EURO

Fundamental Quantum Computing Algorithms and Their Implementation in Qiskit

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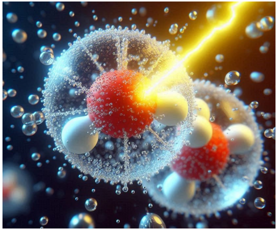
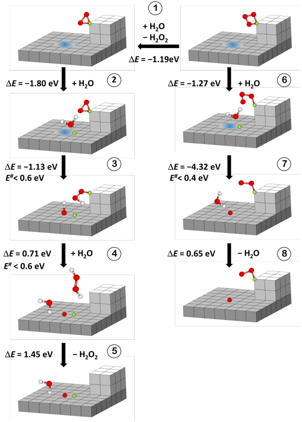
University of Chemistry and Technology Prague (2014-2025):

- Physical chemistry
- Computational chemistry

VŠB-Technical University Ostrava (2024 - present):

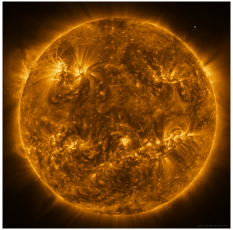
- Quantum Computing Lab



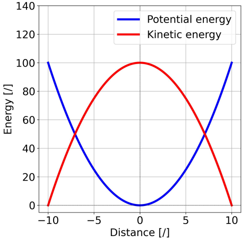


Classical Mechanics

Sun



Chevrolet Impala 1967



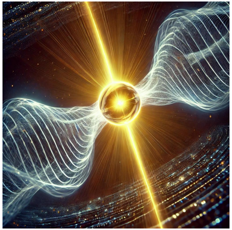
What would happen with the decreasing size?

- Weght: kg $\rightarrow 10^{-31} \times$ kg
- Size: m $\rightarrow 10^{-10} \times$ m

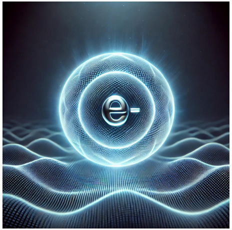
Classical vs Quantum Mechanics

Quantum Mechanics

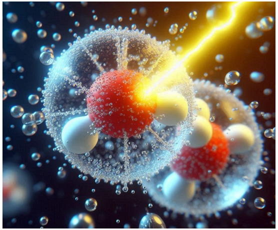
Photon

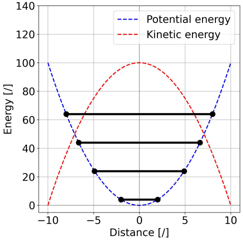


Electron



Light atoms

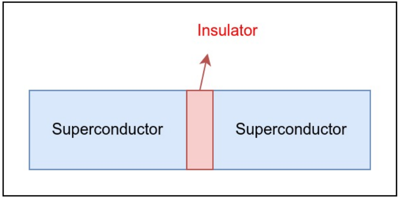


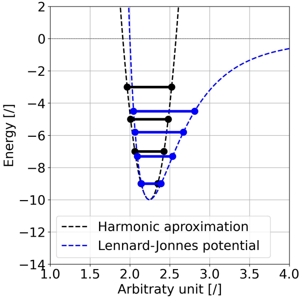


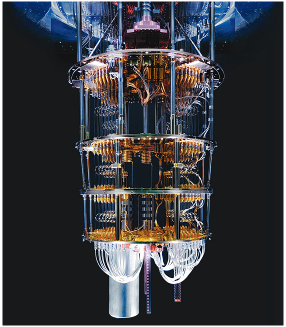
- Stern-Gerlach experiment
- Black-body radiation
- Zeeman effect

