

Womanium Final Project: Development of Novel Quantum Algorithms

Smooth Unitary Operators:

Dimitrios Kranas & Haemanth Velmurugan

Project: Exponential quantum speedup in simulating coupled classical oscillators [Ryan Babbush et al (2023)]

Description

- System of N harmonic oscillators mapped to a system of 2^{2n} qubits.

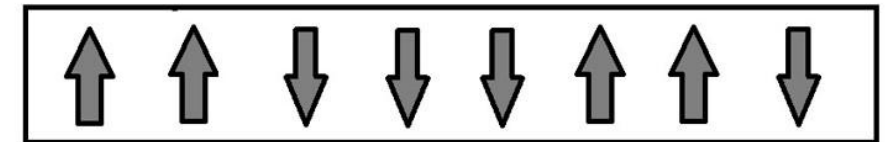
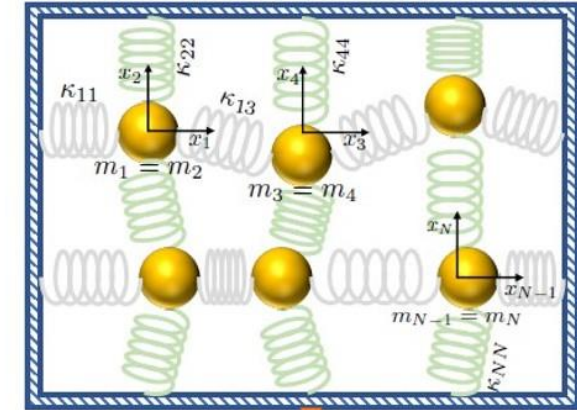
$$|\psi(t)\rangle = \frac{1}{\sqrt{2E}} \begin{pmatrix} \sqrt{M} \dot{\vec{x}}(t) \\ i\vec{\mu}(t) \end{pmatrix}$$

- Mathematical correspondence allows us leverage quantum toolbox:
Hamiltonian Simulation

Result:

Finding an algorithm that produces the state $|\psi(t)\rangle$ efficiently.

Credits: **Ryan Babbush et al**



Tasks achieved

1. Initial state preparation.
2. Construction of the effective Hamiltonian matrix **H**.
3. Decomposition of **H** to a linear combination of unitaries (LCU).
4. Block encoding of **H**.
5. Implementation of the **Hamiltonian simulation** algorithm via the qubitization method.
6. Exploring the parameters space of the model: masses & spring constant values.
7. Optimizing for circuit's **width** & **depth** parameters.
8. Exploring efficiency of several **quantum hardware**s.

Quantum algorithms: extensions proposed

I) Decomposition of an arbitrary $N \times N$ Ham. matrix into Pauli strings (**LCU decomposition**).

LCU Pauli Strings decomposition of the Hamiltonian matrix $\bar{\mathbf{H}}$

Any hermitian operator acting on a Hilbert space \mathcal{H} can be decomposed to a sum of the identity and Pauli matrices tensor products as

$$\mathbf{H} = \sum_{i_1=0}^3 \sum_{i_2=0}^3 \dots \sum_{i_{2n+1}=0}^3 c_{i_1 i_2 \dots i_{2n+1}} \mathbf{P}_{i_1} \otimes \mathbf{P}_{i_2} \otimes \dots \otimes \mathbf{P}_{i_{2n+1}},$$

where $\mathbf{P}_{i_1} \otimes \mathbf{P}_{i_2} \otimes \dots \otimes \mathbf{P}_{i_{2n+1}}$ with $\mathbf{P}_i = (\mathbf{I}, \mathbf{X}, \mathbf{Y}, \mathbf{Z})$ forms a basis with an orthonormal product given by

