Expanding Hardware-Efficiently Manipulable Hilbert Space via Hamiltonian Embedding

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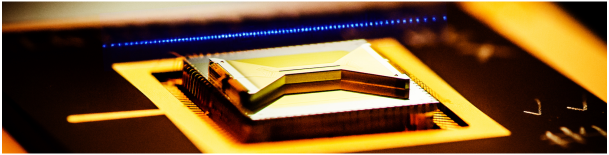
University of Maryland

Motivation

- Bridge the gap between high-level quantum algorithms and implementation on physically realizable quantum hardware platforms



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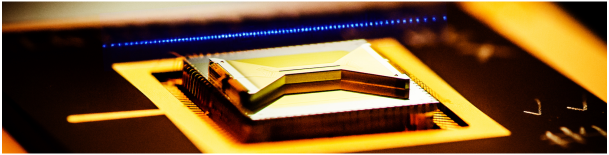
- *Sparse Hamiltonian simulation*: Perform e^{-iAt} for sparse A.



Motivation

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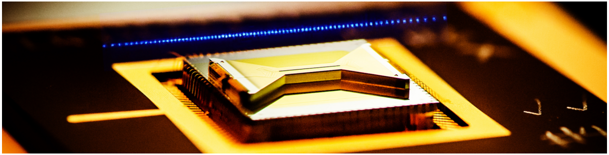
- *Sparse Hamiltonian simulation*: Perform e^{-iAt} for sparse A.
- Can we develop a systematic framework allowing for **hardware-efficient implementations** of quantum algorithms on near-term devices?
  - Make the best use of *native* device operations
  - Commercially available platforms: D-Wave, QuEra, IonQ, etc.



Input models for Hamiltonian simulation

Sparse-matrix oracle access
Construct oracles to query entries of A:

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

Block-encoding
Encode A as a block in unitary

$$U_A = \begin{pmatrix} A & * \\ * & * \end{pmatrix}$$

- **Advantages**: Enables design and analysis of highly efficient algorithms (Childs and Kothari 2011; Low and Chuang 2017; Gilyén et al. 2019, etc.)
- **Limitations**: Very high overheads! Block-encoding an 8×8 banded circulant matrix: 171 one-qubit gates and 114 two-qubit gates for a **single** oracle call (Camps et al. 2022)

Input models for Hamiltonian simulation

Pauli access model (standard binary)
Decompose A as a sum of Pauli operators:

$$A = \sum_j a_j P_j.$$

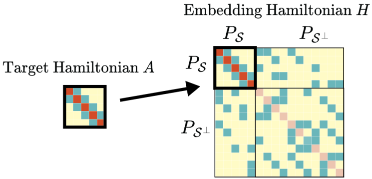
- **Advantages**: Easy for simulation on real devices if matching hardware native operations
  - Analog quantum computers (D-Wave, QuEra) with Ising-like machine Hamiltonian
  - Digital quantum computers (IonQ, IBM, etc.) capable of 1- and 2-qubit operations
- **Limitations**: Can require exponential number of terms even for structured matrices, typically involving more than 2-body interactions

A Unifying Framework for Embedding Hamiltonians

Hamiltonian embedding: Embed the dynamics of the target Hamiltonian A into a larger Hamiltonian H restricted to a subspace $\mathcal{S}$ which we call the *embedding subspace*.

$$H = \begin{pmatrix} A & 0 \\ 0 & * \end{pmatrix} \implies e^{-iHt} = \begin{pmatrix} e^{-iAt} & 0 \\ 0 & * \end{pmatrix}$$

Generalize to "approximately" block-diagonal Hamiltonians:



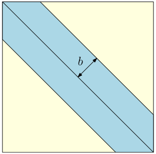
Error depends on off-diagonal blocks $R = P_{\mathcal{S}^\dagger} H P_{\mathcal{S}}$:

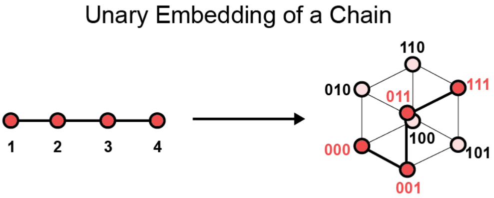
- If $R = 0$, no error
- If $R \neq 0$, introduce a sufficiently large penalty Hamiltonian

