Hamiltonian Embedding

& A Paradigm Shift in Quantum Algorithm Design

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I. Input models of matrices

Input models of a matrix A

Sparse-input oracles

$$O_r : |i\rangle|k\rangle \to |i\rangle|r_{ik}\rangle, \quad O_c : |\ell\rangle|j\rangle \to |c_{\ell j}\rangle|j\rangle$$
$$O_A : |i\rangle|j\rangle|0\rangle^{\otimes b} \to |i\rangle|j\rangle|a_{ij}\rangle$$

- A sparse, not necessarily Hermitian
- Applications: quantum simulation, quantum linear system solvers, Carleman linearization, etc.
- **Limitations**: no guarantee on the actual cost.

Block-encoding

$$U = \begin{bmatrix} A/\alpha & \cdot \\ \cdot & \cdot \end{bmatrix}, \quad A = \alpha(\langle 0| \otimes I)U(|0\rangle \otimes I)$$

- A not necessarily sparse, not necessarily Hermitian
- Applications: quantum signal processing, quantum singular value transformation, etc.
- **Limitations**: no guarantee on the actual cost. Still far from NISQ era.

- Dalzell et. al. *"End-to-end resource analysis for quantum interior point methods and portfolio optimization"*. [arXiv: 2211.12489]. Portfolio optimization with **100** shares (easy for a personal laptop): T-count $\approx 2 \times 10^9$ in a **single** block-encoding, and **repeat** $\sim 10^7$ times.

- Liu et. al. *"An efficient block encoding quantum circuits for a pair Hamiltonian"*. **10** fermions: T-count $\approx 3 \times 10^3$, 2-qubit entanglement gates $\sim 6 \times 10^3$ (can be further improved!)

Input models of a matrix A (Con't)

Pauli basis decomposition (Pauli strings)

$$A = \sum_s a_s P_s, \quad a_s = \frac{1}{2^n}\mathrm{Tr}[AP_s]$$

$\{P_s\}$ = the set of Pauli basis (e.g., I, X, Y, Z)

P_s is ***k*-local** if involving k non-identity Paulis

- **Limitations**: A must be Hermitian. The coefficients a_s could require exponential time to compute.
- **Advantages**: Easy to simulate on real devices if matching the hardware native *instruction set*.

Analog Quantum Computers

Example: Rydberg atoms (QuEra)

$$H = \Omega \sum_j X_j + \Delta \sum_j Z_j + \sum_{j<k} V_{jk} Z_j \otimes Z_k, \quad V_{jk} = C_6 / |r_j - r_k|^6$$

It is efficient to run spin-glass or TFI models on Rydberg atoms.

Digital Quantum Computers

Example: Trapped ions (IonQ)

$$\mathrm{MS}(\phi_0, \phi_1) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 & -ie^{-i(\phi_0+\phi_1)} \\ 0 & 1 & -ie^{-i(\phi_0-\phi_1)} & 0 \\ 0 & -ie^{-i(\phi_0-\phi_1)} & 1 & 0 \\ -ie^{-i(\phi_0+\phi_1)} & 0 & 0 & 1 \end{bmatrix}$$

$$\mathrm{MS}(\phi_0, \phi_1) = e^{-i\frac{\pi}{4}[\cos(\phi_0)X + \sin(\phi_0)Y]\otimes[\cos(\phi_1)X + \sin(\phi_1)Y]}$$

The native Hamiltonians/operations on real devices only involves 1- and 2-local interactions.

Sparse matrices → Pauli strings?

- Finding the Pauli basis decomposition of a matrix is **HARD**!

$$H = \begin{bmatrix} L & 0 \\ 0 & 0 \end{bmatrix}, L = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix}$$

```
from qiskit.quantum_info import SparsePauliOp
H = np.zeros((8, 8))
H[:5, :5] = L_chain
SparsePauliOp.from_operator(H)
```

```
SparsePauliOp(['III', 'IIX', 'IXX', 'IYY', 'XXX', 'XYY', 'YXY', 'YYX', 'ZII', 'ZIX', 'ZIZ', 'ZXX', 'ZYY', 'ZZI',
'ZZZ'],
              coeffs=[ 1.  +0.j, -0.5 +0.j, -0.25+0.j, -0.25+0.j, -0.25+0.j,  0.25+0.j,
 -0.25+0.j, -0.25+0.j,  0.75+0.j, -0.5 +0.j, -0.25+0.j, -0.25+0.j,
 -0.25+0.j, -0.25+0.j, -0.25+0.j])
```

Target Hamiltonian: H

Can we find a Hamiltonian H' (as a sum of Pauli strings), such that the information of e^{-iHt} can be extracted/recovered from $e^{-iH't}$?

