Womanium Final Project: Development of Novel Quantum Algorithms

Smooth Unitary Operators:

Dimitrios Kranas & Haemanth Velmurugan

<u>Project</u>: Exponential quantum speedup in simulating coupled classical oscillators [**Ryan Babbush et al (2023)**]

<u>Description</u>

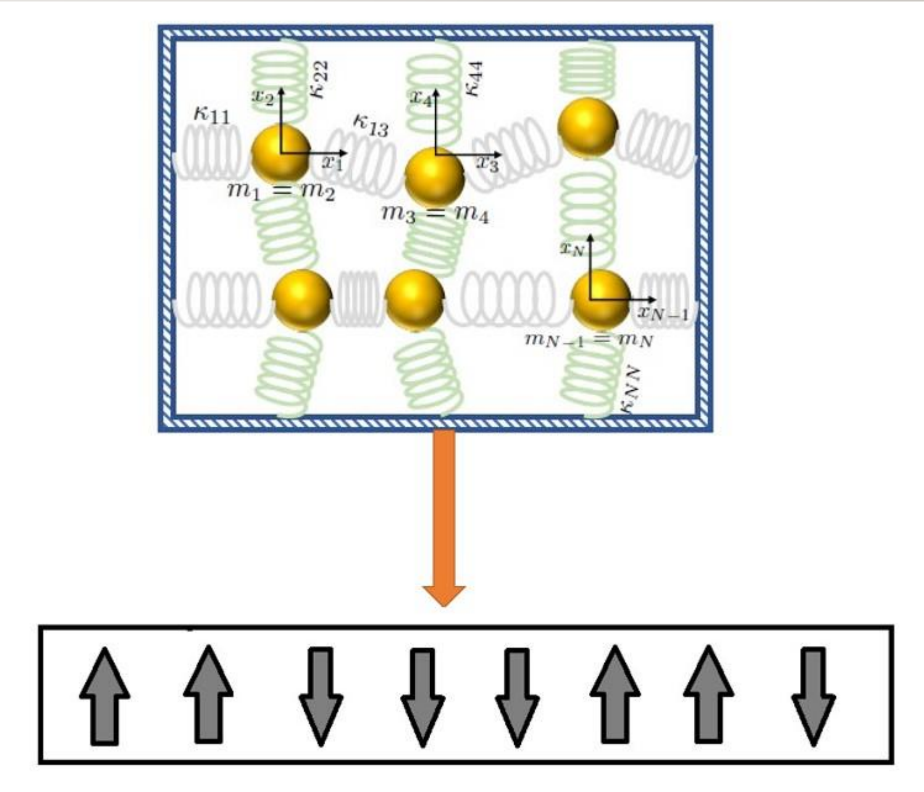
- System of N harmonic oscillators mapped to a system of 2^{2n} qubits.

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

- Mathematical correspondence allows us leverage quantum toolbox: **Hamiltoanian Simulation**

<u>Result</u>:
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 hardwares**.

Quantum algorithms we development

1) 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

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

where $\mathbf{P}_{i_1} \otimes \mathbf{P}_{i_2} \otimes \cdots \otimes \mathbf{P}_{i_{2n+1}}$ 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

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

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 Paili basis $(\mathbf{P}_{i_1} \otimes \mathbf{P}_{i_2} \otimes \cdots \otimes \mathbf{P}_{i_{2n+1}})$ with its expansion coefficients given by

$$\underline{c_{i_1 i_2 \ldots i_{2n+1}} = \frac{1}{2^{2n+1}} \mathrm{Tr}\left[(\mathbf{P}_{i_1} \otimes \mathbf{P}_{i_2} \otimes \cdots \otimes \mathbf{P}_{i_{2n+1}}) \mathbf{H} \right].}$$

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

WOMANIUM | QUANTUM

Quantum algorithms development

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

$$H = \sum_i a_i U_i \,, \qquad a_i \in \mathrm{Re}$$

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

Quantum algorithms development

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

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

❮ WOMANIUM | QUANTUM ❯

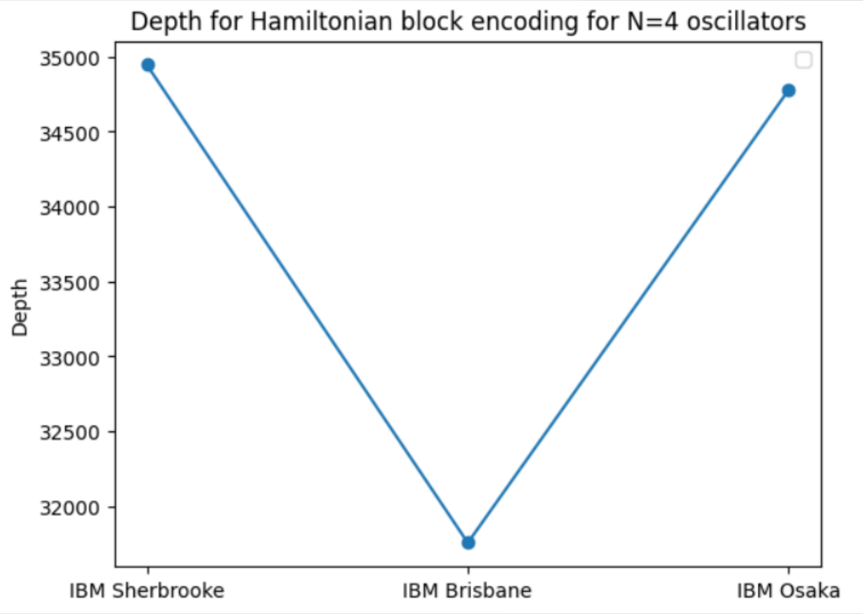
Post-processing

Parameters & Resources

- Our algorithm becomes efficient for mass-to-spring constants ratio: $\boldsymbol{m/\kappa > 10^3}$.
- 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