A Unifying Framework for Embedding Hamiltonians

Embedding scheme	Sparsity structure	Max Pauli weight
Unary	Band	$\max(b, 2)$
Antiferromagnetic	Band	$\max(b, 2)$
Circulant unary	Banded circulant	$\max(b, 2)$
Circulant antiferromagnetic	Banded circulant	$\max(b, 2)$
One-hot (w/ penalty)	Arbitrary sparse	2
Penalty-free one-hot	Arbitrary sparse	2

b is the bandwidth of a banded matrix:





Some embeddings studied before in different contexts (Chancellor 2019; Hadfield et al. 2019; Sawaya et al. 2020)

Example: Embedding a Tridiagonal Matrix

Consider an 5×5 tridiagonal matrix:

$$A = \begin{pmatrix} 0 & 1 & & & \\ 1 & 0 & 1 & & \\ & 1 & 0 & 1 & \\ & & 1 & 0 & 1 \\ & & & 1 & 0 \end{pmatrix}$$

Our framework provides **flexibility** to choose from a collection of different embeddings:

Embedding scheme	**Embedding Hamiltonian** H
Unary	$\sum_{j=1}^{4} X_j + g\left(Z_1 - Z_4 - \sum_{j=1}^{3} Z_j Z_{j+1}\right)$
Antiferromagnetic	$\sum_{j=1}^{4} X_j + g\left(Z_1 + Z_4 + \sum_{j=1}^{3} Z_j Z_{j+1}\right)$
One-hot (w/ penalty)	$\sum_{j=1}^{4} X_j X_{j+1} + g\left(\sum_j \frac{I - Z_j}{2} - 1\right)^2$
Penalty-free one-hot	$\frac{1}{2} \sum_{j=1}^{4} X_j X_{j+1} + Y_j Y_{j+1}$

$g > 0$ is the penalty coefficient for embeddings with a penalty

Hamiltonian Embedding: A New Input Model

- **Advantages**: Embedding certain sparse matrices requires 2-body Hamiltonians $\implies$ enables analog implementations, significantly reduced gate counts for digital implementation
- **Limitations**: Uses $O(n)$ qubits to embed an $n \times n$ matrix (standard binary requires $O(\log n)$ qubits)

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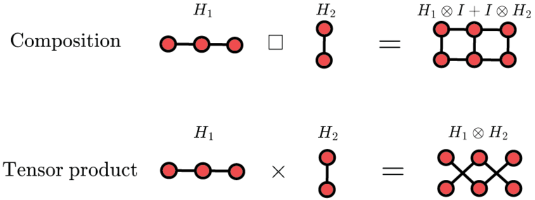
Two embedding Hamiltonians H_1 and H_2 can be composed in different ways:



The dimension of the embedding subspace increases *multiplicatively*.

By composing many such Hamiltonian embeddings, we are able to simulate Hamiltonians with **logarithmically** many resources.

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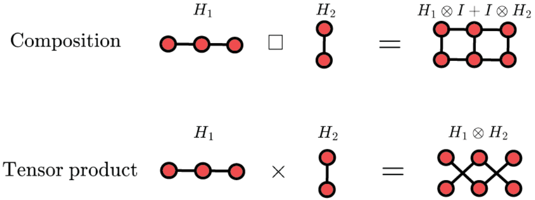

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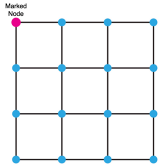
↳ Potential **exponential** quantum speedup!

