EFFICIENT QUANTUM CIRCUITS FOR BLOCK ENCODINGS OF A PAIRING HAMILTONIAN AND BEYOND

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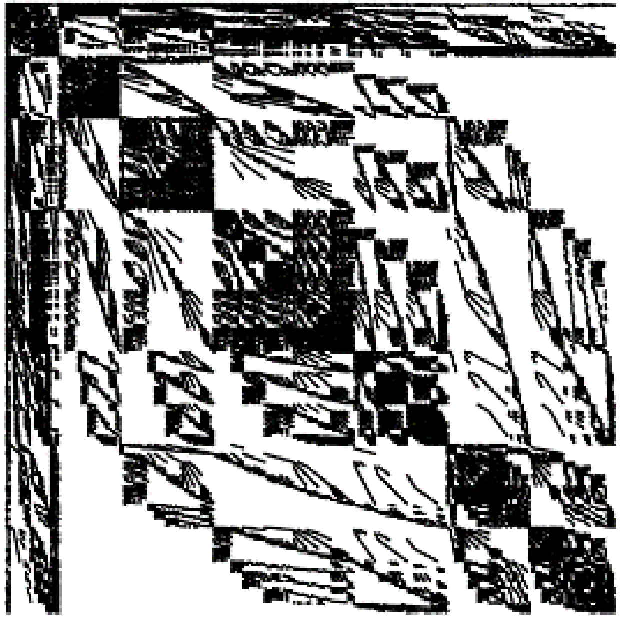
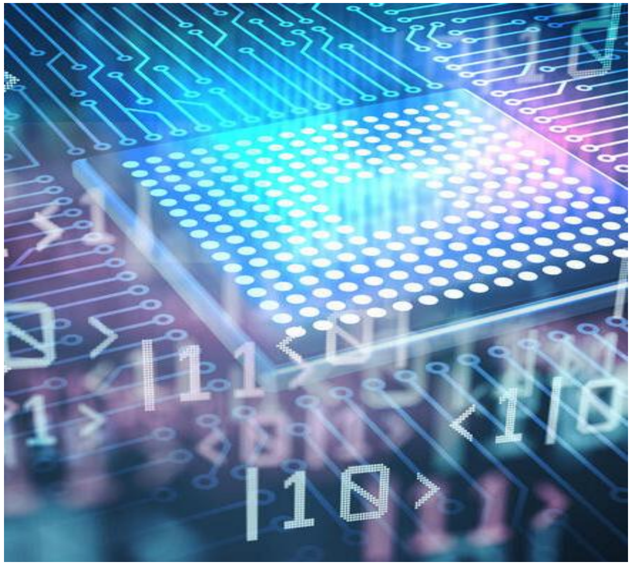
Outline

- Background and motivation
- General template for block encoding sparse matrices
- Examples
- Block encoding circuit for pairing Hamiltonian
- Generalization and further improvement

- D. Camps, L. Lin, R. Van Beeumen, C. Yang, "Explicit Quantum Circuits for Block Encodings of Certain Sparse Matrices", SIMAX, 45(1), 2024.
- D. Liu, W. Du, L. Lin, J. P. Vary and C. Yang, "An Efficient Quantum Circuit for Block Encoding a Pairing Hamiltonian", J. Comp. Sci, 85, 2025

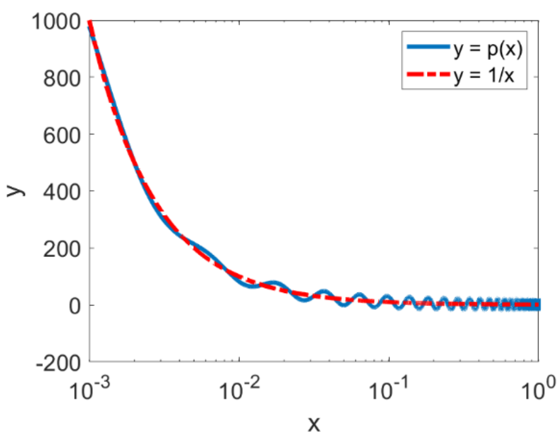


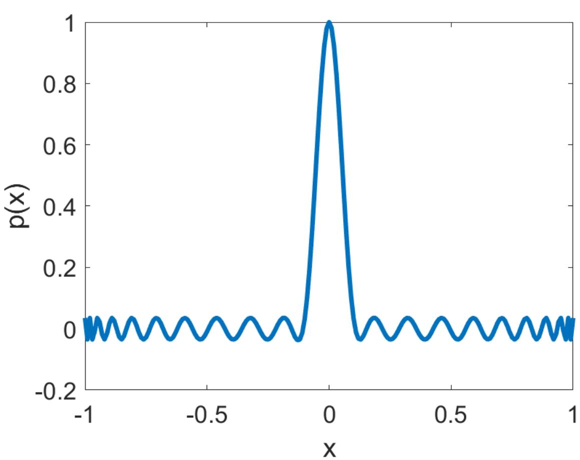


Sparse linear algebra and iterative methods

- Linear systems $Ax = b$, $A \in \mathbb{C}^{N\times N}$, $N = 2^n$
  - $x = A^{-1}b \approx p_k(A)b$
- Least squares $\min_x \|Ax - b\|_2$, $A \in \mathbb{C}^{m\times N}$, $N \geq m$
  - $x = A^{\dagger}b = (A^*A)^{-1}A^*b \approx p_k(A^*A)A^*b$
- Eigenvalue problem: $Ax = \lambda x$
  - $x \approx \delta(A - \lambda I)x_0 = p_k(A)x_0$