II. Hamiltonian Embedding & Quantum Simulation

Mathematical formulation

Suppose that H' is a q-qubit operator, let $\mathcal{S}$ be an n-dim subspace of $\mathbb{C}^{2^q}$. We write

$$H' = \begin{bmatrix} H & R \\ R^\dagger & B \end{bmatrix},$$

with $H = P_{\mathcal{S}} H' P_{\mathcal{S}}, \quad R = P_{\mathcal{S}} H' P_{\mathcal{S}^\perp}, \quad B = P_{\mathcal{S}^\perp} H' P_{\mathcal{S}^\perp}$.

If $\underline{R = 0}$, we have

$$e^{-iH't} = e^{-iHt} \oplus e^{-iBt} \implies \left(e^{-iH't}\right)\Big|_{\mathcal{S}} = e^{-iHt}$$

To simulate H, we only need to look at the **projection** of the *full evolution* in the subspace $\mathcal{S}$.

Mathematical formulation

Suppose that H' is a q-qubit operator, let $\mathscr{S}$ be an n-dim subspace of $\mathbb{C}^{2^q}$. We write

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If $\underline{R \neq 0}$, in general

$$\left(e^{-iH't}\right)\Big|_{\mathscr{S}} \neq e^{-iHt}$$

There will be **leakage** from the subspace $\mathscr{S}$ to $\mathscr{S}^\perp$.

$\boxed{\text{A natural idea: we want to } \textbf{penalize} \text{ the leakage!}}$

Shriefer-Wolff transformation

Suppose that H' is a q-qubit operator, let $\mathcal{S}$ be an n-dim subspace of $\mathbb{C}^{2^q}$. We write

$$H' = \begin{bmatrix} H & R \\ R^\dagger & B \end{bmatrix},$$

with $H = P_{\mathcal{S}} H' P_{\mathcal{S}}, \quad R = P_{\mathcal{S}} H' P_{\mathcal{S}^\perp}, \quad B = P_{\mathcal{S}^\perp} H' P_{\mathcal{S}^\perp}$.

Assume $\Delta = \lambda_{\min}(B) - \lambda_{\max}(H) > 0$. Define $\kappa = \|R\|/\Delta$.

When $\kappa < 1/2$, there exists a **Shriefer-Wolff transformation** U such that $U^\dagger H' U$ is block-diagonal, and

$$H_{\text{eff}} = \left(U^\dagger H' U\right)\Big|_{\mathcal{S}} = H + O\left(\frac{\|R\|^2}{\Delta}\right)$$

Theorem. (Quantum simulation by Hamiltonian embedding)

For any $t \geq 0$, we have $\left\| \left(e^{-iH't}\right)\Big|_{\mathcal{S}} - e^{-iHt} \right\| \leq \left(8\kappa^2 + 4\sqrt{2}\kappa\right) \|R\| t\,.$

Explicit constructions

$$L = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix}$$

= The graph Laplacian of 

Penalty Hamiltonian: $H_{\text{pen}} = Z_1 + Z_4 + \sum_{j=1}^{3} Z_j Z_{j+1}$.

Ground-energy subspace of H_{pen}: $\mathcal{S} = span\{\, |0101>, |0100>, |0110>, |0010>, |1010> \,\}$

Encoding Hamiltonian: $Q = \hat{n}_1 + \hat{n}_4 - \sum_{j=1}^{4} X_j$, where $\hat{n}_j = \frac{1}{2}\left(I - Z_j\right)$.

Consider $H' = Q + gH_{\text{pen}}$.

$$H' = \begin{bmatrix} L & R \\ R^\dagger & B \end{bmatrix} + \text{const.}$$

(1) For sufficiently large $g > 0$, $\underline{0 < \kappa < 1/2}$. Recall that $\kappa = \|R\|/\Delta$, $\Delta = \lambda_{\min}(B) - \lambda_{\max}(L) > 0$.

($g > 0$ is called the ***penalty*** coefficient —> penalizing the leakage from $\mathcal{S}$ to $\mathcal{S}^\perp$)

(2) Easy to check: $\underline{Q|_{\mathcal{S}} = L}$, or $\underline{H'|_{\mathcal{S}} = L + \text{const}}$.

Explicit constructions

$$L = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix} \hookrightarrow H' = \left(-\frac{1}{2} Z_1 - \frac{1}{2} Z_4 - \sum_{j=1}^{4} X_j \right) + g \left(Z_1 + Z_4 + \sum_{j=1}^{4} Z_j Z_{j+1} \right)$$

- We call this the **antiferromagnetic embedding** of the graph Laplacian L.

