Block Encoding

with low gate count for second-quantized Hamiltonians

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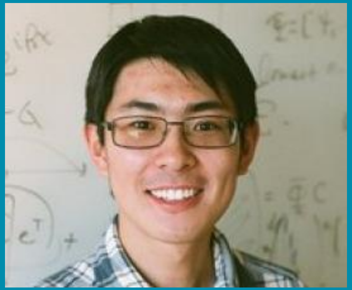

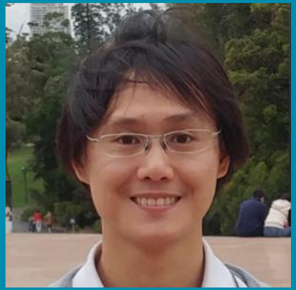

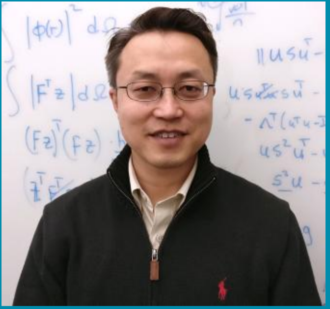

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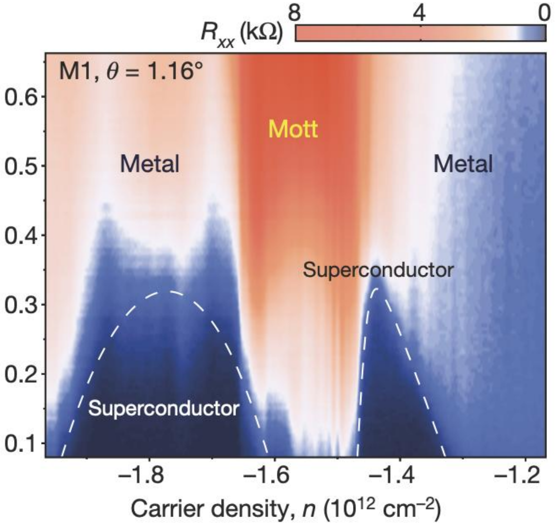
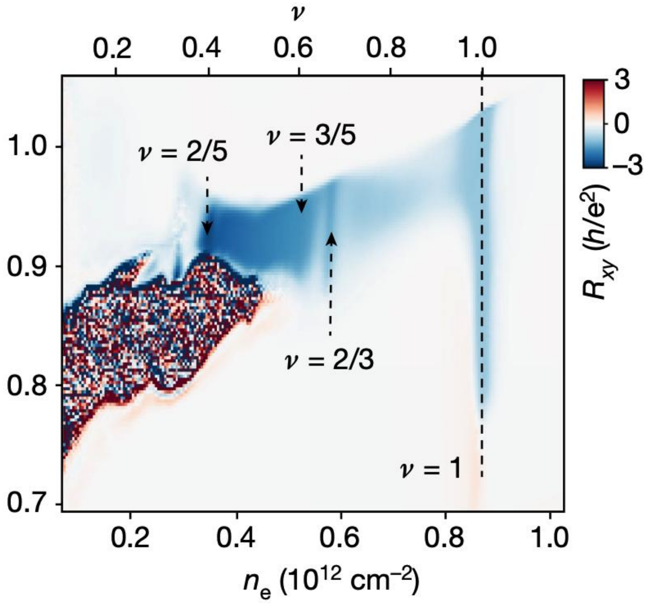
Quantum simulation for Quantum sciences

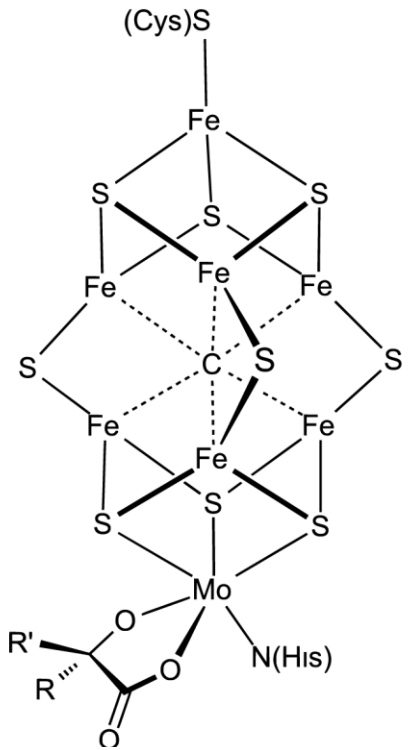
It is hard to understand and predict quantum many-body systems



Superconductivity



Fractional QAH effect



Harber process

Input model of quantum algorithm

Quantum Algorithms often start with a matrix as input

Quantum dynamics

$$e^{-iHt}\psi_0$$

Computing spectral properties

$$Tr(g(H))$$

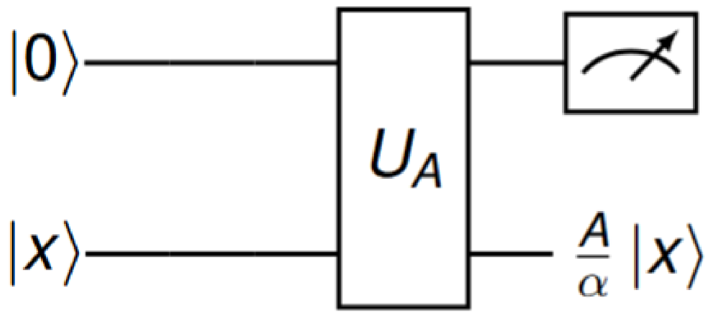
Solving linear systems

$$x = A^{-1}b$$

Definition (General Idea)

Block encoding is a technique for embedding a properly scaled nonunitary matrix $A \in \mathbb{C}^{N\times N}$ into a unitary matrix U_A of the form

$$U_A = \begin{bmatrix} \frac{A}{\alpha} & * \\ * & * \end{bmatrix},$$



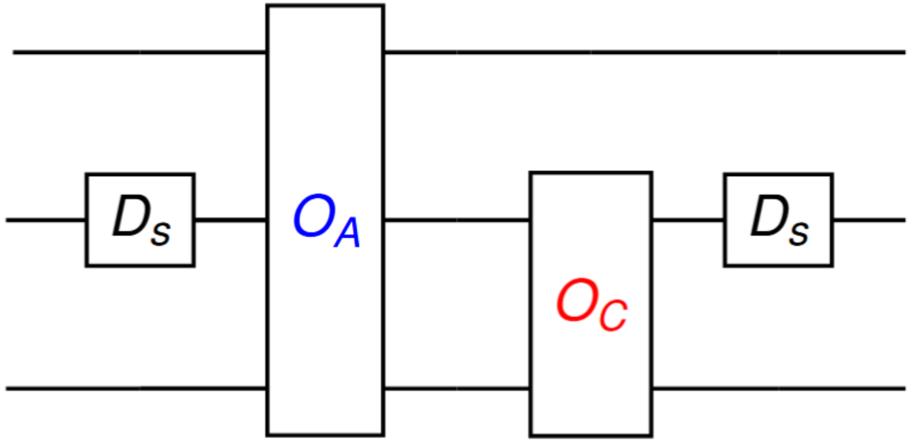
Block Encoding

Definition (Block encoding)

Given an n-qubit matrix $A \in \mathbb{C}^{2^n \times 2^n}$, if we find $\alpha, \epsilon \in \mathcal{R}_+$, and an $(m+n)-$ qubit unitary matrix U_A so that

$$||A - \alpha(\langle 0^m| \otimes I_{2^n})U_A(|0^m\rangle \otimes I_{2^n})|| \leq \epsilon$$

then U_A is called a (α, m, ϵ)-block-encoding of A.