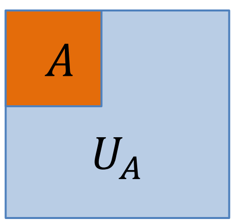
Iterative Methods: A is large but sparse or Av multiplication can be performed efficiently





Quantum (Sparse) Linear Algebra

- Challenge:
  - A is generally not unitary
  - Standard linear algebra operations are non-trivial on a quantum computer, e.g., axpy etc.
- Solution:
  - Embed properly scaled A into a much larger unitary U_A that can be decomposed into an efficient quantum circuit (block encoding)



$$\begin{pmatrix} A & * \\ * & * \end{pmatrix}\begin{pmatrix} \psi \\ 0 \end{pmatrix} = \begin{pmatrix} A\psi \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ * \end{pmatrix} = |0\rangle|A\psi\rangle + |1\rangle| *\rangle$$

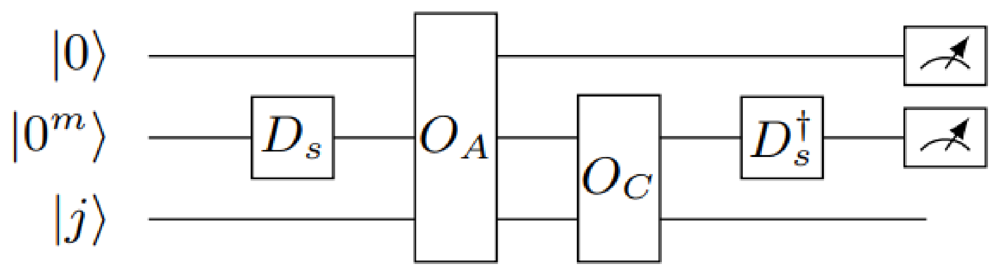
  - Embed $p(A)$ into a much larger unitary U (without forming $p(A)$ explicitly) that can be expressed in terms of U_A and $U_A^\dagger$ (quantum signal processing/quantum singular value transformation)
  - Apply $U_{p(A)}$ to a carefully prepared state, and make measurements

- Childs, Kathari and Somma, SIAM J. Comput, 2017
- Gilyén, Su, Low, and Wiebe, ACM SIGACT STOC., 2019

General template for block encoding for s-sparse A

- Matrix dimension: $N = 2^n$
- Each column of A has $s = 2^m$ nonzero elements (constant or poly(n))

U_A :



- $D_s|0^m\rangle = \frac{1}{\sqrt{s}}\sum_{\ell=0}^{s-1}|\ell\rangle$ (diffusion operator)
- $O_A|0\rangle|\ell\rangle|j\rangle = \left(A_{c(\ell,j),j}|0\rangle + \sqrt{1-\left|A_{c(\ell,j),j}\right|^2}|1\rangle\right)|\ell\rangle|j\rangle$ (numerical)

  $c(\ell, j)$: row index of the ℓth nonzero in the jth column

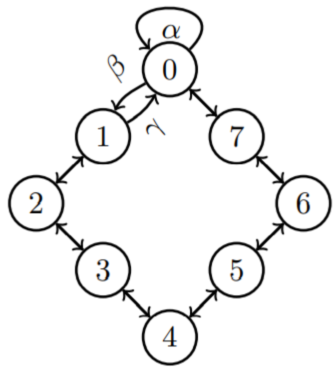
- $O_C|\ell\rangle|j\rangle = |\ell\rangle|c(\ell,j)\rangle$ (symbolic)
- Verify: $\langle 0|\langle 0^m|\langle i|U_A|0\rangle|0^m\rangle|j\rangle = \frac{1}{s}A_{ij}$

Gilyén, Su, Low, and Wiebe, ACM SIGACT STOC., 2019

Examples

Banded circulant matrix

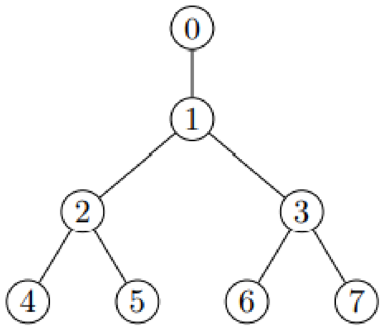
$$A = \begin{pmatrix} \alpha & \gamma & 0 & \cdots & \beta \\ \beta & \alpha & \ddots & \ddots & 0 \\ 0 & \beta & \ddots & \gamma & \vdots \\ \vdots & \ddots & \ddots & \alpha & \gamma \\ \gamma & 0 & \cdots & \beta & \alpha \end{pmatrix}$$



$$c(j,\ell) = \begin{cases} \mathrm{mod}(j-1,N) & \text{if } \ell = 0 \text{ (superdiagonal)}, \\ j & \text{if } \ell = 1 \text{ (diagonal) or } 3, \\ \mathrm{mod}(j+1,N) & \text{if } \ell = 2 \text{ (subdiagonal)}. \end{cases}$$

