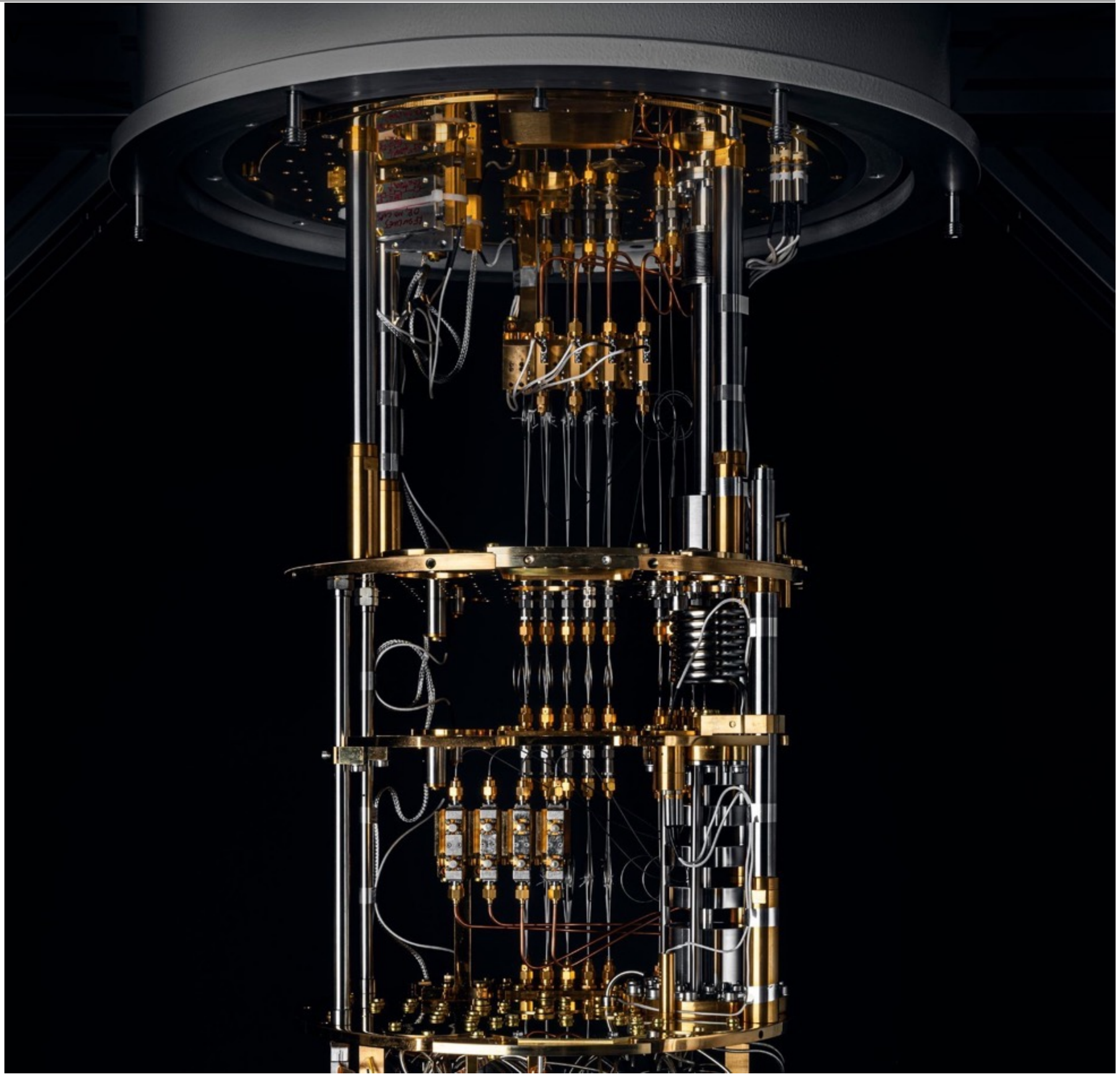
Low-depth simulations of fermionic systems on square-grid quantum hardware

WE BUILD QUANTUM COMPUTERS

Manuel Algaba,
P.V. Sriluckshmy, M. Leib, F. Šimkovic

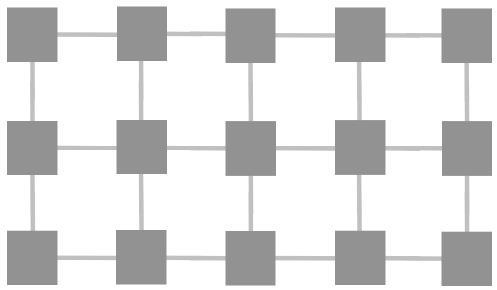
arXiv:2302.01862 arXiv:2303.04498



Objective:

Simulate a single Trotter step of a fermionic system on a realistic quantum computer in minimal circuit depth.

$$e^{-it\mathcal{H}} = \left(\prod_j e^{-i\frac{t}{N}\mathcal{H}_j}\right)^N$$



$$\mathrm{fSIM}_{ij}(\theta,\phi) = e^{i\frac{\theta}{2}(X_iX_j+Y_iY_j)+i\frac{\phi}{4}(Z_i+Z_j-Z_iZ_j)}$$

IQM

1. Fermionic Models

Complexity

$$\mathcal{H}_{\mathrm{ES}} = \sum_{pq} h^{pq} c_p^\dagger c_q + \sum_{pqrs} h^{pqrs} c_p^\dagger c_q^\dagger c_r c_s$$

$$\mathcal{H}_{\mathrm{FH}} = -\sum_{i,j,\sigma} t^{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$\mathcal{H}_{\mathrm{TB}} = -\sum_{i,j} t^{ij} c_i^\dagger c_j$$, 1D FHM

Implementability

IQM

1. Fermionic Models

Complexity

Implementability

$$\mathcal{H}_{\mathrm{ES}} = \sum_{pq} h^{pq} c_p^\dagger c_q + \sum_{pqrs} h^{pqrs} c_p^\dagger c_q^\dagger c_r c_s$$

$$\mathcal{H}_{\mathrm{FH}} = -\sum_{i,j,\sigma} t^{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$\mathcal{H}_{\mathrm{TB}} = -\sum_{i,j} t^{ij} c_i^\dagger c_j$$

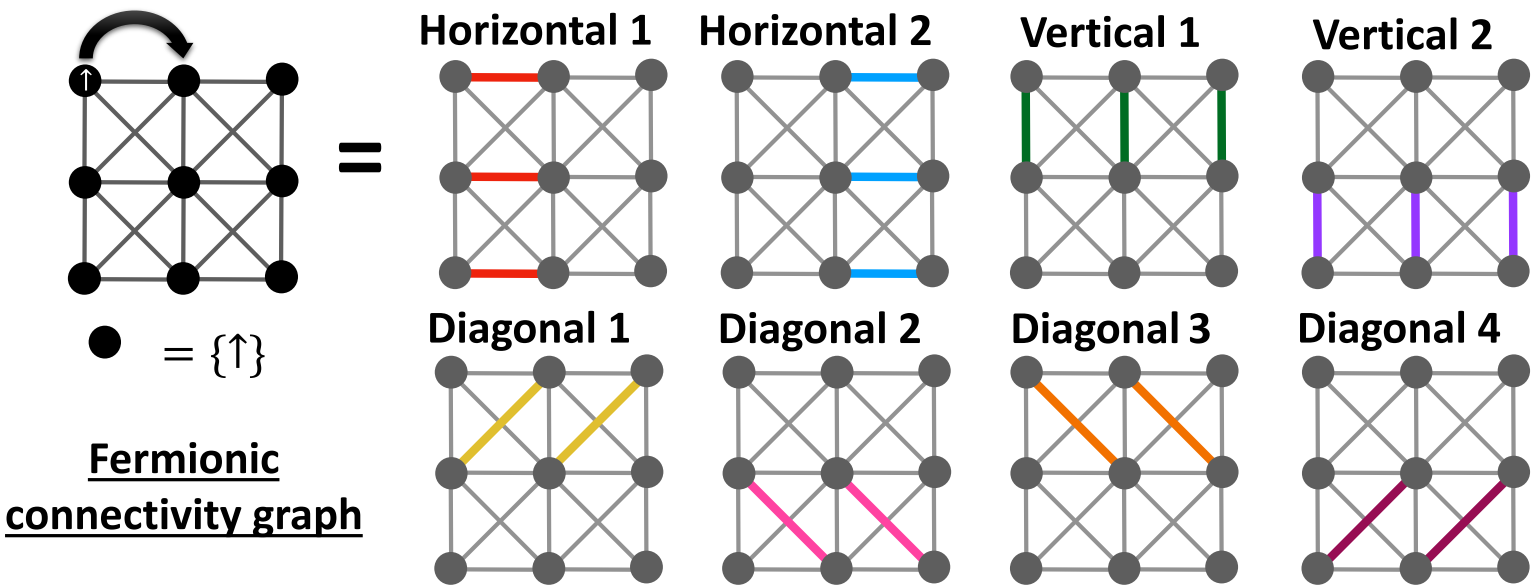
, 1D FHM

TRIVIAL!

2. Fermion-to-qubit mappings

Tight Binding Hamiltonian:

$$\mathcal{H}_{\mathrm{TB}} = \sum_{i,j} t^{ij} c_i^\dagger c_j$$



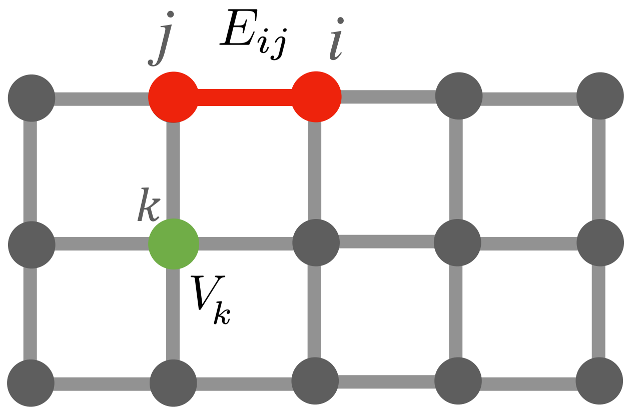
IQM

2. Fermion-to-qubit mappings

$$\mathcal{H}_{\mathrm{TB}} = \sum_{i,j} t^{ij} c_i^\dagger c_j$$

$$\{c_i, c_j^\dagger\} = c_i c_j^\dagger + c_j^\dagger c_i = \delta_{ij}$$

$$\{c_i^\dagger, c_j^\dagger\} = \{c_i, c_j\} = 0$$



Edge and vertex operators:

$$\{E_{ij}, V_i\} = \{E_{ij}, E_{jk}\} = 0$$

$$[E_{ij}, E_{kl}] = [E_{ij}, V_k] = [V_i, V_j] = 0$$

Hopping operators:

$$c_j^\dagger c_k + c_k^\dagger c_j \rightarrow \frac{i}{2}(V_k - V_j)E_{jk}$$

Fermions → Qubits

S. B. Bravyi and A. Y. Kitaev, Ann. Phys. 298, 210 (2002)

IQM

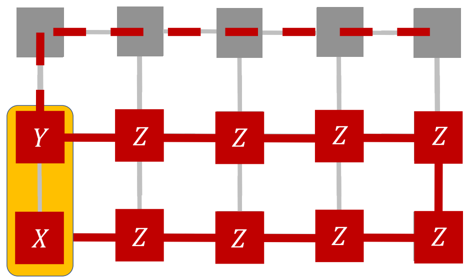
2. Fermion-to-qubit mappings

$$\{E_{ij}, V_i\} = \{E_{ij}, E_{jk}\} = 0$$
$$[E_{ij}, E_{kl}] = [E_{ij}, V_k] = [V_i, V_j] = 0$$
$$c_j^\dagger c_k + c_k^\dagger c_j \to \frac{i}{2}(V_k - V_j)E_{jk}$$

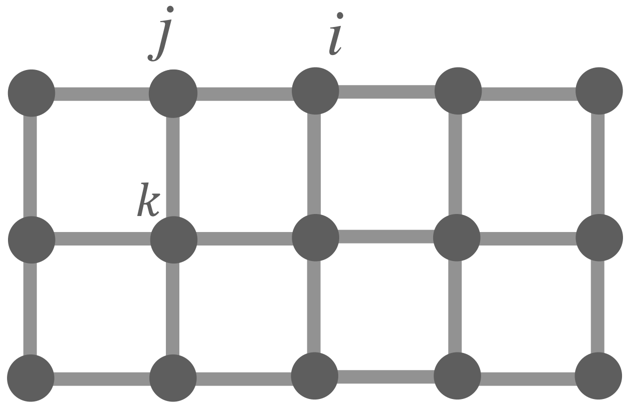
$$\mathcal{H}_{\mathrm{TB}} = \sum_{i,j} t^{ij} c_i^\dagger c_j$$

$$\{c_i, c_j^\dagger\} = c_i c_j^\dagger + c_j^\dagger c_i = \delta_{ij}$$
$$\{c_i^\dagger, c_j^\dagger\} = \{c_i, c_j\} = 0$$

