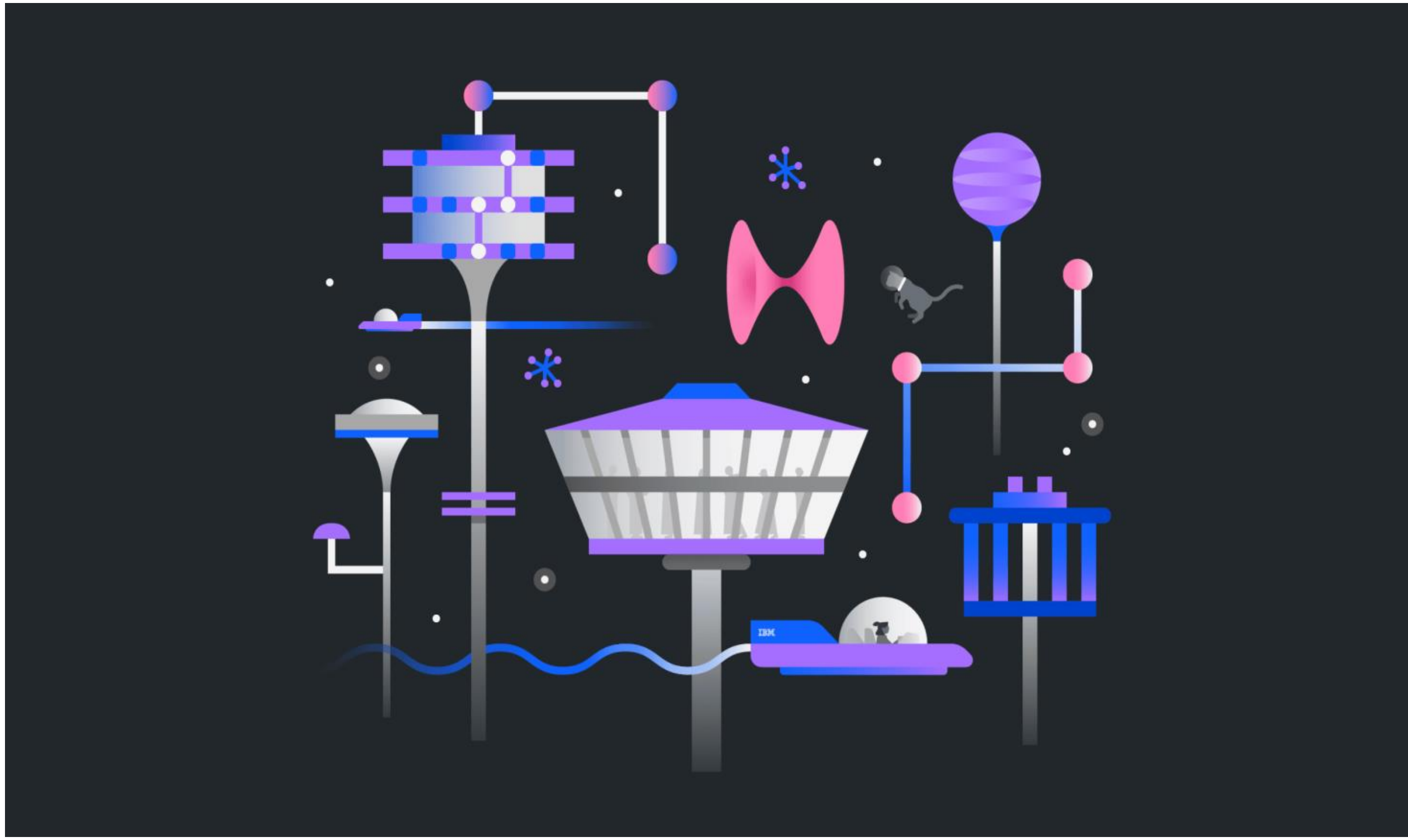
BasQ Qiskit Fall Fest 2024

Implementation of the Jaynes-Cummings Hamiltonian on an IBM quantum computer



Jonathan Sepúlveda
PhD Student

Supervisors: Rubén Esteban, and Javier Aizpurua

IBM Collaborators: Niall Robertson, Sergei Zhuk, and Martin Mevissen

Introduction and motivation

Metallic optical nanoresonators → Enhance and concentrate the optical near fields to small regions

Vincenzo Giannini et al. *Chem. Rev.* 373, 111, 6, 3888 – 3912 (2011).
Francisco J. Garcia-Vidal et al. *Science eabd0336* (2021).

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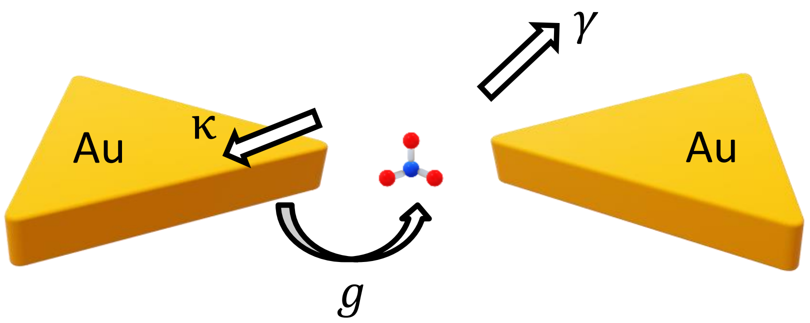

g: Coupling strength

γ: Radiation losses

κ: Nanoantenna losses

This system can be described by

$$\hat{H} = \hbar\omega_c \hat{a}^\dagger \hat{a} + \hbar\frac{\omega_0}{2}\hat{\sigma}_z + \hbar g\left(\hat{\sigma}_+ \hat{a} + \hat{\sigma}_- \hat{a}^\dagger\right)$$

$\hat{a}^\dagger$: Creation operator

$\hat{a}$: Annihilation operator

$\hat{\sigma}_+, \hat{\sigma}_-, \hat{\sigma}_z$: Pauli operators

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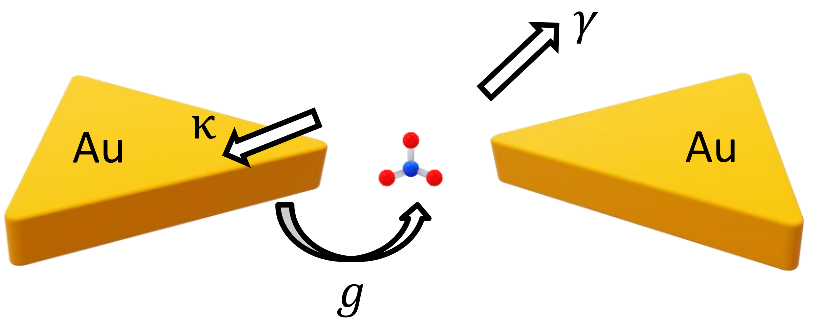

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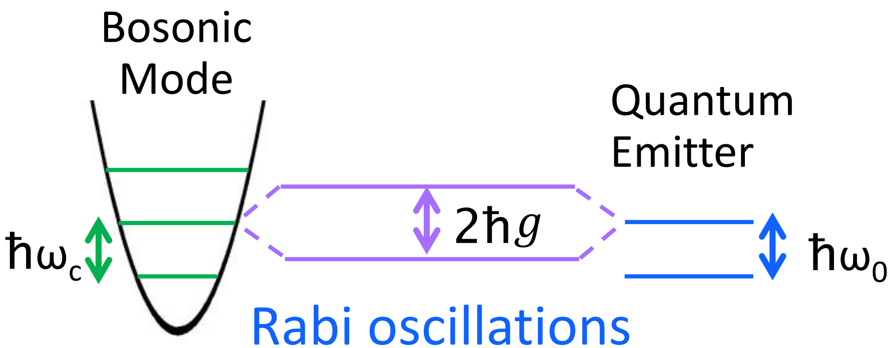
The system can reach the strong coupling regime



Rabi oscillations

Strong coupling criteria

$$\frac{\kappa + \gamma}{4} < g$$

$\hat{a}^\dagger$: Creation operator

$\hat{a}$: Annihilation operator

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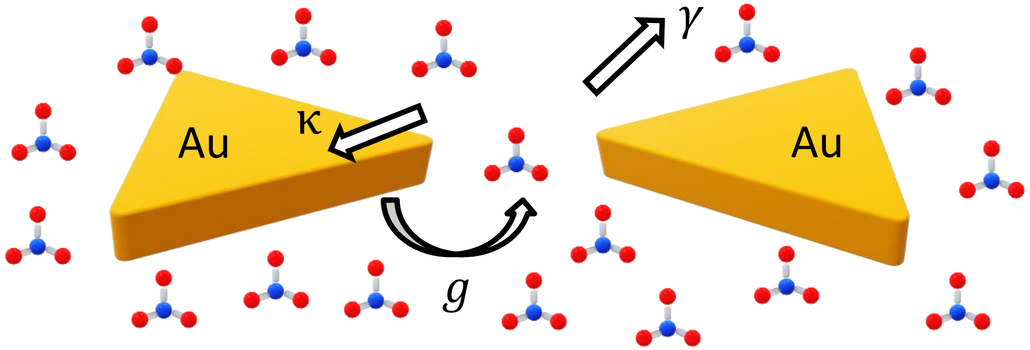
Introduction and motivation

Extension to include more molecules



$$\hat{H} = \hbar\omega_c \hat{a}^\dagger \hat{a} + \hbar \sum_{j} \frac{\omega_{0,i}}{2} \hat{\sigma}_{z,j} + \hbar \sum_{j} g\left(\hat{\sigma}_{+,j}\hat{a} + \hat{\sigma}_{-,j}\hat{a}^\dagger\right)$$

The study of these systems can be useful in molecular sensing and spectroscopic techniques, and also possibly in polaritonic chemistry