- "Antiferromagnetic" $\rightarrow$ the *antiferromagnetic* ordering in the quantum Ising model.

- **Analog quantum simulation**: Rydberg atoms (e.g., QuEra) or spin-glass simulators (e.g., D-Wave).

- **Digital quantum simulation**: H_{pen} is **fast-forwardable** $\rightarrow$ moving to the interaction picture and run **qDRIFT**.

The implementation of this example is available at:
https://github.com/PicksPeng/SimuQ/blob/main/notebooks/tutorials/2-qwalk.ipynb

Rules for building Hamiltonian embeddings

1. *(Addition) For $j = 1, 2$, suppose $H_j^{\mathrm{ebd}} = gH^{\mathrm{pen}} + Q_j$ is an embedding of H_j with the same embedding subspace $\mathcal{S}$. Then, $H^{\mathrm{ebd}} = gH^{\mathrm{pen}} + Q_1 + Q_2$ is an embedding of $H = H_1 + H_2$ with embedding subspace $\mathcal{S}$.*

2. *(Multiplication) Suppose $H^{\mathrm{ebd}} = gH^{\mathrm{pen}} + Q$ is an embedding of H with embedding subspace $\mathcal{S}$. Then, for any real number α, $H'' = gH^{\mathrm{pen}} + \alpha Q$ is an embedding of αH.*

3. *(Composition) For $j = 1, 2$, suppose that the q_j-qubit operator $H_j^{\mathrm{ebd}} = gH_j^{\mathrm{pen}} + Q_j$ is an embedding of H_j with the embedding subspace $\mathcal{S}_j$ being the ground-energy subspace of H_j^{pen}. Then, $H^{\mathrm{ebd}} = gH^{\mathrm{pen}} + Q$ with*

$$H^{\mathrm{pen}} = H_1^{\mathrm{pen}} \otimes \mathbb{I} + \mathbb{I} \otimes H_2^{\mathrm{pen}}, \quad Q = Q_1 \otimes \mathbb{I} + \mathbb{I} \otimes Q_2 \tag{A.14}$$

is an embedding of $H = H_1 \otimes \mathbb{I} + \mathbb{I} \otimes H_2$ with embedding subspace $\mathcal{S} = \mathcal{S}_1 \otimes \mathcal{S}_2$.

4. *(Tensor product) For $j = 1, 2$, suppose that $H_j^{\mathrm{ebd}} = gH_j^{\mathrm{pen}} + Q_j$ is an embedding of H_j with the embedding subspace $\mathcal{S}_j$ being the ground-energy subspace of H_j^{pen}. Then, $H^{\mathrm{ebd}} = gH^{\mathrm{pen}} + Q_1 \otimes Q_2$ with*

$$H^{\mathrm{pen}} = H_1^{\mathrm{pen}} \otimes \mathbb{I} + \mathbb{I} \otimes H_2^{\mathrm{pen}} \tag{A.15}$$

is an embedding of $H = H_1 \otimes H_2$ with embedding subspace $\mathcal{S} = \mathcal{S}_1 \otimes \mathcal{S}_2$.