Amplitude oracle:

$$O_A \,|0\rangle\, |\ell\rangle\, |j\rangle = \left(A_{c(j,\ell),j} \,|0\rangle + \sqrt{1 - |A_{c(j,\ell),j}|^2}\, |1\rangle \right) |\ell\rangle\, |j\rangle$$

Sparsity oracle:

$$O_c \,|\ell\rangle\, |j\rangle = |\ell\rangle\, |c(j,\ell)\rangle$$

$$U_A = (I_2 \otimes D_s \otimes I_N)\,(I_2 \otimes O_c)\, O_A\, (I_2 \otimes D_s \otimes I_N)$$

Guang Hao Low, and Isaac L. Chuang. "**Optimal Hamiltonian simulation by quantum signal processing**" *PRL* (2017).
András Gilyén, Yuan Su, Guang Hao Low, and Nathan Wiebe. "**Quantum singular value transformation and beyond**“ STOC (2019).
Daan Camps, Lin Lin, Roel Van Beeumen, and Chao Yang. "**Explicit quantum circuits for block encodings of certain sparse matrices**" SIAM Matrix Analysis (2024).

Second quantized Hamiltonian

$$\mathcal{H} = \sum_{p,q} h_{pq} a_p^\dagger a_q + \sum_{p<q,\ r<s} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$ General Hamiltonian

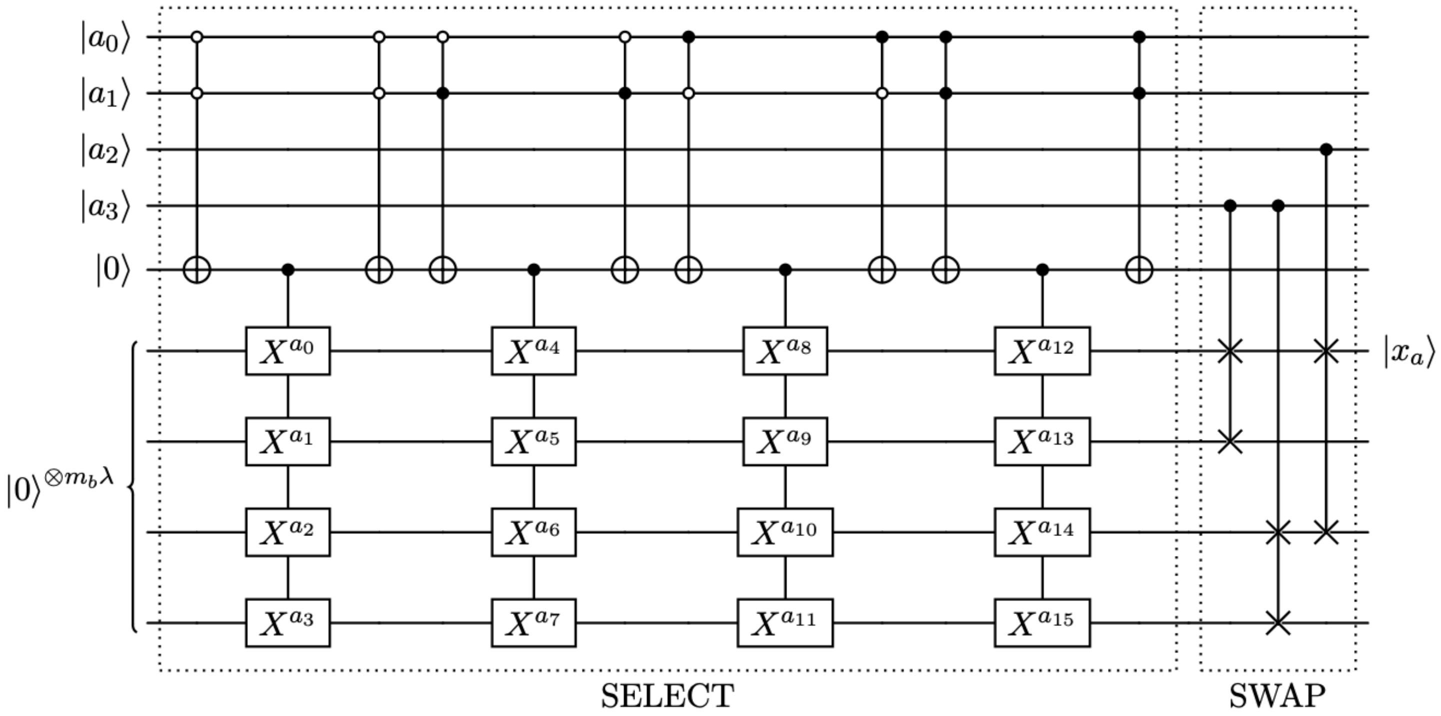
$$\mathcal{H} = \sum_{p,q=0}^{n-1} T(p-q) a_p^\dagger a_q$$ Translational Invariant

$$\mathcal{H} = \sum_{p=0}^{n-1} \sum_{q=0}^{n-1} h_{pq} a_p^\dagger a_q \quad |h_{pq}| \leq C e^{-\alpha|p-q|}$$ Nearest-Neighbour

Model	Reference	Qubit	Subnormalization factor	T count
General	2018 Babbush et al. [1]	$\mathcal{O}(n + \log(\frac{n^4}{\epsilon}))$	$\mathcal{O}(n^4)$	$\mathcal{O}(n^4 + \log(\frac{n^4}{\epsilon}))$
	This paper	$\mathcal{O}(n^2\sqrt{\log(\frac{n^4}{\epsilon})})$	$\mathcal{O}(n^4)$	$\mathcal{O}(n^2\sqrt{\log(\frac{n^4}{\epsilon})})$
Factorized	2018 Kivlichan et al. [2]	N/A	N/A	$\mathcal{O}(n^2\log(\frac{1}{\epsilon}))$
TI Factorized	2018 Babbush et al. [1]	$\mathcal{O}(n + \log(\frac{n^2}{\epsilon}))$	$\mathcal{O}(n^2)$	$\mathcal{O}(n + \log(\frac{n^2}{\epsilon}))$
	This paper	$\mathcal{O}(n + \sqrt{n\log(\frac{n^2}{\epsilon})})$	$\mathcal{O}(n^2)$	$\mathcal{O}(n + \sqrt{n\log(\frac{n^2}{\epsilon})})$
Localized	2021 Wan [3]	$\mathcal{O}(n)$	$\mathcal{O}(n^2)$	$\mathcal{O}(n) + \mathrm{PREP}$
	This paper	$\tilde{\mathcal{O}}(n\sqrt{\log^3(\frac{n^2}{\epsilon})})$	$\mathcal{O}(n^2\log^2(\frac{n^2}{\epsilon}))$	$\tilde{\mathcal{O}}(n\sqrt{\log^3(\frac{n^2}{\epsilon})})$

