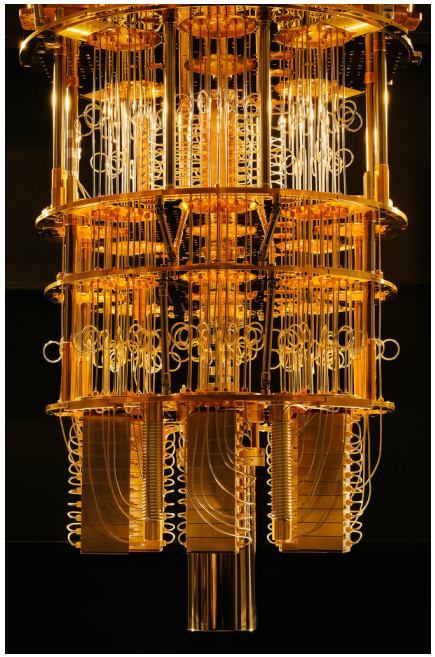
# Quantum Chemistry using Quantum Computers



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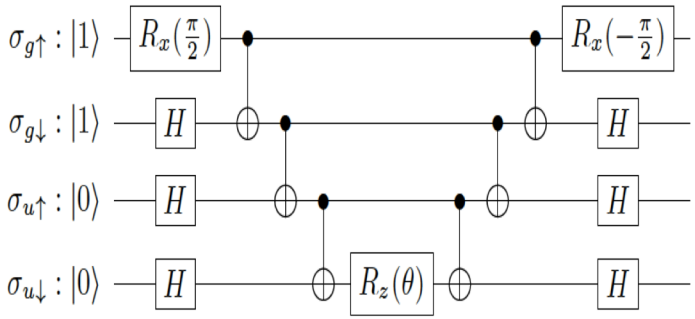


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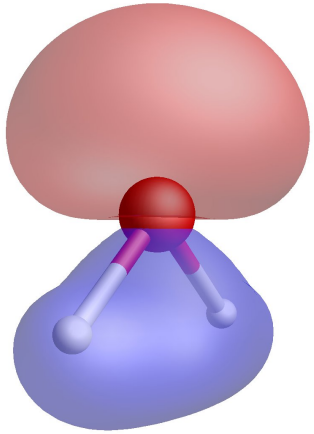

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*Dipartimento di Scienze Fisiche e Chimiche*

# From the Molecular Hamiltonian to Qubits Hamiltonians

- Molecular Hamiltonian with $M$ nuclei, $N$ electrons

$$H_e = -\sum_i \frac{\nabla_i^2}{2} - \sum_{i,I} \frac{Z_I}{\|\mathbf{r}_i - \mathbf{R}_I\|} + \frac{1}{2}\sum_{i \neq j} \frac{1}{\|\mathbf{r}_i - \mathbf{r}_j\|}$$

$r_i$: coordinate elettroni
$R_i$: ccordinate nuclei

- Hamiltonian in second quantization form

$$H_e = \sum_{p,q} h_{pq} a_p^\dagger a_q + \frac{1}{2}\sum_{p,q,r,s} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

$$h_{pq} = \int d\mathbf{x} \phi_p^*(\mathbf{x}) \left( -\frac{\nabla^2}{2} - \sum_I \frac{Z_I}{|\mathbf{r} - \mathbf{R}_I|} \right) \phi_q(\mathbf{x})$$

$$h_{pqrs} = \int d\mathbf{x}_1 d\mathbf{x}_2 \frac{\phi_p^*(\mathbf{x}_1)\phi_q^*(\mathbf{x}_2)\phi_s(\mathbf{x}_1)\phi_r(\mathbf{x}_2)}{|\mathbf{x}_1 - \mathbf{x}_2|}$$

- Mapping the Fermion Fock space into qubits bosons by (for instance) store the occupation number of an orbital in the |0> or |1> state of a qubit:

$$|f_{M-1}, \ldots, f_0\rangle \rightarrow |q_{M-1}, \ldots, q_0\rangle$$

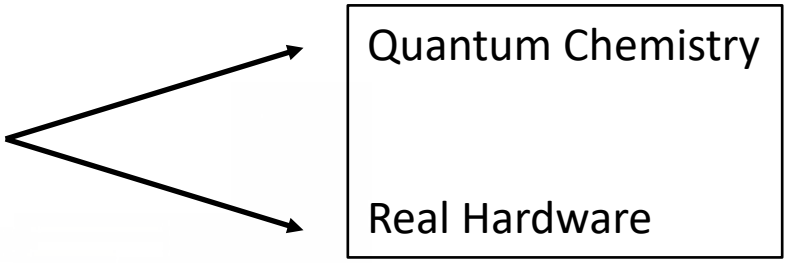
Linear combination of Slater Det. becames superposition of qubit states