Hamiltonian embedding of sparse matrices

1. **Band matrix**: non-zero entries are confined to a diagonal band

- Unary embedding, antiferromagnetic embedding

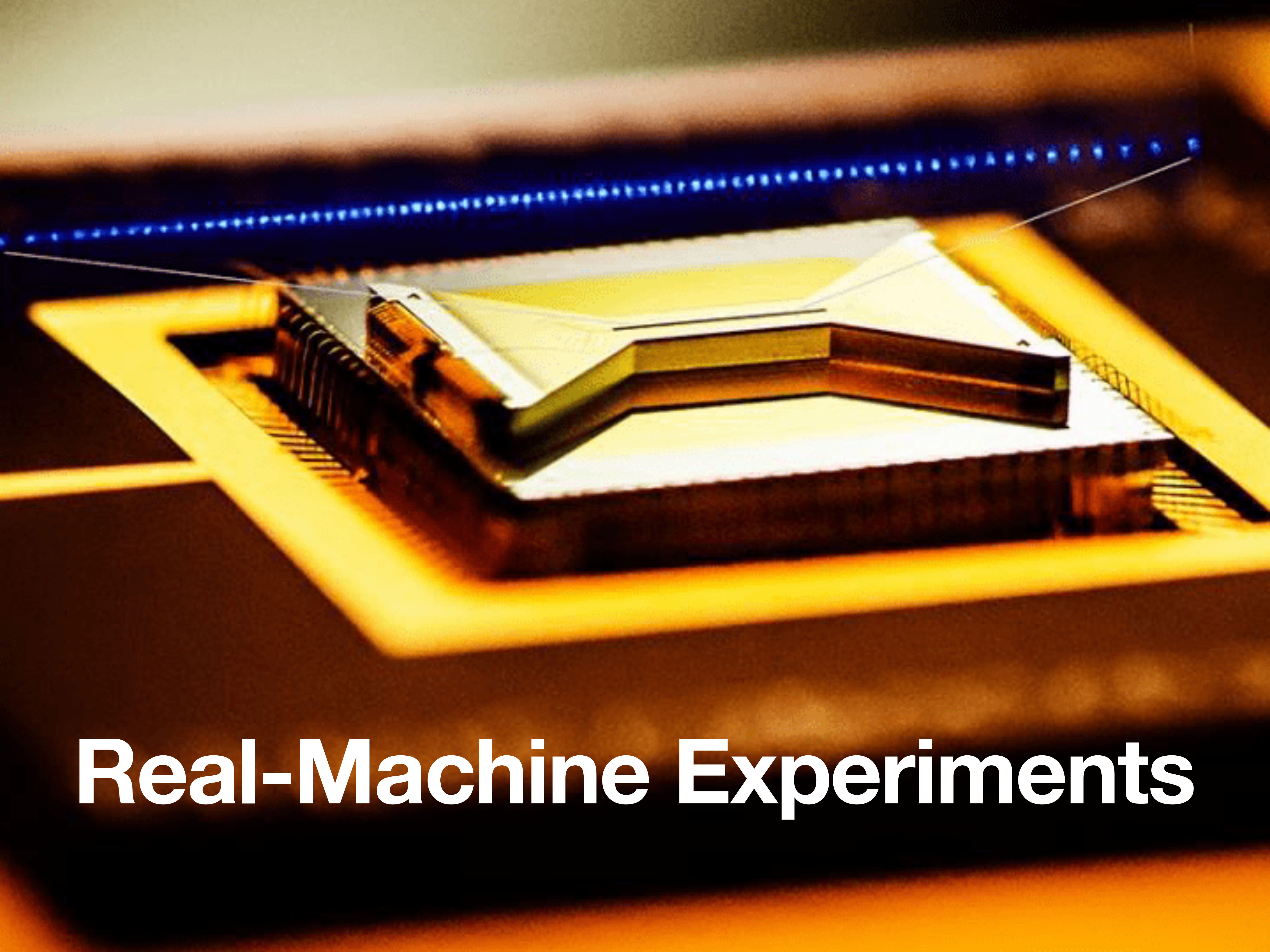
- Embedding Hamiltonian is $\max(2, d)$-local, d = bandwidth

2. **Banded circulant matrix**:

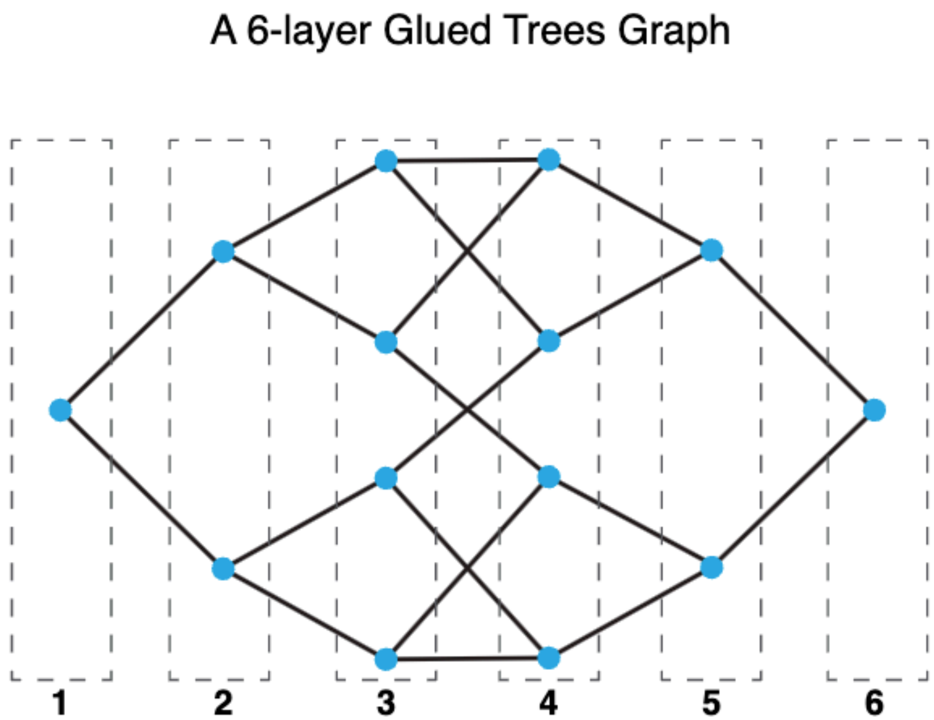
- Circulant unary embedding, circulant antiferromagnetic embedding