Babbush et al. "**Encoding electronic spectra in quantum circuits with linear T complexity**." *PRX* (2018).
Kivlichan et al. "**Quantum simulation of electronic structure with linear depth and connectivity**." *PRL* (2018).
Kianna Wan. "**Exponentially faster implementations of Select(H) for fermionic Hamiltonians**" *Quantum (2021).*

SELECT-SWAP circuit

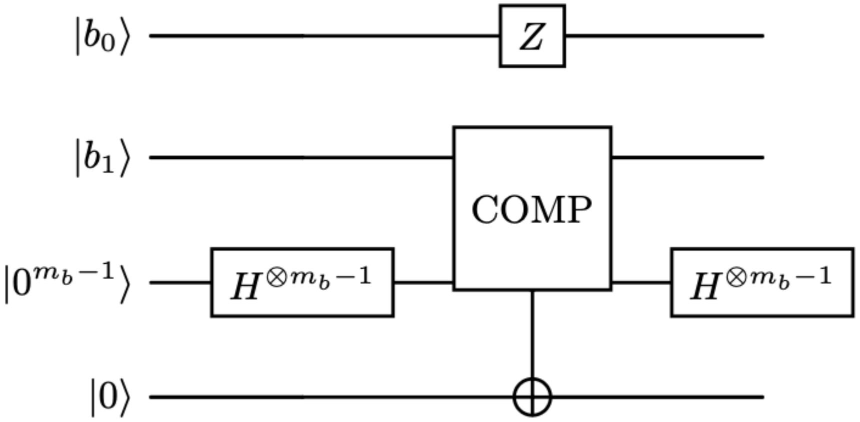


Data lookup $|l\rangle\,|0^{m_b}\rangle \to |l\rangle\,|\mathrm{data}_l\rangle$

Number of Data	L
Word length	m_b
Qubits	$m_b\lambda + 2\lceil \log_2(L) \rceil$
T count	$4\left\lceil \frac{L}{\lambda} \right\rceil + 8m_b\lambda$
T depth	$\frac{L}{\lambda} + \log(\lambda)$

Guang Hao Low, Vadym Kliuchnikov, Luke Schaeffer. "**Trading T gates for dirty qubits in state preparation and unitary synthesis**" *Quantum (2024).*
Shuchen Zhu, Aarthi Sundaram, and Guang Hao Low. "**Unified architecture for a quantum lookup table**“ arXiv:2406.18030.

Construction of amplitude oracle O_A



Direct Sampling

$$|b_0\rangle|b_1\rangle\left|0^{m_b-1}\right\rangle|0\rangle$$

$$\xrightarrow{H^{\otimes m_b-1}} \sum_{i}^{2^{m_b-1}-1} \frac{1}{\sqrt{2^{m_b-1}}}|b_0\rangle|b_1\rangle|i\rangle|0\rangle$$

$$\xrightarrow{\text{COMP}} \frac{1}{\sqrt{2^{m_b-1}}}\sum_{i=0}^{b_1-1}|b_0\rangle|b_1\rangle|i\rangle|0\rangle + \frac{1}{\sqrt{2^{m_b-1}}}\sum_{i=b_1}^{2^{m_b-1}-1}|b_0\rangle|b_1\rangle|i\rangle|1\rangle$$

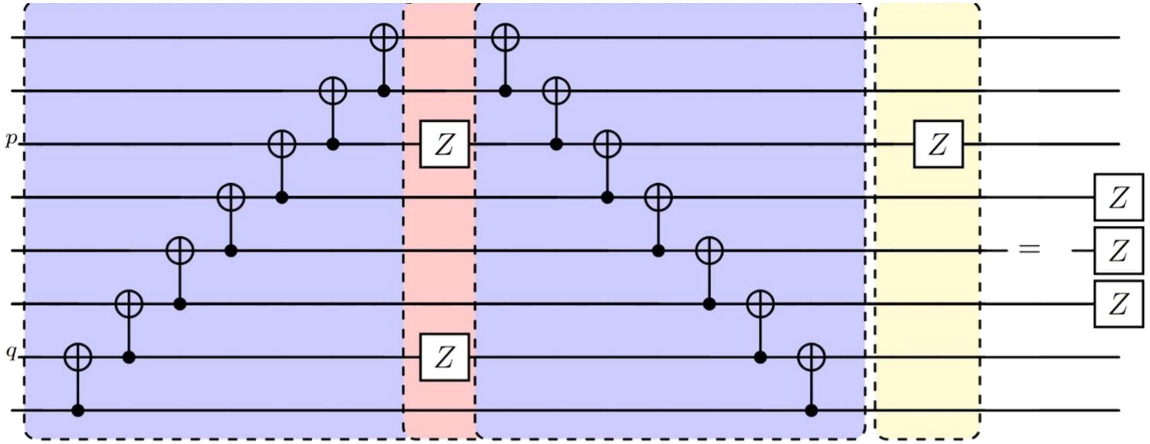
$$\xrightarrow{H^{\otimes m_b-1},\, Z} |b_0\rangle|b_1\rangle\left|0^{m_b-1}\right\rangle\left(r_b|0\rangle+\sqrt{1-r_b^2}\,|1\rangle\right)+|b\rangle|\Psi\rangle$$

Babbush et al. "**Encoding electronic spectra in quantum circuits with linear T complexity**." *PRX* (2018).