Jordan-Wigner mapping



$$c_i^\dagger c_j + c_j^\dagger c_i = X_i Z_{i-1} \ldots Z_{j+1} Y_j + Y_i Z_{i-1} \ldots Z_{j+1} X_j$$



IQM

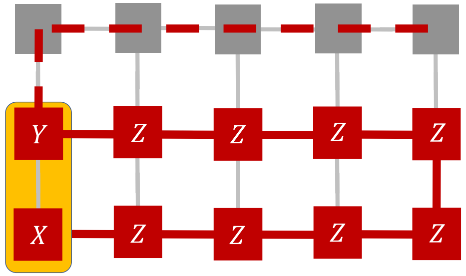
2. Fermion-to-qubit mappings

$$\{E_{ij}, V_i\} = \{E_{ij}, E_{jk}\} = 0$$
$$[E_{ij}, E_{kl}] = [E_{ij}, V_k] = [V_i, V_j] = 0$$
$$c_j^\dagger c_k + c_k^\dagger c_j \to \frac{i}{2}(V_k - V_j)E_{jk}$$

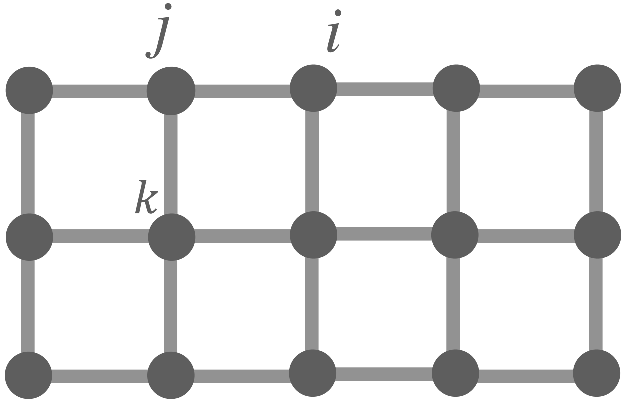
$$\mathcal{H}_{\mathrm{TB}} = \sum_{i,j} t^{ij} c_i^\dagger c_j$$

$$\{c_i, c_j^\dagger\} = c_i c_j^\dagger + c_j^\dagger c_i = \delta_{ij}$$
$$\{c_i^\dagger, c_j^\dagger\} = \{c_i, c_j\} = 0$$

Jordan-Wigner mapping



$$c_i^\dagger c_j + c_j^\dagger c_i = X_i Z_{i-1} \ldots Z_{j+1} Y_j + Y_i Z_{i-1} \ldots Z_{j+1} X_j$$



Local mappings

Bravyi-Kitaev mapping

Verstraete-Cirac mapping

Derby-Klassen mapping

⋮

Black arrows

2. Fermion-to-qubit mappings

$$\{E_{ij}, V_i\} = \{E_{ij}, E_{jk}\} = 0$$
$$[E_{ij}, E_{kl}] = [E_{ij}, V_k] = [V_i, V_j] = 0$$
$$c_j^\dagger c_k + c_k^\dagger c_j \to \frac{i}{2}(V_k - V_j)E_{jk}$$

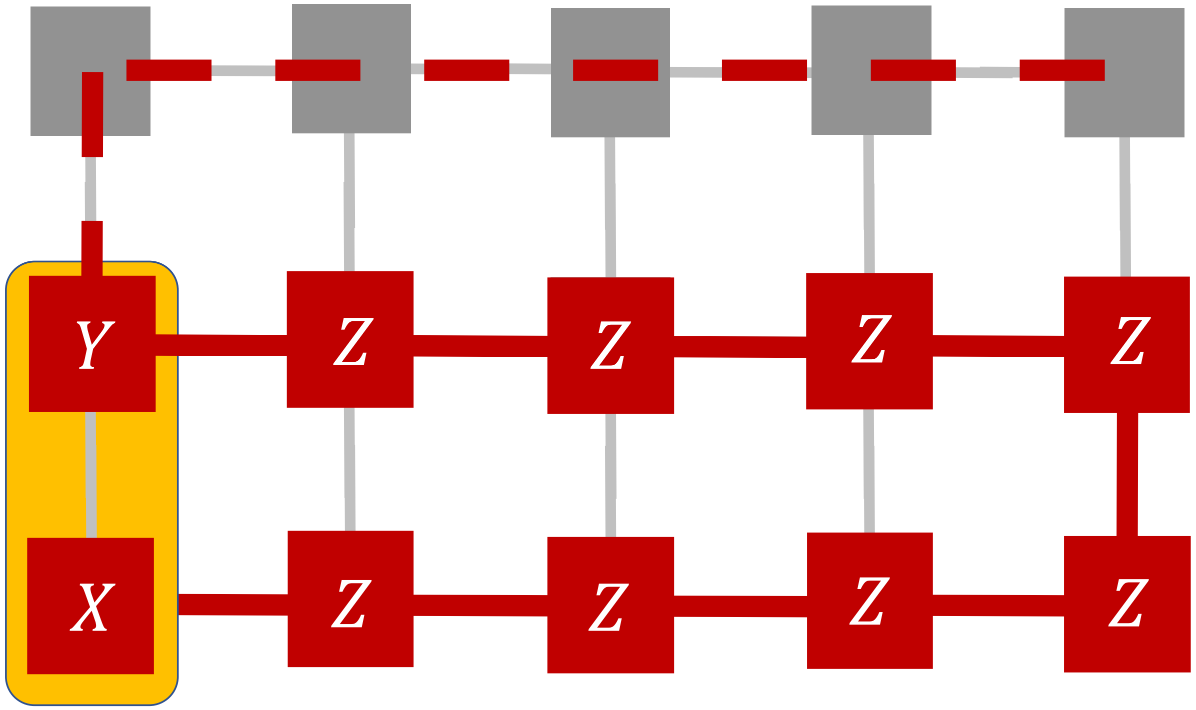
Local mappings

Bravyi-Kitaev mapping

Verstraete-Cirac mapping

Derby-Klassen mapping

⋮



IQM

2. Fermion-to-qubit mappings

$$\{E_{ij}, V_i\} = \{E_{ij}, E_{jk}\} = 0$$
$$[E_{ij}, E_{kl}] = [E_{ij}, V_k] = [V_i, V_j] = 0$$
$$c_j^\dagger c_k + c_k^\dagger c_j \to \frac{i}{2}(V_k - V_j)E_{jk}$$

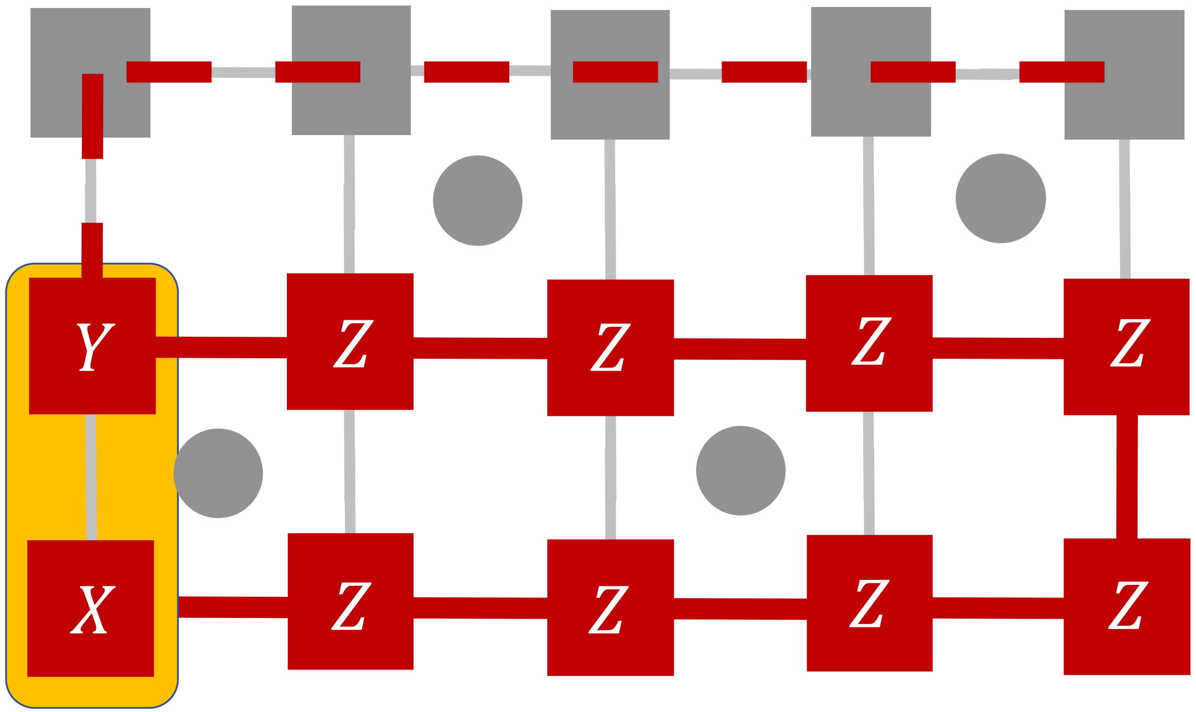
Local mappings

Bravyi-Kitaev mapping

Verstraete-Cirac mapping

Derby-Klassen mapping

⋮



IQM

2. Fermion-to-qubit mappings

$$\{E_{ij}, V_i\} = \{E_{ij}, E_{jk}\} = 0$$
$$[E_{ij}, E_{kl}] = [E_{ij}, V_k] = [V_i, V_j] = 0$$
$$c_j^\dagger c_k + c_k^\dagger c_j \rightarrow \frac{i}{2}(V_k - V_j)E_{jk}$$

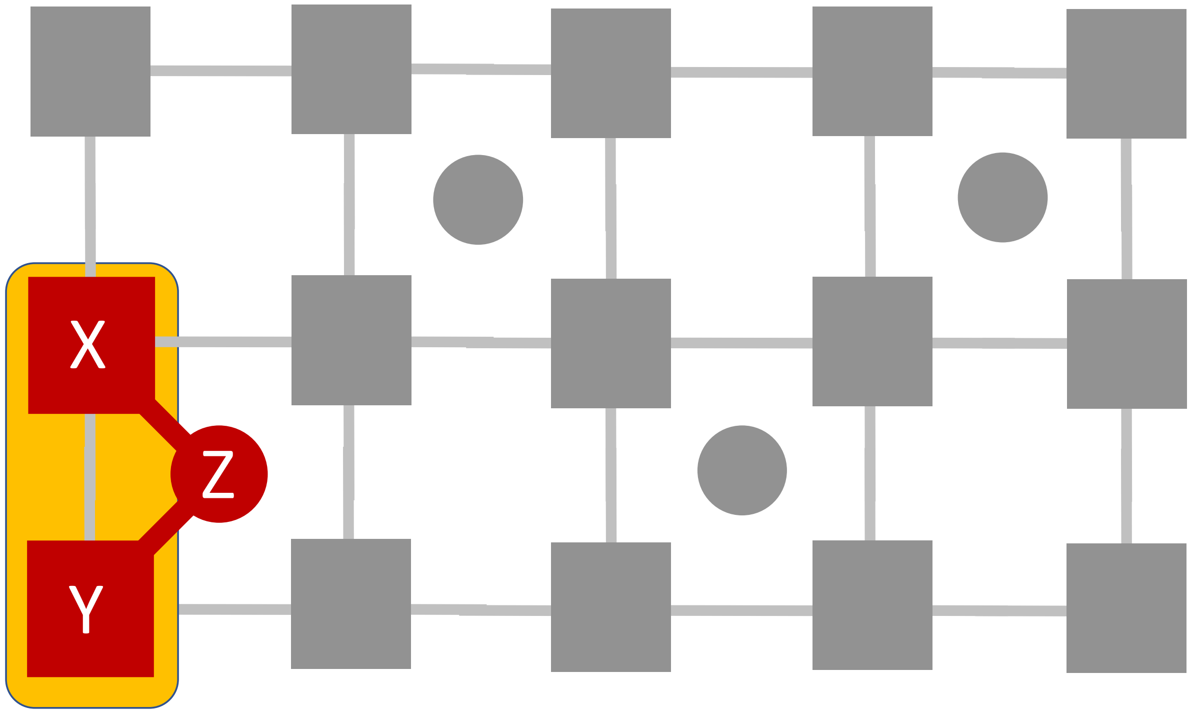
Local mappings

Bravyi-Kitaev mapping

Verstraete-Cirac mapping

Derby-Klassen mapping

⋮



C. Derby *et al.* Phys. Rev. Res. 104 (2021)

2. Fermion-to-qubit mappings

Why local mappings are better when no ATA couplings?

- Local fermionic operators ⟶ Local two-qubit gates
- Less depth
- Less number of gates
- Error correction/mitigation properties

I. D. Kivlichan *et al.* PRL (2018)

IQM

2. Fermion-to-qubit mappings

Why local mappings are better when no ATA couplings?