Tomáš Neuman, et. al. J. Phys. Chem. C. 119, 26652, (2015).
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Thomas W. Ebbesen. Acc. Chem. Res. 49, 2403, (2016).
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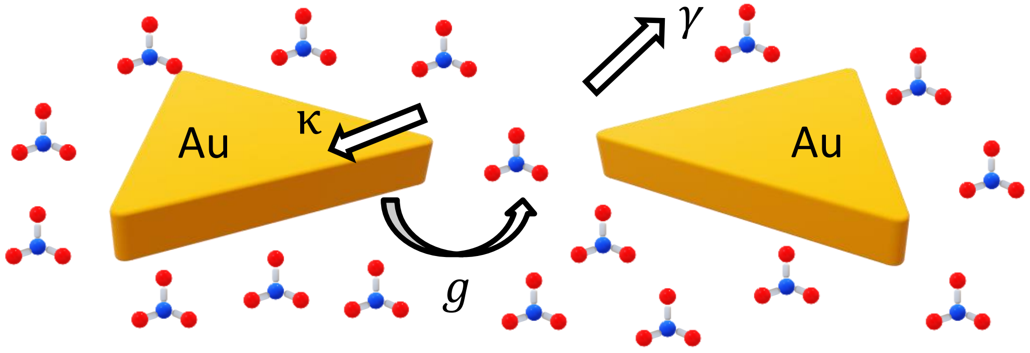
Introduction and motivation

Extension to include more molecules → Simulations become very demanding in classical computers



$$\hat{H} = \hbar\omega_c \hat{a}^\dagger \hat{a} + \hbar \sum_j \frac{\omega_{0,i}}{2} \hat{\sigma}_{z,j} + \hbar \sum_j g \left(\hat{\sigma}_{+,j} \hat{a} + \hat{\sigma}_{-,j} \hat{a}^\dagger \right)$$

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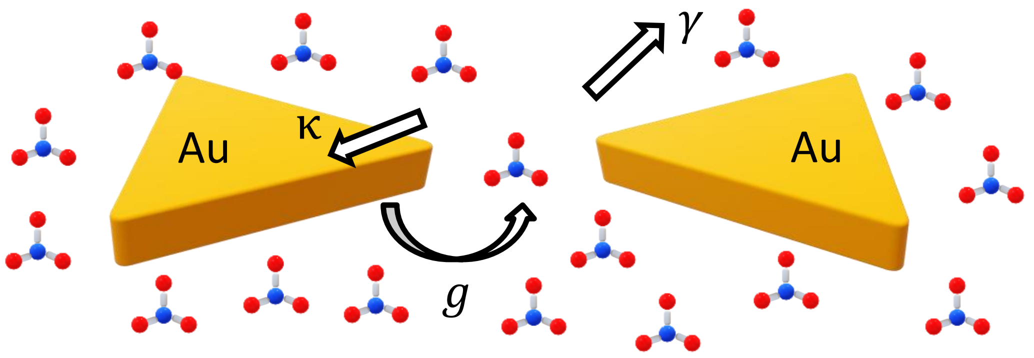

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↓ Explore the implementation of these systems in a quantum computer

The study of these systems can be useful in molecular sensing and spectroscopic techniques, and also possibly in polaritonic chemistry

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Qubitization of the optical (bosonic) mode

Example of mapping 4 Fock states

$$|0\rangle_p \rightarrow |1_0 0_1 0_2 0_3\rangle$$
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$$|2\rangle_p \rightarrow |0_0 0_1 1_2 0_3\rangle$$
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R. Somma. Quantum Computation, Complexity and many-body physics. Phd Thesis, 2005.
R. Somma, et. al., Proc. SPIE 5105, Quantum Information and Computation 96, 2003.
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Qubitization of the optical (plasmonic) mode

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$$\hat{a}^\dagger \to \tilde{a}^\dagger = \sum_{n=0}^{N_{Fock}-1} \sqrt{n+1}\hat{\sigma}_-^n \hat{\sigma}_+^{n+1}$$

$$\tilde{a}^\dagger |1_0 0_1 0_2 0_3\rangle = |0_0 1_1 0_2 0_3\rangle$$
$$\tilde{a}^\dagger |0_0 0_1 0_2 1_3\rangle = 0$$
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$$\hat{H} = \hbar\omega_c \left[\left(\frac{1+\hat{\sigma}_{z'}^0}{2}\right)\left(\frac{1-\hat{\sigma}_{z'}^1}{2}\right) + 2\left(\frac{1+\hat{\sigma}_{z'}^1}{2}\right)\left(\frac{1-\hat{\sigma}_{z'}^2}{2}\right) + 3\left(\frac{1+\hat{\sigma}_{z'}^2}{2}\right)\left(\frac{1-\hat{\sigma}_{z'}^3}{2}\right)\right] + \hbar\frac{\omega_0}{2}\hat{\sigma}_{z'}^{QE} +$$
$$+\frac{\hbar g}{4}\left[\hat{\sigma}_x^{QE}\left(\hat{\sigma}_x^1\hat{\sigma}_x^0 + \hat{\sigma}_y^1\hat{\sigma}_y^0\right) + \hat{\sigma}_y^{QE}\left(\hat{\sigma}_y^1\hat{\sigma}_x^0 - \hat{\sigma}_x^1\hat{\sigma}_y^0\right) + \sqrt{2}\hat{\sigma}_x^{QE}\left(\hat{\sigma}_x^2\hat{\sigma}_x^1 + \hat{\sigma}_y^2\hat{\sigma}_y^1\right) + \sqrt{2}\hat{\sigma}_y^{QE}\left(\hat{\sigma}_y^2\hat{\sigma}_x^1 - \hat{\sigma}_x^2\hat{\sigma}_y^1\right) +\right.$$
$$\left.+\sqrt{3}\hat{\sigma}_x^{QE}\left(\hat{\sigma}_x^3\hat{\sigma}_x^2 + \hat{\sigma}_y^3\hat{\sigma}_y^2\right) + \sqrt{3}\hat{\sigma}_y^{QE}\left(\hat{\sigma}_y^3\hat{\sigma}_x^2 - \hat{\sigma}_x^3\hat{\sigma}_y^2\right)\right]$$

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Trotterization for one quantum emitter

After trotterization for $\omega_c = \omega_0$ (zero detuning) the time dynamics is given by

$$e^{-\frac{it}{\hbar}\hat{H}^{RF}} = e^{-\frac{itg}{4}\hat{\sigma}_x^{QE}\hat{\sigma}_x^1\hat{\sigma}_x^0} e^{-\frac{itg}{4}\hat{\sigma}_x^{QE}\hat{\sigma}_y^1\hat{\sigma}_y^0} e^{-\frac{itg}{4}\hat{\sigma}_y^{QE}\hat{\sigma}_y^1\hat{\sigma}_x^0} e^{\frac{itg}{4}\hat{\sigma}_y^{QE}\hat{\sigma}_x^1\hat{\sigma}_y^0} e^{-\sqrt{2}\frac{itg}{4}\hat{\sigma}_x^{QE}\hat{\sigma}_x^2\hat{\sigma}_x^1} e^{-\sqrt{2}\frac{itg}{4}\hat{\sigma}_x^{QE}\hat{\sigma}_y^2\hat{\sigma}_y^1} e^{-\sqrt{2}\frac{itg}{4}\hat{\sigma}_y^{QE}\hat{\sigma}_y^2\hat{\sigma}_x^1} e^{\sqrt{2}\frac{itg}{4}\hat{\sigma}_y^{qE}\hat{\sigma}_x^2\hat{\sigma}_y^1}$$

$$e^{-\sqrt{3}\frac{itg}{4}\hat{\sigma}_x^{QE}\hat{\sigma}_x^3\hat{\sigma}_x^2} e^{-\sqrt{3}\frac{itg}{4}\hat{\sigma}_x^{QE}\hat{\sigma}_y^3\hat{\sigma}_y^2} e^{-\sqrt{3}\frac{itg}{4}\hat{\sigma}_y^{QE}\hat{\sigma}_y^3\hat{\sigma}_x^2} e^{\sqrt{3}\frac{itg}{4}\hat{\sigma}_y^{QE}\hat{\sigma}_x^3\hat{\sigma}_y^2}$$

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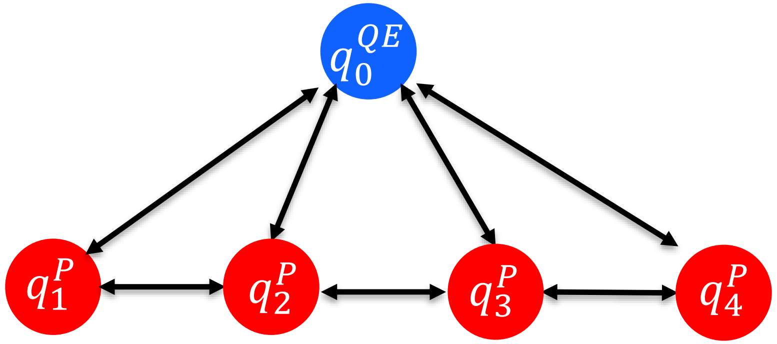
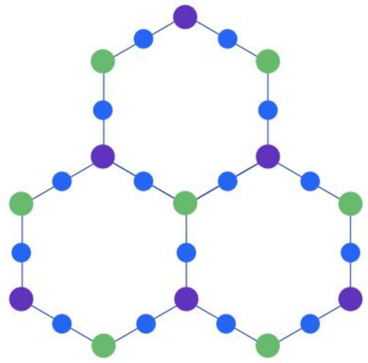
Non-local Hamiltonian