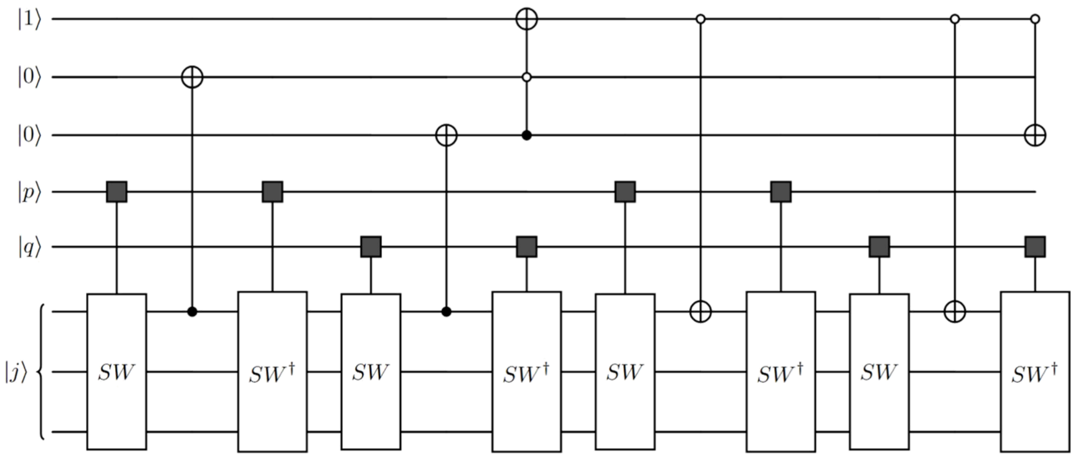
Construction of sparsity oracle O_C

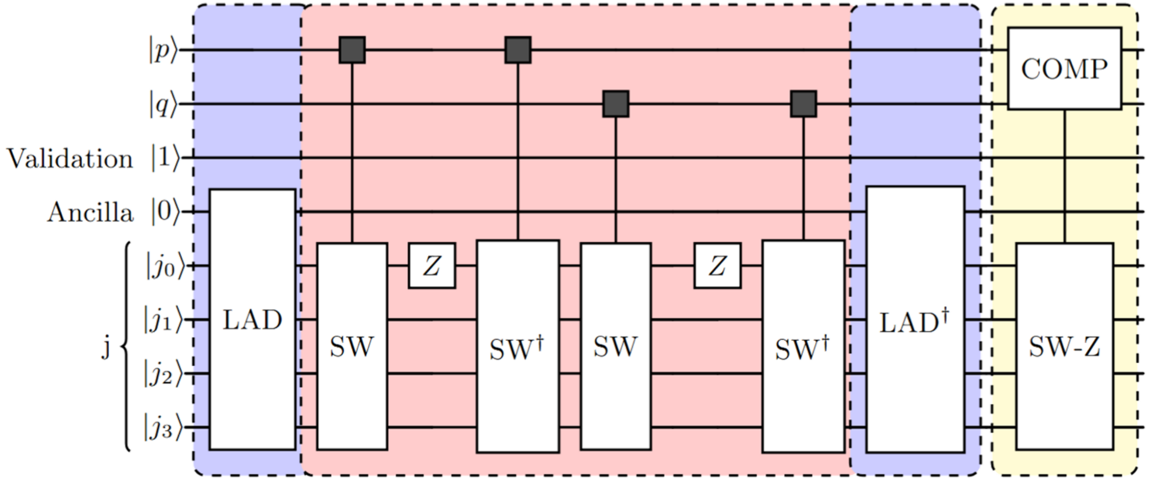
$$a_2^\dagger a_0 |110\rangle = a_2^\dagger a_0 a_0^\dagger a_1^\dagger |vac\rangle = a_2^\dagger a_1^\dagger |vac\rangle = -|011\rangle$$

$$\sum_{p,q=0}^{n-1} |o(j,p,q)\rangle \langle 0| \otimes |i\rangle \langle i| \otimes a_p^\dagger a_q$$



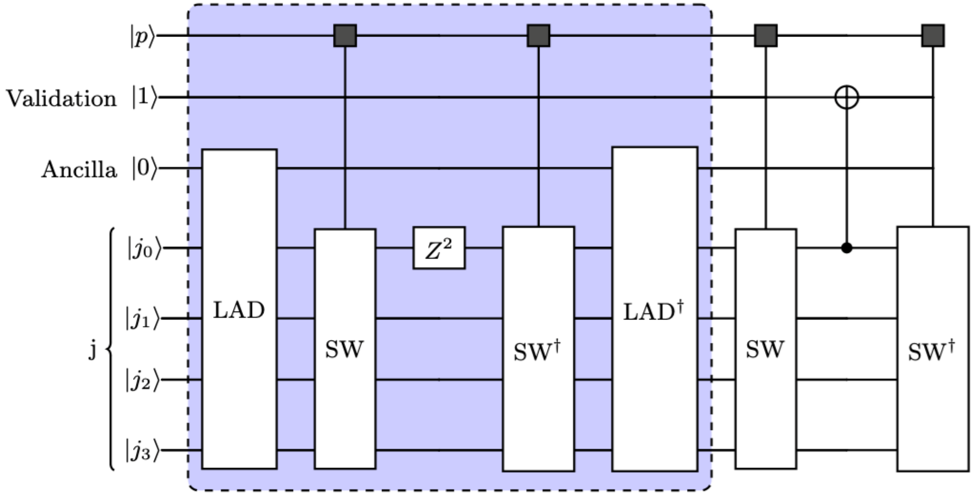
LAD OPERATOR





SW-Z ORACLE

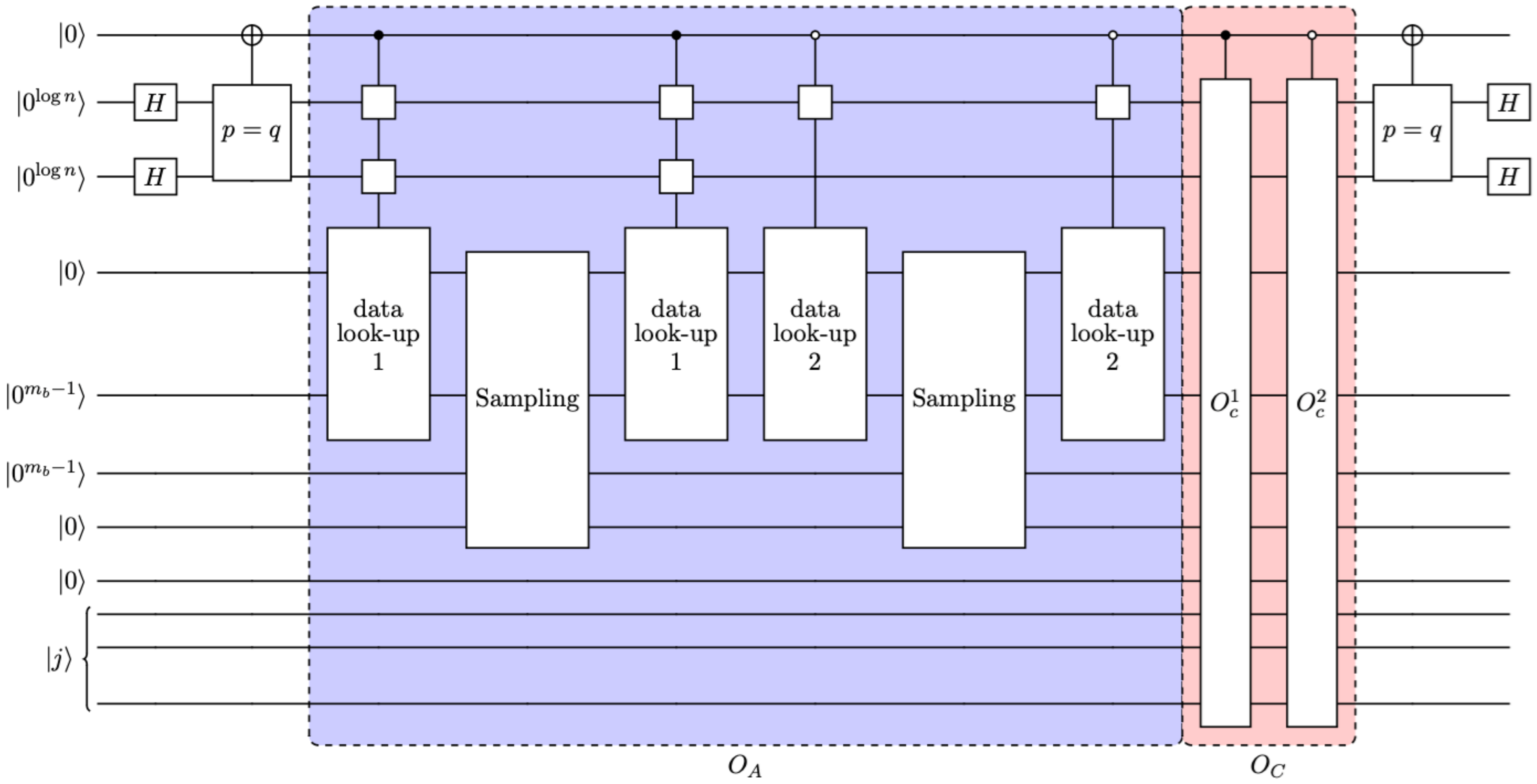
$Z_{\min(p,q)}$



IDENTITY OPERATOR

Diyi Liu, Weijie Du, Lin Lin, James P Vary, Chao Yang. "**An efficient quantum circuit for block encoding a pairing Hamiltonian**" Journal of Computational Science 2025