3. **Arbitrary sparse matrix**:

- One-hot embedding (with or without penalty Hamiltonian)

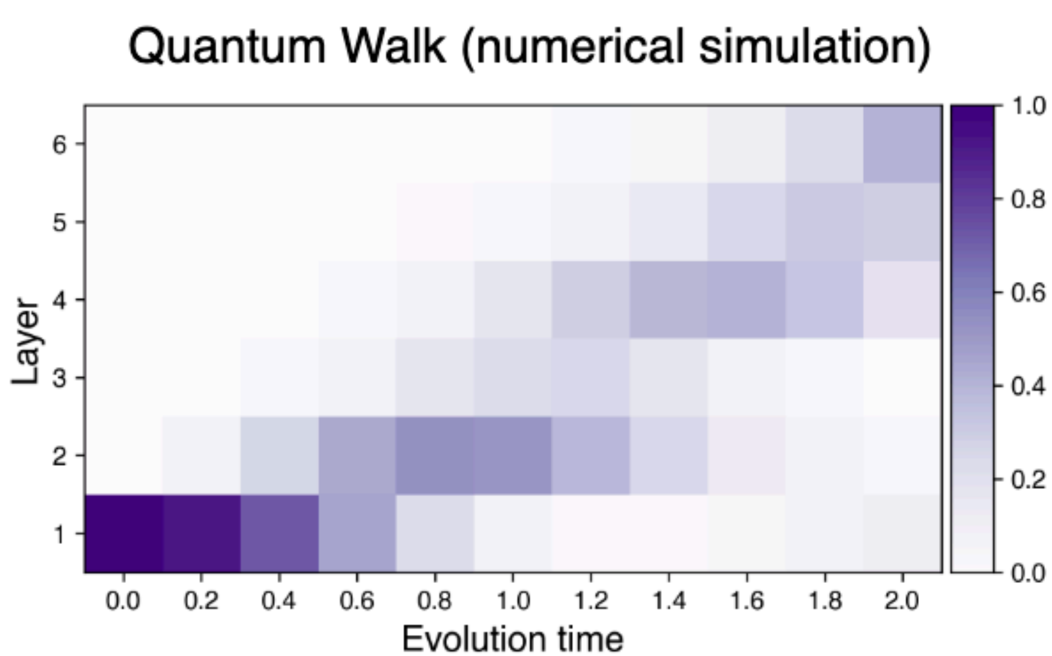

Real-Machine Experiments

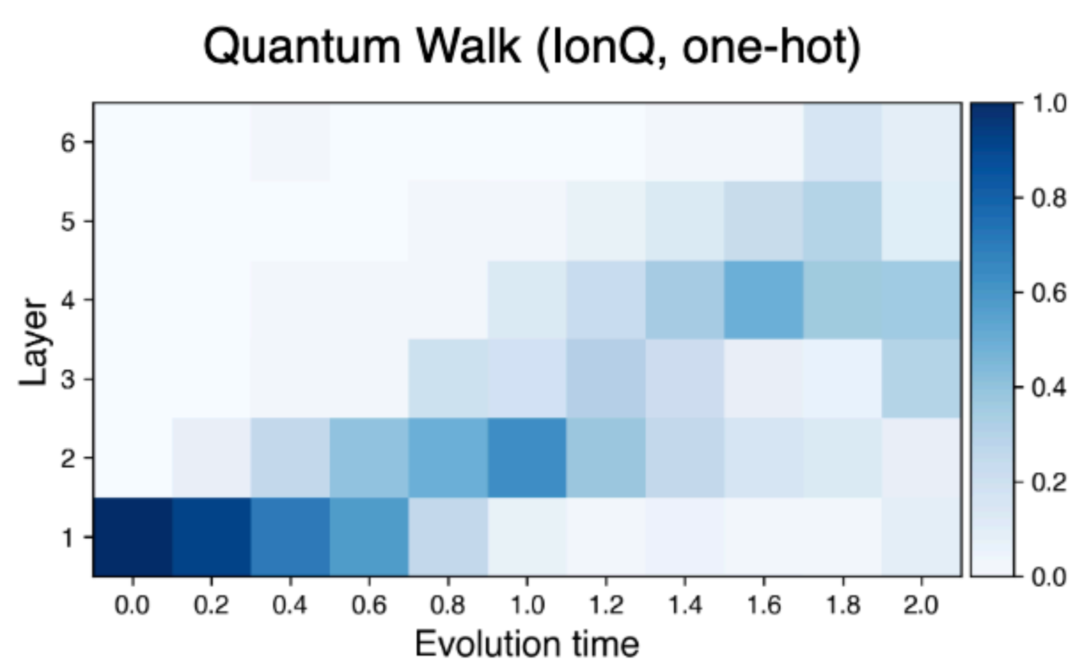
Traversing the glued trees graph



Childs et. al. "Exponential algorithmic speedup by quantum walk". arXiv:quant-ph/0209131

Task: to simulate e^{-iLt}, L = graph Laplacian