Topology of all active IBM quantum devices



Heavy hex lattice

: Qubits that represent the quantum emitter

: Qubits that represent the boson

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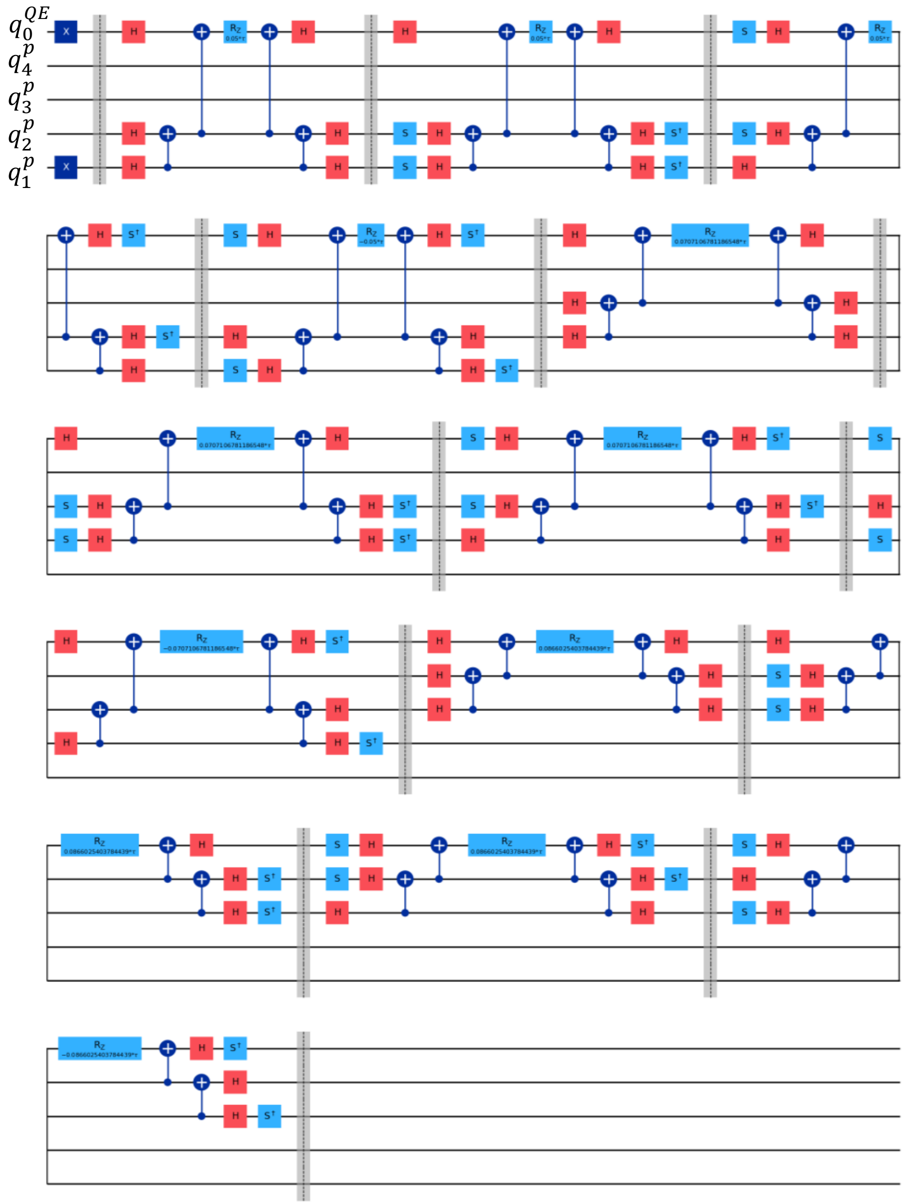
Quantum circuit for one quantum emitter



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Basque Quantum

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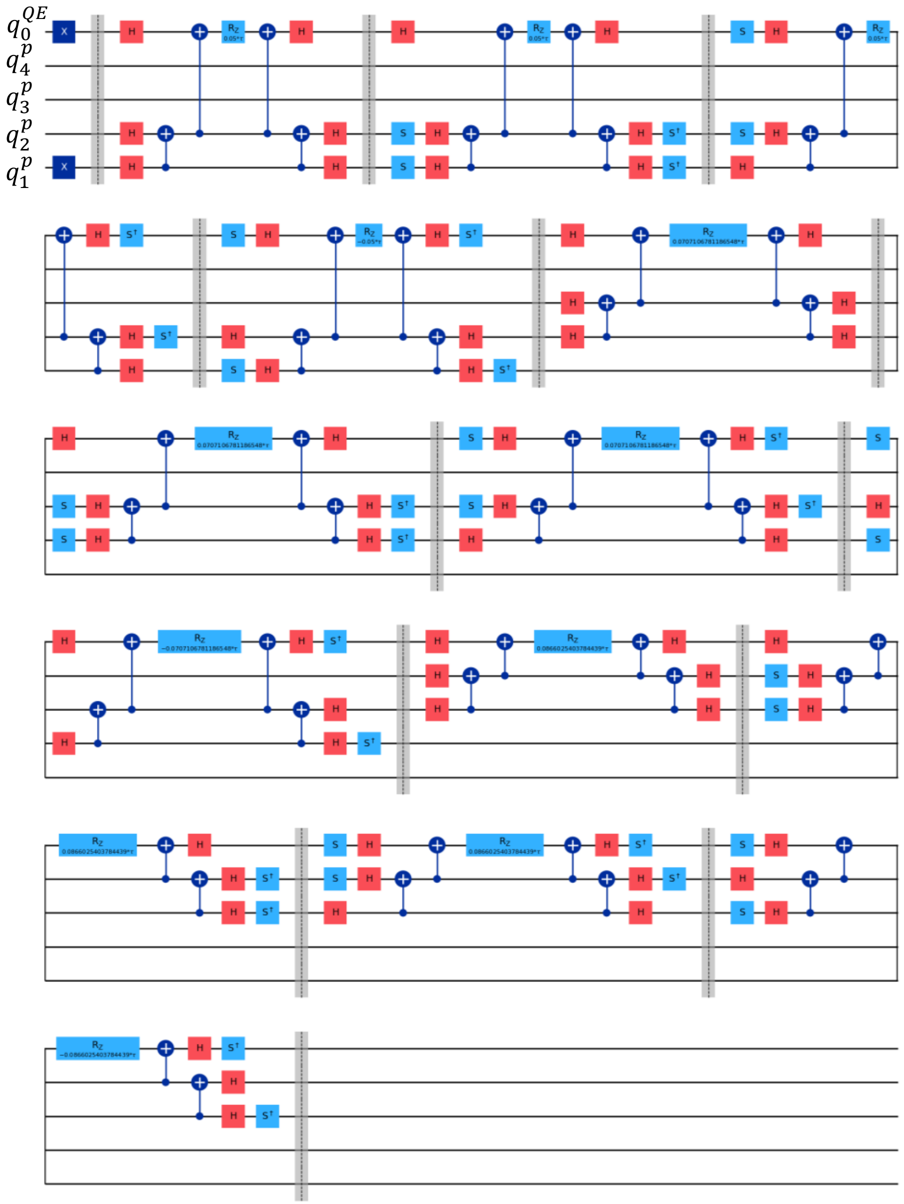

Example of mapping 4 Fock states

For 5 qubits we obtain a 2-qubit depth of 48 (for 4 Fock states, before transpilation)

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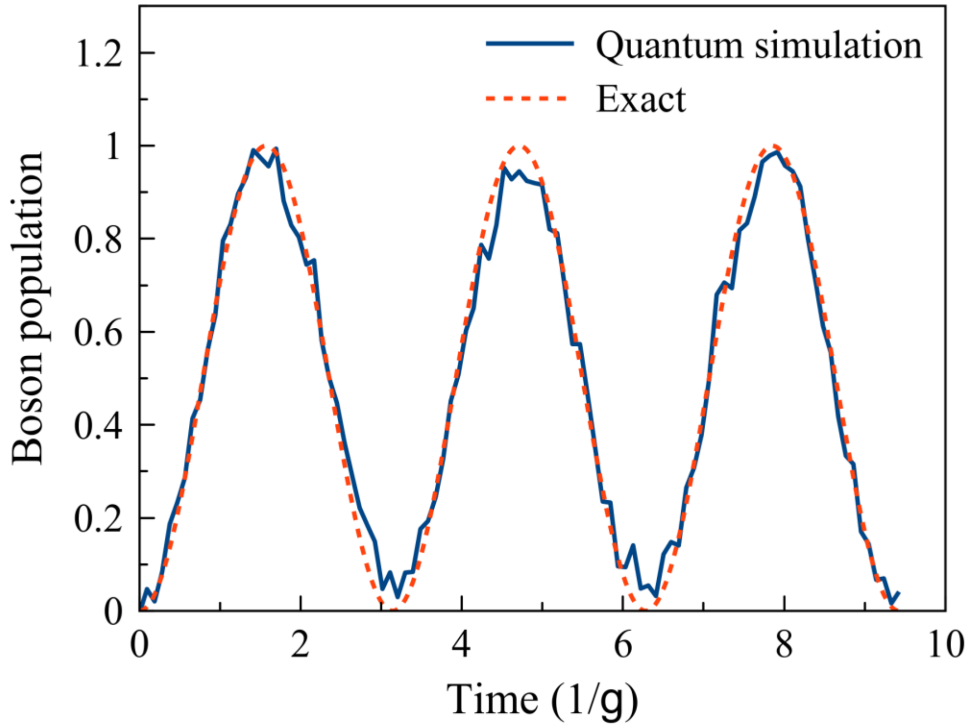
BasQ Basque Quantum

Quantum simulation with IBM Torino

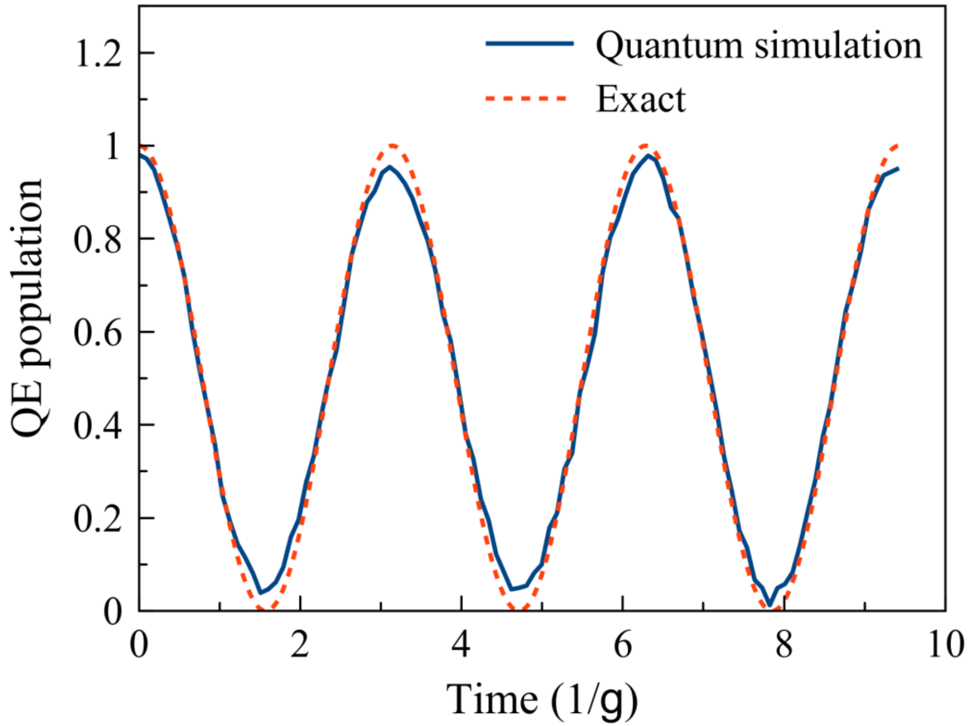
Estimator primitive: We have used a resilience level 2 and optimization level 1