- Local fermionic operators ⟶ Local two-qubit gates
- Less depth
- Less number of gates
- Error correction/mitigation properties

But more ancillas? I prefer Jordan-Wigner

- Number of qubits are not the limiting step nowadays

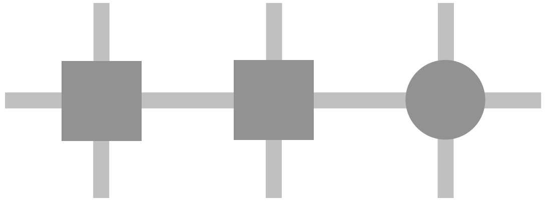
I. D. Kivlichan *et al.* PRL (2018)

IQM

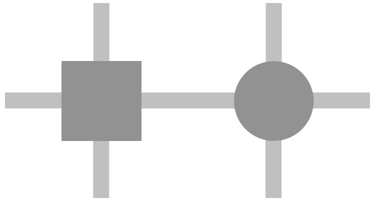
2. Fermion-to-qubit mappings

$$\{E_{ij}, V_i\} = \{E_{ij}, E_{jk}\} = 0$$
$$[E_{ij}, E_{kl}] = [E_{ij}, V_k] = [V_i, V_j] = 0$$
$$c_j^\dagger c_k + c_k^\dagger c_j \to \frac{i}{2}(V_k - V_j)E_{jk}$$

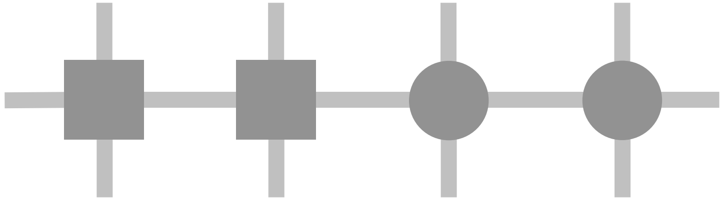
PPA



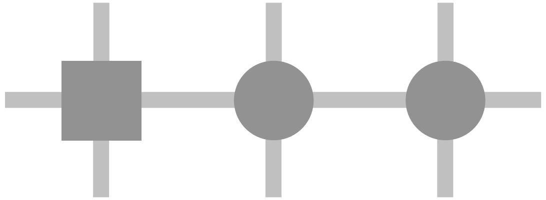
PA



PPAA



PAA

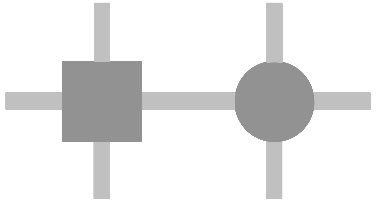


MA et al. (2023), arXiv:2302.01862

2. Fermion-to-qubit mappings

$$\{E_{ij}, V_i\} = \{E_{ij}, E_{jk}\} = 0$$
$$[E_{ij}, E_{kl}] = [E_{ij}, V_k] = [V_i, V_j] = 0$$
$$c_j^\dagger c_k + c_k^\dagger c_j \to \frac{i}{2}(V_k - V_j)E_{jk}$$

PA

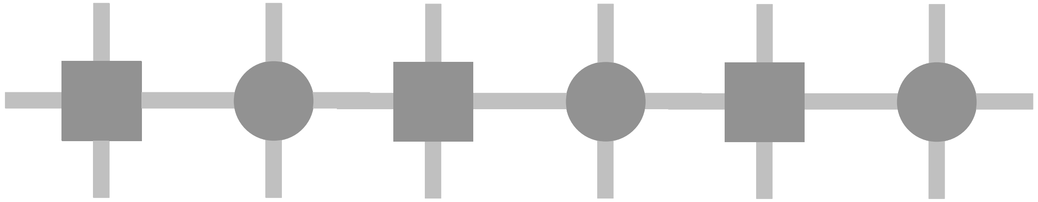


MA et al. (2023), arXiv:2302.01862

2. Fermion-to-qubit mappings

$$\{E_{ij}, V_i\} = \{E_{ij}, E_{jk}\} = 0$$
$$[E_{ij}, E_{kl}] = [E_{ij}, V_k] = [V_i, V_j] = 0$$
$$c_j^\dagger c_k + c_k^\dagger c_j \rightarrow \frac{i}{2}(V_k - V_j)E_{jk}$$

PA

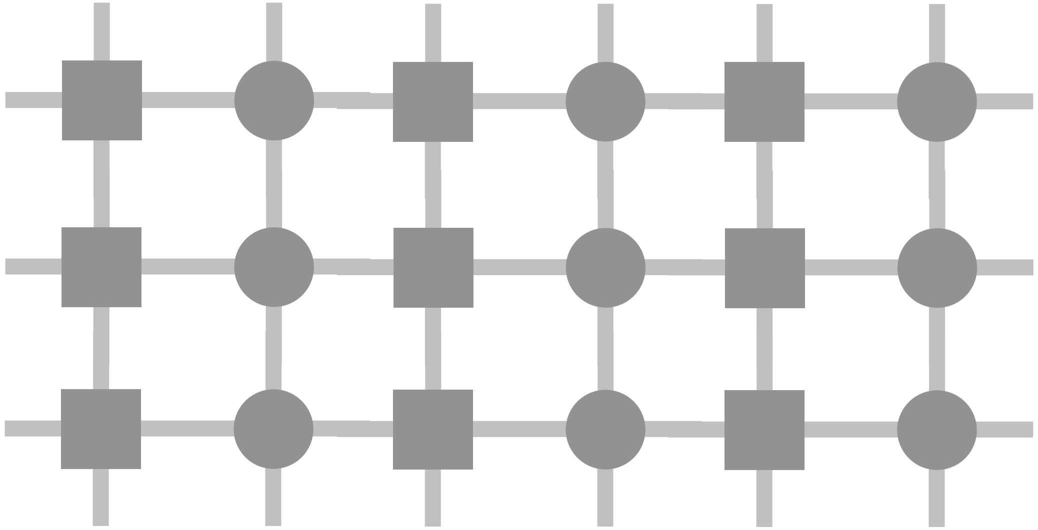


MA et al. (2023), arXiv:2302.01862

2. Fermion-to-qubit mappings

$$\{E_{ij}, V_i\} = \{E_{ij}, E_{jk}\} = 0$$
$$[E_{ij}, E_{kl}] = [E_{ij}, V_k] = [V_i, V_j] = 0$$
$$c_j^\dagger c_k + c_k^\dagger c_j \to \frac{i}{2}(V_k - V_j)E_{jk}$$

PA



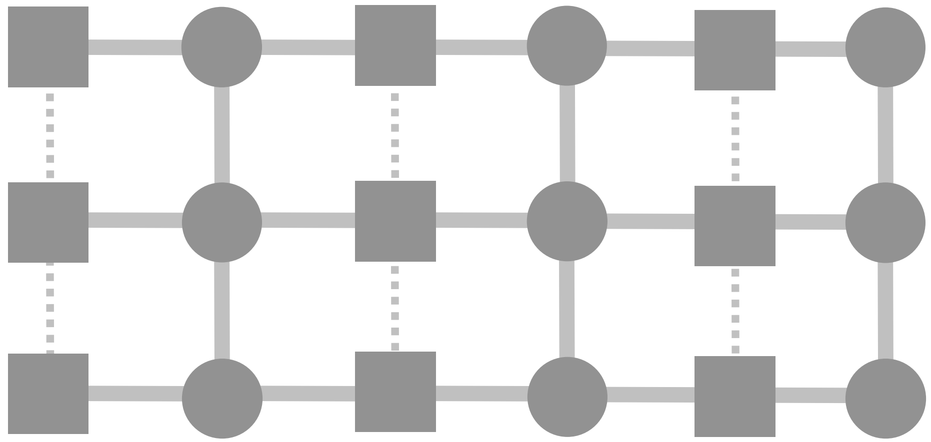
MA et al. (2023), arXiv:2302.01862

IQM

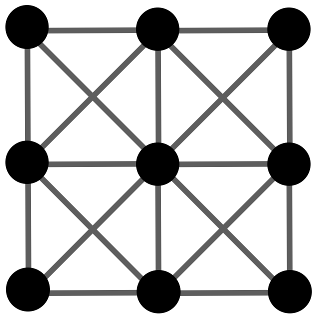
2. Fermion-to-qubit mappings

$$\{E_{ij}, V_i\} = \{E_{ij}, E_{jk}\} = 0$$
$$[E_{ij}, E_{kl}] = [E_{ij}, V_k] = [V_i, V_j] = 0$$
$$c_j^\dagger c_k + c_k^\dagger c_j \rightarrow \frac{i}{2}(V_k - V_j)E_{jk}$$

PA



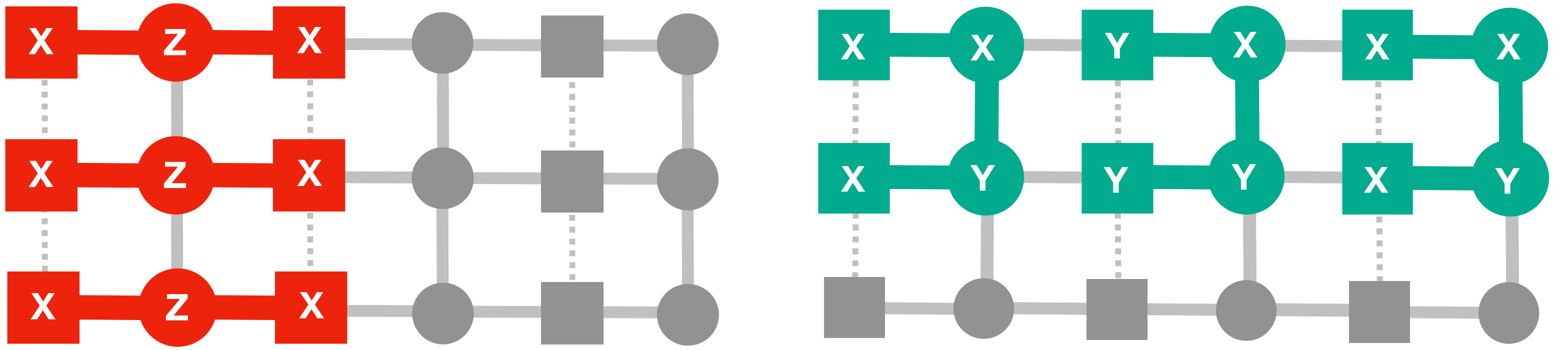
=



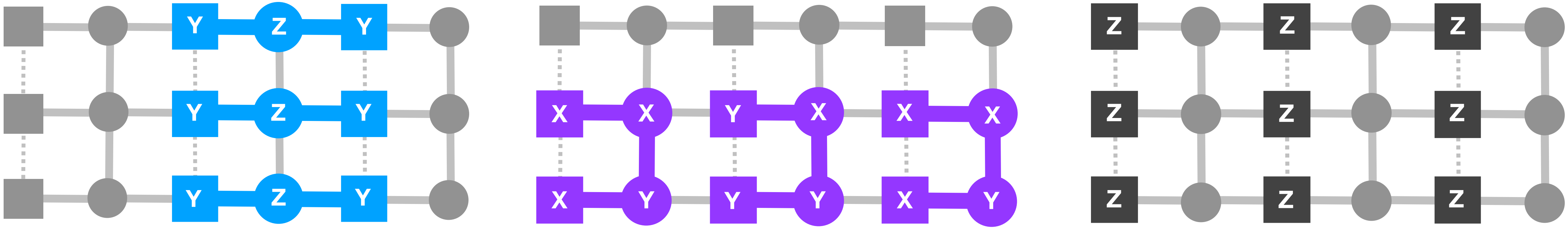
MA et al. (2023), arXiv:2302.01862

IQM

2. Fermion-to-qubit mappings



$$\{E_{ij}, V_i\} = \{E_{ij}, E_{jk}\} = 0$$
$$[E_{ij}, E_{kl}] = [E_{ij}, V_k] = [V_i, V_j] = 0$$
$$c_j^\dagger c_k + c_k^\dagger c_j \to \frac{i}{2}(V_k - V_j)E_{jk}$$

