Expanding Hardware-Efficiently Manipulable Hilbert Space via Hamiltonian Embedding

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Abstract

We propose Hamiltonian embedding, a technique for simulating a desired sparse Hamiltonian by embedding it into the evolution of a larger and more structured quantum system, allowing for more efficient simulation through hardware-efficient operations. We conduct a systematic study of this new technique and demonstrate significant savings in computational resources for implementing prominent quantum applications. As a result, we experimentally realize quantum walks on complicated graphs (e.g., binary trees, glued-tree graphs), quantum spatial search, and the simulation of real-space Schrödinger equations on current trapped-ion and neutral-atom platforms. Given the fundamental role of Hamiltonian evolution in the design of quantum algorithms, our technique markedly expands the horizon of implementable quantum advantages in the NISQ era.

Motivation: Sparse Hamiltonian simulation

Sparse Hamiltonian simulation plays a fundamental role in quantum computation. Although several theoretically appealing quantum algorithms have been proposed for this task, they typically require a black-box query model of the sparse Hamiltonian, rendering them impractical for near-term implementation on quantum devices.

To avoid sophisticated oracle constructions, we propose to use the quantum Hamiltonian to model native operations in a quantum computer, thereby enabling efficient Hamiltonian simulation without going through a hardware-agnostic compilation process. We develop a general framework with rigorous error analysis and a flexible construction approach with concrete instances, allowing us to demonstrate interesting quantum applications on both digital and analog quantum computers.

General formulation and error analysis

Given $\eta, \epsilon > 0$, we say H is a (q, η, ϵ)-**embedding** of A if there exists a subspace $\mathcal{S} \subset \mathbb{C}^{2^q}$ and a unitary operator U such that

1. $P_{\mathcal{S}}(U^\dagger H U)P_{\mathcal{S}^\perp} = 0$, i.e., $U^\dagger H U$ is block-diagonal in $\mathcal{S}$ and $\mathcal{S}^\perp$,
2. $\|I - U\| \leq \eta$, where I is the identity operator in $\mathbb{C}^{2^q}$,
3. $\|(U^\dagger H U)|_{\mathcal{S}} - A\| \leq \epsilon$, where $(\cdot)|_{\mathcal{S}} \coloneqq P_{\mathcal{S}}(\cdot)P_{\mathcal{S}}$.

We call the subspace $\mathcal{S}$ as the **embedding subspace**.

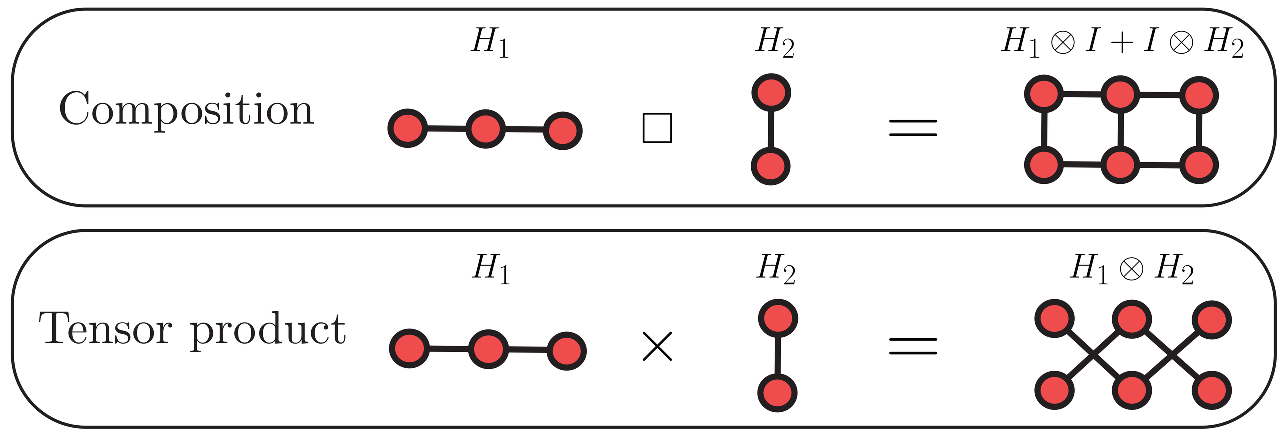
Theorem 1. (Hamiltonian simulation with Hamiltonian embedding)
Suppose that H is a (q, η, ϵ)-embedding of A. Then, for a fixed evolution time $t \geq 0$, we have that