Block Encoding of one-body interactions



Kianna Wan. "**Exponentially faster implementations of Select(H) for fermionic Hamiltonians**" *Quantum (2021).*

Second quantized Hamiltonian

$$\mathcal{H} = \sum_{p,q} h_{pq} a_p^\dagger a_q + \sum_{p<q,\ r<s} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

General Hamiltonian [H, n]=0

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

Translational Invariant

$$\mathcal{H} = \sum_{p=0}^{n-1} \sum_{q=0}^{n-1} h_{pq} a_p^\dagger a_q \qquad |h_{pq}| \leq C e^{-\alpha|p-q|}$$

Nearest-Neighbour

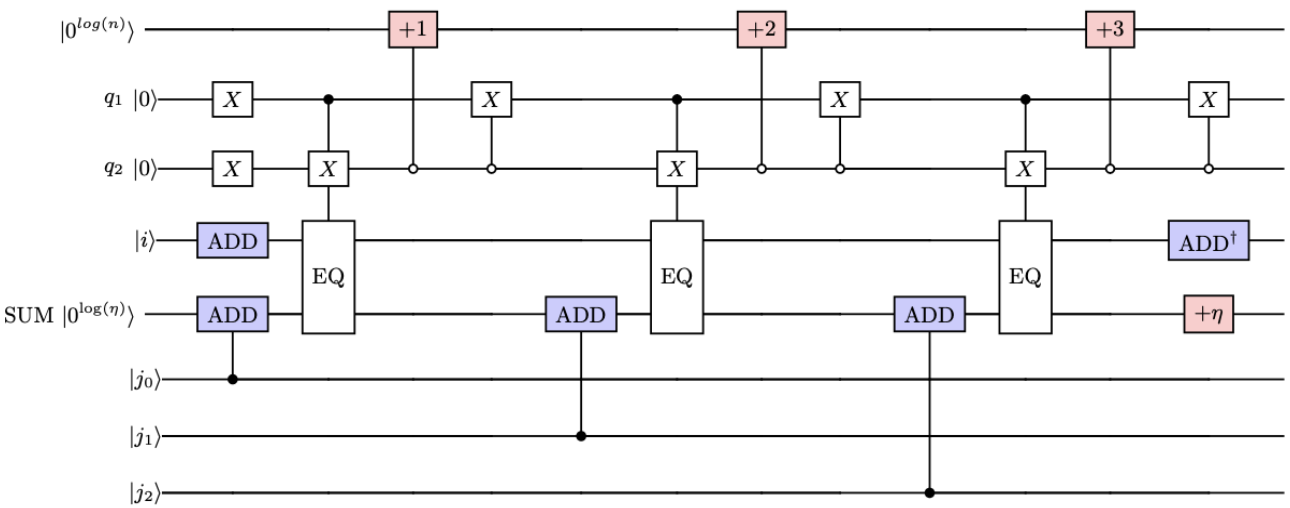
Model	Reference	Qubit	Subnormalization factor	T count
General	2018 Babbush et al. [1]	$\mathcal{O}(n + \log(\frac{n^4}{\epsilon}))$	$\mathcal{O}(n^4)$	$\mathcal{O}(n^4 + \log(\frac{n^4}{\epsilon}))$
	This paper	$\mathcal{O}(n + \lambda_1 \log(\frac{n^4}{\epsilon}))$	$\mathcal{O}(n^4)$	$\mathcal{O}(\frac{n^4}{\lambda_1} + \lambda_1 \log(\frac{n^4}{\epsilon}))$
Factorized	2018 Kivlichan et al. [2]	N/A	N/A	$\mathcal{O}(n^2 \log(\frac{1}{\epsilon}))$
TI Factorized	2018 Babbush et al. [1]	$\mathcal{O}(n + \log(\frac{n^2}{\epsilon}))$	$\mathcal{O}(n^2)$	$\mathcal{O}(n + \log(\frac{n^2}{\epsilon}))$
	This paper	$\mathcal{O}(n + \lambda_2 \log(\frac{n^2}{\epsilon}))$	$\mathcal{O}(n^2)$	$\mathcal{O}(n + \frac{n}{\lambda_2} + \lambda_2 \log(\frac{n^2}{\epsilon}))$
Localized	2021 Wan [3]	$\mathcal{O}(n)$	$\mathcal{O}(n^2)$	$\mathcal{O}(n) + \text{PREP}$
	This paper	$\tilde{\mathcal{O}}(n + \lambda_3 \log(\frac{n^2}{\epsilon}))$	$\mathcal{O}(n^2 \log^2(\frac{n^2}{\epsilon}))$	$\tilde{\mathcal{O}}\left(\frac{n^2}{\lambda_3} \log^2(\frac{n^2}{\epsilon}) + \lambda_3 \log(\frac{n^2}{\epsilon})\right)$

η −particle Hamiltonian Block Encoding

$$H = \sum_{p=0}^{n-1} h_p a_p^\dagger a_p.$$

$$|0\rangle\,|0^{log(\eta)}\rangle\,|j\rangle \xrightarrow[O_A]{H} \frac{1}{\sqrt{\eta}}\sum_{i=0}^{\eta-1}\left(h_{add_i(j)}\,|0\rangle + \sqrt{1-h^2_{add_i(j)}}\,|1\rangle\right)|i\rangle\,|j\rangle$$

State-dependent amplitude oracle O_A



$$\left|0^{\log(\eta)}\right\rangle\left|0^{\log(n)}\right\rangle|j\rangle \xrightarrow{H^{\otimes \log(\eta)}} \frac{1}{\sqrt{\eta}}\sum_{i=0}^{\eta-1}|i\rangle\left|0^{\log(n)}\right\rangle|j\rangle$$

$$|i\rangle\left|0^{\log(n)}\right\rangle|j\rangle \xrightarrow{O_{occ}} |i\rangle\,|add_i(j)\rangle\,|j\rangle$$

$$\xrightarrow{O_{\mathrm{IDF}}} \frac{1}{\sqrt{\eta}}\sum_{i=0}^{\eta}|i\rangle\,|add_i(j)\rangle\,|j\rangle$$