Extended binary tree

$$A = \begin{pmatrix} \gamma & \beta & & & & & & \\ \beta & \alpha & \beta & \beta & & & & \\ & \beta & \alpha & & \beta & \beta & & \\ & \beta & & \alpha & & & \beta & \beta \\ & & \beta & & \gamma & & & \\ & & \beta & & & \gamma & & \\ & & & \beta & & & \gamma & \\ & & & \beta & & & & \gamma \end{pmatrix}$$

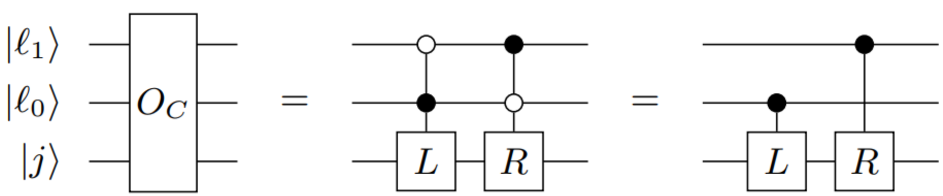


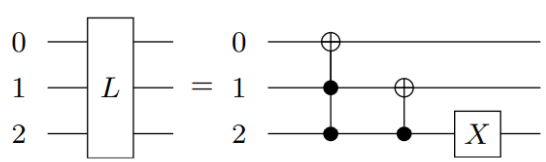
$$c(j,\ell) = \begin{cases} 2j & \text{if } \ell = 0 \text{ and } j < 2^{n-1} \text{ (left child)}, \\ 2j+1 & \text{if } \ell = 1 \text{ and } j < 2^{n-1} \text{ (right child)}, \\ j/2 & \text{if } \ell = 2 \text{ and } j \text{ even (parent)}, \\ (j-1)/2 & \text{if } \ell = 3 \text{ and } j \text{ odd (parent)}, \\ j & \text{if } 3 < \ell < 8 \text{ (diagonal)}, \end{cases}$$

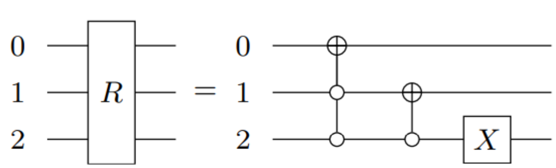
O_C circuits

Banded circulant matrix

$$c(j,\ell) = \begin{cases} j & \text{if } \ell = 0 \text{ (diagonal) or } 3, \\ \mathrm{mod}(j+1, N) & \text{if } \ell = 1 \text{ (subdiagonal)}, \\ \mathrm{mod}(j-1, N) & \text{if } \ell = 2 \text{ (superdiagonal)}, \end{cases}$$

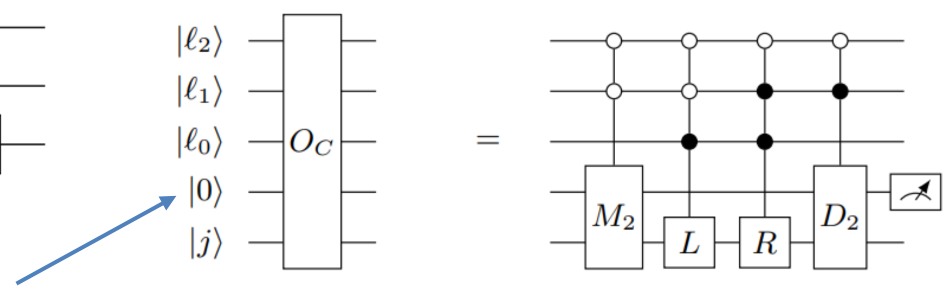




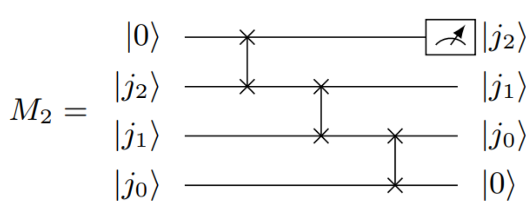


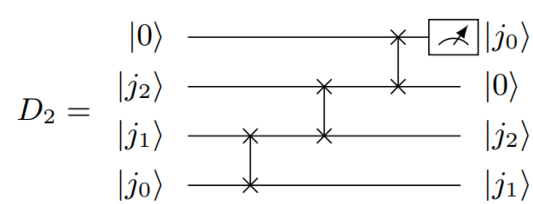
Extended binary tree

$$c(j,\ell) = \begin{cases} 2j & \text{if } \ell = 0 \text{ and } j < 2^{n-1} \text{ (left child)}, \\ 2j+1 & \text{if } \ell = 1 \text{ and } j < 2^{n-1} \text{ (right child)}, \\ j/2 & \text{if } \ell = 2 \text{ and } j \text{ even (parent)}, \\ (j-1)/2 & \text{if } \ell = 3 \text{ and } j \text{ odd (parent)}, \\ j & \text{if } 3 < \ell < 8 \text{ (diagonal)}, \end{cases}$$