- Hamiltonian in the qubit space as sum of Pauli matrices

$$H = c_1 IIII + c_2 ZZII + c_3 XZXZ + \ldots$$

# Variational Quantum Eigensolver

- Ansatz ? $|\psi(\vec{\theta})\rangle$

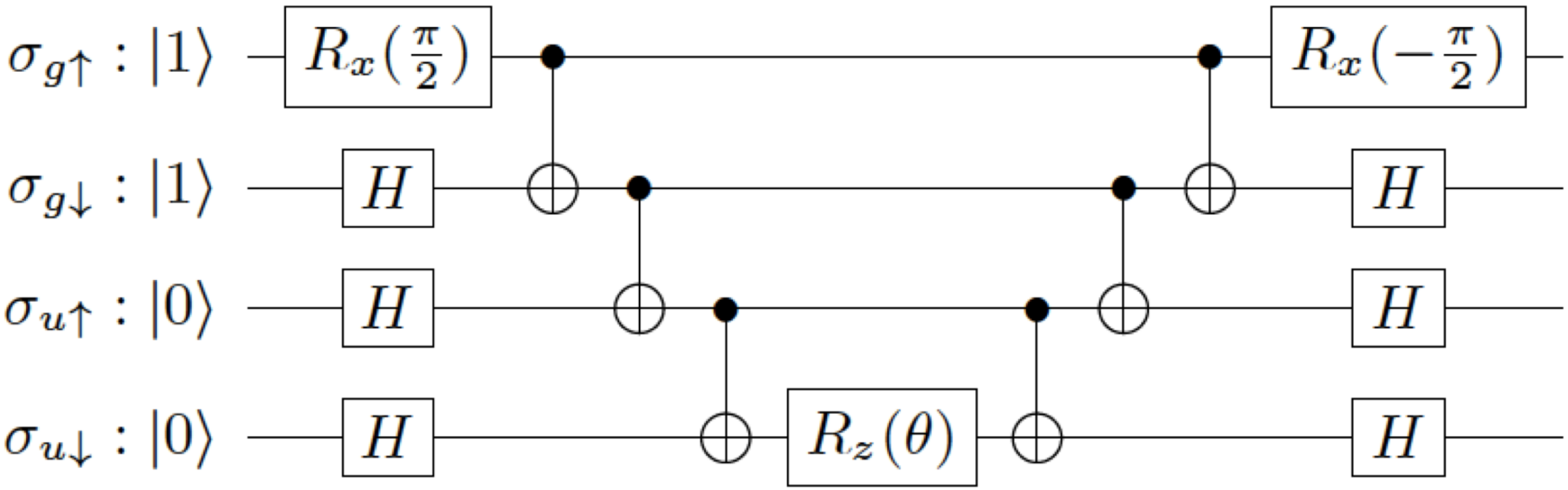



- Variational principle $\langle\psi(\vec{\theta})|H|\psi(\vec{\theta})\rangle \geq E_0$

  where $E_0$ is the lowest energy eigenvalue of the Hamiltonian $H$, and $\vec{\theta}$ is a vector of parameters used to construct the qubit state.

- Uses a classical computer to optimize the parameters $\vec{\theta}$ and a quantum computer to measure the expectation value

# Wave Function Ansatz inspired by Quantum Chemistry




$$U(\vec{\theta}) = e^{T-T^\dagger}$$

UCCSD operator for H2 in the STO-3G basis

$$T = \sum_i T_i$$

☺ **Accurate**

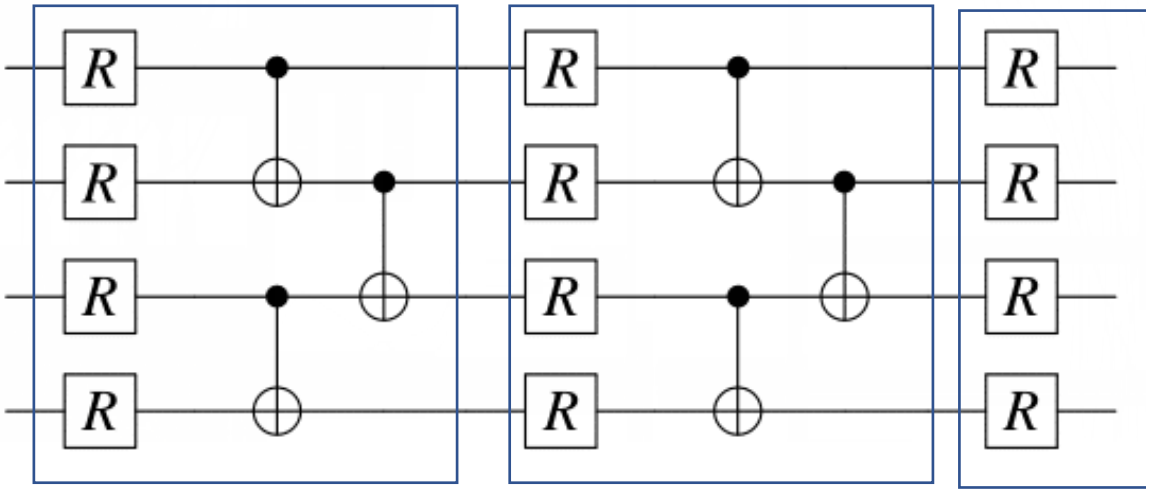
☹ Bad scaling for the number of gates

# Wave Function Ansatz from heuristic approach

- The heuristic ansatz wavefunction is:

$$|\psi(\vec{\theta})\rangle = \underbrace{R_y(\vec{\theta_D})U_{ent}\ldots R_y(\vec{\theta_1})U_{ent}}_{\text{D times}} R_y(\vec{\theta_0})\,|00\ldots0\rangle$$

