University of Minho
School of Engineering

Quantum Simulation

Leander Reascos

Quantum Computing School @ Yachay

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Introduction

Simulate Natural Systems

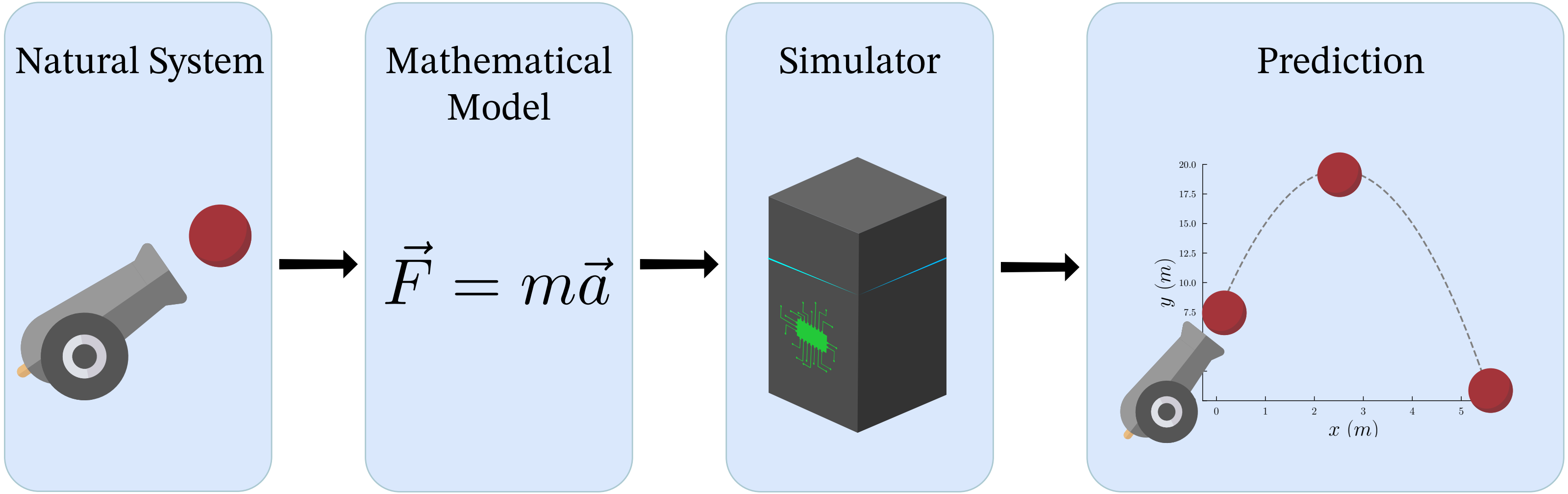


Figure 1: Scheme of a simulation.

Simulate Quantum Systems

Figure 2: Richard Phillips Feynman (1965). *Source:* *The Nobel Prize*

$$N = 2^n \text{ (Complex Numbers)}$$

Beyond Classical Capacities

$$n = 50 \rightarrow N \approx 10^{15}$$

$$n = 300 \rightarrow N \approx 10^{90} > N_{\text{Universe}}$$

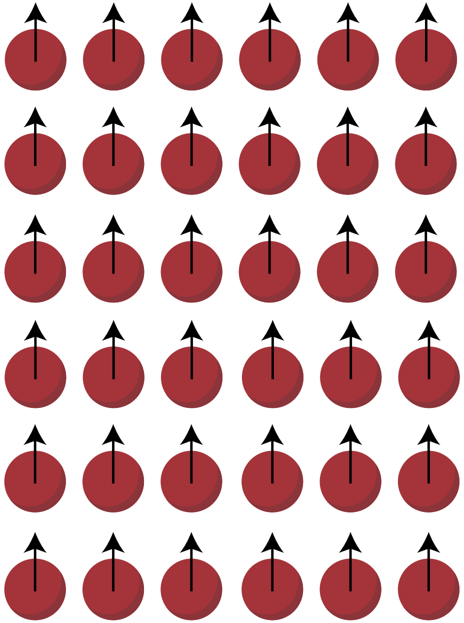


Figure 3: System of n electrons (qubits).