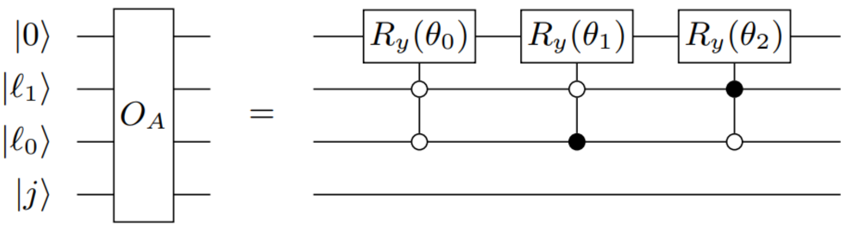
Additional ancilla qubit used to
1) Encode the fact that leaf nodes do not have children
2) Perform division only when j is even





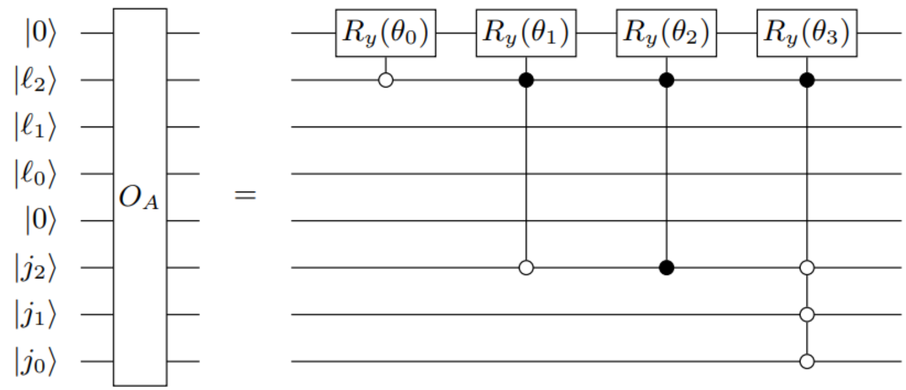
O_A circuits

Banded circulant matrix
(rotation independent of $|j\rangle$)



- $\theta_0 = 2\cos^{-1}\gamma$
- $\theta_1 = 2\cos^{-1}(1-\alpha)$
- $\theta_2 = 2\cos^{-1}\beta$

Extended binary tree
(Rotation depends on both $|\ell\rangle$ and $|j\rangle$)



- $\theta_0 = 2\cos^{-1}\beta$
- $\theta_1 = 2\cos^{-1}\frac{\alpha}{4}$
- $\theta_2 = 2\cos^{-1}\frac{\gamma}{4}$
- $\theta_3 = 2\cos^{-1}(\frac{\gamma}{4}-\frac{\beta}{2})$

$$\langle 0|\langle 0^m|\langle i|U_A|0\rangle|0^m\rangle|j\rangle = \frac{1}{s}A_{ij}$$

Pairing Hamiltonian

- Fermionic Hamiltonian in second quantization

$$\mathcal{H} = \sum_{i,j} h_{i,j}\, c_i^\dagger c_j + \sum_{i<j,k<l} g_{i,j,k,l}\, c_i^\dagger\, c_j^\dagger\, c_k\, c_l$$

- Pairing Hamiltonian

$$\mathcal{H} = \sum_{p=0}^{n-1} \sum_{q=0}^{n-1} g_{2p,2p+1,2q,2q+1}\, c_{2p}^\dagger\, c_{2p+1}^\dagger\, c_{2q}\, c_{2q+1}$$

  - Simplified model used in nuclear physics to model pairwise correlations among nucleons

- Simplified representation

$$\mathcal{H} = \sum_{p=0}^{n-1} \sum_{q=0}^{n-1} v_{p,q}\, a_p^\dagger\, a_q$$

Pseudo creation/annihilation: $a_p^\dagger \equiv\ c_{2p}^\dagger\ c_{2p+1}^\dagger,\ \ a_q \equiv c_{2q}\ c_{2q+1}$

O_C for Pairing Hamiltonian

- The sparsity structure of $H = \sum_{p=0}^{n-1} \sum_{q=0}^{n-1} v_{p,q}\, a_p^\dagger\, a_q$ is determined by $\sum_{p=0}^{n-1} \sum_{q=0}^{n-1} a_p^\dagger\, a_q$
- $|j\rangle = |j_0 j_1 \cdots j_{m-1}\rangle,\ j_i \in \{0,1\}$
- $a_p^\dagger\, a_q |j\rangle = 0$ unless $|j\rangle_\mathrm{p} = |0\rangle$ and $|j\rangle_\mathrm{q} = |1\rangle$
- If $|j\rangle_\mathrm{p} = |0\rangle$ and $|j\rangle_\mathrm{q} = |1\rangle$

$$\left[a_p^\dagger\, a_q |j\rangle\right]_p = |1\rangle,\ \left[a_p^\dagger\, a_q |j\rangle\right]_q = |0\rangle$$

i.e., $a_p^\dagger\, a_q |j\rangle$ simply swaps the p-th and q-th qubits of $|j\rangle$

- Define $l \equiv (p, q)$ and $c(l, j)$ as

$$c(l,j) = \begin{cases} \mathrm{SWAP}(j; p, q), & \text{if } |j\rangle_\mathrm{p} = |0\rangle \text{ and } |j\rangle_\mathrm{q} = |1\rangle \\ \text{invalid}, & \text{otherwise} \end{cases}$$