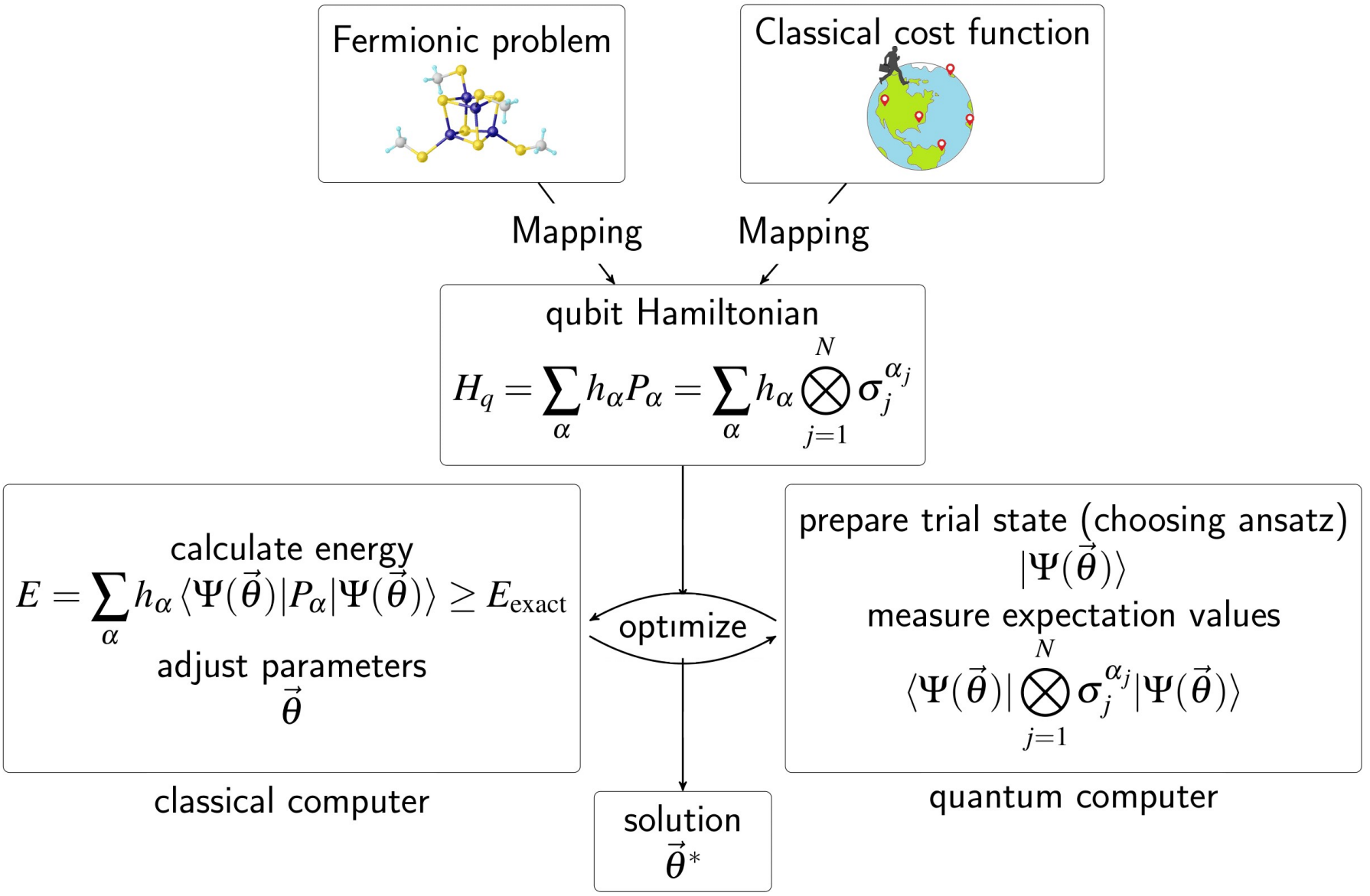
where $R_y(\vec{\theta_i})$ is a rotation around axis $y$ (generated by the Pauli matrix $Y$) on all qubits, and $U_{ent}$ is an entangling block (CNOTs between neighbors)