$$\left\| \left(e^{-iHt}\right)\Big|_{\mathcal{S}} - e^{-iAt} \right\| \leq (2\eta\|H\| + \epsilon)t.$$

Building Hamiltonian embeddings

Theorem 2. (Rules for building Hamiltonian embeddings)

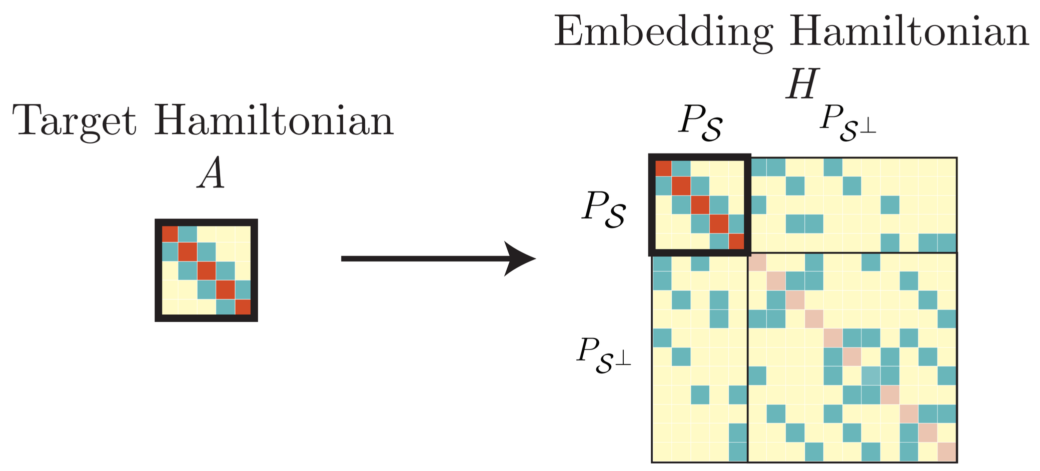
1. (Addition) For $j = 1, 2$, let H_j be a (q, η, ϵ_j)-embedding of A_j, then $H_1 + H_2$ is a $(q, \eta, \epsilon_1 + \epsilon_2)$-embedding of $A_1 + A_2$.
2. (Multiplication) Let H be a (q, η, ϵ_j)-embedding of A, then for a real scalar α, αH is a $(q, \eta, |\alpha|\epsilon)$-embedding of αA.
3. (Composition) For $j = 1, 2$, let H_j be a $(q_j, \eta_j, \epsilon_j)$-embedding of A_j, then $H_1 \otimes I + I \otimes H_2$ is a $(q_1 + q_2, \eta_1 + \eta_2, \epsilon_1 + \epsilon_2)$-embedding of $A_1 \otimes I + I \otimes A_2$.
4. (Tensor product) For $j = 1, 2$, let H_j be a $(q_j, \eta_j, \epsilon_j)$-embedding of A_j, then $H_1 \otimes H_2$ is a $(q_1 + q_2, \eta_1 + \eta_2, \|A_1\|\epsilon_2 + \|A_2\|\epsilon_1 + \epsilon_1\epsilon_2)$-embedding of $A_1 \otimes A_2$.