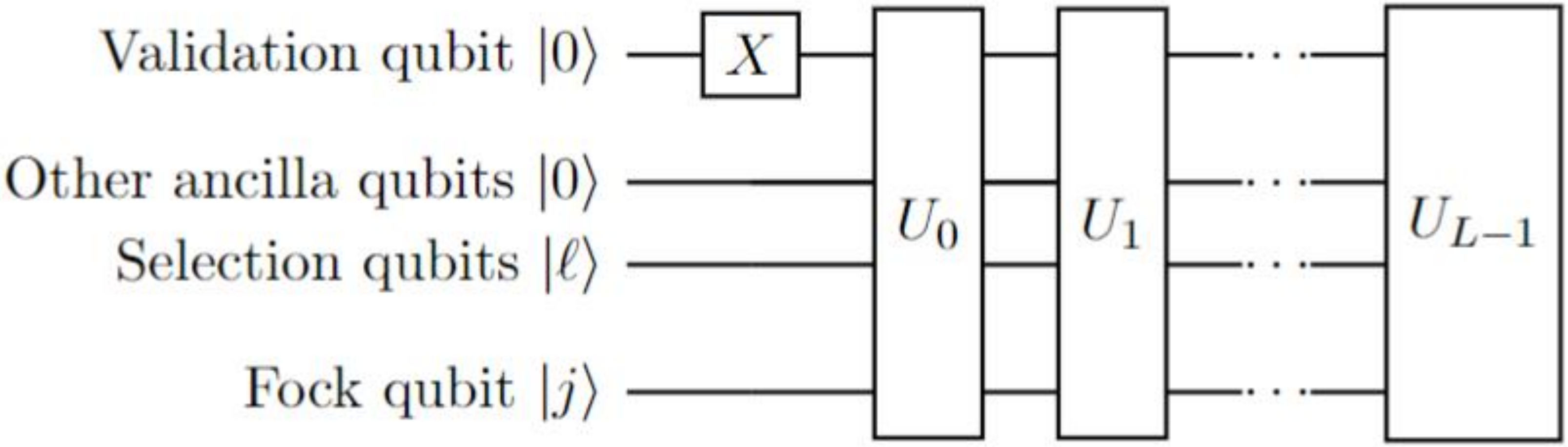
O_C as a select oracle

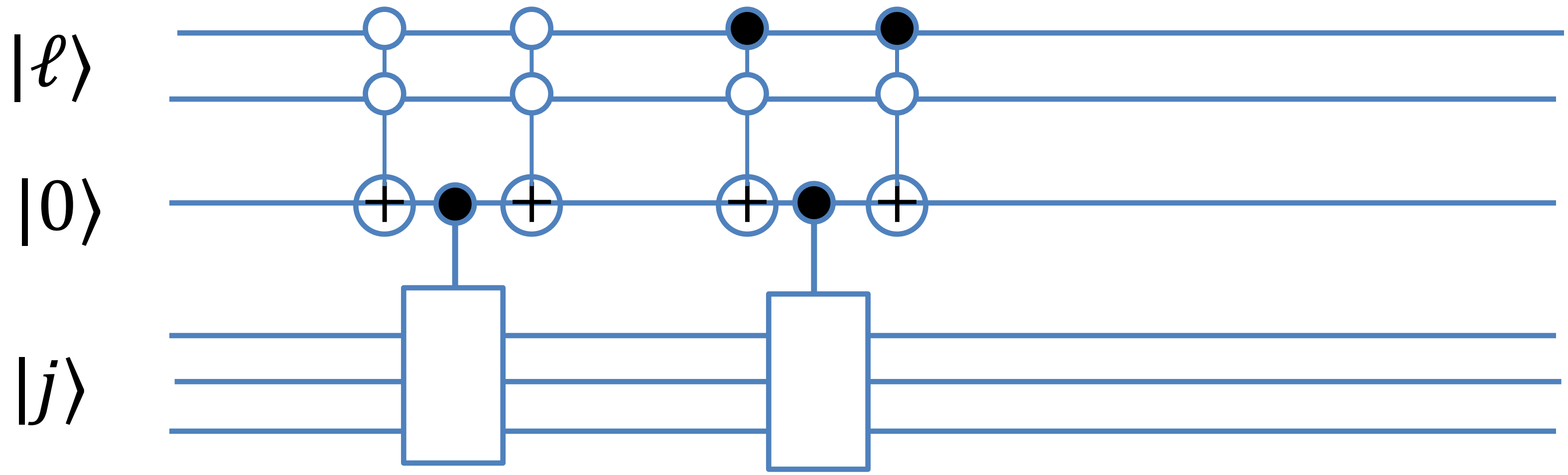
- Notation simplification:
  - ✓Define $l \equiv (p, q)$
  - ✓Define $H_l = a_p^\dagger a_q$
- $\sum_{l=0}^{L-1} H_l$ can be encoded by a select oracle (similar to LCU except that H_l is not unitary)