Initial state: $(|0\rangle_p \otimes |1\rangle_{QE} = |1_0 0_1 0_2 0_3 1_{QE}\rangle)$

Population of the boson



Population of the emitter



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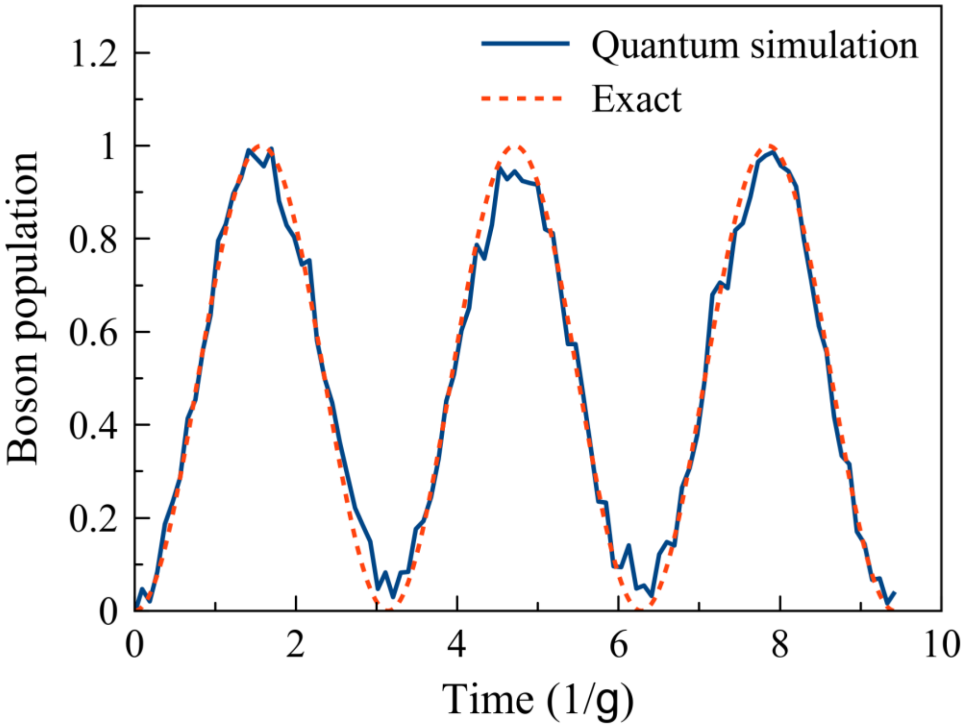

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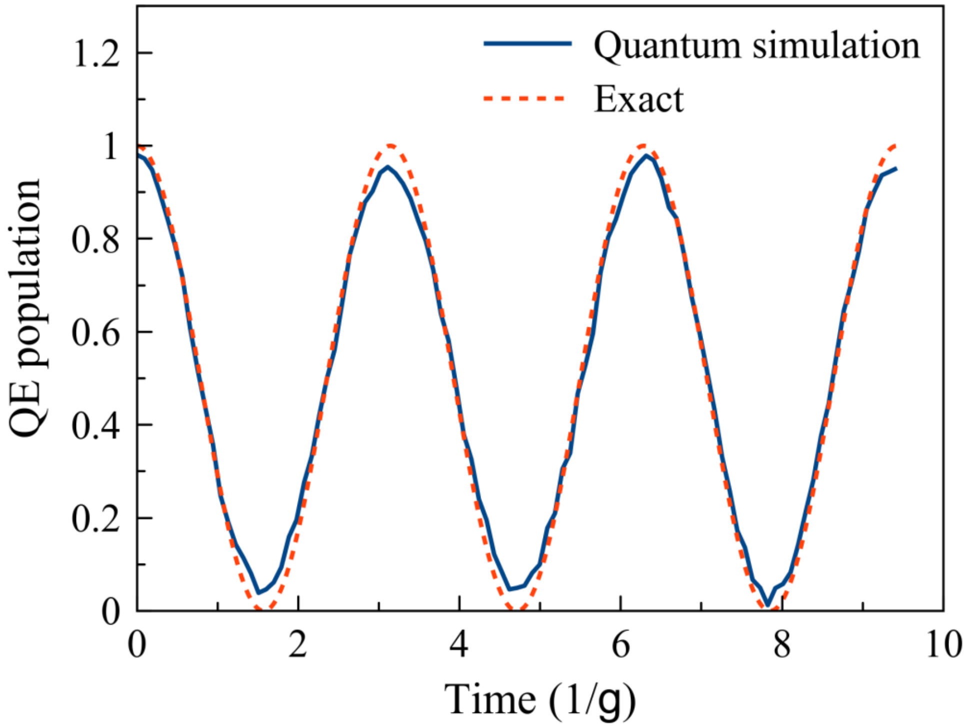

We obtain an excellent agreement between the classical and quantum simulations

We observe 3 clear Rabi oscillations

Extension to many quantum emitters

The really interesting part is including j quantum emitters ($\omega_c = \omega_0$)

$$\hat{H}_T^{RF} = \hbar g \sum_j \left(\hat{\sigma}_{+,j} \hat{a} + \hat{\sigma}_{-,j} \hat{a}^\dagger \right)$$

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$$\Downarrow$$

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$$\prod_j \Big[e^{-\frac{itg}{4}\hat{\sigma}_x^{QE_j}\hat{\sigma}_x^1\hat{\sigma}_x^0} e^{-\frac{itg}{4}\hat{\sigma}_x^{QE_j}\hat{\sigma}_y^1\hat{\sigma}_y^0} e^{-\frac{itg}{4}\hat{\sigma}_y^{QE_j}\hat{\sigma}_y^1\hat{\sigma}_x^0} e^{\frac{itg}{4}\hat{\sigma}_y^{QE_j}\hat{\sigma}_x^1\hat{\sigma}_y^0} e^{-\sqrt{2}\frac{itg}{4}\hat{\sigma}_x^{QE_j}\hat{\sigma}_x^2\hat{\sigma}_x^1} e^{-\sqrt{2}\frac{itg}{4}\hat{\sigma}_x^{QE_j}\hat{\sigma}_y^2\hat{\sigma}_y^1}$$

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We need to add more terms

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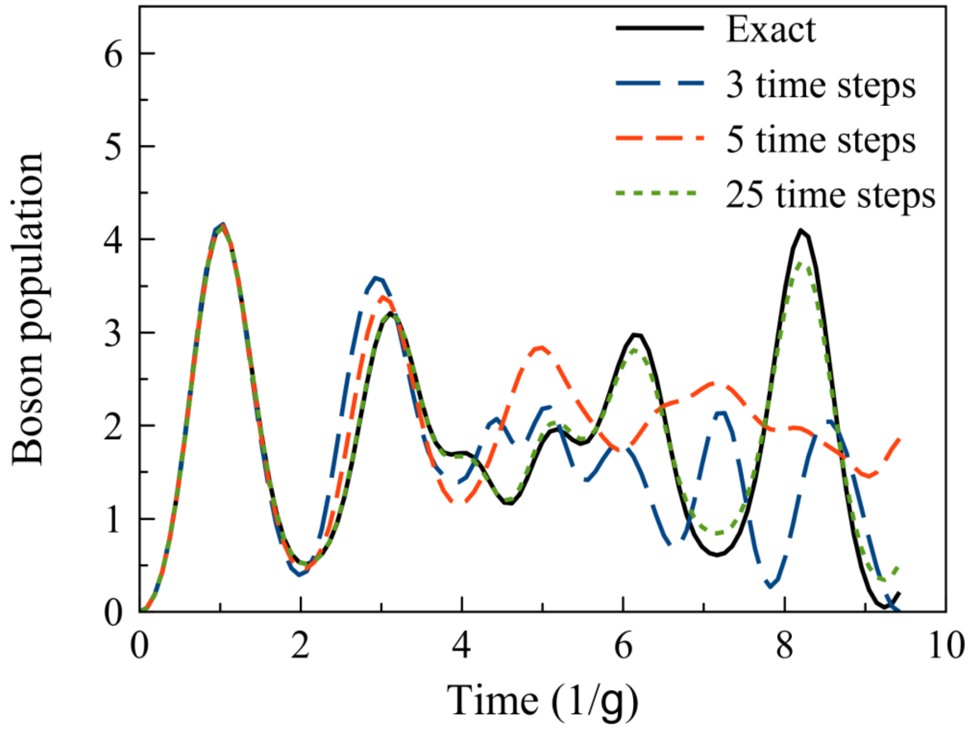
We need to add more terms

Strongly non-local Hamiltonian

Results for 5 quantum emitters (classical simulation)