Initial state: $|\mathrm{node1}\rangle$
Embedding scheme: penalty-free one-hot
Device: IonQ Aria-1
Resources: 14 qubits, 1 single-qubit gate, 120 two-qubit gates.
Budget: < \$100.





Heat map on layers over evolution time

Simulating real-space quantum dynamics

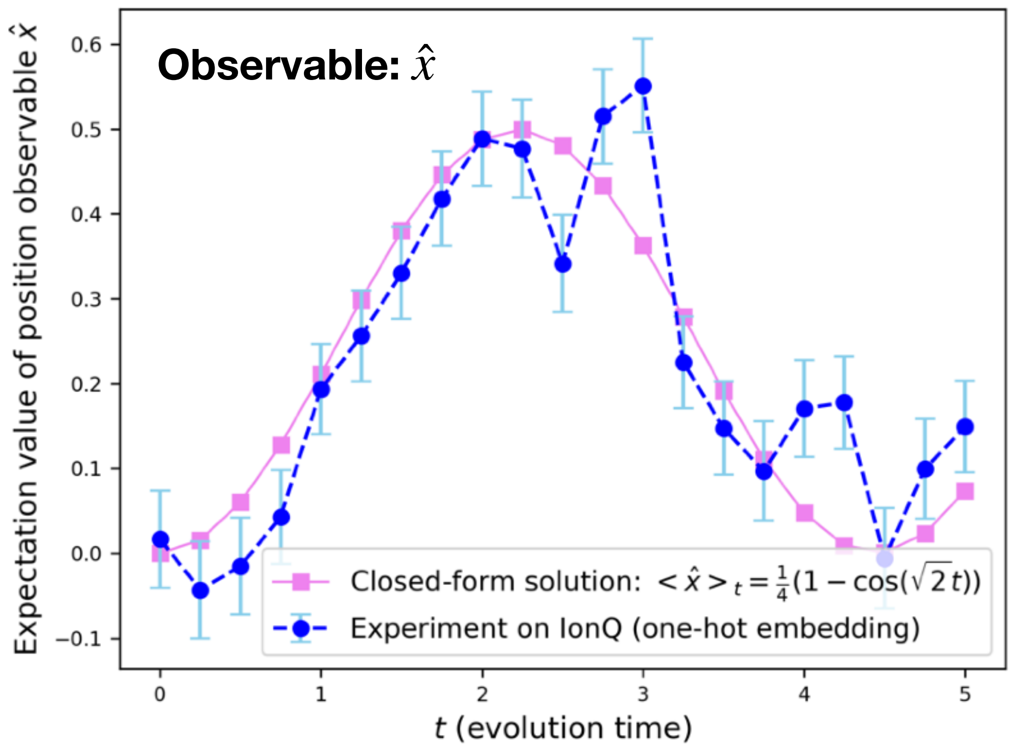
Task: to simulate the following 1D Schrodinger equation (1 Bosonic mode),