Quantum Simulators

Analog Quantum Simulator (AQS)

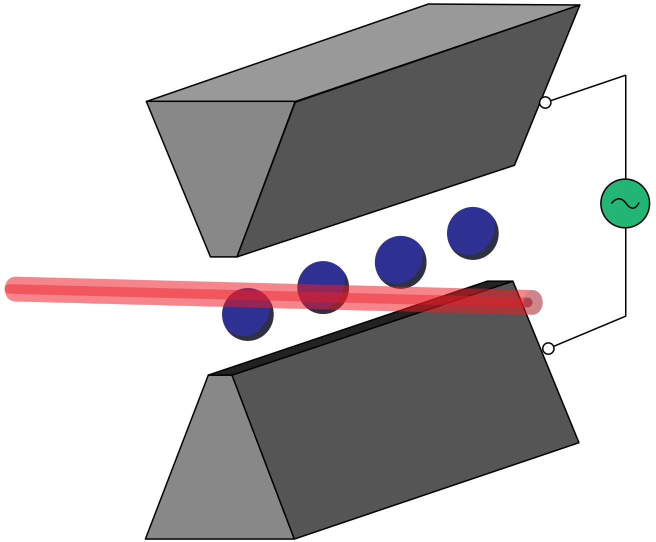


Figure 4: Scheme of Analog Quantum Simulation using trapped ions.

$$\hat{H} \approx \hat{\mathcal{H}}$$

- The target system's interactions are replicated by the simulator.
- The simulation is limited to the type of interactions the system can replicate.

Digital Quantum Simulator (DQS)

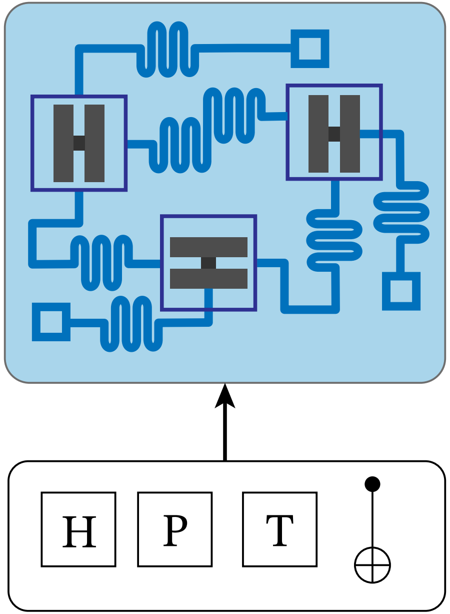


Figure 5: Scheme of Digital Quantum Computer using superconducting qubits.

$$\hat{U}_{\hat{H}}(t) \approx \hat{U}_{\hat{\mathcal{H}}}(t)$$

- The DQS approach uses digital quantum computers to have a general-purpose quantum simulator.
- Attempts to accurately approximate the unitary evolution $\hat{U}_{\hat{\mathcal{H}}}(t)$.