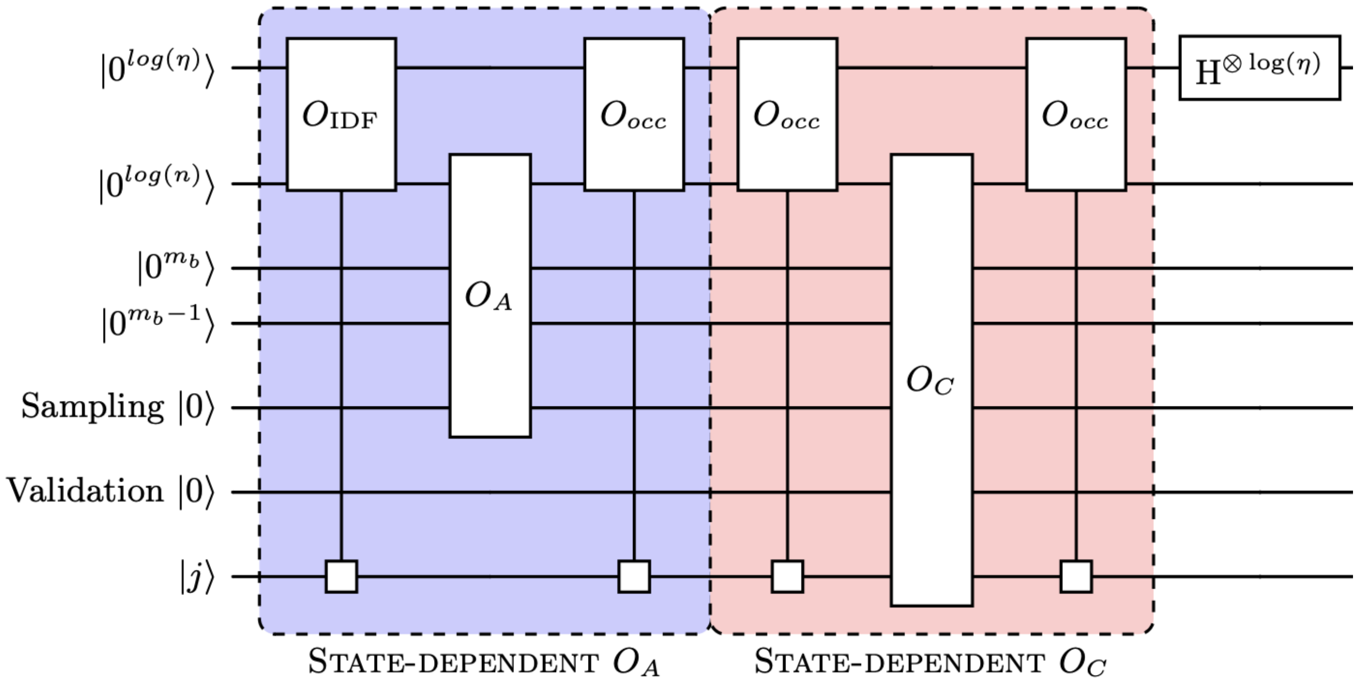
Indirect diffusion

η −particle Hamiltonian Block Encoding

$$H = \sum_{p=0}^{n-1} h_p a_p^\dagger a_p.$$

$$\sum_{i=0}^{\eta-1} |o(j, add_i(j)))\rangle \langle 0| \otimes |i\rangle \langle i| \otimes a^\dagger_{add_i(j)} a_{add_i(j)}$$

State-dependent sparse oracle O_C



$$\xrightarrow{X} \frac{1}{\sqrt{\eta}} \sum_{i=0}^{\eta-1} |1\rangle |i\rangle |add_i(j)\rangle |j_0\rangle |j_1\rangle \ldots |j_{n-1}\rangle$$

$$\xrightarrow{SW} \frac{1}{\sqrt{\eta}} \sum_{i=0}^{\eta-1} |1\rangle |i\rangle |add_i(j)\rangle \left|j_{add_i(j)}\right\rangle * * \ldots$$

$$\xrightarrow{CNOT} \frac{1}{\sqrt{\eta}} \sum_{i=0}^{\eta-1} |o(j, add_i(j)))\rangle |i\rangle |add_i(j)\rangle \left|j_{add_i(j)}\right\rangle * * \ldots$$

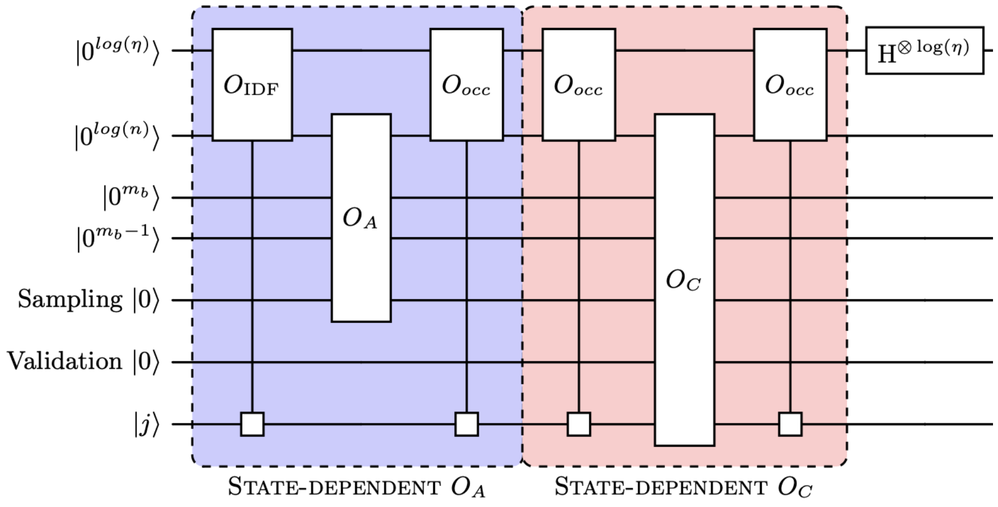
$$\xrightarrow{SW^\dagger} \frac{1}{\sqrt{\eta}} \sum_{i=0}^{\eta-1} |o(j, add_i(j))\rangle |i\rangle |add_i(j)\rangle |j\rangle$$

η −particle Hamiltonian Block Encoding

$$H = \sum_{p=0}^{n-1} h_p a_p^\dagger a_p.$$

$$\sum_{i=0}^{\eta-1} |o(j, add_i(j)))\rangle \langle 0| \otimes |i\rangle \langle i| \otimes a^\dagger_{add_i(j)} a_{add_i(j)}$$

