)} \prod_{\ell:(\ell,j)<(k,j)} Z_{(\ell,j)} \prod_{s:(s,k)<(j,k)} Z_{(s,k)}, \quad \widetilde{V}_k = \prod_{j:(j,k)\in\mathcal{E}} Z_{(j,k)}.$$

5. Find the independent loops in the graph. Define stabilizers for these loops.
6. Use the stabilizers to find the relevant subspace that fermionic states get mapped to:

$$\text{span}\left\{ |\psi\rangle : \widetilde{C}_{j_1,j_2,\ldots,j_p}|\psi\rangle = |\psi\rangle \quad \text{for all closed paths } (j_1, j_2, \ldots, j_p) \text{ in the graph} \right\},$$

where

$$\widetilde{C}_{j_1,j_2,\ldots,j_p} = \mathrm{i}^p \widetilde{E}_{j_1,j_2} \widetilde{E}_{j_2,j_3} \cdots \widetilde{E}_{j_{p-1},j_p} \widetilde{E}_{j_p,j_1}.$$

The new mapping for a square lattice [arXiv:2003.06939, arXiv:2101.10735]

⋆ Put qubits on the vertices and odd faces instead.

⇒ number of qubits for $L_1 \times L_2$ lattice is $m + \frac{n_F}{2}$, where $m = L_1 L_2$ (# of modes) and $n_F = (L_1 - 1)(L_2 - 1)$ (# of faces).

$$\widetilde{V}_j = Z_j,$$

$$\widetilde{E}_{i,j} = \begin{cases} X_i Y_j X_{f(i,j)} & (i,j) \text{ oriented downwards,} \\ -X_i Y_j X_{f(i,j)} & (i,j) \text{ oriented upwards,} \\ X_i Y_j Y_{f(i,j)} & (i,j) \text{ horizontal,} \end{cases}$$

where $f(i,j) =$ the unique odd face adjacent to (i,j).

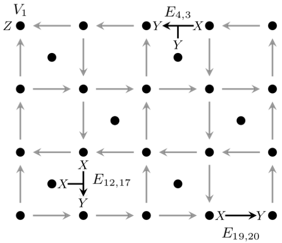

FIG. 1. Qubit assignment, edge orientation, and examples of mapped edge and vertex operators for a 4 × 5 square lattice. Vertices are numbered in snaking order, left to right, top to bottom.

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Qubit to Mode Ratio	$2 - \frac{2}{L}$	2	$2 - \frac{2}{L}$	$2 - \frac{1}{L}$	3	$1.5 - \frac{2}{L}$	$1.5 - \frac{2}{L} - \frac{1}{2L^2}$	$1.5 - \frac{2}{L} + \frac{1}{2L^2}$
Max Weight Hopping	6	4	4	5	4	3	3	3
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Encoded Fermionic Space	Even	Full	Even	Full	Even	Full	Even	Full Plus Qubit
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