Basic idea: To facilitate the discrete energetic levels

Superconducting technology - Josephson junction

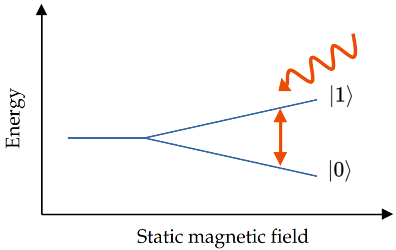


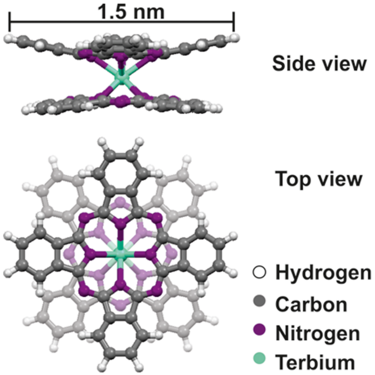




QC based on molecular spin

- Single-ion Magnets
- f-block ion in the middle – 1 “unpaired electron”
- Highly adjustable ligands

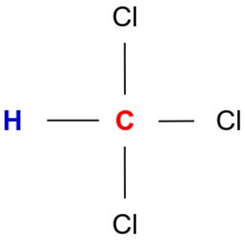


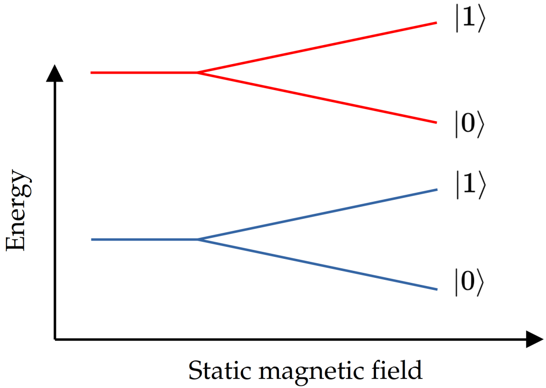


https://pubs.acs.org/doi/pdf/10.1021/acs.jpcc.6b03676

QC based on NMR

- Atoms with odd number of protons and/or neutrons.
- ^{1}H, ^{13}C...^{19}F,^{31}P





Qiskit

- Qiskit = Quantum Information Software Kit
- open-source software development kit (SDK) for working with quantum Computers

Bloch sphere

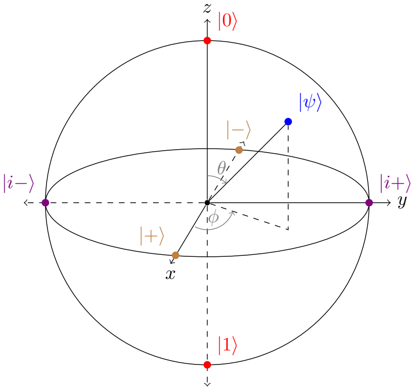
Other interesting point on Bloch sphere:

$$|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

$$|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

$$|i+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + i\,|1\rangle)$$

$$|i-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - i\,|1\rangle)$$



One-Qubit Quantum Gates

Definition: A one-qubit gate is represented by a 2×2 unitary matrix U acting on a single qubit:

$$U|\psi\rangle = U \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

Important One-Qubit Gates:

- **Pauli Gates:**

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

- **Hadamard Gate:**

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

- **Phase Gates:**

$$S = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}, \quad T = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$$

Actions of One-Qubit Quantum Gates

Example:

- Pauli-X (NOT gate): $X|0\rangle = |1\rangle, \quad X|1\rangle = |0\rangle$
- Hadamard on $|0\rangle$:

$$H|0\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}\begin{bmatrix}1\\ 0\end{bmatrix} = \frac{1}{\sqrt{2}}\left(\begin{bmatrix}1\\ 0\end{bmatrix} + \begin{bmatrix}0\\ 1\end{bmatrix}\right) = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\ 1\end{bmatrix} = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

- Hadamard on $|1\rangle$:

$$H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

- Z-gate on superposition state:

$$Z\left(\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\right) = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

Actions of One-Qubit Quantum Gates II

Initial State: The superposition state

$$|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

Action of the S Gate:

$$S|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle) = |i+\rangle$$

Quantum Circuit:

$$|0\rangle \;\text{—}\boxed{H}\text{—}\boxed{S}\text{——}\; |i+\rangle$$

The S gate introduces a phase factor i to $|1\rangle$, transforming $|+\rangle$ into $|i+\rangle$, an eigenstate of the Y operator.