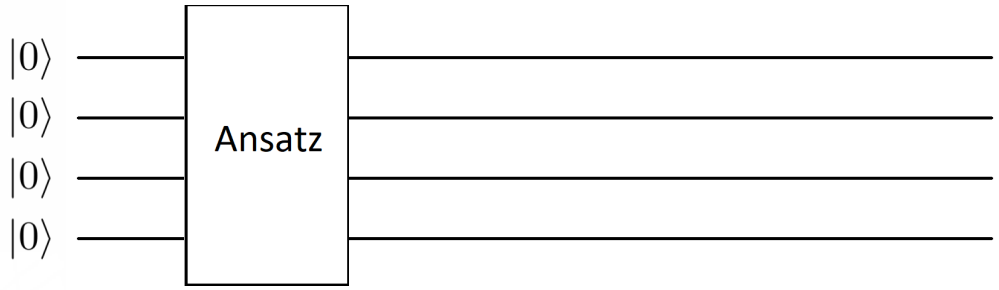

☺ Very compact

☹ Lost of the chemical meaning

# Variational Quantum Eigensolver



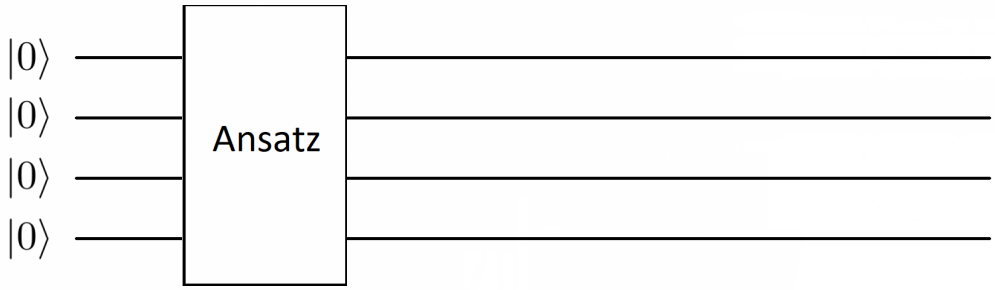
# The Variational Quantum Eigensolver



# The Variational Quantum Eigensolver

- The Hamiltonian is a sum of Pauli strings, each with its coefficient:

$$H = c_1 IIII + c_2 ZZII + c_3 XZXZ + \ldots$$



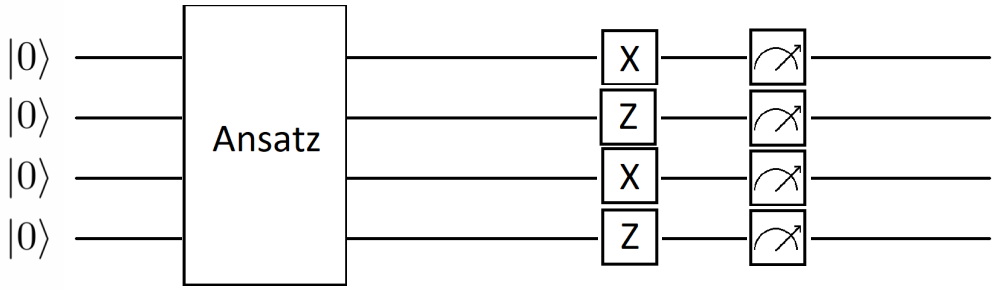

- Pick one Pauli string to measure it:

$$H = c_1 IIII + c_2 ZZII + c_3 XZXZ + \ldots$$

# The Variational Quantum Eigensolver

- The Hamiltonian is a sum of Pauli strings, each with its coefficient:

$$H = c_1 IIII + c_2 ZZII + c_3 XZXZ + \ldots$$




- Measure the Pauli string

$$< \Psi | XZXZ | \Psi >$$

# Non-unitary ansatz for VQE

$$\underbrace{|\Psi^J(\vec{\theta})\rangle}_{\text{Non-unitary Wave function}} = \underbrace{J}_{\text{Non-unitary Operator}} \underbrace{|\Psi(\vec{\theta})\rangle}_{\text{Unitary Wave function}}$$

- We can study non-unitary operators if we divide the expectation value of the Hamiltonian by the normalization of the state. The estimated energy on the state is now

$$E = \frac{\langle \Psi^J(\vec{\theta})|H|\Psi^J(\vec{\theta})\rangle}{\langle \Psi^J(\vec{\theta})|\Psi^J(\vec{\theta})\rangle} = \frac{\langle \Psi(\vec{\theta})|J^\dagger H J|\Psi(\vec{\theta})\rangle}{\langle \Psi(\vec{\theta})|J^\dagger J|\Psi(\vec{\theta})\rangle}$$

- We use a Quantum Monte-Carlo inspired operator to introduce some qubit correlation outside of the quantum computer; this acts as a ‘projector’ reducing the contribution of unphysical states

# Jastrow operator

- The operator is inspired by the one-body and two-body Jastrow factors

$$J = J_1 + J_2$$

$$J_1 = \exp\left[-\sum_{i=1}^{N} \alpha_i Z_i\right] \qquad J_2 = \exp\left[-\sum_{i<j=1}^{N} \lambda_{ij} Z_i Z_j\right]$$

- This would add an exponentially growing number of measurements! So instead we use the linearization