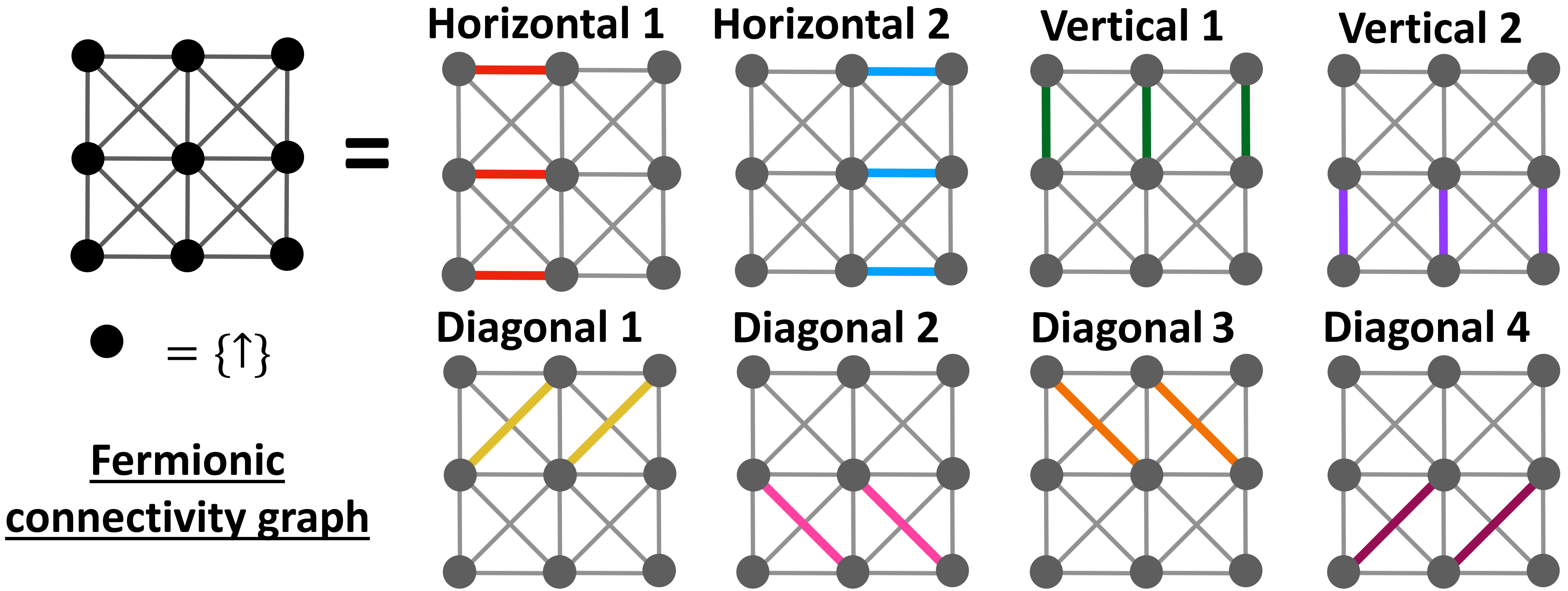


Edge operators

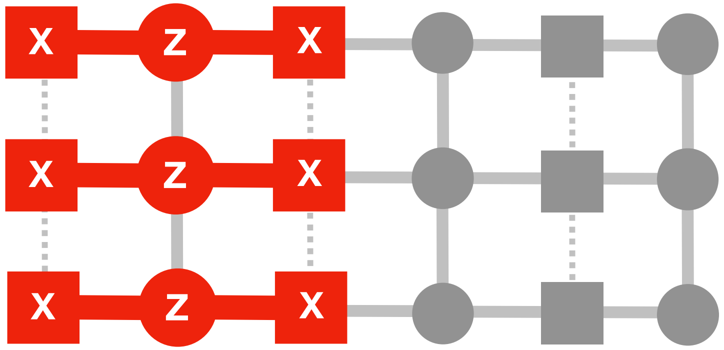
Vertex operators

2. Fermion-to-qubit mappings

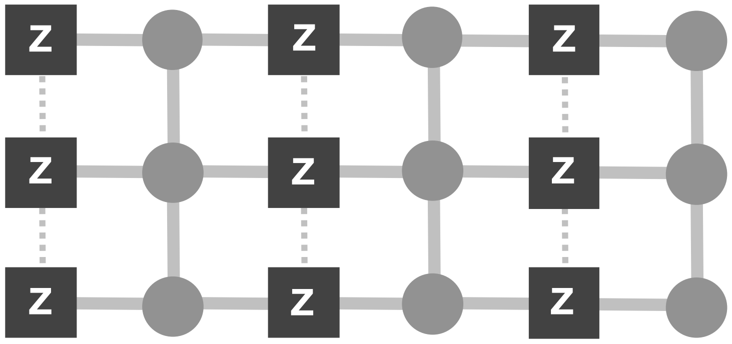
$$\{E_{ij}, V_i\} = \{E_{ij}, E_{jk}\} = 0$$
$$[E_{ij}, E_{kl}] = [E_{ij}, V_k] = [V_i, V_j] = 0$$
$$c_j^\dagger c_k + c_k^\dagger c_j \to \frac{i}{2}(V_k - V_j)E_{jk}$$