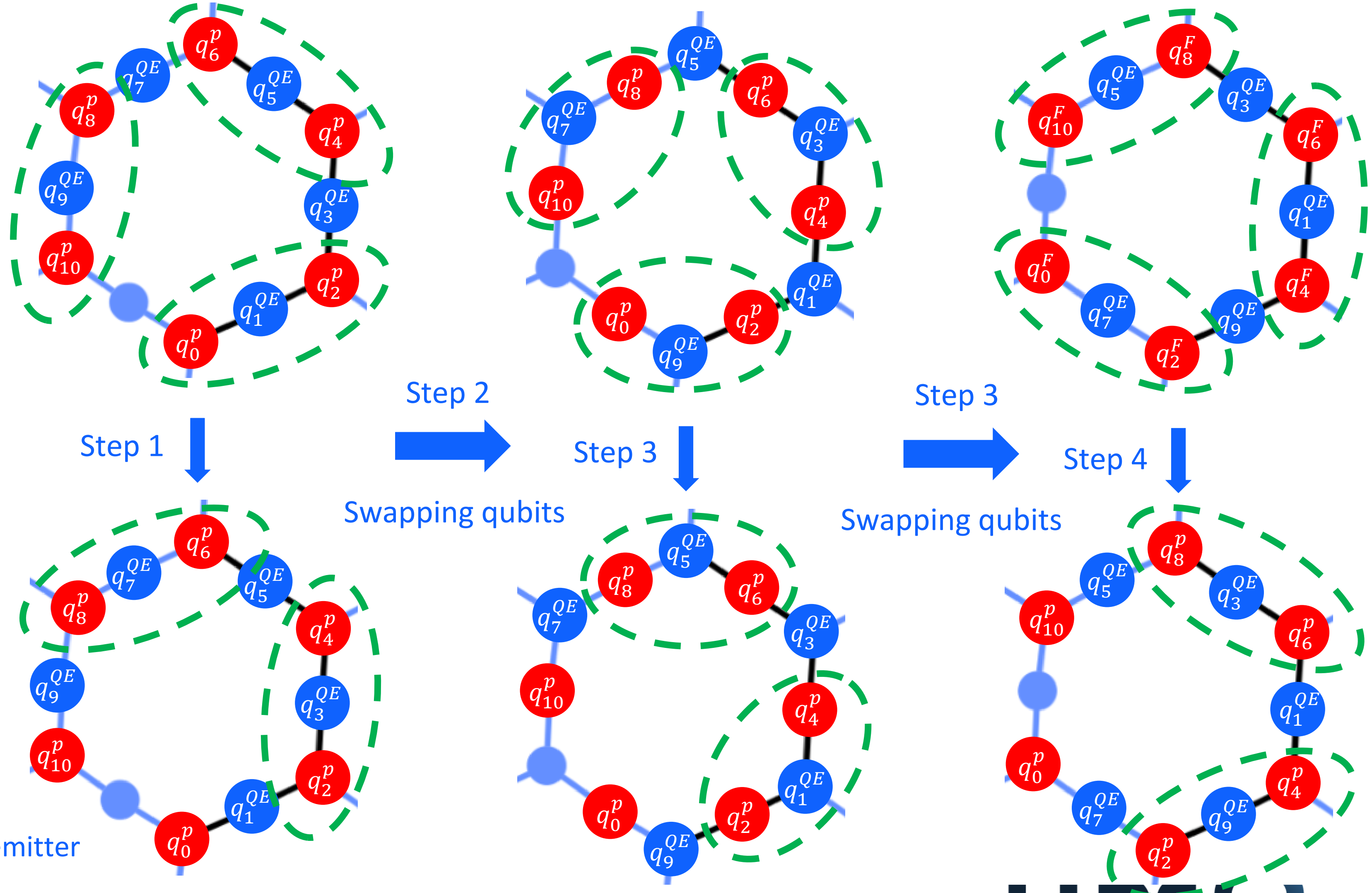
Automatic circuit



For 1 time step:
2-qubit depth = 208
We need to include more time steps

Parallelize the quantum circuit

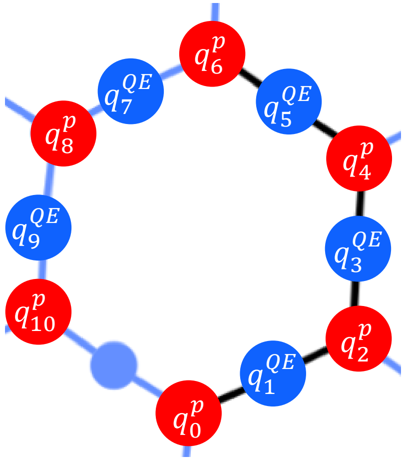
Example of 5 quantum emitters and 6 bosonic states



- Blue circle: Qubits that describe the quantum emitter
- Red circle: Qubits that describe the boson

Parallelize the quantum circuit

Example of 5 quantum emitters and 6 bosonic states



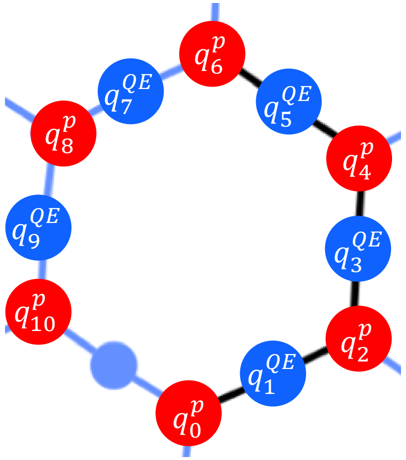
: Qubits that describe the quantum emitter

: Qubits that describe the boson

2-qubit Depth = $\left(N_{qubits} - N_{QE} - (N_P - 2)\right)(N_{QE} - 1)N_{steps} + 32N_{QE}N_{steps}$

Parallelize the quantum circuit

Example of 5 quantum emitters and 6 bosonic states



: Qubits that describe the quantum emitter

: Qubits that describe the plasmon

$$\text{2-qubit Depth} = \underbrace{\overbrace{\left(N_{qubits} - N_{QE} - (N_P - 2)\right)}^{\approx 1 \text{ or } 3}\left(N_{QE} - 1\right)N_{steps}}_{\text{Number of swaps gates}} + \overbrace{32 N_{QE} N_{steps}}^{\text{Scaling of the quantum circuit}}$$

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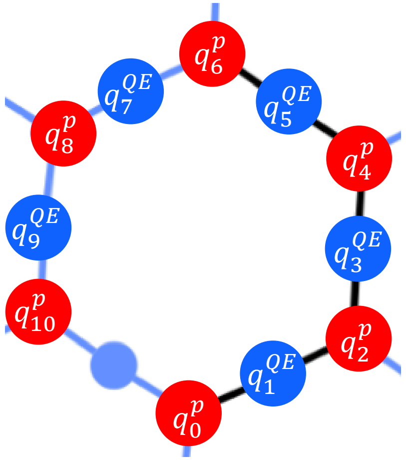
Parallelize the quantum circuit

Example of 5 quantum emitters and 6 plasmonic states



: Qubits that describe the quantum emitter

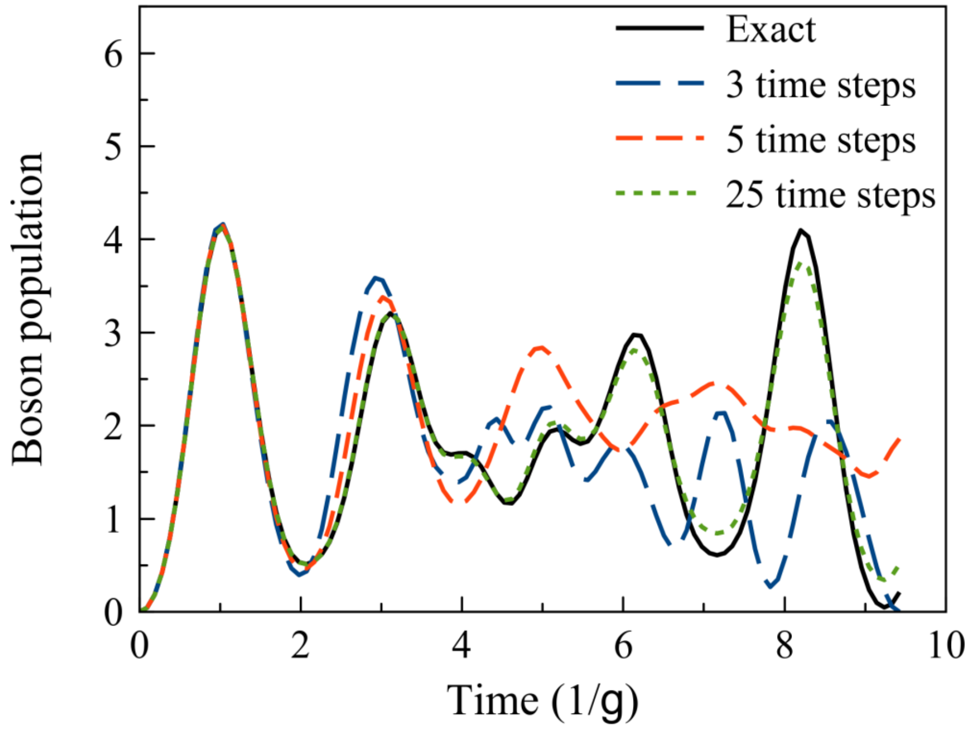
: Qubits that describe the plasmon

2-qubit Depth = $\left(N_{qubits} - N_{QE} - (N_P - 2)\right)(N_{QE} - 1)N_{steps} + 32N_{QE}N_{steps}$

This equation scales linearly with the number of the quantum emitters and the number of time steps

Results for 5 quantum emitters (classical simulation)