State-dependent sparse oracle O_C



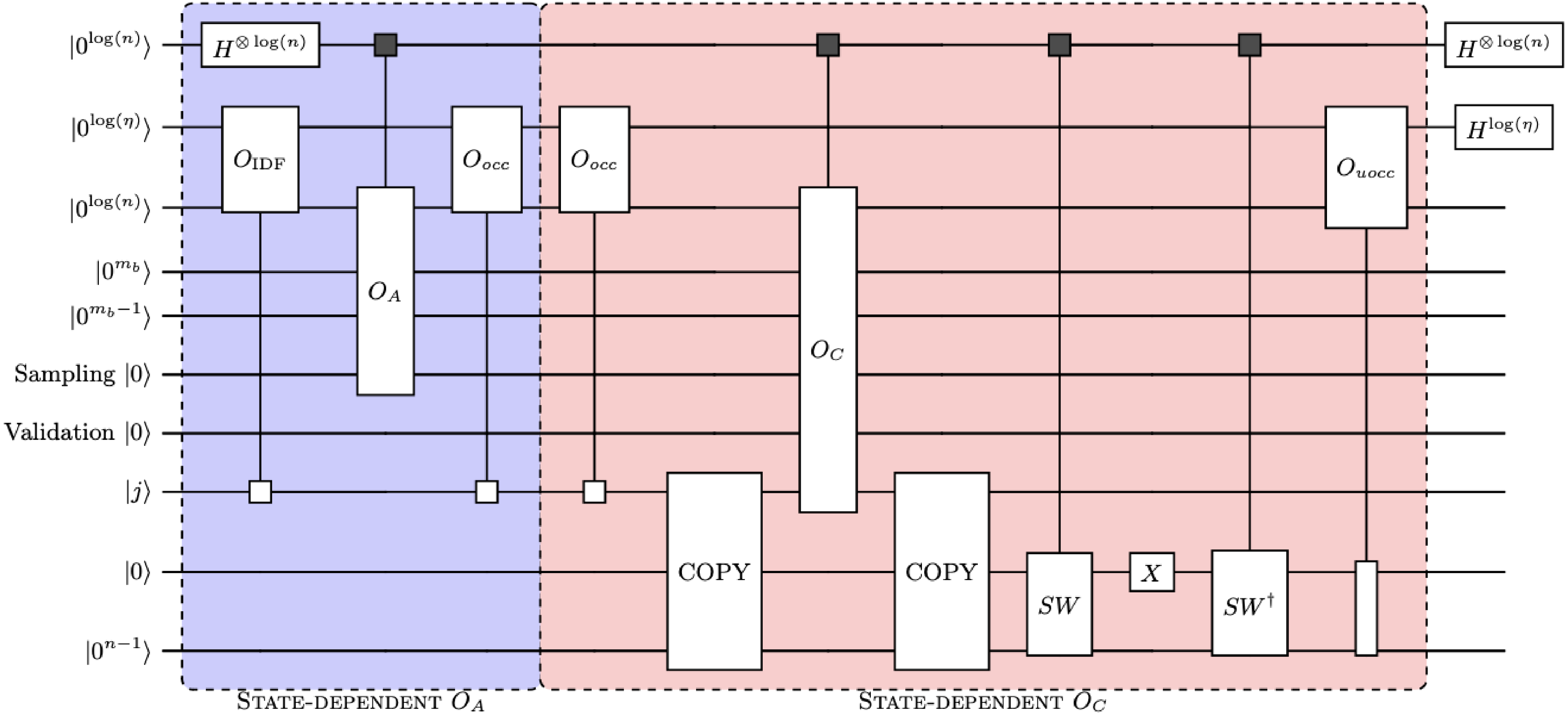
$$\xrightarrow{O_{\text{IDF}}, O_A} \frac{1}{\sqrt{\eta}} \sum_{i=0}^{\eta-1} |0\rangle |i\rangle \left(h_{add_i(j)} |0\rangle + \sqrt{1 - h^2_{add_i(j)}} |1\rangle \right) |j\rangle$$

$$\xrightarrow{O_C} \frac{1}{\sqrt{\eta}} \sum_{i=0}^{\eta-1} |o(j, add_i(j))\rangle |i\rangle \left(h_{add_i(j)} |0\rangle + \sqrt{1 - h^2_{add_i(j)}} |1\rangle \right) a^\dagger_{add_i(j)} a_{add_i(j)} |j\rangle$$

$$= \frac{1}{\sqrt{\eta}} \sum_{i=0}^{\eta-1} |0\rangle |i\rangle \left(h_{add_i(j)} |0\rangle + \sqrt{1 - h^2_{add_i(j)}} |1\rangle \right) a^\dagger_{add_i(j)} a_{add_i(j)} |j\rangle$$

$$\xrightarrow{H} \frac{1}{\eta} \sum_{i=0}^{\eta-1} |0\rangle \left|0^{\log(\eta)}\right\rangle |0\rangle \left(h_{add_i(j)} a^\dagger_{add_i(j)} a_{add_i(j)} \right) |j\rangle + *$$

$$= \frac{1}{\eta} |0\rangle \left|0^{\log(\eta)}\right\rangle |0\rangle \sum_{p=0}^{n-1} h_p a_p^\dagger a_p |j\rangle + *$$



$|0^{\log(n)}\rangle$
$|0^{\log(\eta)}\rangle$
$|0^{\log(n)}\rangle$
$|0^{m_b}\rangle$
$|0^{m_b-1}\rangle$
Sampling $|0\rangle$
Validation $|0\rangle$
$|j\rangle$
$|0\rangle$
$|0^{n-1}\rangle$
$H^{\otimes \log(n)}$
O_{IDF}
O_A
O_{occ}
O_{occ}
COPY
O_C
COPY
SW
X
$SW^\dagger$
O_{uocc}
$H^{\otimes \log(n)}$
$H^{\log(\eta)}$
State-dependent O_A
State-dependent O_C