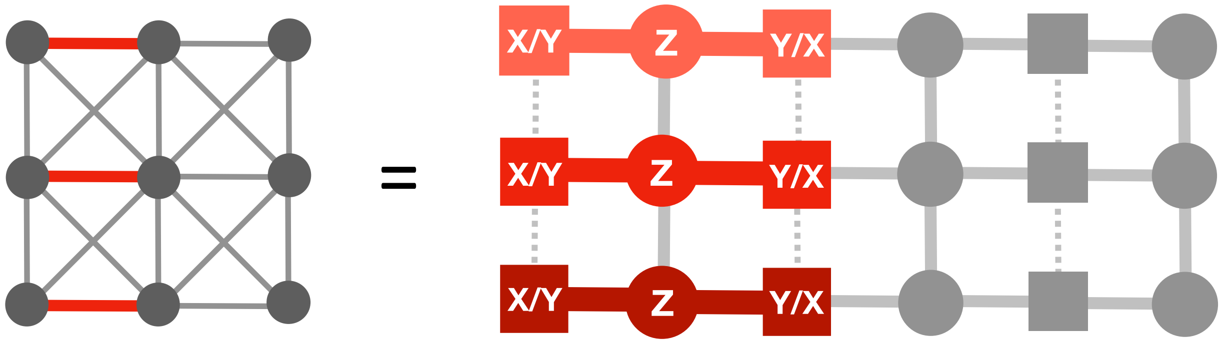
2. Fermion-to-qubit mappings



Edge operators



Vertex operators



Hopping operators

$$\{E_{ij}, V_i\} = \{E_{ij}, E_{jk}\} = 0$$

$$[E_{ij}, E_{kl}] = [E_{ij}, V_k] = [V_i, V_j] = 0$$

$$c_j^\dagger c_k + c_k^\dagger c_j \rightarrow \frac{i}{2}(V_k - V_j)E_{jk}$$

$$\downarrow$$

$$(Z_k - Z_j)X_k Z_a X_j$$

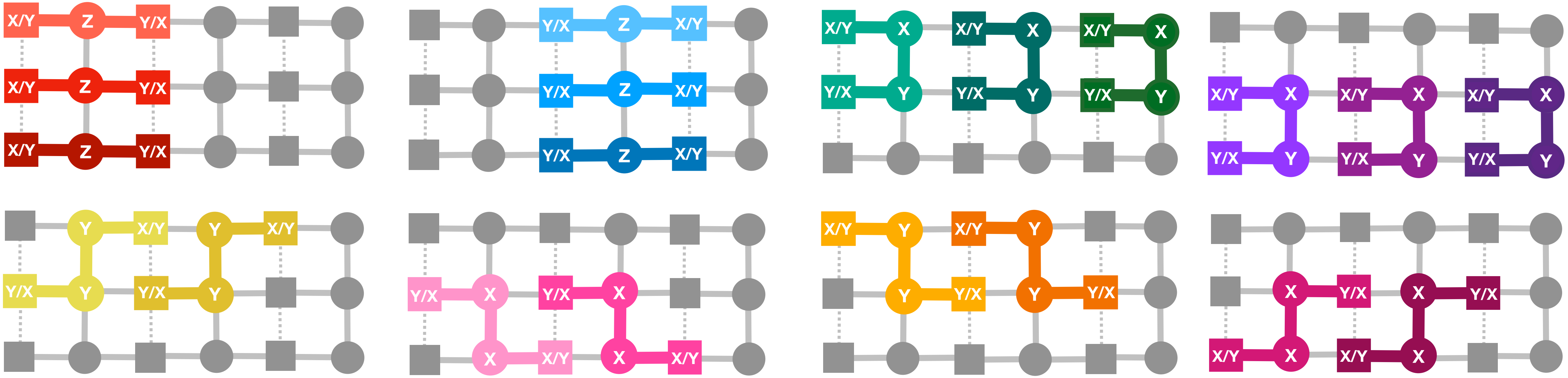
$$\downarrow$$

$$Y_k Z_a X_j + X_k Z_a Y_j$$

IQM

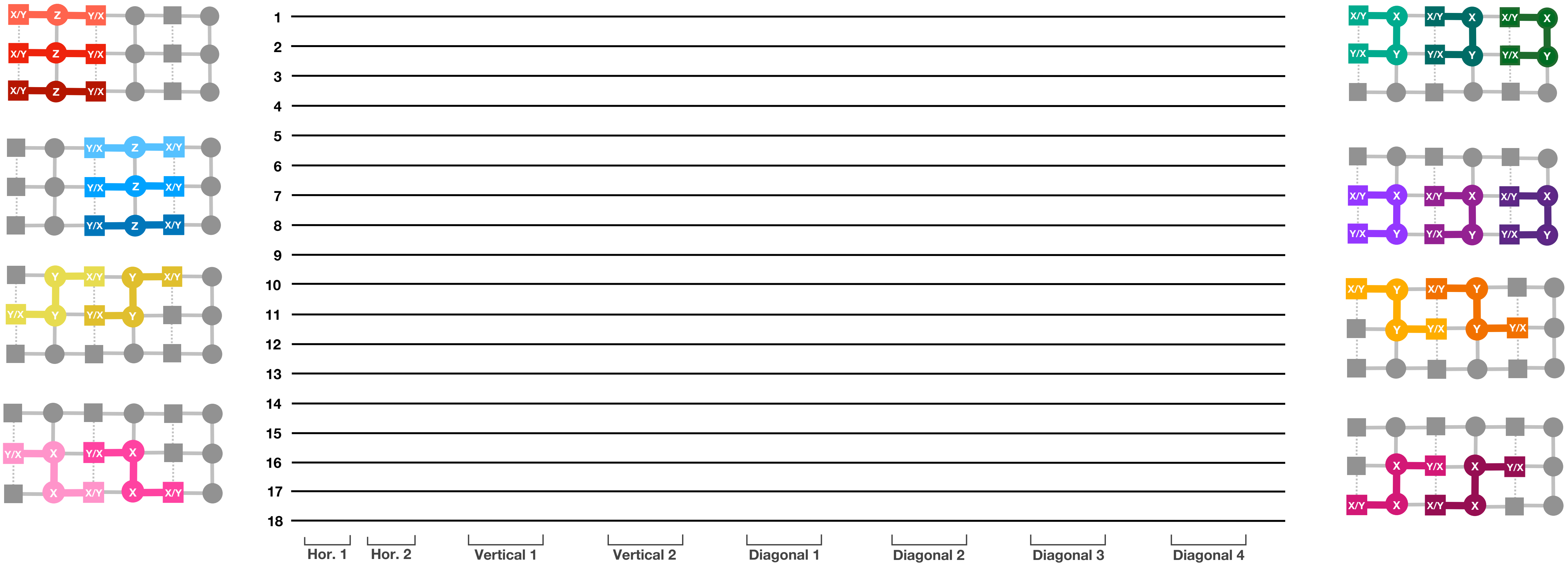
2. Fermion-to-qubit mappings

$$c_j^\dagger c_k + c_k^\dagger c_j \rightarrow \frac{i}{2}(V_k - V_j)E_{jk}$$

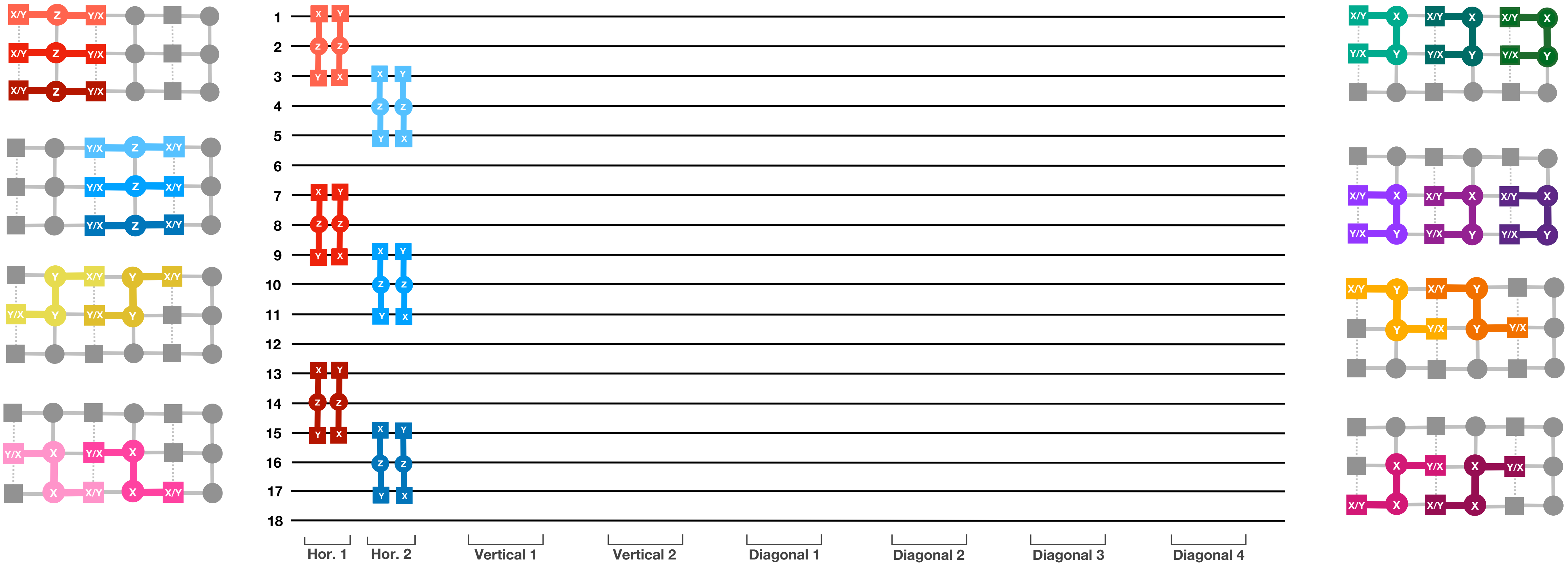


IQM

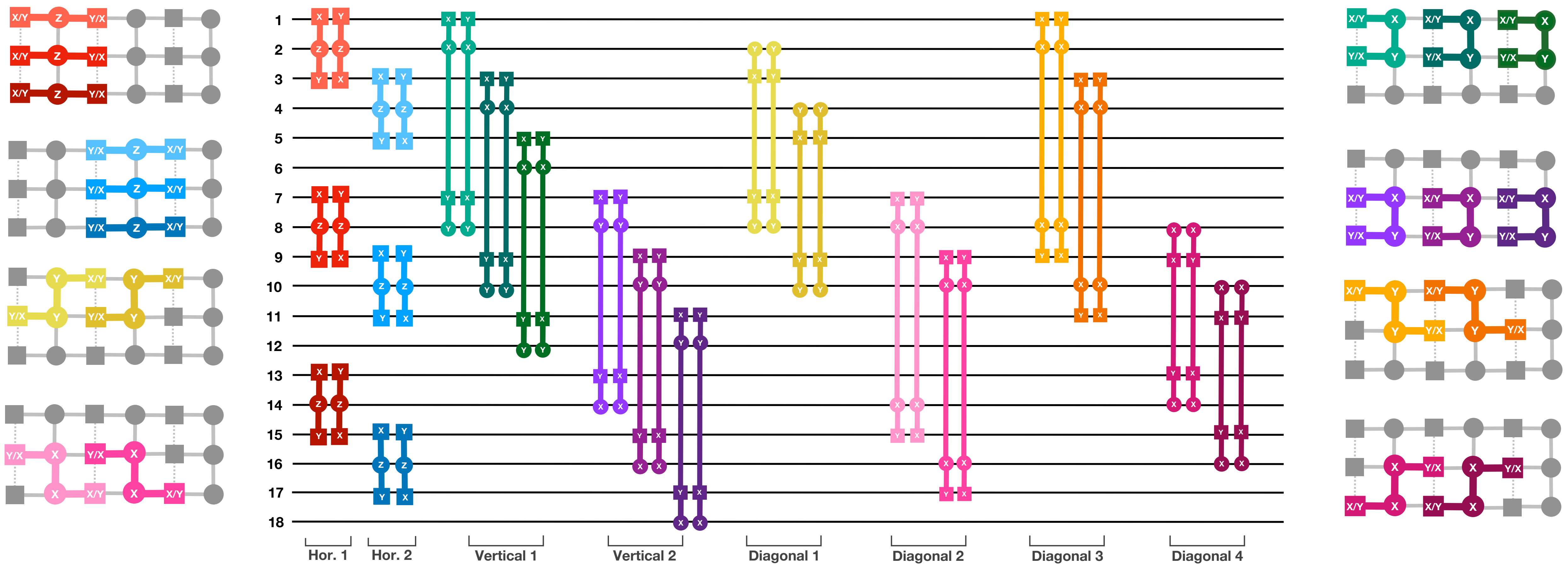
2. Fermion-to-qubit mappings



2. Fermion-to-qubit mappings



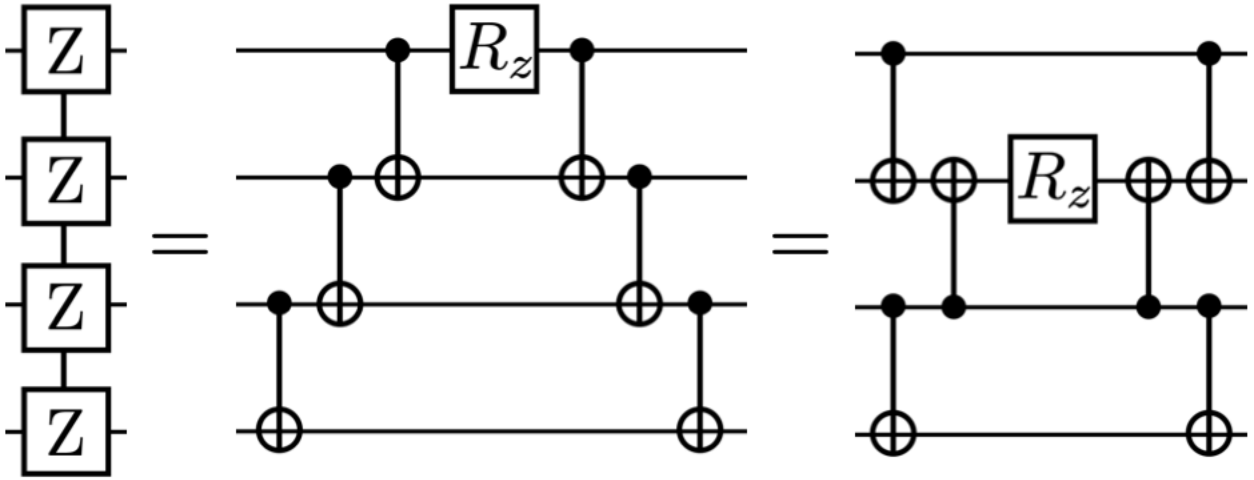
2. Fermion-to-qubit mappings



IQM

3. XYZ decomposition

$$e^{i\alpha Z_1 Z_2 Z_3 Z_4} =$$



Standard decomposition

3. XYZ decomposition

P. V. Sriluckshmy, MA et al. (2023) arXiv:2303.04498

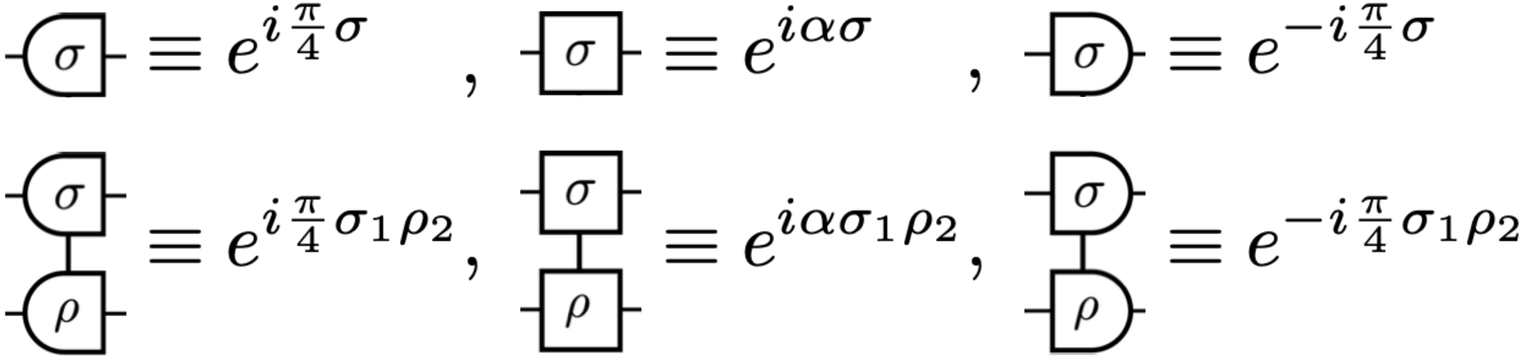
XYZ decomposition

$$e^{i\alpha\mathcal{O}} = e^{i\frac{\pi}{4}\mathcal{O}_1} e^{i\alpha\mathcal{O}_2} e^{-i\frac{\pi}{4}\mathcal{O}_1}$$

$$\mathcal{O} = \frac{i}{2}[\mathcal{O}_1, \mathcal{O}_2]$$

$$\mathcal{O}^2 = \mathbb{1}$$

Graphical notation



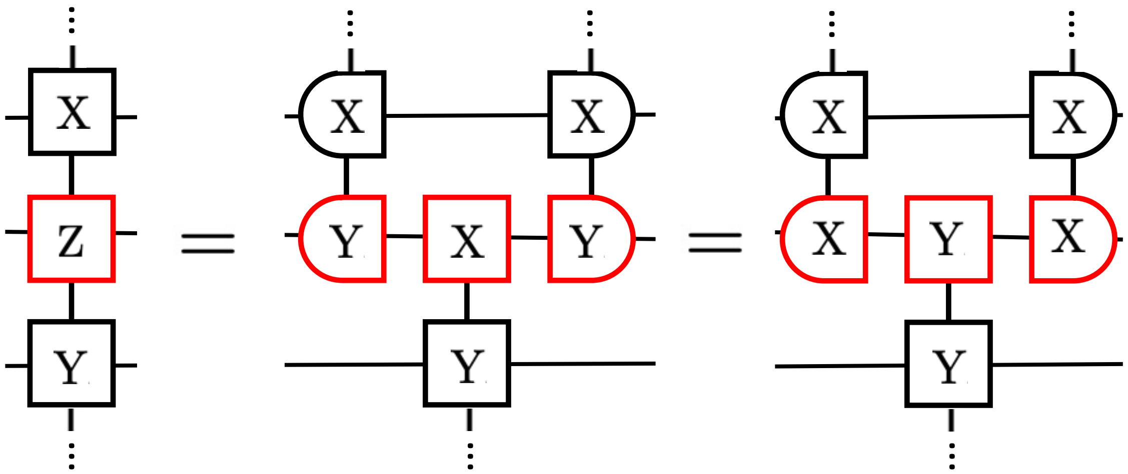
$$\equiv e^{i\frac{\pi}{4}\sigma}, \quad \equiv e^{i\alpha\sigma}, \quad \equiv e^{-i\frac{\pi}{4}\sigma}$$

$$\equiv e^{i\frac{\pi}{4}\sigma_1\rho_2}, \quad \equiv e^{i\alpha\sigma_1\rho_2}, \quad \equiv e^{-i\frac{\pi}{4}\sigma_1\rho_2}$$

IQM

3. XYZ decomposition

$$e^{i\alpha\mathcal{O}} = e^{i\frac{\pi}{4}\mathcal{O}_1} e^{i\alpha\mathcal{O}_2} e^{-i\frac{\pi}{4}\mathcal{O}_1}$$
$$\mathcal{O} = \frac{i}{2}[\mathcal{O}_1, \mathcal{O}_2]$$
$$\mathcal{O}^2 = \mathbb{1}$$

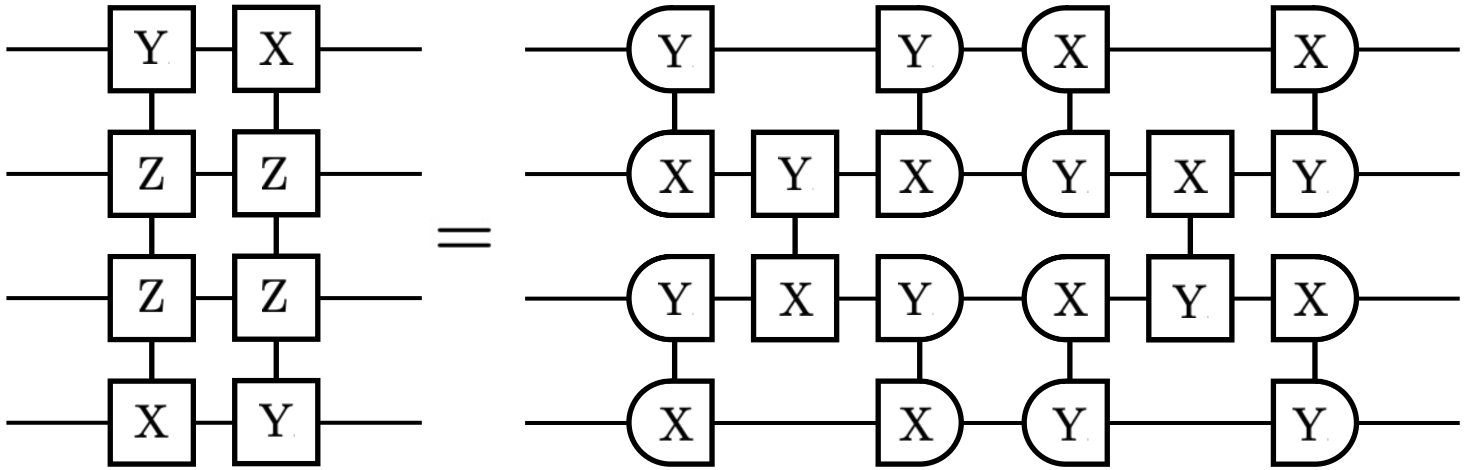


IQM

$$e^{i\alpha\mathcal{O}} = e^{i\frac{\pi}{4}\mathcal{O}_1} e^{i\alpha\mathcal{O}_2} e^{-i\frac{\pi}{4}\mathcal{O}_1}$$
$$\mathcal{O} = \frac{i}{2}[\mathcal{O}_1, \mathcal{O}_2]$$
$$\mathcal{O}^2 = \mathbb{1}$$