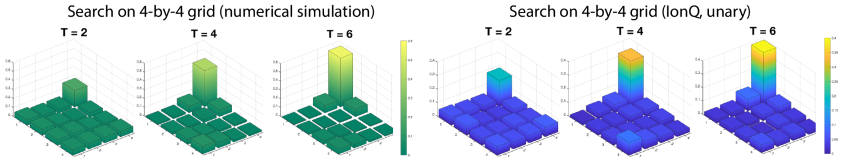
Quantum spatial search on 2D lattices

Task: Starting from uniform superposition state, simulate

$$H = -\gamma L - |w\rangle\langle w|$$

to find the *marked node* $|w\rangle$ (Childs and Goldstone 2004).
Embedding scheme: unary embedding
Resources: 6 qubits, 132 1-qubit gates, 114 2-qubit gates
Budget: $< \$100$ (AWS Braket pricing)





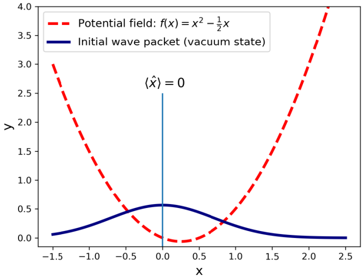
Standard binary: **831 1-qubit and 123 2-qubit gates** on 4 qubits.

Real-space quantum dynamics - IonQ

Task: Simulate the 1D Schrödinger equation with a quadratic potential:

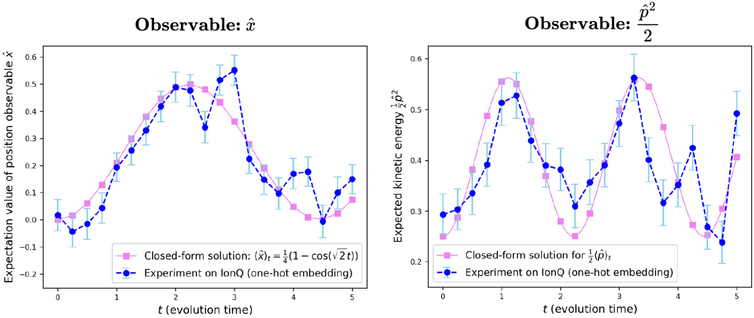
$$i\frac{\partial}{\partial t}\Psi = \left[-\frac{1}{2}\nabla^2 + \left(x^2 - \frac{1}{2}x\right)\right]\Psi(t,x)$$

with Gaussian initial state $\Psi(0,x) \propto e^{-\frac{x^2}{4\sigma^2}}$.



Real-space quantum dynamics - IonQ

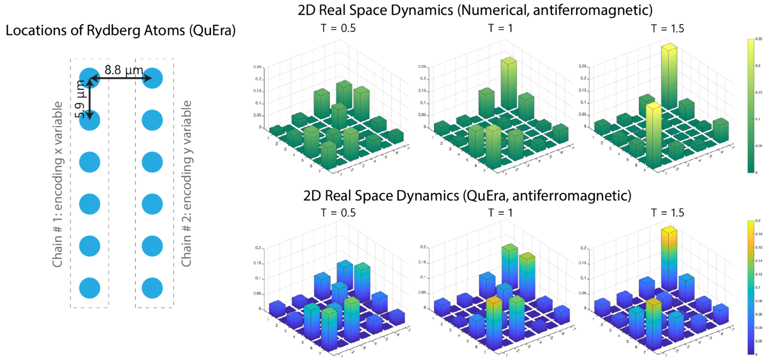
Method: Fock space truncation
Embedding scheme: penalty-free one-hot embedding
Resources: 5 qubits, 1 single-qubit gate, 154 two-qubit gates.
Budget: $< \$1300$ (AWS Braket pricing)



Standard binary: requires over **1800 1-qubit gates** and **200 2-qubit gates** on 3 qubits.

Real-space quantum dynamics - QuEra

Method: Finite differences
Embedding scheme: antiferromagnetic embedding
Resources: 12 qubits, 2 μs evolution time
Budget: $< \$100$ (AWS Braket pricing)



Standard binary: analog implementation not possible

Summary and Outlook

- We developed a **unifying framework** for mapping sparse problem Hamiltonians to embedding Hamiltonians accessible to quantum hardware, applicable to analog and digital devices
- Our framework allows for *hardware-aware* design of algorithms and leads to **significantly improved resource usage** (gate count), enabling the deployment of quantum algorithms for interesting scientific problems

Future directions:

- Applications to other problems? (condensed matter physics, quantum chemistry, differential equations, etc.)
- Finding new task-oriented Hamiltonian embeddings for problems with less regular structure?

Acknowledgement

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https://github.com/jiaqileng/hamiltonian-embedding

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