Designing a Quantum Simulation

Designing a Quantum Simulation

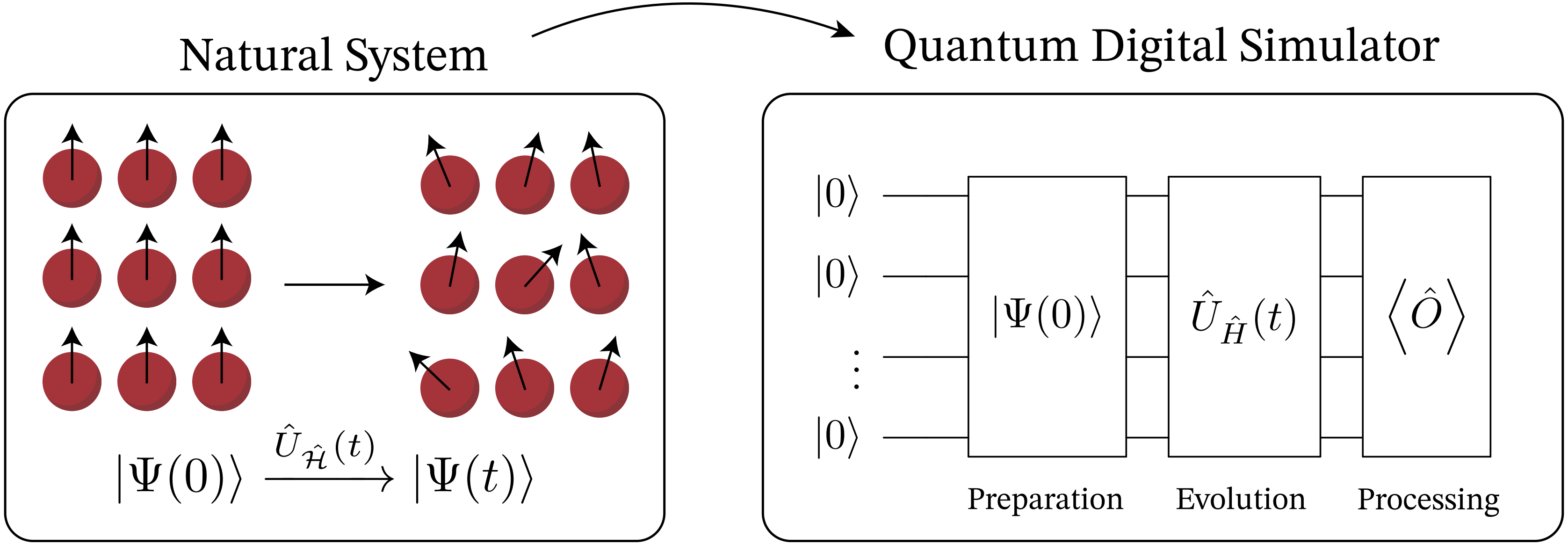


Figure 6: Scheme of digital quantum simulation using a quantum computer.

Initial State

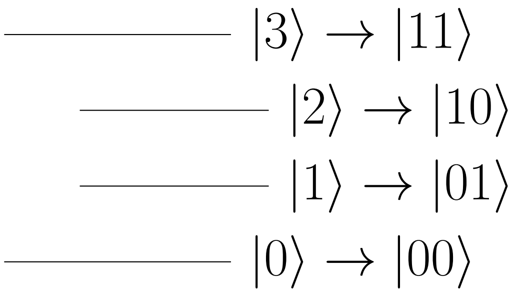


Figure 7: Energy level diagram in a 4 level laser codified with two qubits.

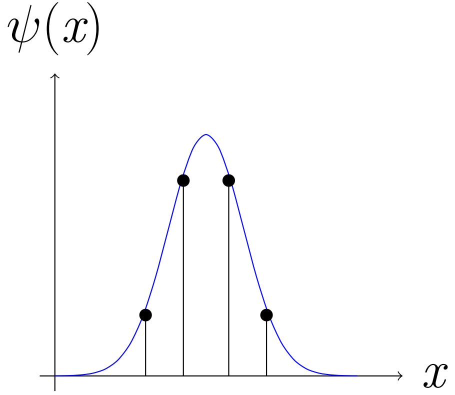


Figure 8: Wave function of a particle.

Methods for Initial State Preparation

- **Adiabatic State Preparation:** The system is initialized in the ground state of a Hamiltonian $\hat{H}_0$ and then the Hamiltonian is changed to the target Hamiltonian $\hat{\mathcal{H}}$.
- **Variational State Preparation:** The system is initialized in a trial state $\left|\psi(\vec{\theta})\right\rangle$ and then the parameters $\vec{\theta}$ are optimized to minimize the energy of the trial state.
- **Quantum Phase Estimation:** The system is initialized in a superposition of eigenstates of the target Hamiltonian $\hat{\mathcal{H}}$ and then the eigenvalues are measured.