4. Fermionic Simulation

Hopping operators $c_j^\dagger c_k + c_k^\dagger c_j$



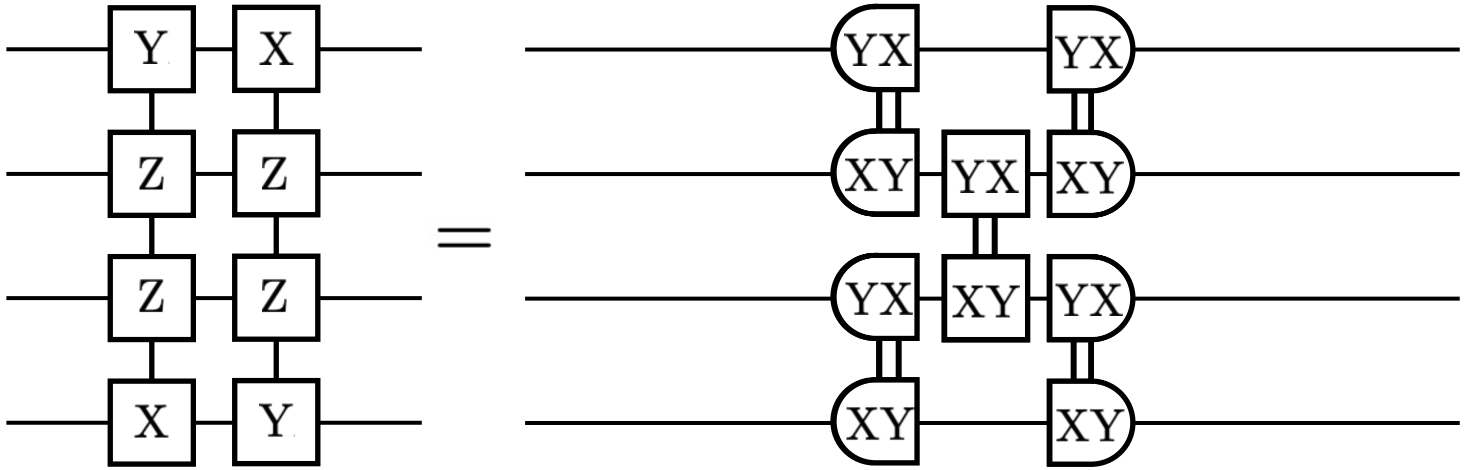
Remember we are using fSIM: $e^{i\frac{\theta}{2}(X_iX_j+Y_iY_j)+i\frac{\phi}{4}(Z_i+Z_j-Z_iZ_j)}$

IQM

$$e^{i\alpha\mathcal{O}} = e^{i\frac{\pi}{4}\mathcal{O}_1} e^{i\alpha\mathcal{O}_2} e^{-i\frac{\pi}{4}\mathcal{O}_1}$$
$$\mathcal{O} = \frac{i}{2}[\mathcal{O}_1, \mathcal{O}_2]$$
$$\mathcal{O}^2 = \mathbb{1}$$

4. Fermionic Simulation

Hopping operators $c_j^\dagger c_k + c_k^\dagger c_j$



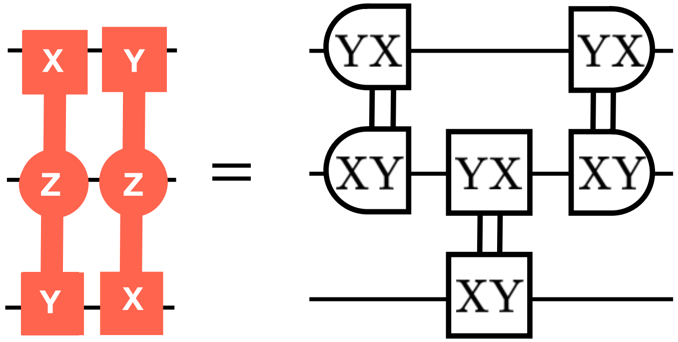
Remember we are using fSIM: $e^{i\frac{\theta}{2}(X_iX_j+Y_iY_j)+i\frac{\phi}{4}(Z_i+Z_j-Z_iZ_j)}$

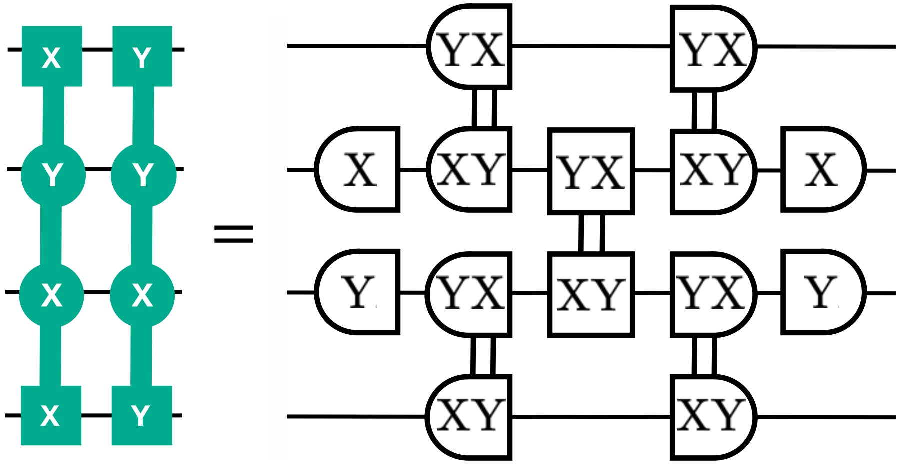
IQM

$$e^{i\alpha\mathcal{O}} = e^{i\frac{\pi}{4}\mathcal{O}_1} e^{i\alpha\mathcal{O}_2} e^{-i\frac{\pi}{4}\mathcal{O}_1}$$
$$\mathcal{O} = \frac{i}{2}[\mathcal{O}_1, \mathcal{O}_2]$$
$$\mathcal{O}^2 = \mathbb{1}$$

4. Fermionic Simulation

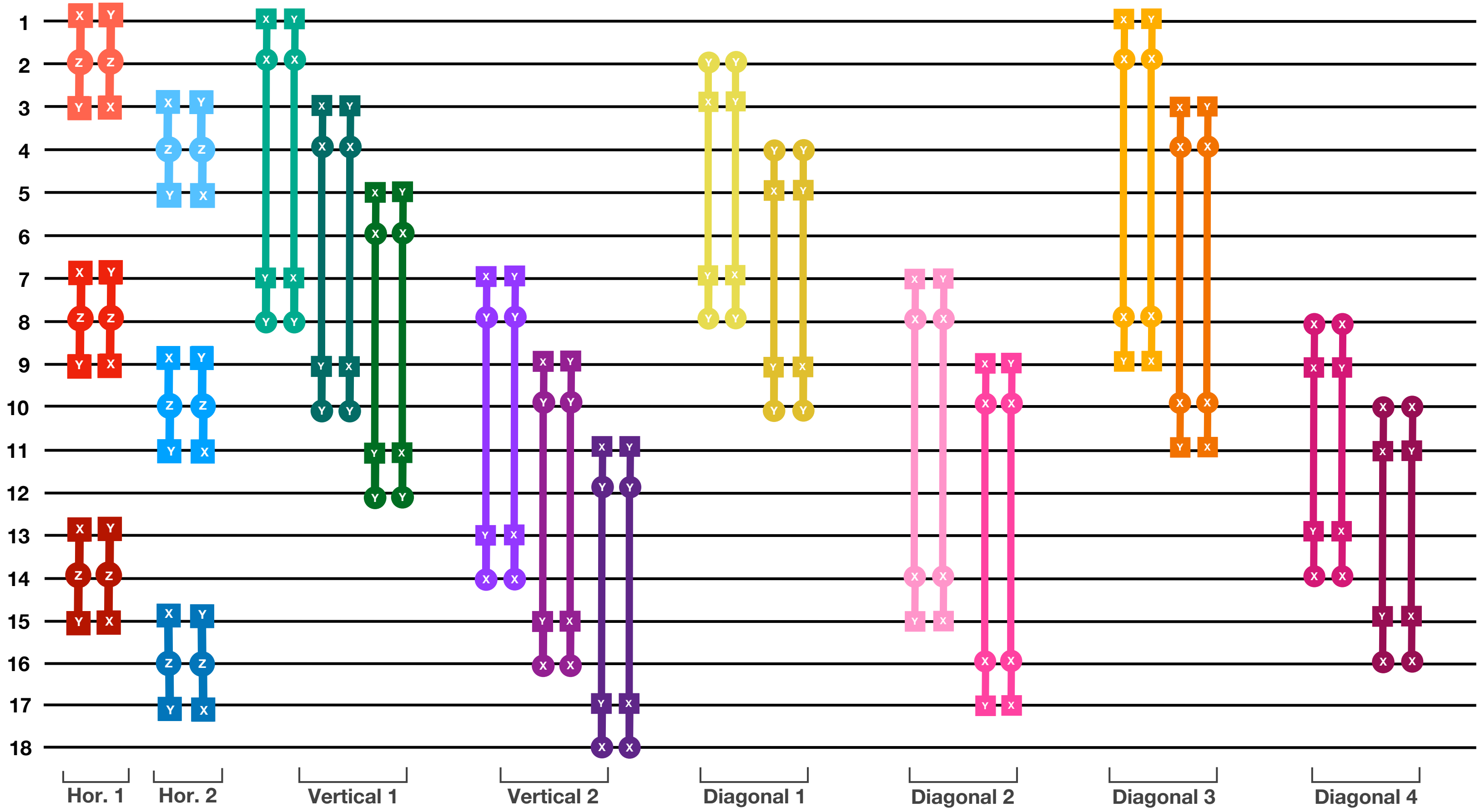
Hopping operators $c_j^\dagger c_k + c_k^\dagger c_j$