$$SELECT \equiv \sum_l |l\rangle\langle l| \otimes H_l$$

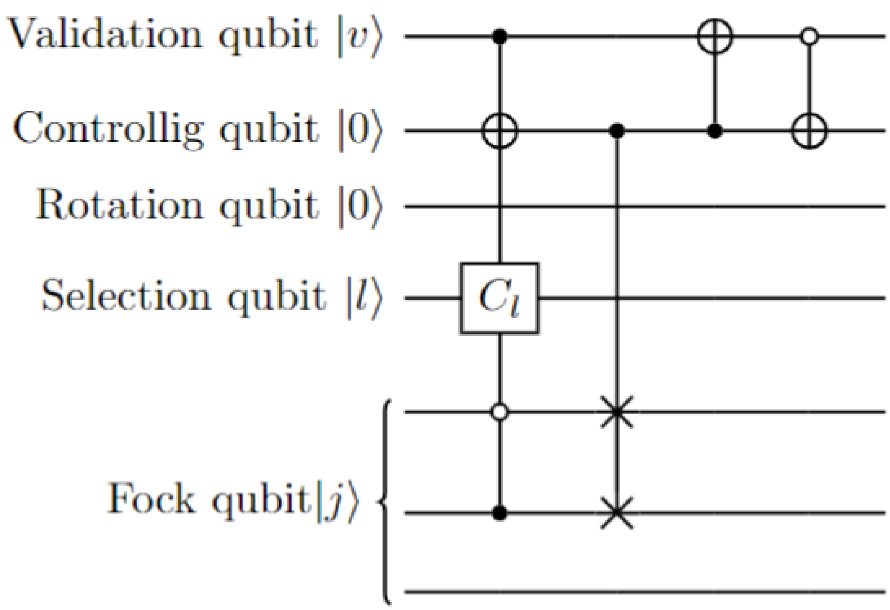
- Need additional ancilla qubits to invalidate $H_l\ |j\rangle$ for $j's$ that don't satisfy $|j\rangle_\mathrm{p} = |0\rangle$ and $|j\rangle_\mathrm{q} = |1\rangle$

The general structure of O_C circuit



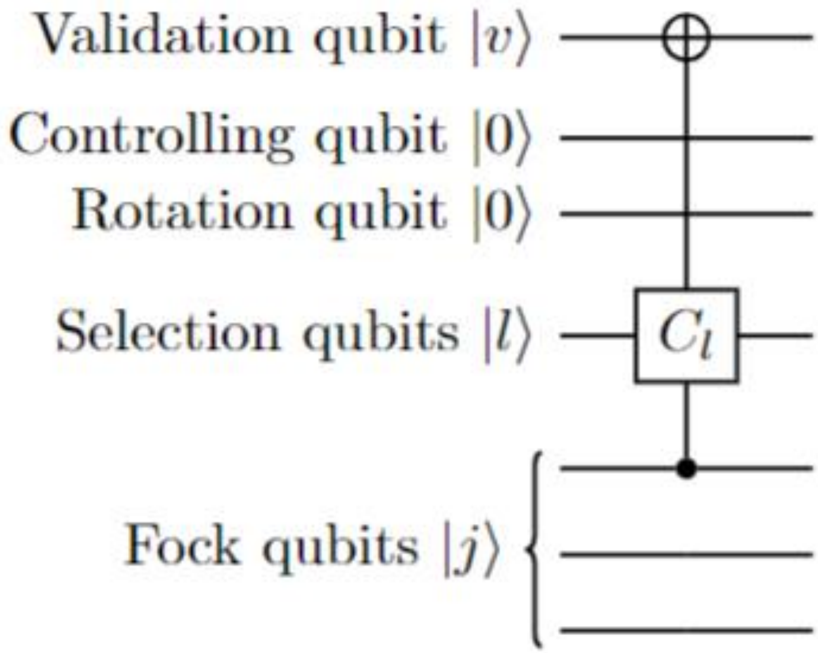


The U_l circuit



- Turn the controlling qubit from $|0\rangle$ to $|1\rangle$ when
  $|j\rangle_{\mathrm{p}} = |0\rangle$ and $|j\rangle_{\mathrm{q}} = |1\rangle$
  with controls on both the selection and Fock qubits
- Perform a controlled swap
- Restore validation and controlling qubits to $|0\rangle$ (uncompute)