Phase Transformations

$$P(\lambda)\left|\psi\right\rangle = \begin{bmatrix}1 & 0\\ 0 & e^{i\lambda}\end{bmatrix}\begin{bmatrix}\alpha\\ \beta\end{bmatrix} = \begin{bmatrix}\alpha\\ e^{i\lambda}\beta\end{bmatrix}$$

$$Z\left|\psi\right\rangle = \begin{bmatrix}1 & 0\\ 0 & e^{i\pi}\end{bmatrix}\begin{bmatrix}\alpha\\ \beta\end{bmatrix} = \begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}\begin{bmatrix}\alpha\\ \beta\end{bmatrix} = \begin{bmatrix}\alpha\\ -\beta\end{bmatrix}$$

$$S\left|\psi\right\rangle = \begin{bmatrix}1 & 0\\ 0 & e^{i\frac{\pi}{2}}\end{bmatrix}\begin{bmatrix}\alpha\\ \beta\end{bmatrix} = \begin{bmatrix}1 & 0\\ 0 & i\end{bmatrix}\begin{bmatrix}\alpha\\ \beta\end{bmatrix} = \begin{bmatrix}\alpha\\ i\beta\end{bmatrix}$$

$$T\left|\psi\right\rangle = \begin{bmatrix}1 & 0\\ 0 & e^{i\frac{\pi}{4}}\end{bmatrix}\begin{bmatrix}\alpha\\ \beta\end{bmatrix} = \begin{bmatrix}\alpha\\ e^{i\frac{\pi}{4}}\beta\end{bmatrix} = \begin{bmatrix}\alpha\\ \frac{1}{\sqrt{2}}(1+i)\beta\end{bmatrix}$$

Action of Gates on Special States:

$$Z\left|+\right\rangle = \left|-\right\rangle, \quad Z\left|-\right\rangle = \left|+\right\rangle, \quad S\left|+\right\rangle = \left|i+\right\rangle$$

$$Z\left|i-\right\rangle = SS\left|i-\right\rangle = TTTT\left|i-\right\rangle = \left|i+\right\rangle$$

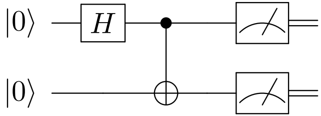
Quantum Circuits

Definition: A quantum circuit is a computational model in which quantum gates are applied to qubits to perform quantum computations.

Components of a Quantum Circuit:

- Qubits
- Quantum Gates (e.g., H, X, Z, $CNOT$, T)
- Measurements (collapsing qubits into classical bits)

Example: Bell State Circuit



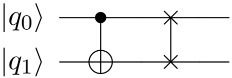
Common Two-Qubit Quantum Gates

- CNOT (Controlled-NOT) Gate:

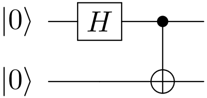
$$\text{CNOT}\,|11\rangle = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} |11\rangle = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} = |10\rangle$$

- SWAP Gate:

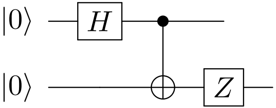
$$\text{SWAP} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

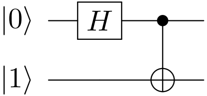


Bell States



$$CX|H\,|00\rangle = CX\left(\frac{1}{\sqrt{2}}\,|00\rangle + \frac{1}{\sqrt{2}}\,|01\rangle\right) = \frac{1}{\sqrt{2}}CX\,|00\rangle + \frac{1}{\sqrt{2}}CX\,|01\rangle =$$
$$= \frac{1}{\sqrt{2}}\,|00\rangle + \frac{1}{\sqrt{2}}\,|11\rangle = \left|\Phi^+\right\rangle$$





$$\begin{aligned}
|\Phi^+\rangle &= \tfrac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \\
|\Phi^-\rangle &= \tfrac{1}{\sqrt{2}}(|00\rangle - |11\rangle) \\
|\Psi^+\rangle &= \tfrac{1}{\sqrt{2}}(|10\rangle + |01\rangle) \\
|\Psi^-\rangle &= \tfrac{1}{\sqrt{2}}(|10\rangle - |01\rangle)
\end{aligned}$$