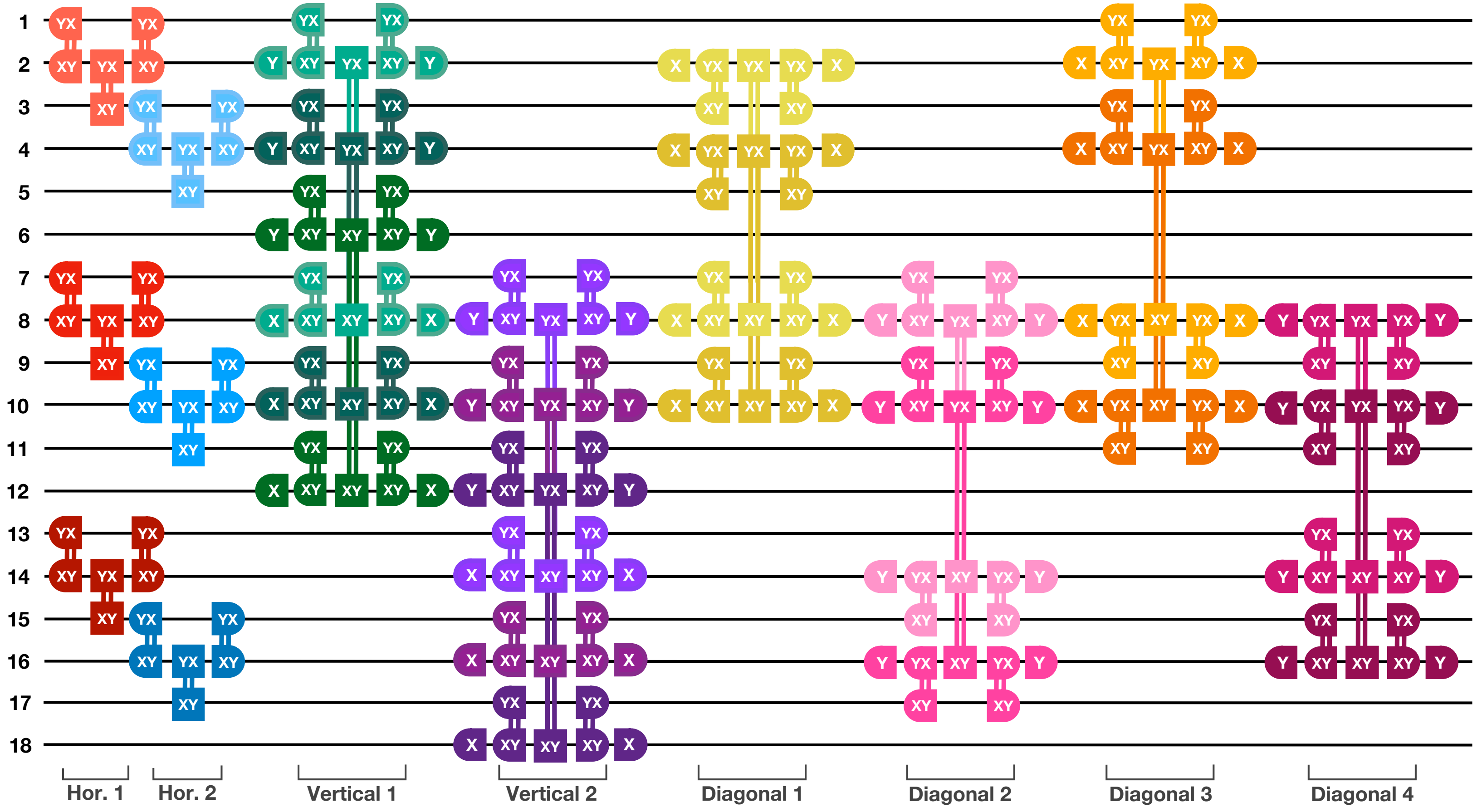
IQM

4. Fermionic Simulation



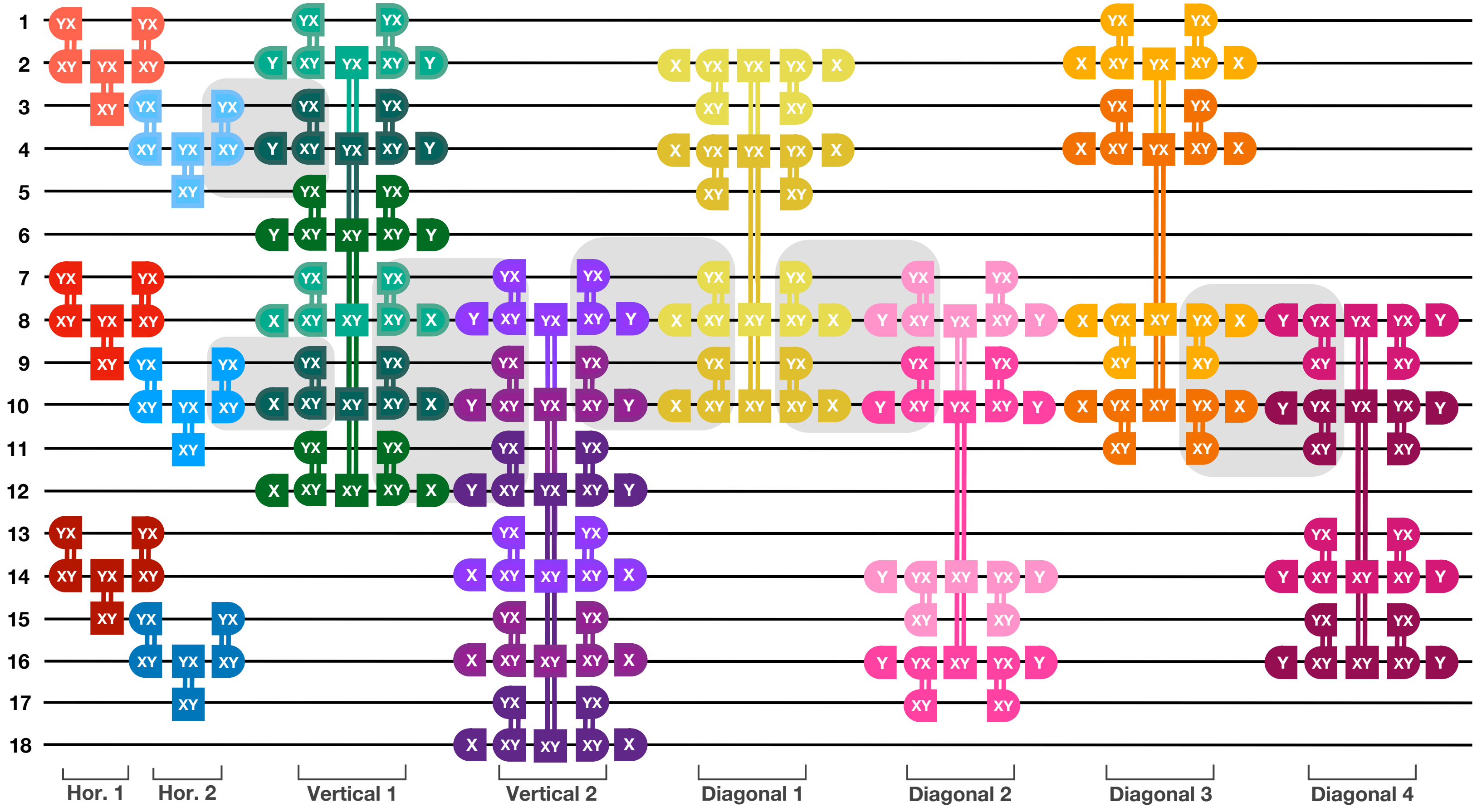
IQM

4. Fermionic Simulation

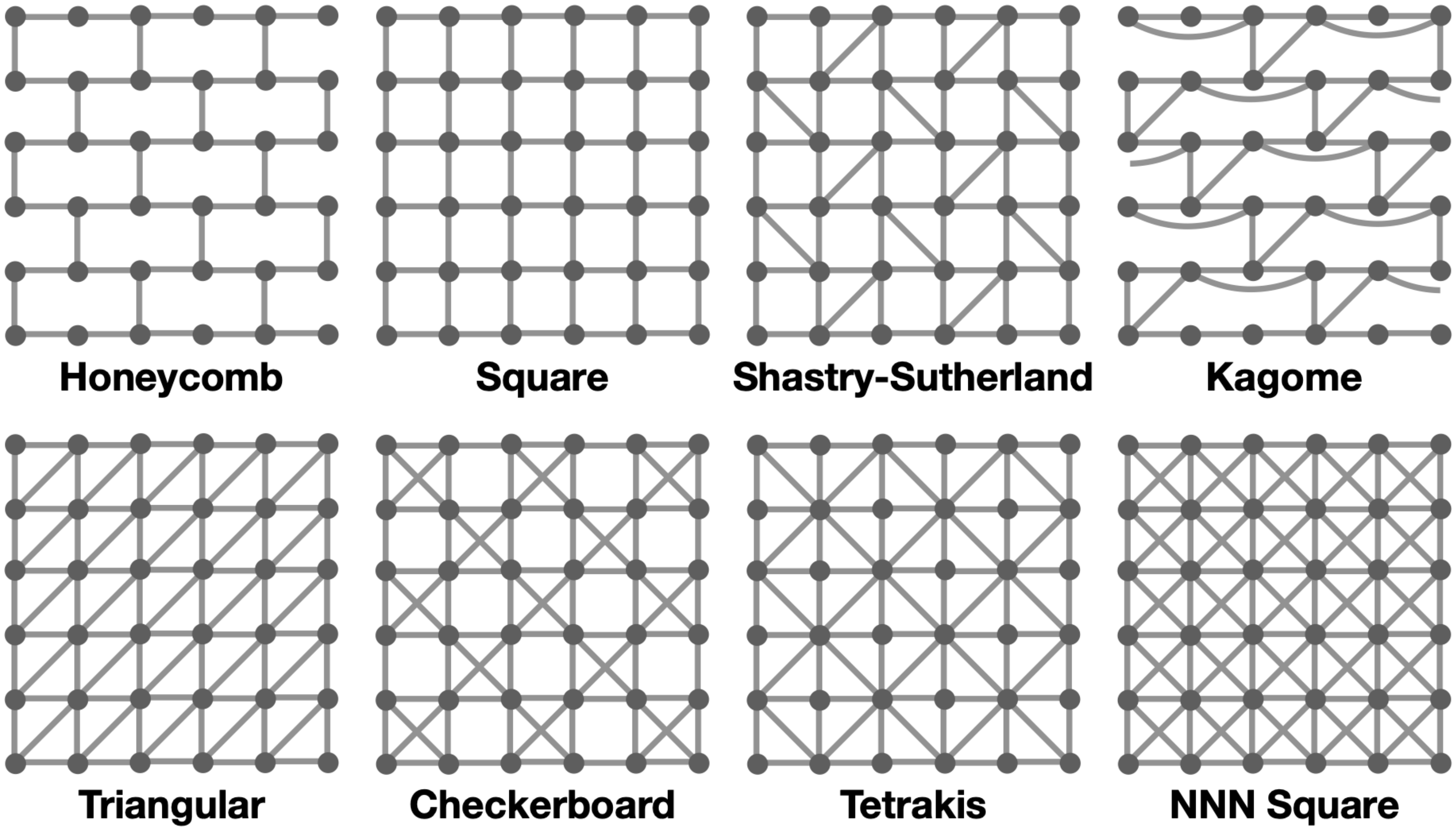


IQM

4. Fermionic Simulation



4. Fermionic Simulation

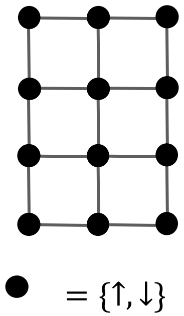


IQM

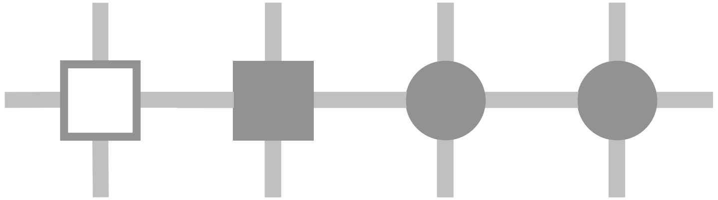
4. Fermionic Simulation

$$\mathcal{H}_{\mathrm{FH}} = \sum_{i,j,\sigma} t^{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Fermionic connectivity graph



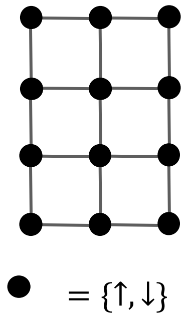
P̃AA



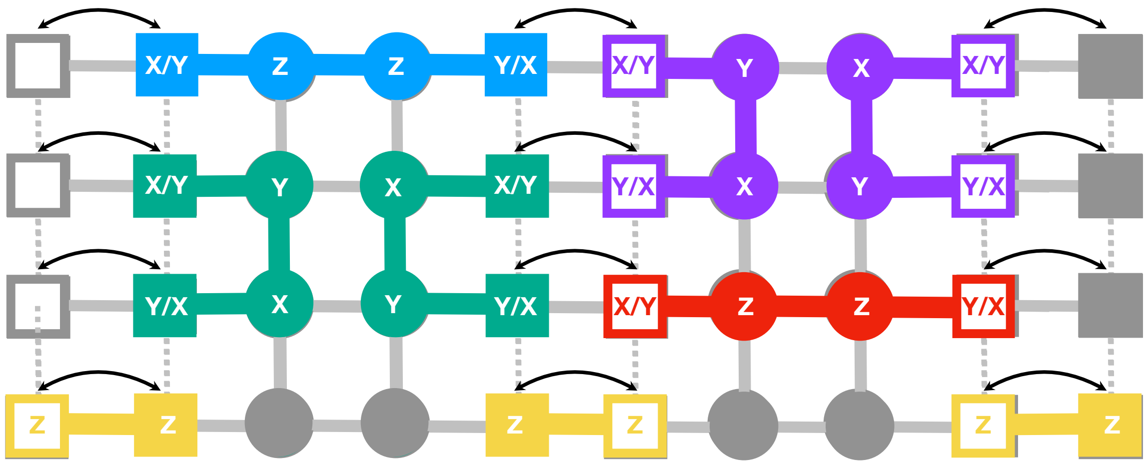
4. Fermionic Simulation

$$\mathcal{H}_{\mathrm{FH}} = \sum_{i,j,\sigma} t^{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Fermionic connectivity graph



Qubit layout

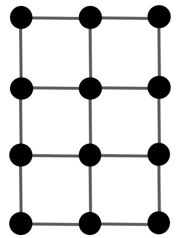


IQM

4. Fermionic Simulation

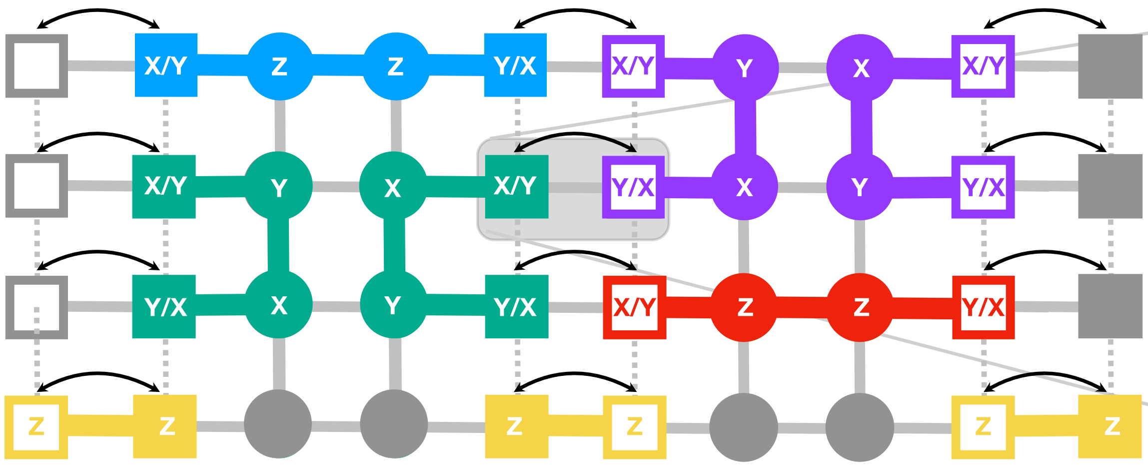
$$\mathcal{H}_{\mathrm{FH}} = \sum_{i,j,\sigma} t^{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Fermionic connectivity graph