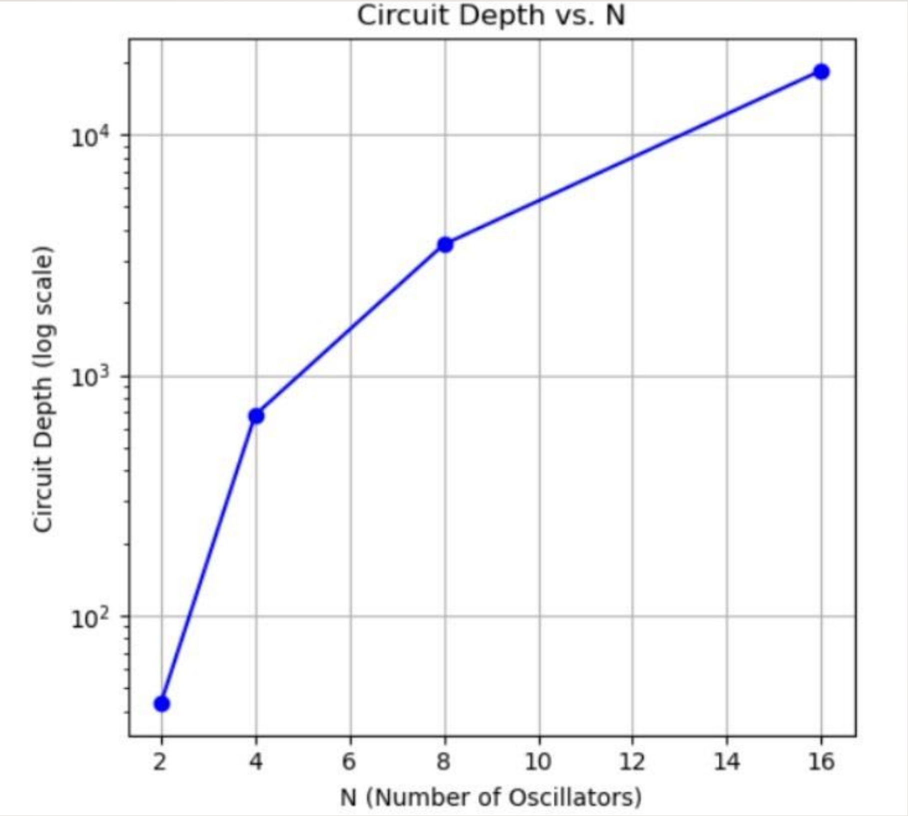
WOMANIUM | QUANTUM

Future Directions

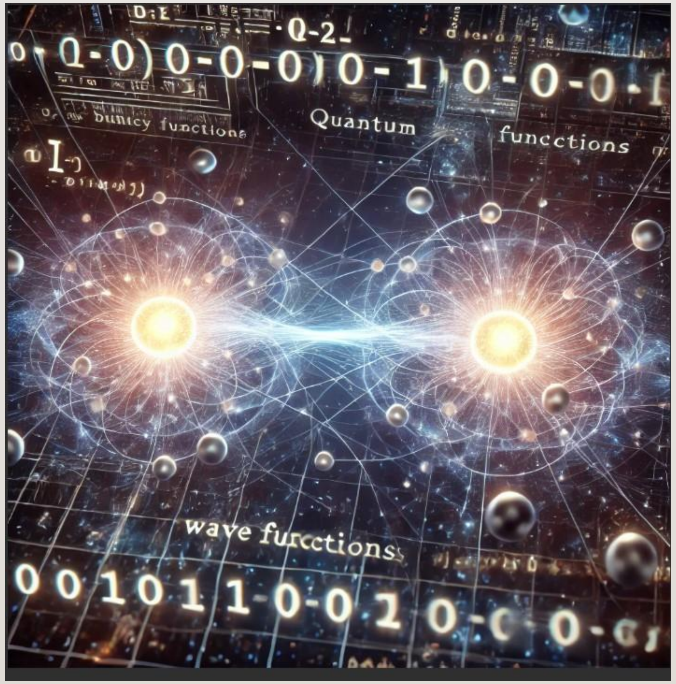
- Study in greater detail the **optimal model parameters** (masses, spring constants) & **initial conditions** (velocities, displacements).
- In-depth investigation of the **scalability** of our quantum algorithm, i.e. **depth**, **gate counts**, etc. vs the number N of oscillators.
- Compare Classiq's **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!!



WOMANIUM | QUANTUM