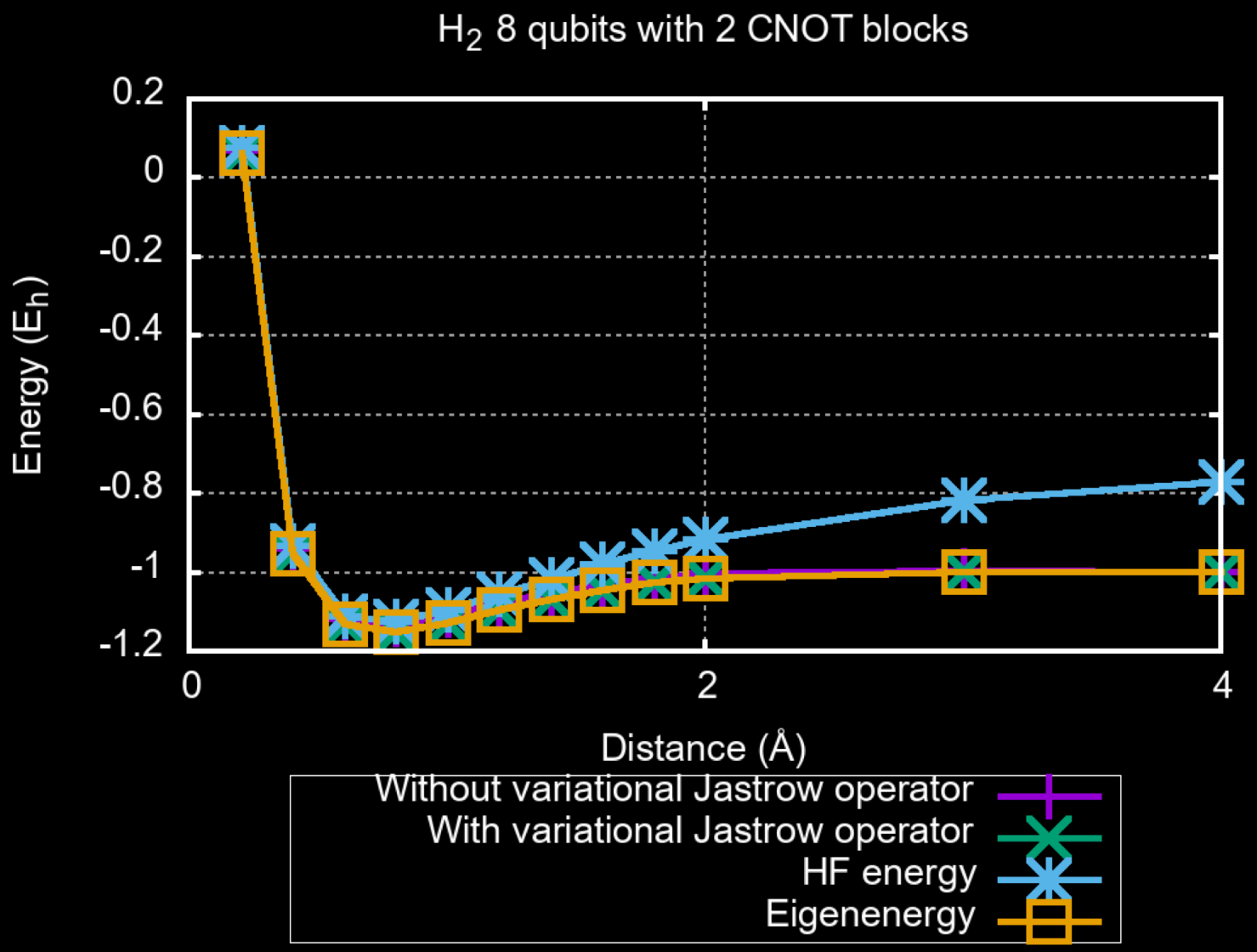
$$J(\vec{\alpha}, \vec{\lambda}) = 1 - \sum_{i=1}^{N} \alpha_i Z_i - \sum_{i<j=1}^{N} \lambda_{ij} Z_i Z_j$$

- This only adds a polinomial number of parameters (and additional measurements)

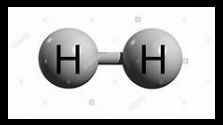
Mazzola et al. PRL 123, 130501 (2019).