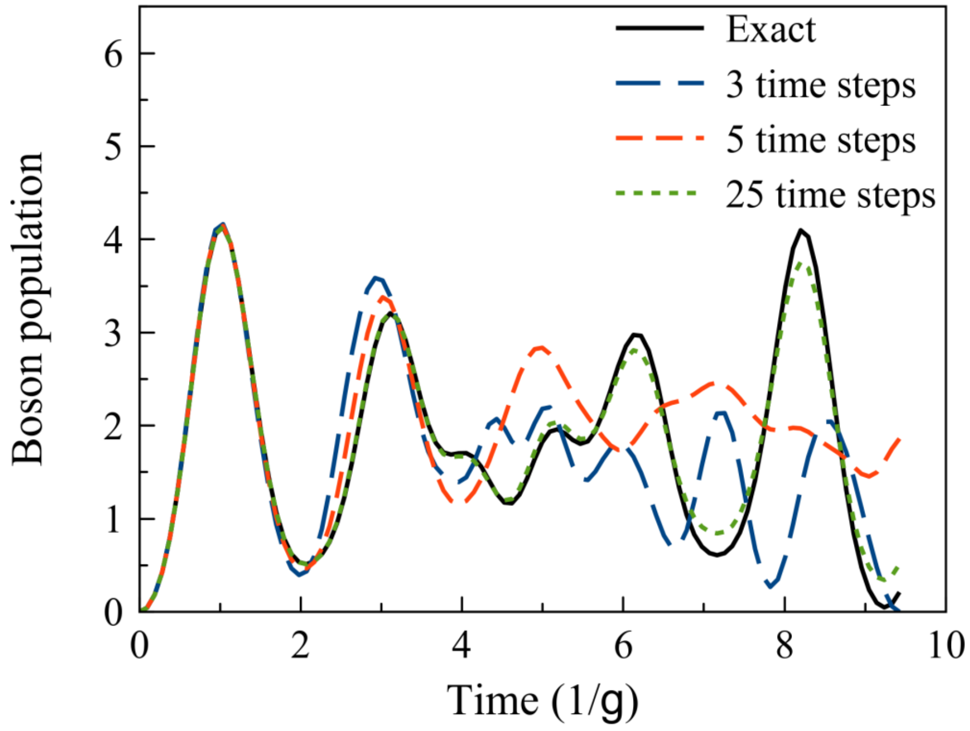
Automatic circuit



For 1 time step:
2-qubit depth = 208

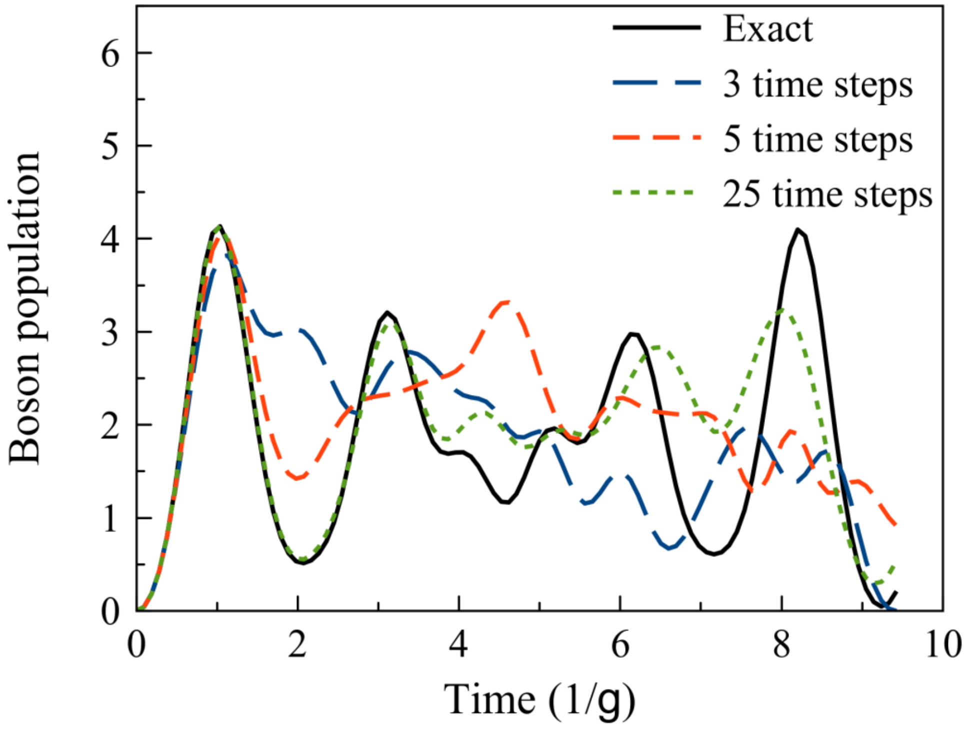
Results for 5 quantum emitters (classical simulation)

Automatic circuit



For 1 time step:
2-qubit depth = 208

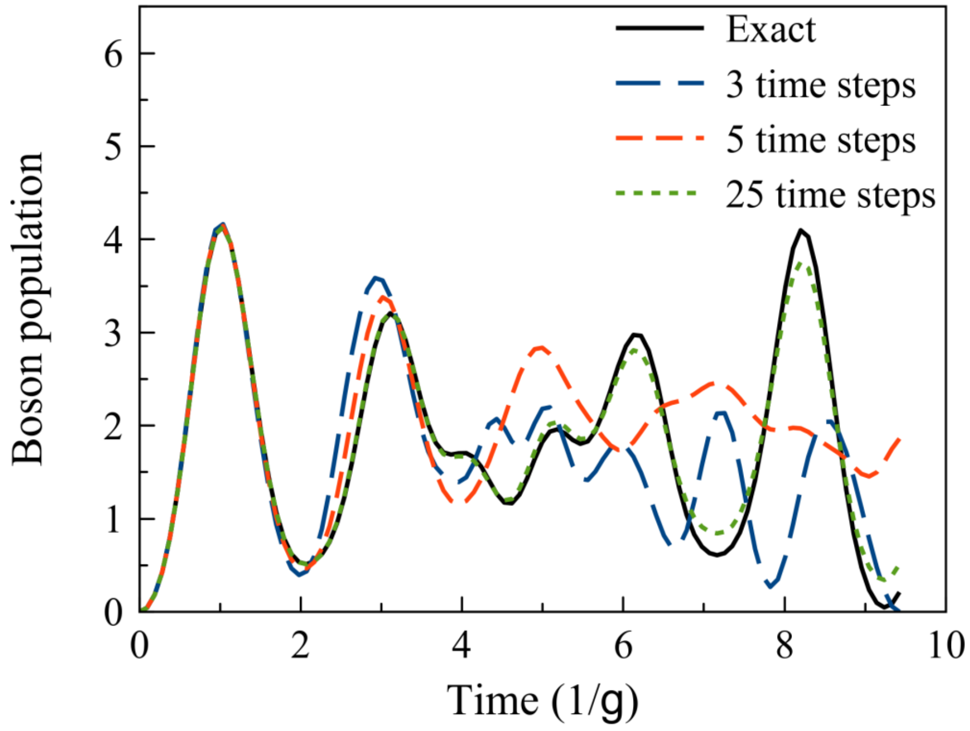
Parallelize circuit



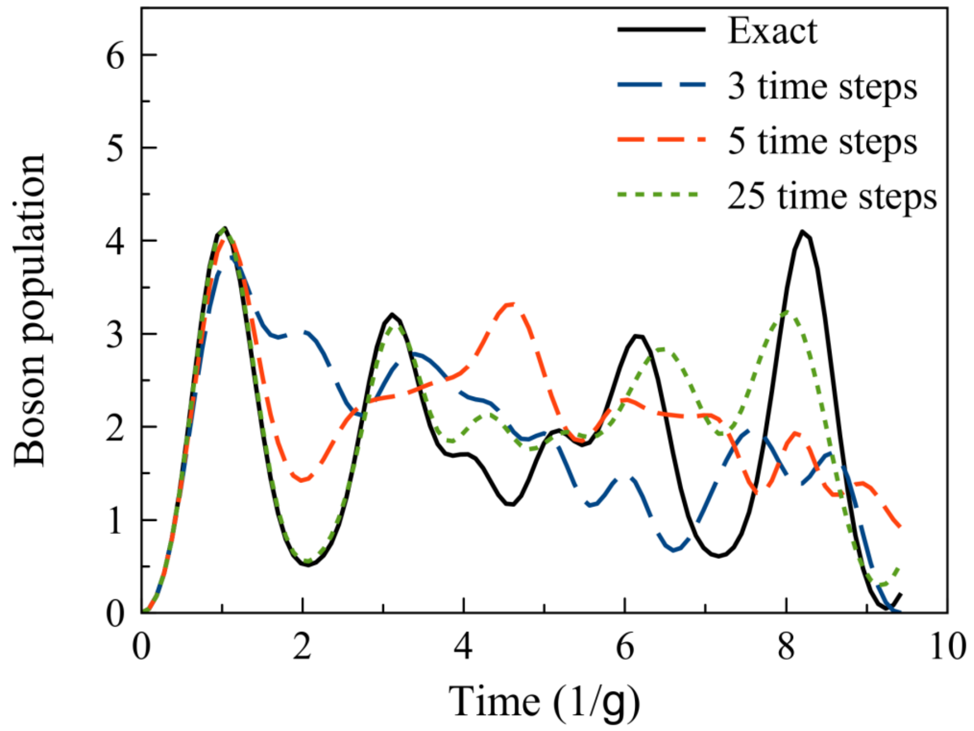
For 1 time step:
2-qubit depth = 160

Results for 5 quantum emitters (classical simulation)

Automatic circuit



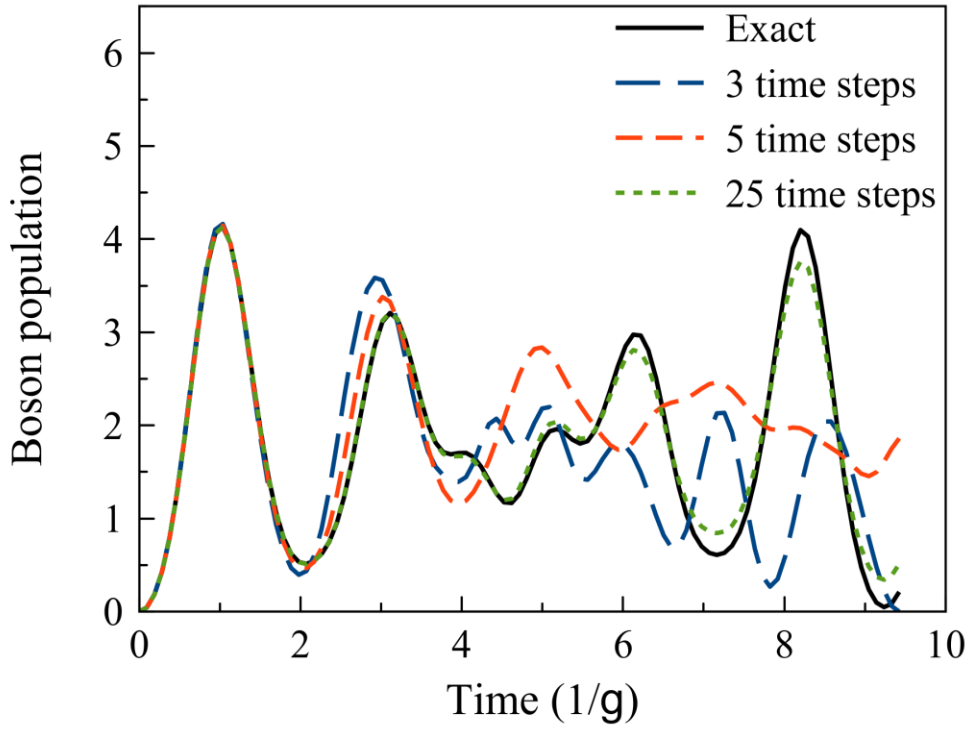
Parallelize circuit



Quantum emitters	Automatic circuit 2-qubit depth	Parallelize circuit 2-qubit depth
5	208	160
7	304	224
10	448	320
15	688	480