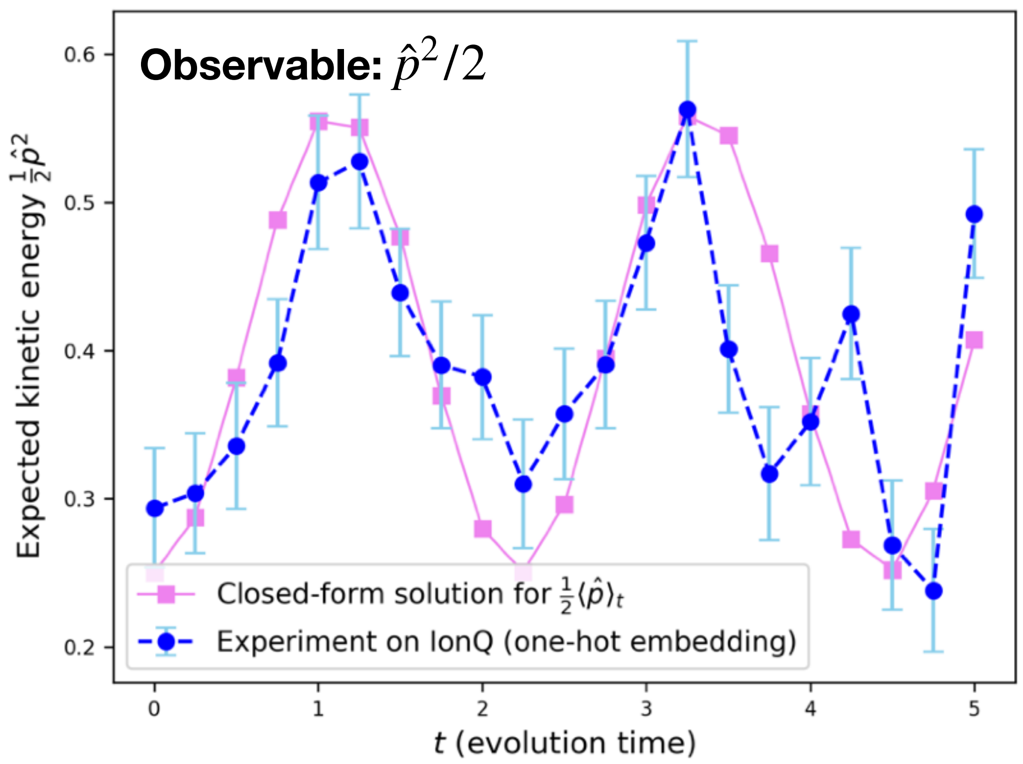
$$i\frac{\partial}{\partial t}\Psi(t,x) = \left[-\frac{1}{2}\frac{\partial^2}{\partial x^2} + \left(\frac{1}{2}ax^2 + bx\right)\right]\Psi(t,x)$$

We choose
$a = 2, \quad b = -1/2.$

with Gaussian initial state $\Psi(0,x) = \left(\frac{1}{2\pi\sigma^2}\right)^{1/4} e^{-\frac{x^2}{4\sigma^2}}$

Embedding scheme: penalty-free one-hot
Device: IonQ Aria-1
Resources: 5 qubits, 1 single-qubit gate, 154 two-qubit gates.
Budget: < $1,300.