Evolution Operator

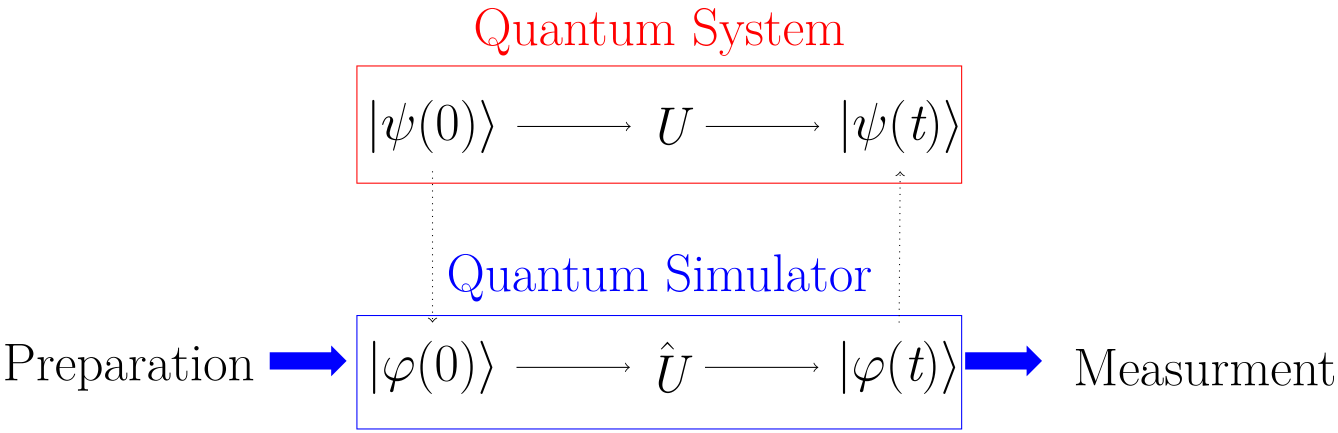


Figure 9: Scheme of a quantum simulation.

Useful methods for $U(t)$

- **Trotterization:** The evolution operator is approximated by a product of unitary operators.

$$U(t) \approx \prod_{j=1}^{M} e^{-i\hat{\mathcal{H}}_j \Delta t}$$

- **Linear Combination of Unitaries:** The evolution operator is approximated by a linear combination of unitary operators.

$$U(t) \approx \sum_{j=1}^{M} c_j e^{-i\hat{\mathcal{H}}_j \Delta t}$$

Measurment

- **Hamiltonian Simulation:** The Hamiltonian is measured at the end of the simulation.
- **An Observable:** The expectation value of an observable is measured at the end of the simulation.
- **Quantum Phase Estimation:** The eigenvalues of the Hamiltonian are measured at the end of the simulation.
- **Quantum State Tomography:** The state of the system is measured at the end of the simulation.
- **Indirect Measurment:** The system is coupled to an ancilla and the ancilla is measured at the end of the simulation.

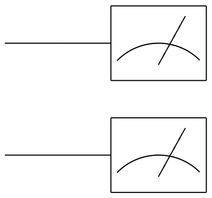
Measure an Observable

The Observable can be written as a linear combination of Pauli operators.

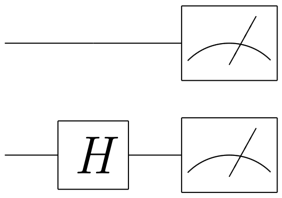
$$\hat{O} = \sum_{j=1}^{M} c_j \hat{\sigma}_j, \quad \hat{\sigma}_j \in \{\hat{I}, \hat{X}, \hat{Y}, \hat{Z}\}$$

For example to measure the Observables:

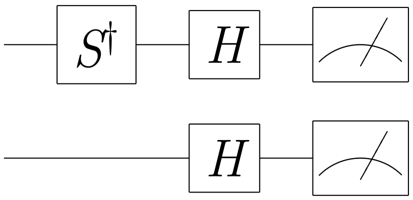
$Z \otimes Z$



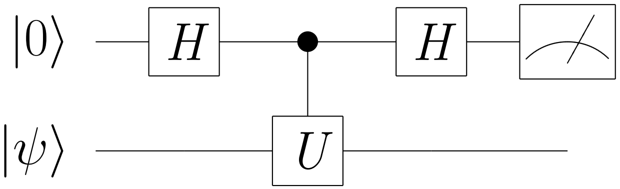
$X \otimes Z$

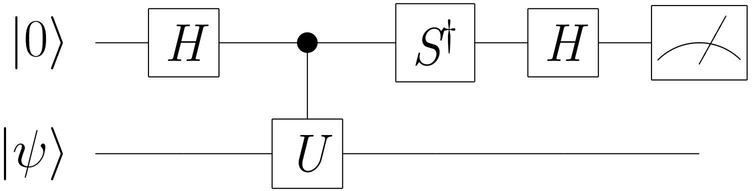


$X \otimes Y$

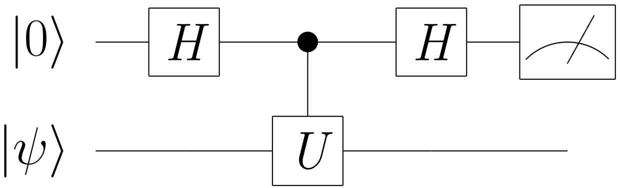


Indirect Measurement

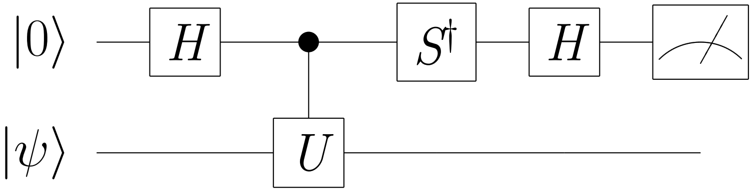




Hadamard Test

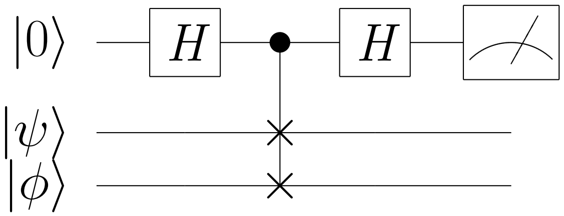


$$\langle Z \rangle = \mathrm{Re}\{\langle U \rangle\} \tag{1}$$



$$\langle Z \rangle = \mathrm{Im}\{\langle U \rangle\} \tag{2}$$

Swap Test



Other Applications

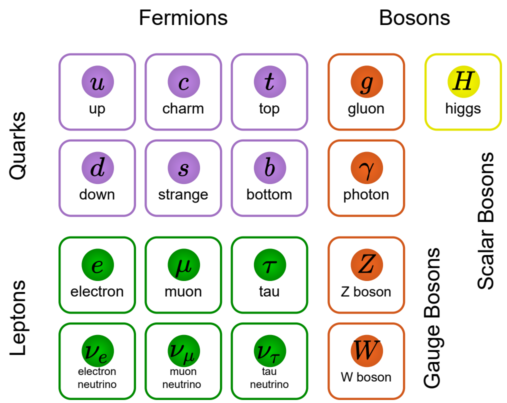
Open Quantum Systems

A open quantum system is a quantum system that interacts with its environment. It is described by a density matrix $\hat{\rho}$ that evolves according to the Lindblad equation.

$$\frac{d\hat{\rho}}{dt} = -i[\hat{\mathcal{H}}, \hat{\rho}] + \sum_{j=1}^{M} \left(\hat{L}_j \hat{\rho} \hat{L}_j^\dagger - \frac{1}{2}\{\hat{L}_j^\dagger \hat{L}_j, \hat{\rho}\} \right) \tag{3}$$

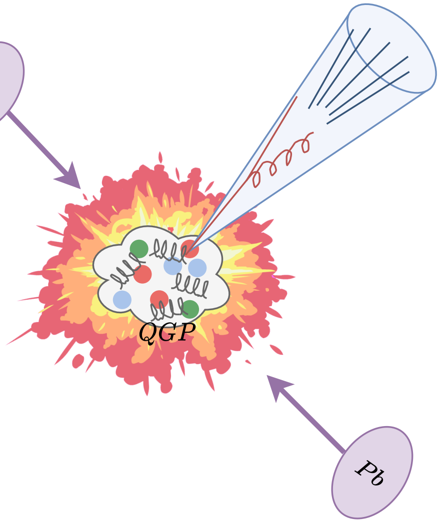
Quantum Field Theory

Quantum Field Theory (QFT) is the union of quantum mechanics and special relativity.