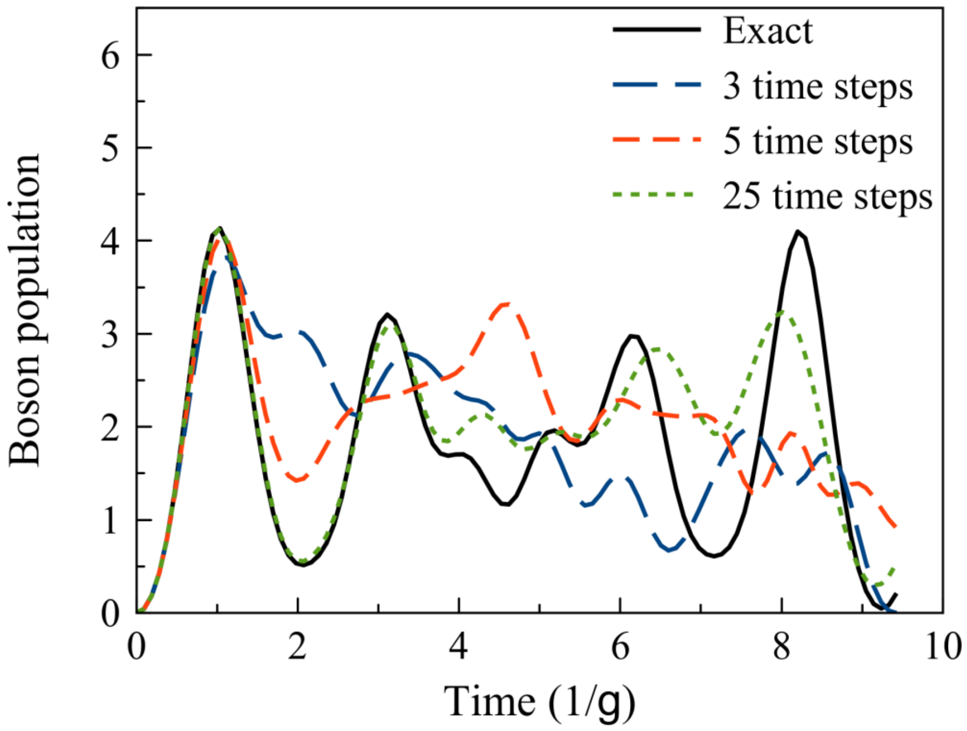
Results for 5 quantum emitters (classical simulation)

Automatic circuit



For 1 time step:
2-qubit depth = 208

Parallelize circuit



For 1 time step:
2-qubit depth = 160

We reduce the 2-qubit depth but at the cost of increasing the Trotter error

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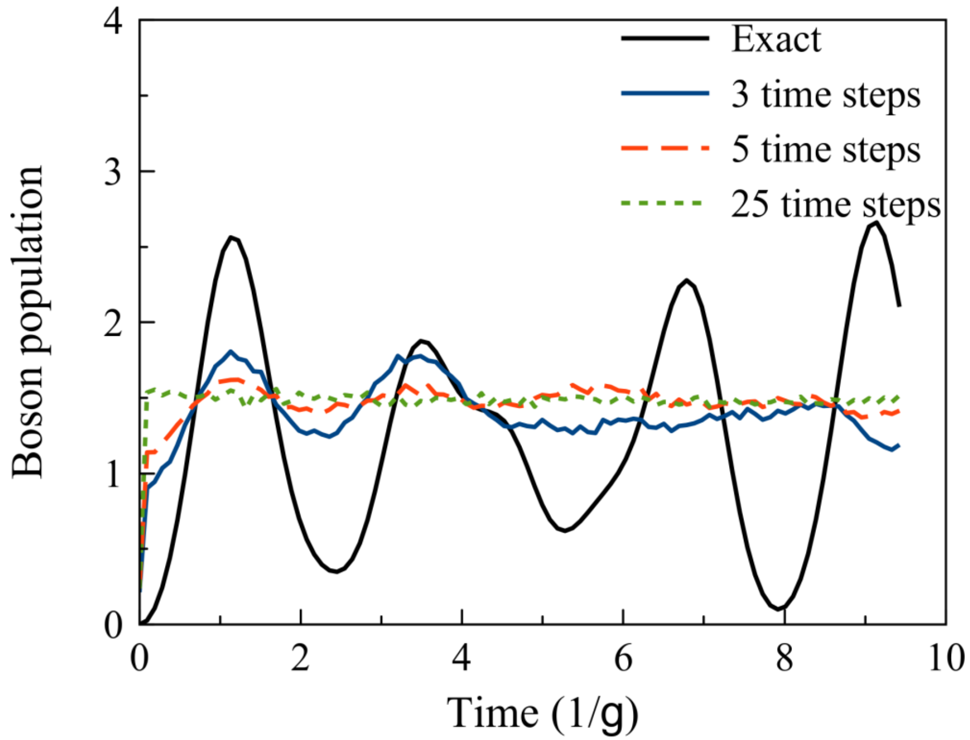
Quantum simulation with IBM Torino

Quantum simulation with 3 molecules

Estimator primitive: We have used a resilience level 2 and optimization level 1

Automatic circuit

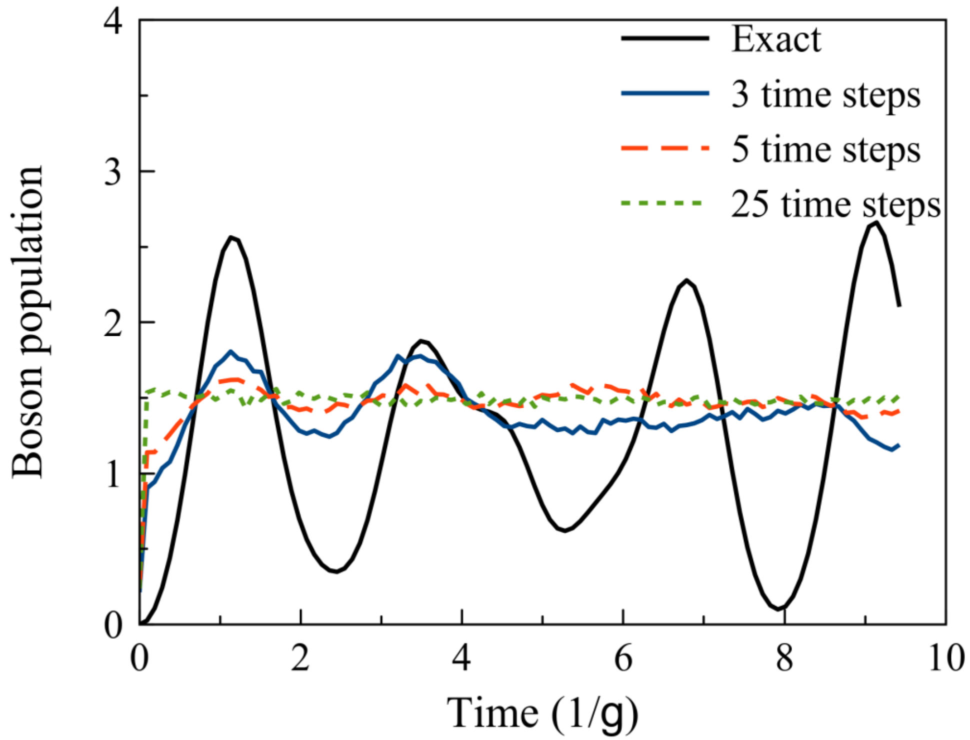


Quantum simulation with IBM Torino

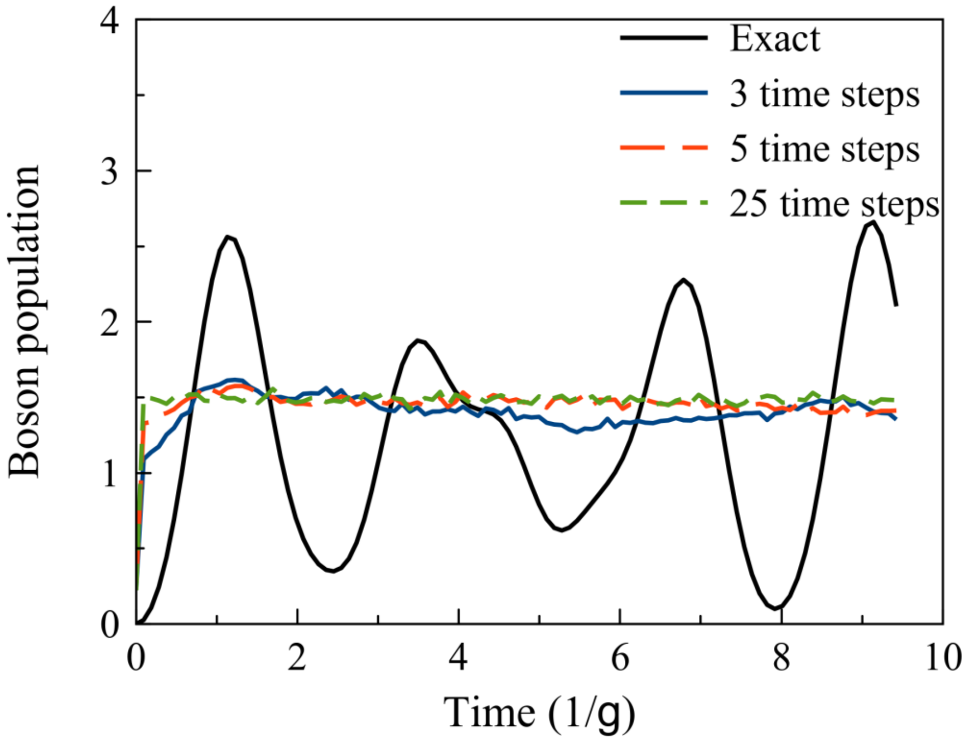
Quantum simulation with 3 molecules

Estimator primitive: We have used a resilience level 2 and optimization level 1

Automatic circuit



Parallelize circuit



Quantum simulation becomes very demanding

We want to implement the Qiskit Addons Multi-Product Formula (MPF) to obtain lower trotter errors

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Conclusions

We have implemented the Jaynes-Cumming Hamiltonian in a quantum circuit.

- Excellent agreement with the exact results.
- We observe three clear Rabi oscillations.

- We have extended the model to include more quantum emitters
  - We obtain very deep circuits.
  - Linear scaling with the number of emitters and time steps.

Acknowledgements

- Grant "(SCOM-Q)", funded by the BasQ initiative in the framework of the collaboration agreement signed between MPC and Ikerbasque.
- Grant PID2022-139579NB-I00 funded by MICIU/AEI /10.13039/501100011033/ERDF.
- Grant IT1526-22 from the Basque Government for consolidated groups of the Basque University.
- Material Physics Center predoctoral research grant.