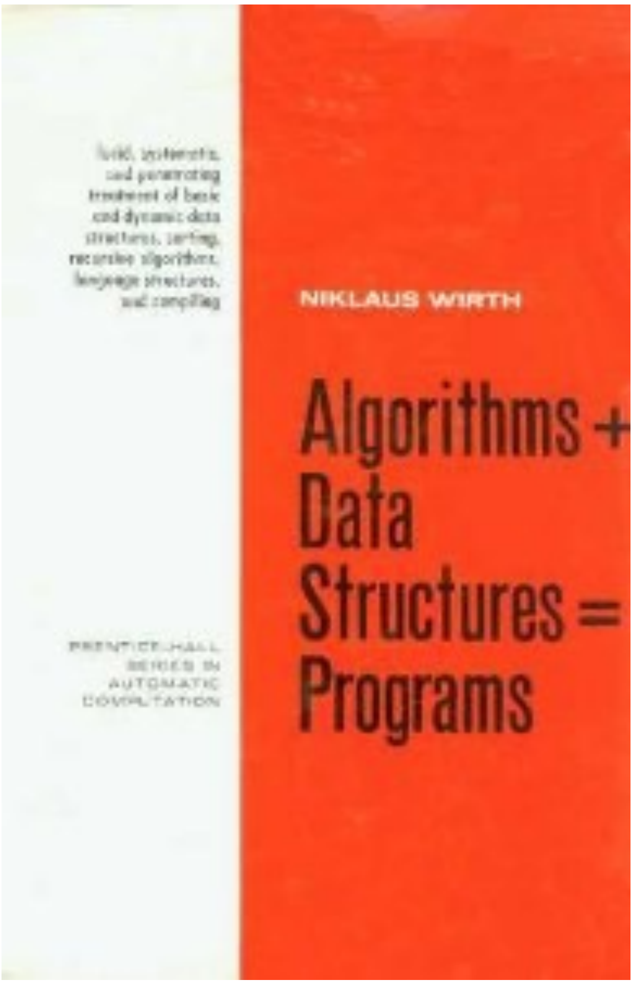




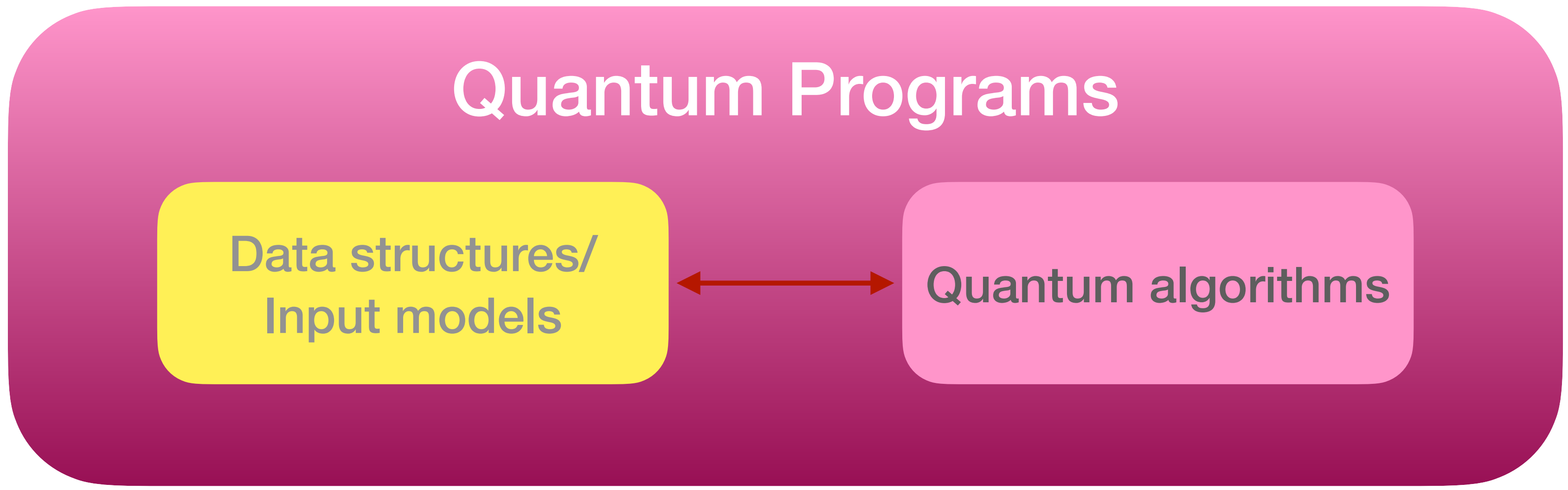
II. Hamiltonian-oriented Quantum Algorithms

A New Paradigm in Quantum Algorithm Design

Programs = Algorithms + Data Structures



By Niklaus Wirth, 1976.



* Output/measurement is also important in quantum algorithm design!

- **Algorithms** and **data structures (input models)** are *inherently* related!
- Classical scientific computing → "matrix-oriented" algorithms (using **numerical linear algebra** as major subroutines)
- Block-encodings → QSP/QSVT
- **Hamiltonian embeddings** → **Hamiltonian-oriented Quantum Algorithms** (using *Hamiltonian simulation* as a major subroutine)

Hamiltonian-oriented Quantum Algorithms

* Feasible on NISQ devices and even early fault-tolerant devices

- Quantum adiabatic algorithms (for discrete optimization)
- (Continuous-time) quantum walk
- Phase estimation (Trotterized controlled evolution, arXiv:1512.06860)
- Linear combination of Hamiltonian Simulations (non-unitary dynamics, arXiv:2303.01029)
- Schrodingerization (non-unitary PDEs, arXiv:2212.13969)
- Quantum Hamiltonian Descent (for continuous optimization, arXiv:2303.01471)
- Pulse-level variational quantum algorithms & quantum optimal control (arXiv:2210.15812)
- And many more …

SimuQ: SIMULation language for Quantum

arXiv:2303.02775. Yuxiang Peng, Jacob Young, Pengyu Liu (CMU), and Xiaodi Wu. Accepted by POPL 2024.

Domain Problems

Quantum chemistry,
Condensed matter,
Optimization, etc.

Hamiltonian-oriented Algorithm

Hamiltonian Simulation

Analog/Hamiltonian compilation

Programmable Quantum Systems

|QuEra⟩ COMPUTING INC.

IBM Q

IONQ

SimuQ

A domain-specific language for quantum simulation with analog compilation

```
pip install simuq
```