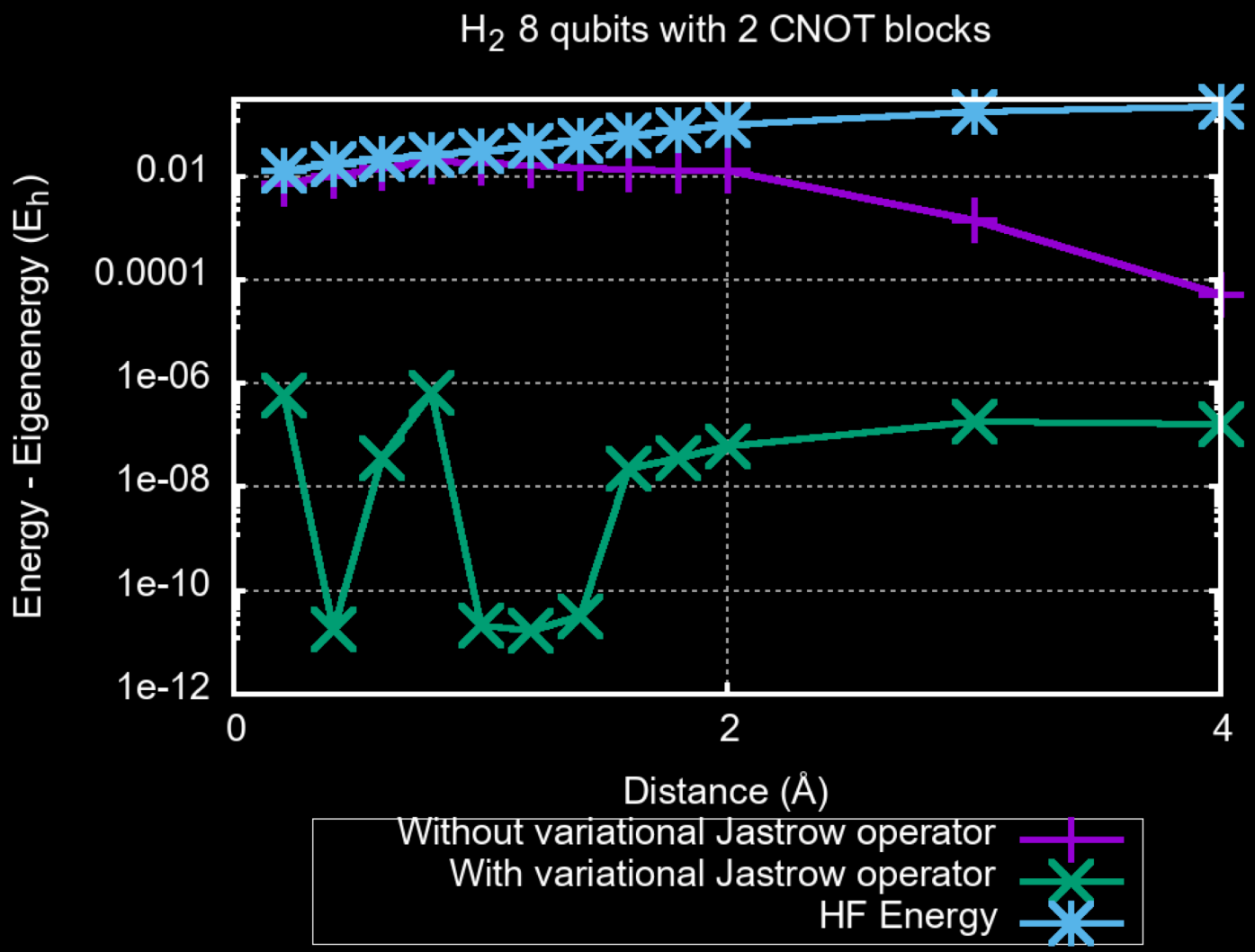
# Procedure

- Choose a hardware efficient ansatz (rotations on each qubit, blocks of entangling CNOTs)
- Given a set of parameters (rotation angles), initialize the wavefunction on the quantum computer
- Measure the Pauli strings composing $J^\dagger H J$ and $J^\dagger J$
- Calculate the expectation value $$E = \frac{\langle \Psi(\vec{\theta}) | J^\dagger H J | \Psi(\vec{\theta}) \rangle}{\langle \Psi(\vec{\theta}) | J^\dagger J | \Psi(\vec{\theta}) \rangle}$$
- Optimize all the parameters together (the rotation angles and the coefficients in the Jastrow operator) like in the normal VQE