For the N -oscillators, resulting to the $2n + 1$ -qubits case, as we explained in the 2_oscilators notebook, the orthonormality reads

$$\langle \mathbf{P}_{i_1} \otimes \mathbf{P}_{i_2} \otimes \dots \otimes \mathbf{P}_{i_{2n+1}}, \mathbf{P}_{i'_1} \otimes \mathbf{P}_{i'_2} \otimes \dots \otimes \mathbf{P}_{i'_{2n+1}} \rangle = \frac{1}{2^{2n+1}} \text{Tr} [(\mathbf{P}_{i_1} \otimes \mathbf{P}_{i_2} \otimes \dots \otimes \mathbf{P}_{i_{2n+1}}) (\mathbf{P}_{i'_1} \otimes \mathbf{P}_{i'_2} \otimes \dots \otimes \mathbf{P}_{i'_{2n+1}})] = \delta_{i_1 i'_1} \delta_{i_2 i'_2} \dots \delta_{i_{2n+1} i'_{2n+1}}.$$

The (padded) $2N^2 \times N^2$ Hamiltonian of the N oscillators that maps the evolution to that of a $2n + 1$ -qubit system is decomposed to the LCU Pauli basis $(\mathbf{P}_{i_1} \otimes \mathbf{P}_{i_2} \otimes \dots \otimes \mathbf{P}_{i_{2n+1}})$ with its expansion coefficients given by

$$c_{i_1 i_2 \dots i_{2n+1}} = \frac{1}{2^{2n+1}} \text{Tr} [(\mathbf{P}_{i_1} \otimes \mathbf{P}_{i_2} \otimes \dots \otimes \mathbf{P}_{i_{2n+1}}) \mathbf{H}].$$

The code below computes the $c_{i_1 i_2 \dots i_{2n+1}}$ coefficients from which it constructs the LCU decomposition of the Hamiltonian.

Quantum algorithms: extensions proposed

2) Block encoding of Hamiltonians with **negative** LCU decomposition coefficients.

$$H = \sum_i a_i U_i, \quad a_i \in \text{Re}$$

Classiq's "apply_pauli_term" $\frac{1}{2} X \cdot Z$ $\xrightarrow{U = -I}$ $-\frac{1}{2} X \cdot Z$

Quantum algorithms: extensions proposed

3) We combined Classiq's functions "prepare_amplitude()" & "unitary()" to **prepare** the **initial state**.

$$|0\rangle \xrightarrow{\text{prepare_amplitude()}} \begin{pmatrix} \sqrt{M}\dot{\vec{y}}(0) \\ \vec{y}(0) \end{pmatrix} \xrightarrow{U = \begin{pmatrix} I & 0 \\ 0 & iI \end{pmatrix}} \begin{pmatrix} \sqrt{M}\dot{\vec{y}}(0) \\ i\vec{y}(0) \end{pmatrix}$$