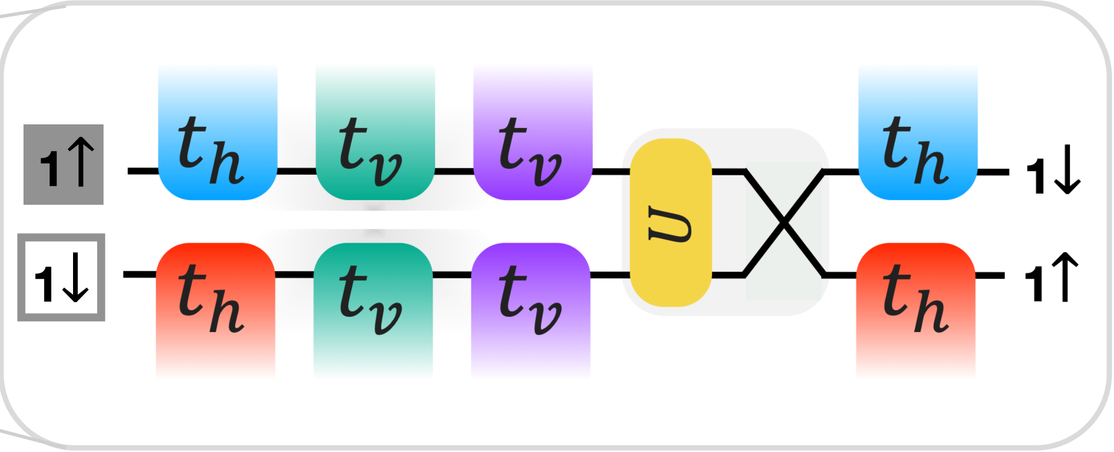


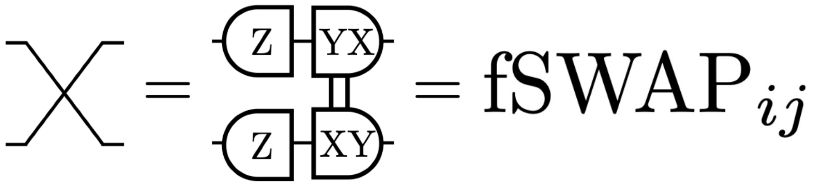
$= \{\uparrow, \downarrow\}$

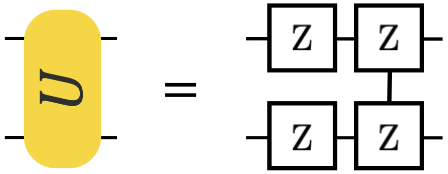
Qubit layout



Quantum circuit





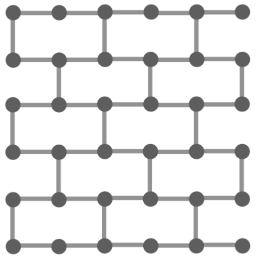


4. Fermionic Simulation

So, what's the improvement?

- Least number of TQGs with DK + XYZ decomposition
- Up to 72% depth reduction (3.2x).
- Shallowest single-Trotter-step circuits for these condensed matter Hamiltonians in literature:

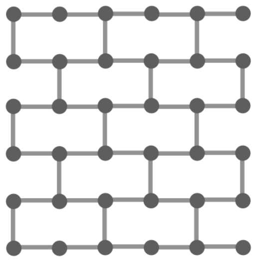
TB: 6



Honeycomb

● = {1↑}

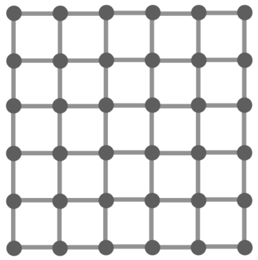
FH: 9



Honeycomb

● = {1↑, 1↓}

HK: 35



Square

● = {1↑, 1↓, 2↑, 2↓, 3↑, 3↓}

Thank you for your attention!

manuel.algaba@meetiqm.com
@ManuQPhys

IQM

Backup I

But, where is the advantage coming from?

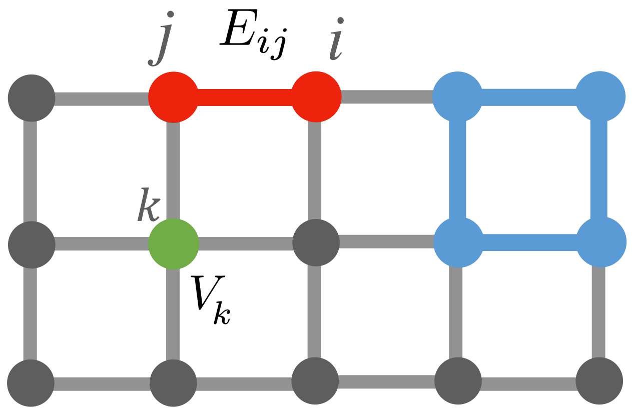
Decomp.	Native TQGs	TB NNN PA	FH NNN PAA	FH NNN DK	HK NN PAA
XYZ	fSIM	18	30	74	55
Standard	fSIM	31	68	97	84
XYZ	CNOT	31	53	125	100
Standard	CNOT	47	93	130	132

IQM

Backup II

$$\mathcal{H}_{\text{TB}} = \sum_{i,j} t^{ij} c_i^\dagger c_j$$

$$\{c_i, c_j^\dagger\} = c_i c_j^\dagger + c_j^\dagger c_i = \delta_{ij}$$
$$\{c_i^\dagger, c_j^\dagger\} = \{c_i, c_j\} = 0$$



Edge and vertex operators:

$$\{E_{ij}, V_i\} = \{E_{ij}, E_{jk}\} = 0$$
$$[E_{ij}, E_{kl}] = [E_{ij}, V_k] = [V_i, V_j] = 0$$

Eigenspace condition:

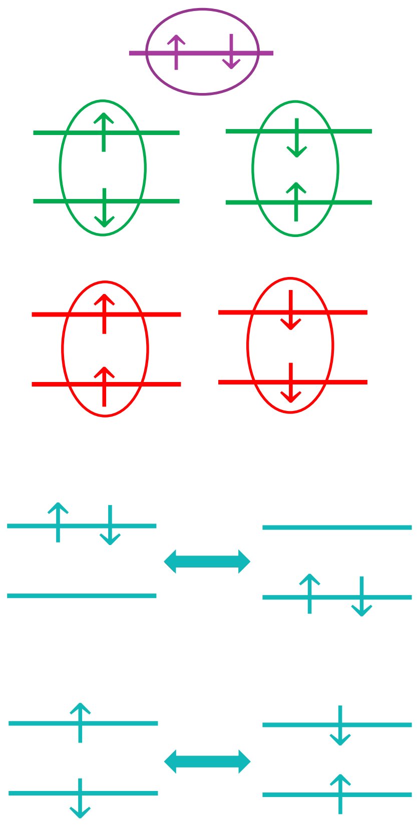
$$i^{(|p|-1)} \prod_{j}^{|p|-1} E_{p_j, p_{j+1}} = \mathbb{1}$$

S. B. Bravyi and A. Y. Kitaev, Ann. Phys. 298, 210 (2002)

Backup III

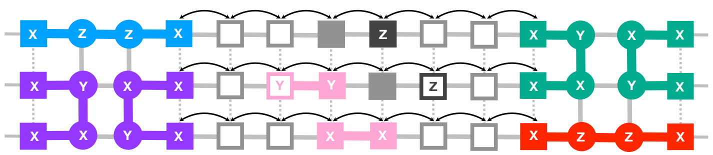
Hubbard-Kanamori Hamiltonian:

$$\mathcal{H}_{\mathrm{HK}} = \sum_{i,j,m,\sigma} t^{ijm\sigma} c^{\dagger}_{im\sigma} c_{jm\sigma} + \sum_{i,m} U^{im} n_{im\uparrow} n_{im\downarrow}$$
$$+ \sum_{i,m<\bar{m}} U_1^{im\bar{m}} \left(n_{im\uparrow} n_{i\bar{m}\downarrow} + n_{im\downarrow} n_{i\bar{m}\uparrow} \right)$$
$$+ \sum_{i,m<\bar{m}} U_2^{im\bar{m}} \left(n_{im\uparrow} n_{i\bar{m}\uparrow} + n_{im\downarrow} n_{i\bar{m}\downarrow} \right)$$
$$+ \sum_{i,m<\bar{m}} J^{im\bar{m}} \left(c^{\dagger}_{im\uparrow} c^{\dagger}_{im\downarrow} c_{i\bar{m}\downarrow} c_{i\bar{m}\uparrow} + c^{\dagger}_{i\bar{m}\uparrow} c^{\dagger}_{i\bar{m}\downarrow} c_{im\downarrow} c_{im\uparrow} \right.$$
$$\left. + c^{\dagger}_{im\uparrow} c^{\dagger}_{i\bar{m}\downarrow} c_{im\downarrow} c_{i\bar{m}\uparrow} + c^{\dagger}_{i\bar{m}\uparrow} c^{\dagger}_{im\downarrow} c_{i\bar{m}\downarrow} c_{im\uparrow} \right)$$



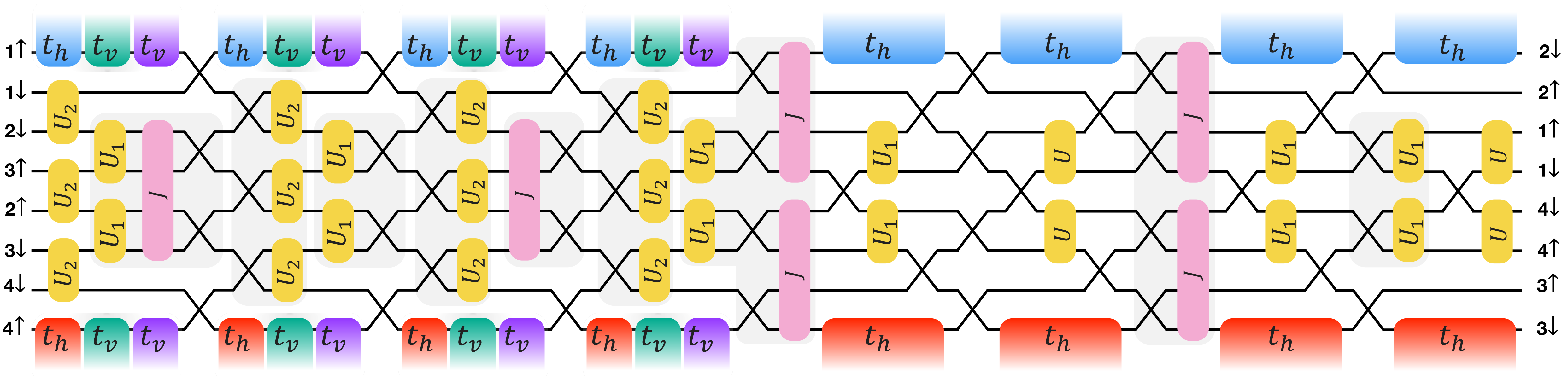
IQM

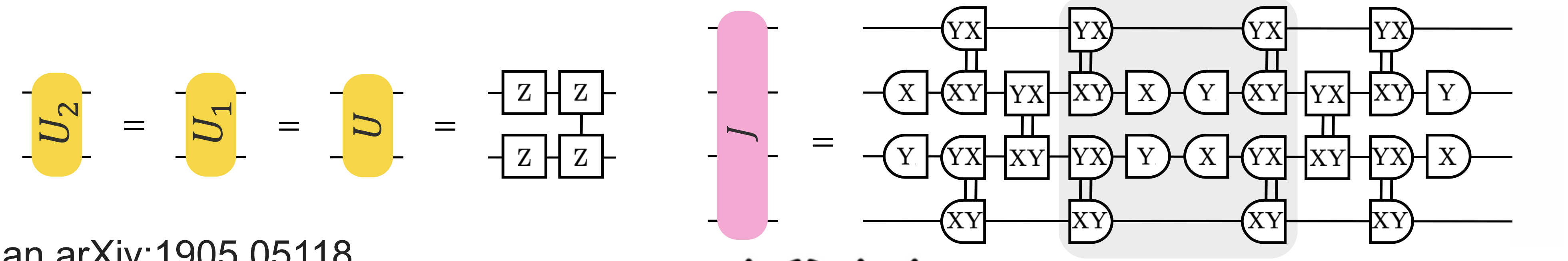
Backup IV



Qubit layout

Quantum circuit





B. O'Gorman arXiv:1905.05118