How does the subspace influence complexity

$$\mathcal{H} = \sum_{p=0}^{n-1} h_p a_p^\dagger a_p$$

$$\mathcal{H} = \sum_{p=0}^{n-1}\sum_{q=0}^{n-1} h_{pq} a_p^\dagger a_q.$$

Number of data : n

Word length m_b : $\log\left(\frac{\eta}{\epsilon}\right)$

α : η

Number of data : n^2

Word length m_b : $\log\left(\frac{n\eta}{\epsilon}\right)$

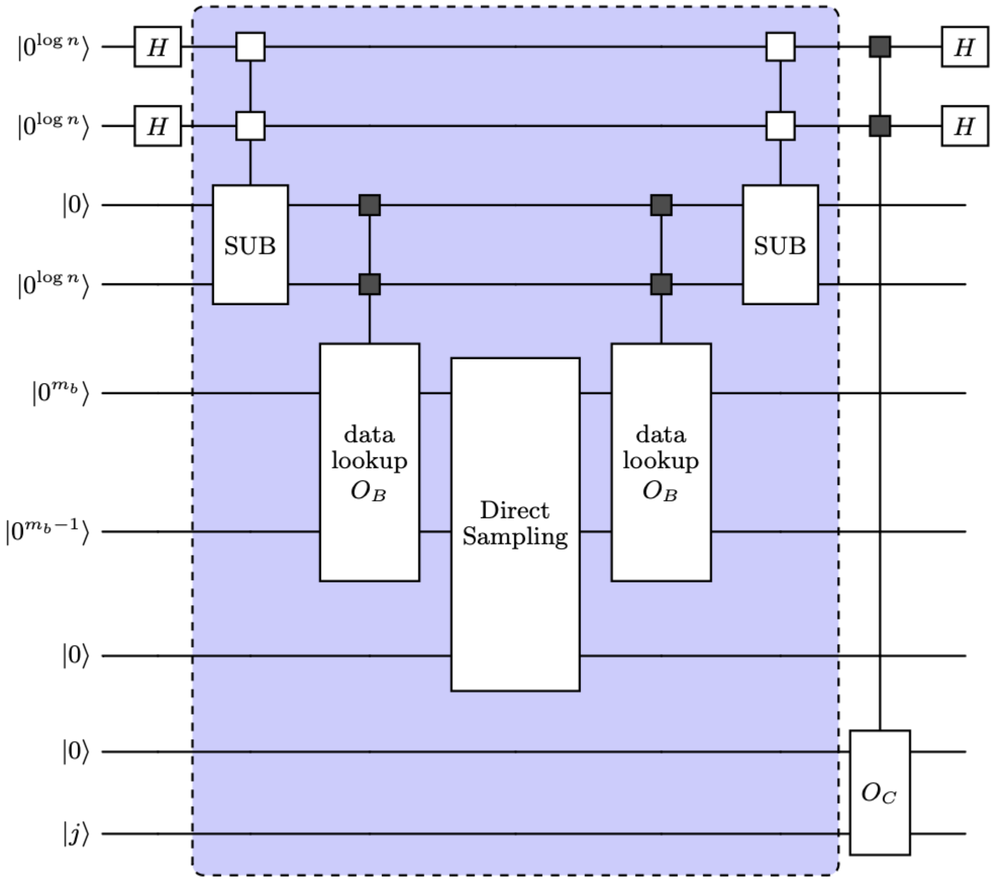
α : $n\eta$

Model	Reference	Qubit	Subnormalization factor	T count
General	2018 Babbush et al. [1]	$\mathcal{O}(n+\log(\frac{n^4}{\epsilon}))$	$\mathcal{O}(n^4)$	$\mathcal{O}(n^4+\log(\frac{n^4}{\epsilon}))$
	This paper	$\mathcal{O}(n+\tilde{\lambda}_1\log(\frac{n^2\eta^2}{\epsilon}))$	$\mathcal{O}(n^2\eta^2)$	$\mathcal{O}(n\log(\eta)+\frac{n^4}{\tilde{\lambda}_1}+\tilde{\lambda}_1\log(\frac{n^2\eta^2}{\epsilon}))$
Factorized	2018 Kivlichan et al. [2]	N/A	N/A	$\mathcal{O}(n^2\log(\frac{1}{\epsilon}))$
TI Factorized	2018 Babbush et al. [1]	$\mathcal{O}(n+\log\frac{n^2}{\epsilon})$	$\mathcal{O}(n^2)$	$\mathcal{O}(n+\log(\frac{1}{\epsilon}))$
	This paper	$\mathcal{O}(n+\tilde{\lambda}_2\log(\frac{n\eta}{\epsilon}))$	$\mathcal{O}(n\eta)$	$\mathcal{O}(n\log(\eta)+\frac{n}{\tilde{\lambda}_2}+\tilde{\lambda}_2\log(\frac{n\eta}{\epsilon}))$
Localized	2021 Wan [3]	$\mathcal{O}(n)$	$\mathcal{O}(n^2)$	$\mathcal{O}(n)+\text{PREP}$
	This paper	$\tilde{\mathcal{O}}(n+\tilde{\lambda}_3\log(\frac{\eta^2}{\epsilon}))$	$\mathcal{O}(\eta^2\log^2(\frac{\eta^2}{\epsilon}))$	$\tilde{\mathcal{O}}(n\log(\eta)+\frac{n^2}{\tilde{\lambda}_3}\log(\frac{\eta^2}{\epsilon})+\tilde{\lambda}_3\log(\frac{\eta^2}{\epsilon}))$

Block Encoding for Structured Hamiltonian

Translational Invariant

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



O_A for translation invariance

Number of data : n

Word length m_b : $\log\left(\frac{n^2}{\epsilon}\right)$

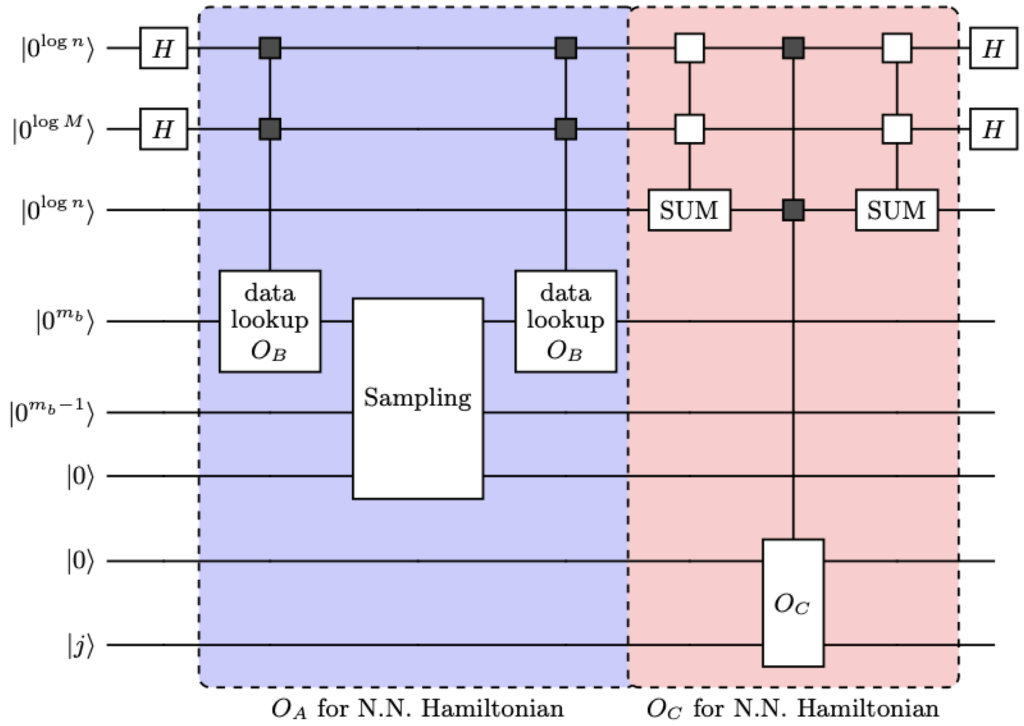
α : n^2

Block Encoding for Structured Hamiltonian

Nearest-Neighbour

$$\mathcal{H} = \sum_{p=0}^{n-1} \sum_{q=0}^{n-1} h_{pq} a_p^\dagger a_q \qquad |h_{pq}| \leq C e^{-\alpha|p-q|}$$

Less data $\quad |p-q| \leq C' \log\left(\frac{n}{\epsilon}\right)$



Number of data : $\quad n \log\left(\frac{n}{\epsilon}\right)$

Word length m_b : $\quad \log\left(\frac{n}{\epsilon}\right) + \log\left(\log\left(\frac{n}{\epsilon}\right)\right)$

α : $\quad n \log\left(\frac{n}{\epsilon}\right)$

Large α $\quad \frac{1}{\sqrt{2n}} \sum_{p=0}^{n-1} |p\rangle |p-1\rangle |0\rangle + \frac{1}{\sqrt{2n}} \sum_{p=0}^{n-1} |p\rangle |p+1\rangle |1\rangle$

Conclusion

- We develop Block Encoding with reduced T gate count for general second-quantized Hamiltonian
- We develop η particle Hamiltonian with state-dependent O_A and state-dependent O_C , through indirect diffusion. This gives smaller subnormalization factor and smaller T gate count.
- We extend the frameworks to structured Hamiltonians

Future work

- Non-binary block encoding
- More structured Hamiltonians: lower bound and construction

Thank You