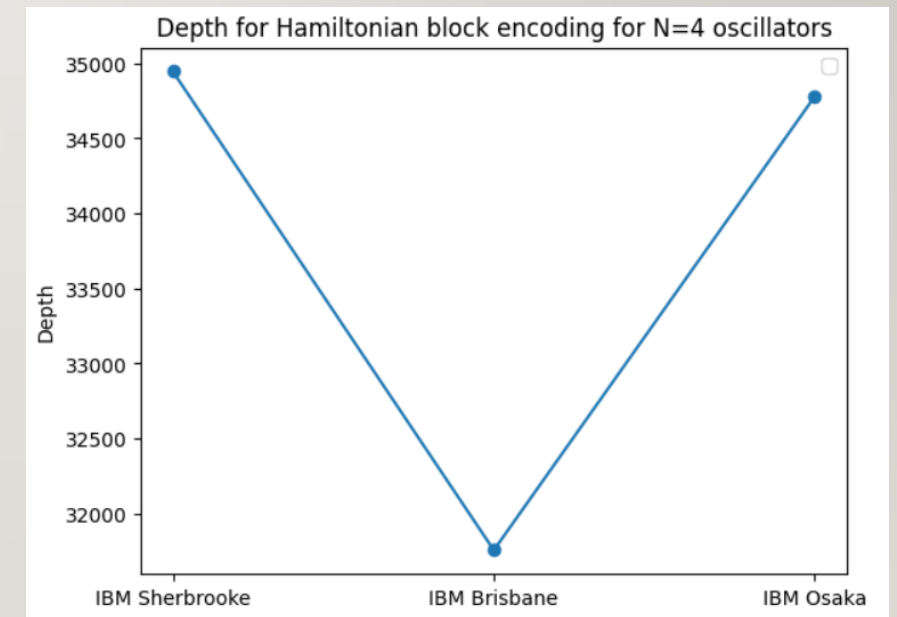
Analysis

Parameters & Resources

- Our algorithm becomes efficient for mass-to-spring constants ratio: $m/\kappa > 10^3$.
- We **optimized** our circuit for **width & depth**.
- We explored the **performance** of different **quantum hardware**.

Case of N=2 oscillators

S.No	Method	Width	Depth	U	CX
1.	Default	12	7886	5817	5507
2.	Optimize Width	10	14628	11013	10347
3.	Optimize Depth	267	4433	4100	3555

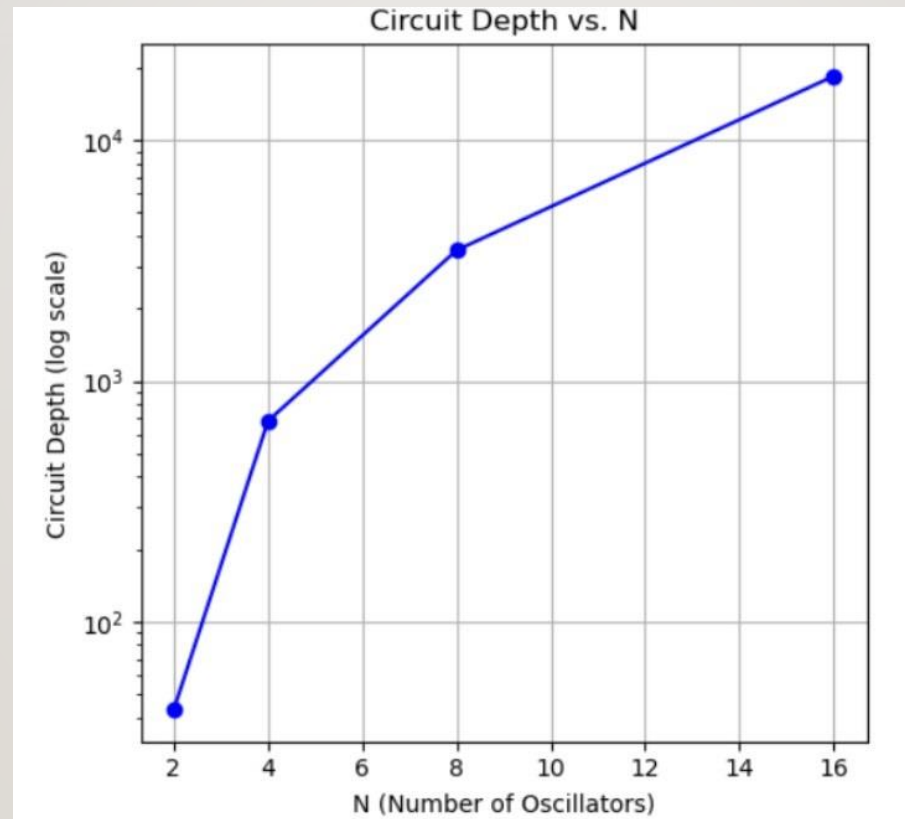


Future Directions

- ❖ Study in greater detail the **optimal model parameters** (masses, spring constants) & **initial conditions** (velocities, displacements).
- ❖ In-depth investigation of the **scalability** of our quantum algorithm, i.e. **depth, gate counts**, etc. vs the number N of oscillators.
- ❖ Compare Classiq's **optimization parameters** with the papers' theoretical **bounds of complexity**.
- ❖ Include **dissipation (energy losses)** in the analysis.

Future Directions

Analysis for initial state preparation



**Thank you for the wonderful quantum
journey this summer!!**