Simplified circuit for $p = q$

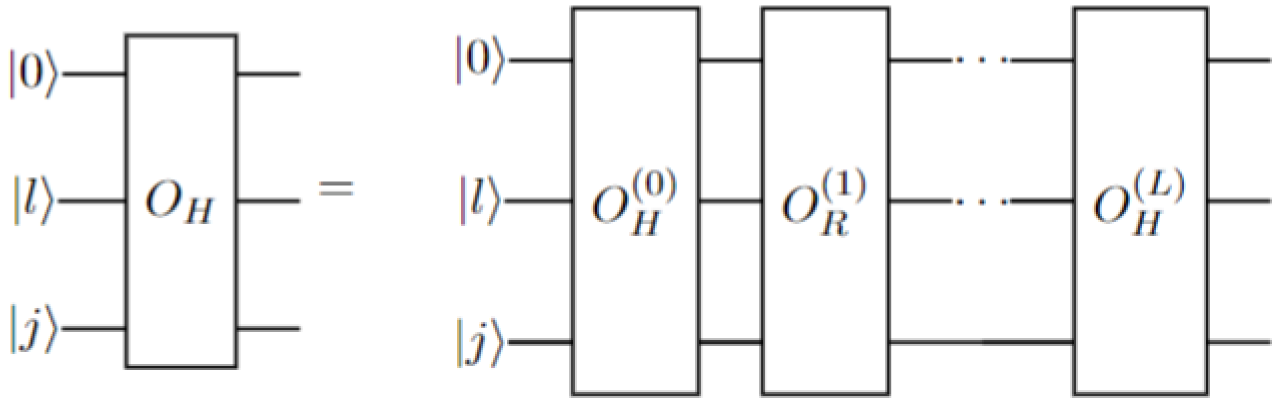


The $O_{\mathcal{H}}$ circuit

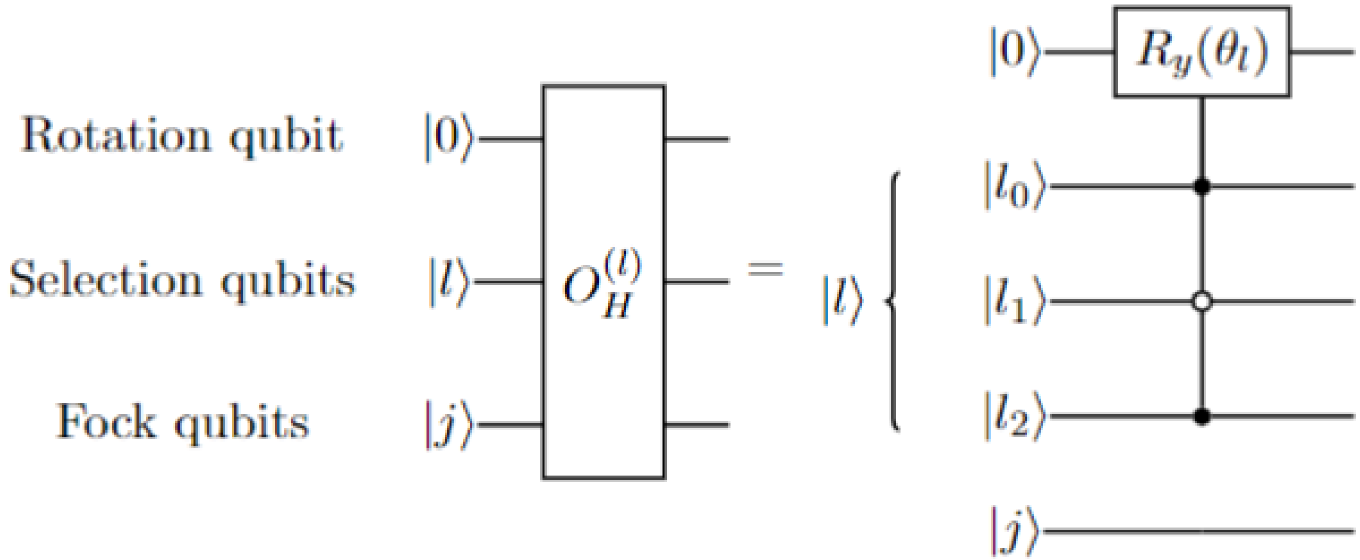
- If $|j\rangle_{\mathrm{p}} = |0\rangle$ and $|j\rangle_{\mathrm{q}} = |1\rangle$, $l = (p, q)$

$$O_H|0\rangle|l\rangle|j\rangle = \left(H_{c(l,j),j}|0\rangle + \sqrt{1 - \left|H_{c(l,j),j}\right|^2}|1\rangle\right)|l\rangle|j\rangle$$

- Otherwise, the output is to be discarded
- The general structure is a product of controlled rotations



The $O_{\mathcal{H}}^{(l)}$ circuit



General 2nd quantized fermionic Hamiltonian

- $\mathcal{H} = \sum_{p,q} h_{p,q}\, a_p^\dagger a_q + \sum_{p<q,r<s} g_{p,q,r,s}\, a_p^\dagger\, a_q^\dagger\, a_r\, a_s$
- Phase factor:

$$\{a_p, a_q^\dagger\} = \delta_{p,q}$$

$$a_p^\dagger\, a_q |j\rangle = (-1)^{d_j(p,q)} |\mathrm{FLIP}(j;p,q)\rangle$$

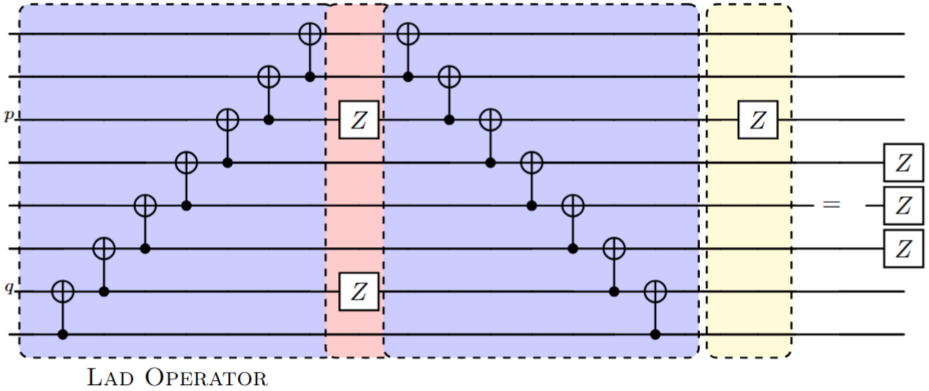
  if $|j\rangle_p = |0\rangle$ and $|j\rangle_q = |1\rangle$
- $d_j(p,q) = j_{p+1} + j_{p+2} + \cdots + j_{q-1}$

  where $(j_0, j_1, \ldots, j_n)$ is the binary representation of j.
- $\mathrm{FLIP}(j;p,q)$ (the $c(\ell, j)$ function) is obtained from j by flipping the pth and qth bits in the binary representation (or swapping the pth and qth bits)