Quark Gluon Plasma

Quark Gluon Plasma (QGP) is a state of matter where quarks and gluons are not confined inside hadrons.



Other

- Quantum Chemistry
- Quantum Many-Body Systems
- Quantum Optics
- Superconductivity
- Quantum Gravity?

Discussion

References I

[1] R. P. Feynman, "Simulating physics with computers," *International Journal of Theoretical Physics*, vol. 21, no. 6, pp. 467–488, Jun. 1, 1982, ISSN: 1572-9575. DOI: 10.1007/BF02650179. [Online]. Available: https://doi.org/10.1007/BF02650179.

[2] R. Blatt and C. F. Roos, "Quantum simulations with trapped ions," *Nature Physics*, vol. 8, no. 4, pp. 277–284, Apr. 1, 2012, ISSN: 1745-2481. DOI: 10.1038/nphys2252. [Online]. Available: https://doi.org/10.1038/nphys2252.

References II

[3] S. Singh, P. Chawla, A. Sarkar, and C. M. Chandrashekar, "Universal quantum computing using single-particle discrete-time quantum walk," *Scientific Reports*, vol. 11, no. 1, p. 11 551, Jun. 2, 2021, ISSN: 2045-2322. DOI: 10.1038/s41598-021-91033-5. [Online]. Available: https://doi.org/10.1038/s41598-021-91033-5.

[4] S. Lloyd, "Universal Quantum Simulators," *Science*, vol. 273, no. 5278, pp. 1073–1078, 1996. DOI: 10.1126/science.273.5278.1073. [Online]. Available: https://www.science.org/doi/abs/10.1126/science.273.5278.1073.

References III

[5] B. Murta, P. M. Q. Cruz, and J. Fernández-Rossier, "Preparing valence-bond-solid states on noisy intermediate-scale quantum computers," *Phys. Rev. Res.*, vol. 5, p. 013 190, 1 Mar. 2023. DOI: 10.1103/PhysRevResearch.5.013190. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevResearch.5.013190.

[6] P. M. Q. Cruz and B. Murta, "Shallow unitary decompositions of quantum Fredkin and Toffoli gates for connectivity-aware equivalent circuit averaging," *arXiv:2305.18128*, 2023. [Online]. Available: https://arxiv.org/abs/2305.18128.

References IV

[7] M. A. Nielsen and I. L. Chuang, *Quantum computation and quantum information*. Cambridge university press, 2010.

[8] S. Lloyd, "Universal quantum simulators," *Science*, vol. 273, no. 5278, pp. 1073–1078, Aug. 23, 1996, ISSN: 0036-8075, 1095-9203. DOI: 10.1126/science.273.5278.1073. [Online]. Available: https://www.science.org/doi/10.1126/science.273.5278.1073 (visited on 12/09/2022).

References V

[9] A. J. Daley, I. Bloch, C. Kokail, *et al.*, "Practical quantum advantage in quantum simulation," *Nature*, vol. 607, no. 7920, pp. 667–676, Jul. 2022, Number: 7920 Publisher: Nature Publishing Group, ISSN: 1476-4687. DOI: 10.1038/s41586-022-04940-6. [Online]. Available: https://www.nature.com/articles/s41586-022-04940-6 (visited on 12/14/2022).

[10] P. Shor, "Algorithms for quantum computation: Discrete logarithms and factoring," in *Proceedings 35th Annual Symposium on Foundations of Computer Science*, 1994, pp. 124–134. DOI: 10.1109/SFCS.1994.365700.

References VI

[11] L. K. Grover, *A fast quantum mechanical algorithm for database search*, 1996. DOI: 10.48550/ARXIV.QUANT-PH/9605043. [Online]. Available: https://arxiv.org/abs/quant-ph/9605043.

[12] J. Preskill, "Quantum computing in the NISQ era and beyond," *Quantum*, vol. 2, p. 79, Aug. 6, 2018, ISSN: 2521-327X. DOI: 10.22331/q-2018-08-06-79. arXiv: 1801.00862[cond-mat,physics:quant-ph]. [Online]. Available: http://arxiv.org/abs/1801.00862 (visited on 12/09/2022).