MPC Materials Physics Center

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Thank you for your attention

An interesting finding

The terms of the Hamiltonian do **not commute**. However, for zero detuning $\Delta = \omega_0 - \omega_c = 0$

$$\hbar\omega_c \hat{a}^\dagger \hat{a} + \hbar\frac{\omega_0}{2}\hat{\sigma}_{z'} \xrightarrow{\text{Rotating frame}} 0$$

Further, if we write the remaining terms in the order

$$\hbar g\left(\hat{\sigma}_-^{(\mathrm{QE})}\hat{a}^\dagger + \hat{\sigma}_+^{(\mathrm{QE})}\hat{a}\right) = \frac{\hbar g}{4}\Big[\hat{\sigma}_x^{(\mathrm{QE})}\hat{\sigma}_x^1\hat{\sigma}_x^0 + \hat{\sigma}_x^{(\mathrm{QE})}\hat{\sigma}_y^1\hat{\sigma}_y^0 + \hat{\sigma}_y^{(\mathrm{QE})}\hat{\sigma}_y^1\hat{\sigma}_x^0 - \hat{\sigma}_y^{(\mathrm{QE})}\hat{\sigma}_x^1\hat{\sigma}_y^0 + \sqrt{2}\hat{\sigma}_x^{(\mathrm{QE})}\hat{\sigma}_x^2\hat{\sigma}_x^1 + \sqrt{2}\hat{\sigma}_x^{(\mathrm{QE})}\hat{\sigma}_y^2\hat{\sigma}_y^1 + \sqrt{2}\hat{\sigma}_y^{(\mathrm{QE})}\hat{\sigma}_y^2\hat{\sigma}_x^1 - \sqrt{2}\hat{\sigma}_y^{(\mathrm{QE})}\hat{\sigma}_x^2\hat{\sigma}_y^1 + \sqrt{3}\hat{\sigma}_x^{(\mathrm{QE})}\hat{\sigma}_x^3\hat{\sigma}_x^2 + \sqrt{3}\hat{\sigma}_x^{(\mathrm{QE})}\hat{\sigma}_y^3\hat{\sigma}_y^2 + \sqrt{3}\hat{\sigma}_y^{(\mathrm{QE})}\hat{\sigma}_y^3\hat{\sigma}_x^2 - \sqrt{3}\hat{\sigma}_y^{(\mathrm{QE})}\hat{\sigma}_x^3\hat{\sigma}_y^2\Big]$$

We find **zero trotterization error**

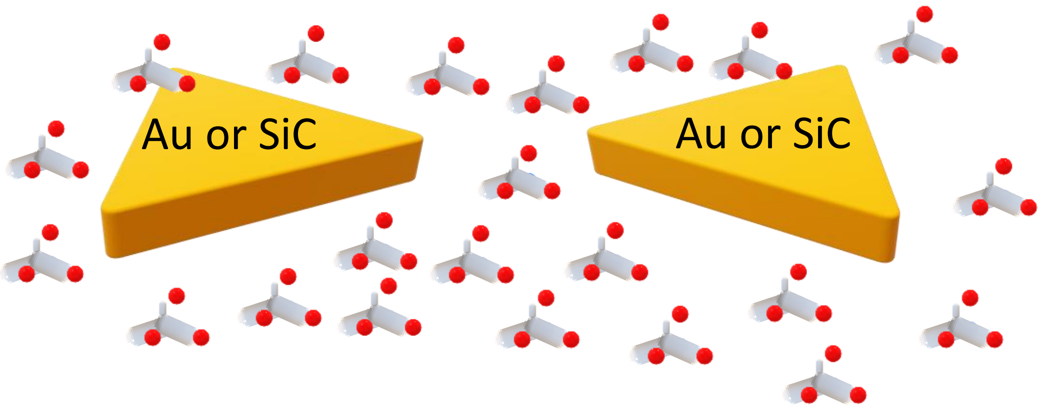
PRELIMINARY EXPLANATION

Terms $\{H_1, H_2, H_3, H_4\}$ commute, as well as $\{H_5, H_6, H_7, H_8\}$ terms and $\{H_9, H_{10}, H_{11}, H_{12}\}$ terms.

$H_5 + H_6 + H_7 + H_8$ commute with $H_1 + H_2 + H_3 + H_4$ and $H_9 + H_{10} + H_{11} + H_{12}$.

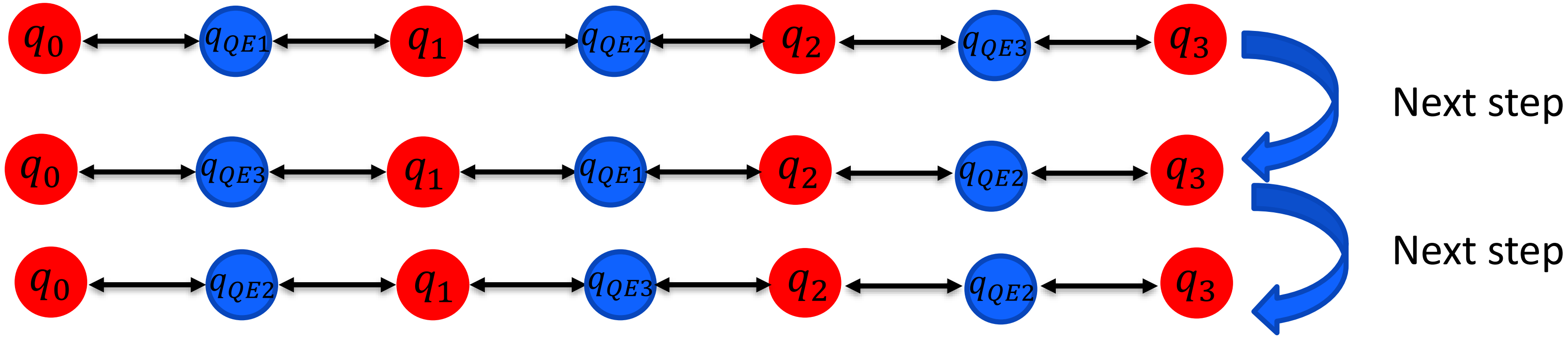
$H_1 + H_2 + H_3 + H_4$ 'almost commutes' with $H_9 + H_{10} + H_{11} + H_{12}$ (the result applied to any plasmonic state gives zero)

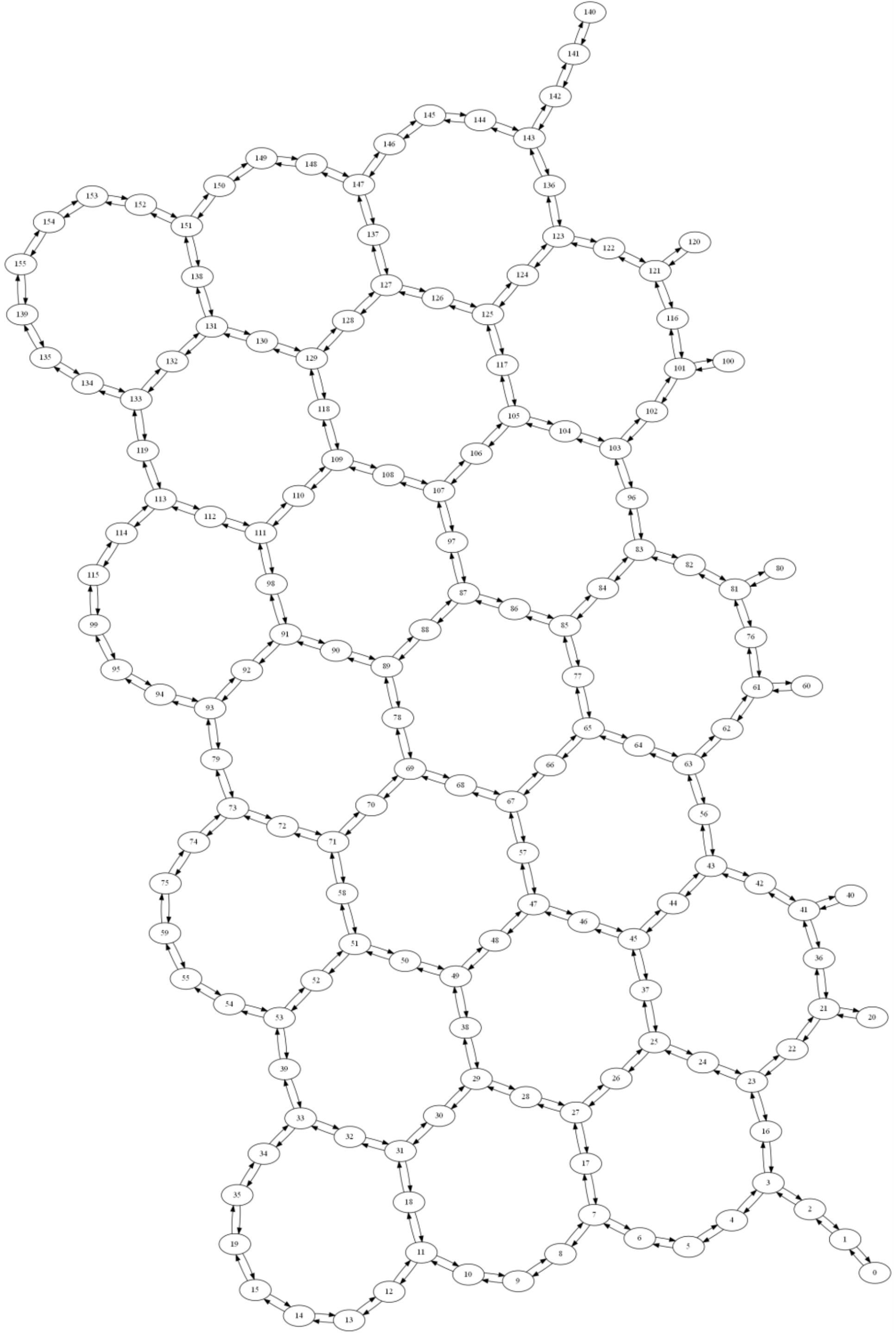
$$e^{-iHt} = e^{-i(H_1+H_2+H_3+H_4+H_5+H_6+H_7+H_8+H_9+H_{10}+H_{12}+H_{12})t} =$$
$$e^{-i(H_1+H_2+H_3+H_4)t}e^{-i(H_5+H_6+H_7+H_8)t}e^{-i(H_9+H_{10}+H_{12}+H_{12})t} =$$
$$e^{-iH_1t}e^{-iH_2t}e^{-iH_3t}e^{-iH_4t}e^{-iH_5t}e^{-iH_6t}e^{-iH_7t}e^{-iH_8t}e^{-iH_9t}e^{-iH_{10}t}e^{-iH_{11}t}e^{-iH_{12}t}$$



Scaling

$$\left(N_{qubits} - N_{QE} - (N_{Fock} - 2)\right)(N_{QE} - 1)N_{steps} + 32N_{QE}N_{steps}$$





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