Perturbative Hamiltonian embedding

Let Q be a q-qubit operator such that $Q\big|_{\mathcal{S}} = A$, and let H^{pen} be a q-qubit operator such that the ground-energy subspace is $\mathcal{S}$. For $g > 0$, we construct $H = gH^{\text{pen}} + Q$ to be a **perturbative Hamiltonian embedding** of A with penalty coefficient g.

Theorem 3. (Perturbative Hamiltonian embedding, informal)
Let H and A be as above, and let $R = P_{\mathcal{S}^\perp} Q P_{\mathcal{S}}$, where $P_{\mathcal{S}}$ and $P_{\mathcal{S}^\perp}$ are projections onto $\mathcal{S}$ and $\mathcal{S}^\perp$. Then for sufficiently large $g > 0$, the Hamiltonian H is a (q, η, ϵ)-embedding of A, where $\eta \sim 1/g$, $\epsilon \sim \|R\|/g$.



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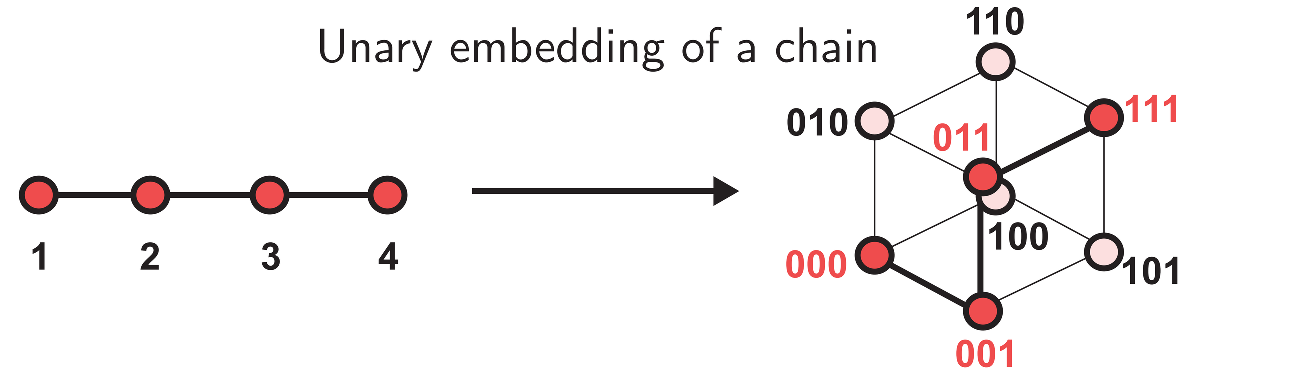
Hamiltonian embedding of sparse matrices

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)

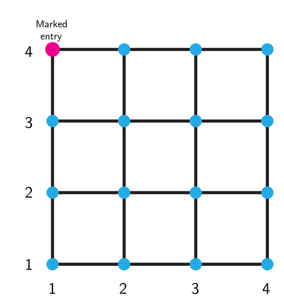


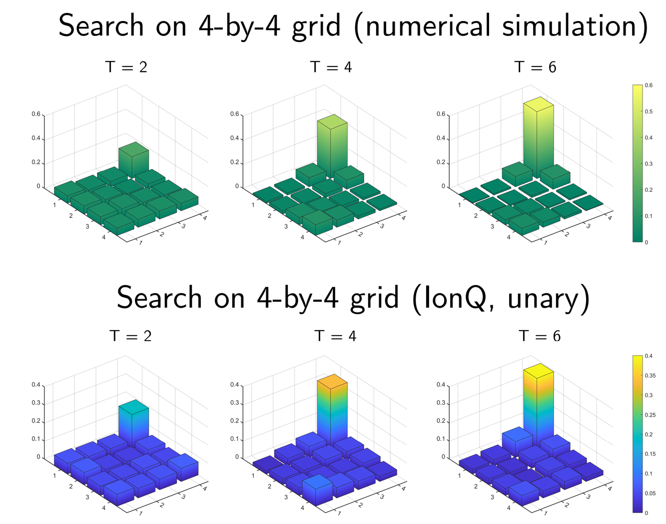
Real-machine experiments

Quantum spatial search on a 2D lattice.
Starting from the uniform superposition state, we simulate

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

to find the *marked node* $|w\rangle$ on a 2D lattice (L is the graph Laplacian).