Phase oracle

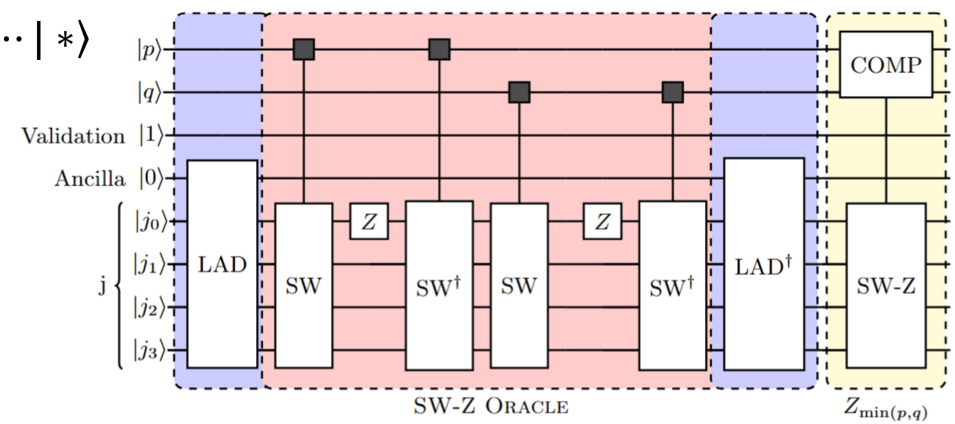
- Rewriting a product of Z's using three Z's and CNOT ladder circuits

$(-1)^{d(j;p,q)}$ implemented by $Z_{p+1}Z_{p+2}\cdots Z_{q-1}$



- SWAP-UP selection

SW(p): $|p\rangle\,|j_0\rangle\,|j_1\rangle\cdots|j_{n-1}\rangle \to |p\rangle\,|j_p\rangle\,|*\rangle\cdots|*\rangle$



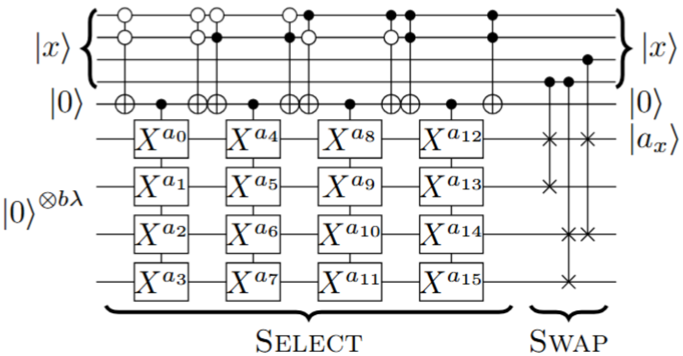
K. Wan, "Exponentially faster implementations of Select(H) for fermionic Hamiltonians", Quantum, 5, 2021

Prepare oracle $O_{\mathcal{H}}$ through data lookup

- Replace controlled rotation (not available as native gates) by quantum data lookup to encode approximate coefficients $\tilde{h}_x$, $\tilde{g}_x$ ($x \equiv (p,q)$ or $x \equiv (p,q,r,s)$)
- Two steps:
  1. Map x to the binary representation of $\tilde{h}_x$, denoted by a_x using a SELECT-SWAP circuit

$$O_a: |x\rangle\left|0^k\right\rangle \to |x\rangle|a_x\rangle$$

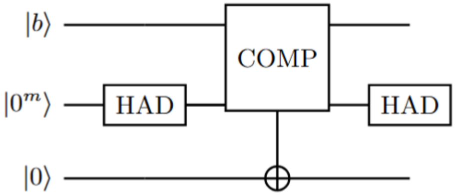
G. H. Low et al, "Trading T-gates for dirty qubits in state preparation and unitary synthesis", Quantum 8, 1375, 2024.



  2. Use a_x to generate $\tilde{h}_x$ as a probability amplitude through "direct sampling"

HAD: $|b\rangle|0^m\rangle|0\rangle \to \frac{1}{\sqrt{2^m}}\sum_{i=0}^{2^m-1}|b\rangle|i\rangle|0\rangle$

COMP: $\frac{1}{\sqrt{2^m}}\sum_{i=0}^{2^m-1}|b\rangle|i\rangle|0\rangle \to \frac{1}{\sqrt{2^m}}\left[\sum_{i=0}^{b-1}|b\rangle|i\rangle|0\rangle + \sum_{i=b}^{2^m-1}|b\rangle|i\rangle|1\rangle\right]$



Conclusion

- Second quantized fermionic Hamiltonians can be efficiently block encoded without using Jordan-Wigner transformation
- Creation and annihilation can be directly encoded as controlled bit flips or swaps
- Using SWAP-UP can reduce the number of controls in the SELECT oracle
- Data lookup based PREPARE oracle via SELECT-SWAP and “direct sampling” can further reduce gate count