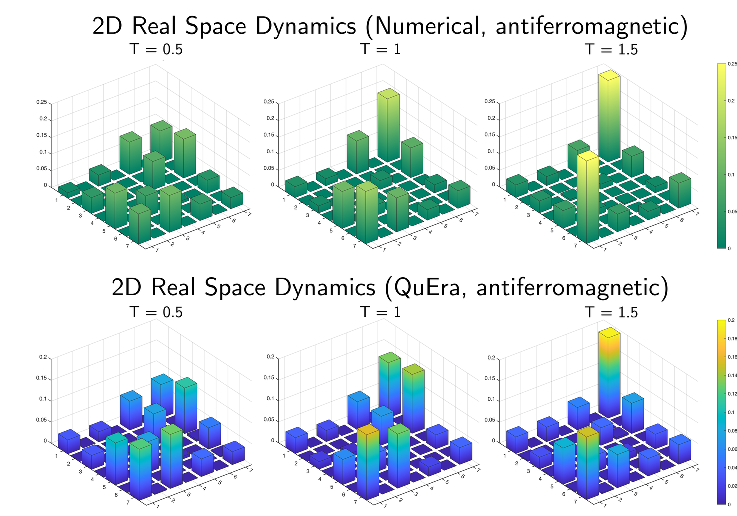


Spatial search on IonQ Aria-1

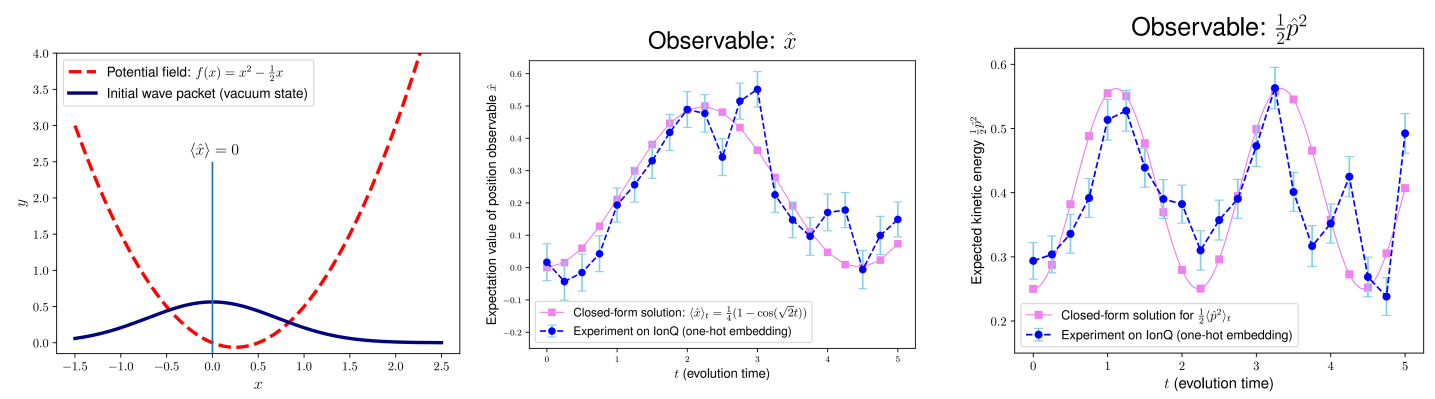
Real-space quantum simulation.
We simulate the Schrödinger equation over d-dimensional Euclidean space:

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

with initial state $\Psi(0, x) = \Psi_0(x)$.



Real-space simulation on QuEra Aquila



Real-space simulation on IonQ Aria-1