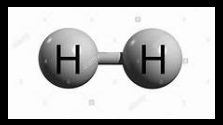


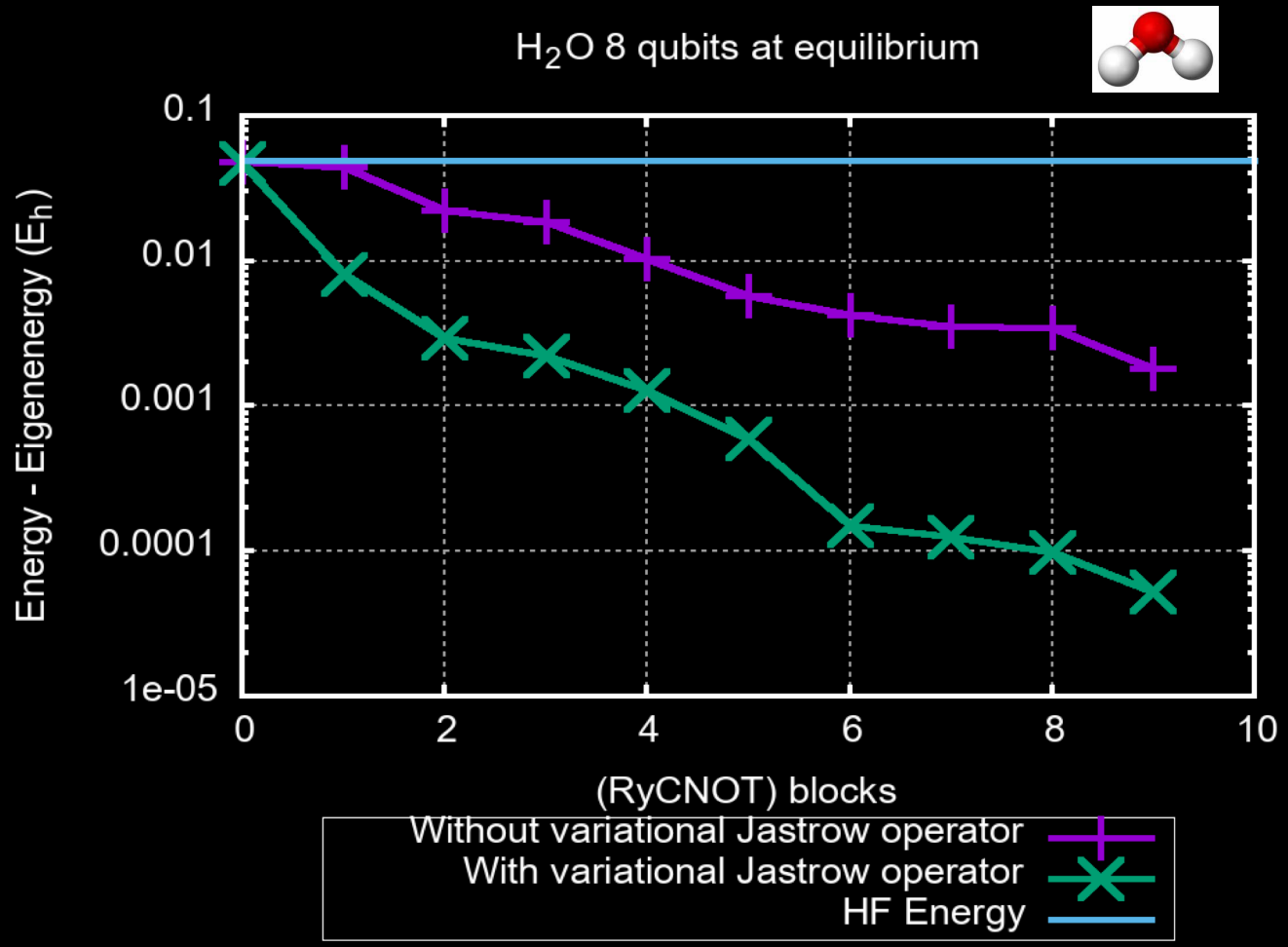

# Dissociation curve for $H_2$



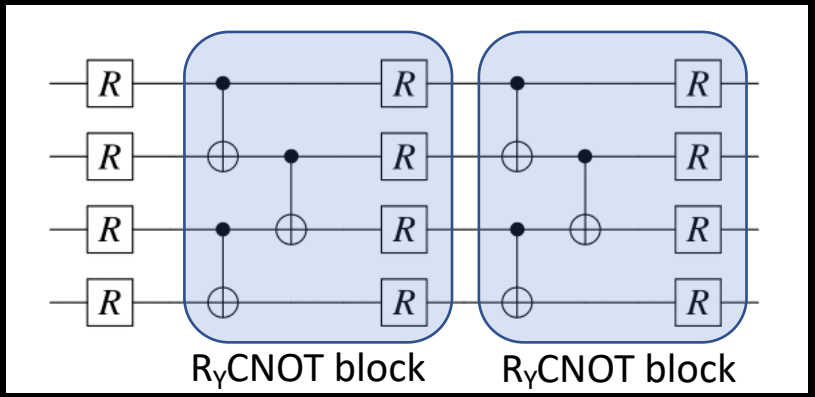


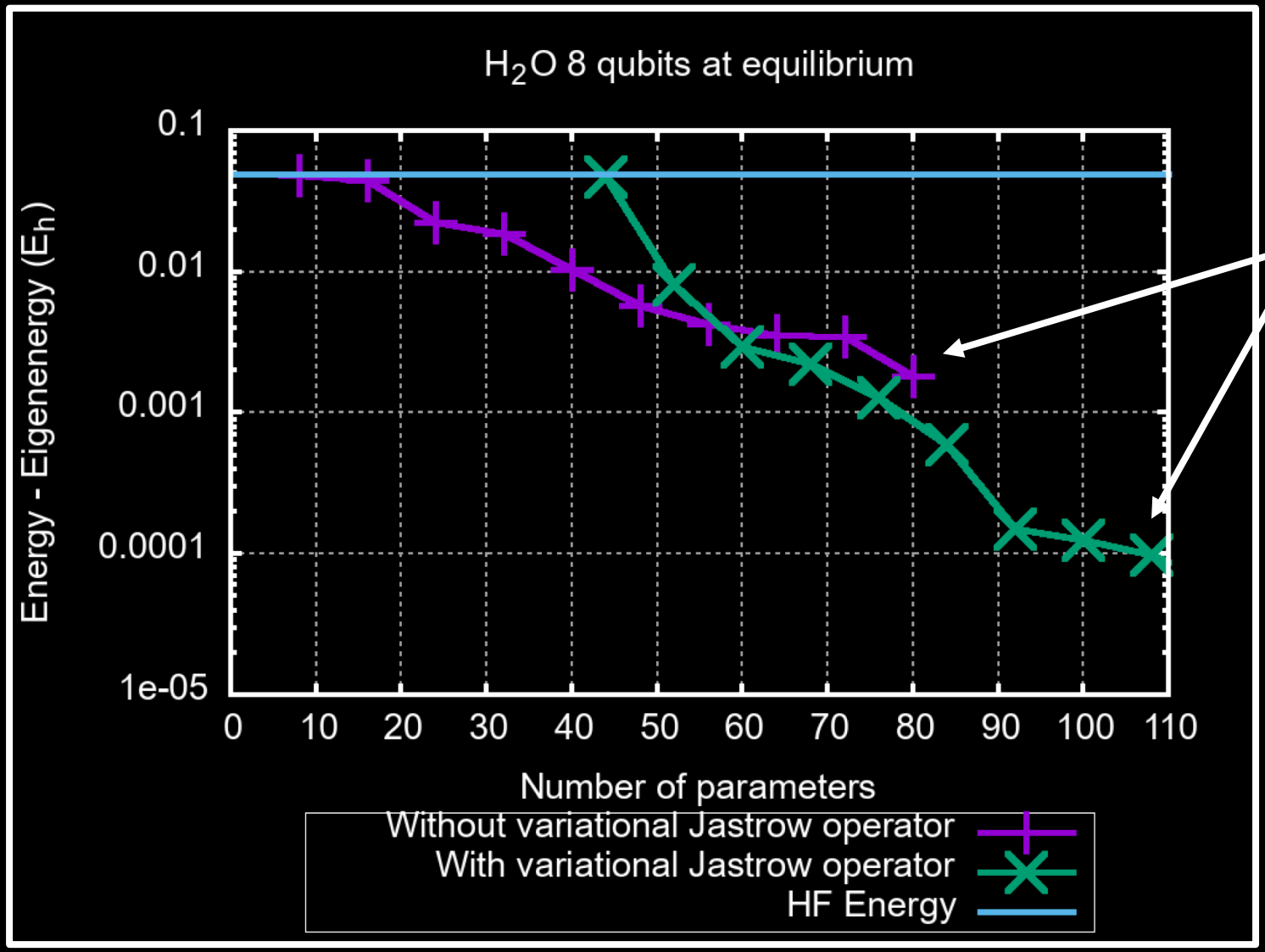

# Dissociation curve for $H_2$






The improvement grows with the number of entangling blocks!

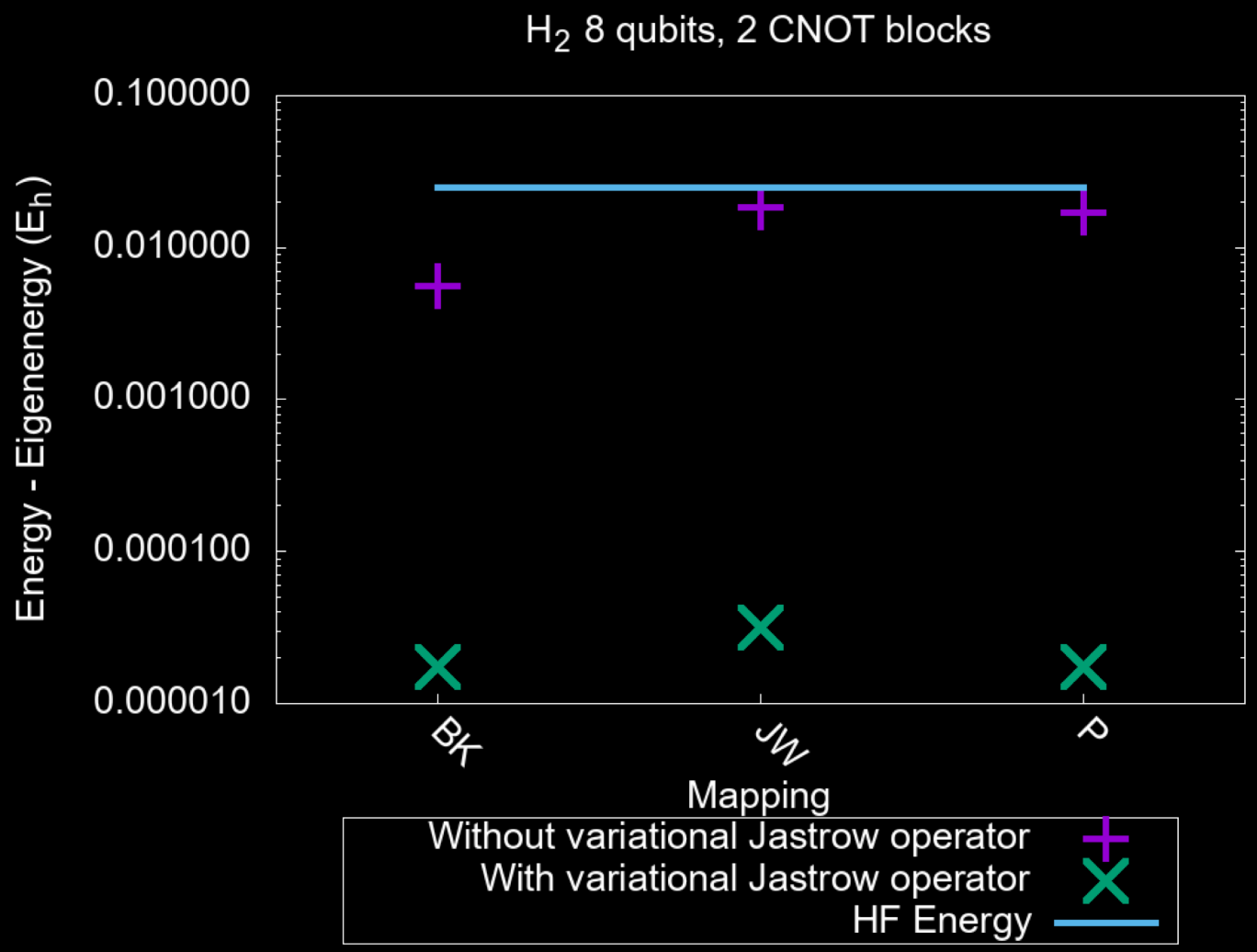





The number of total parameters grows as

$\alpha\ (N_{qubits}+N^2_{qubits}) + \beta\ N_{blocks}$

# The method works with all qubit mappings



# Conclusions

$$|\Psi^J(\vec{\theta})\rangle = J\,|\Psi(\vec{\theta})\rangle$$

- Effective procedure to introduce non-unitary wavefunctions in VQE
- The advantage increases with the number of blocks of the wave function
- Results are robusts with respect to chemistry → qubits mapping


# Computational Biophysics
## Biochemistry and Chemistry Group

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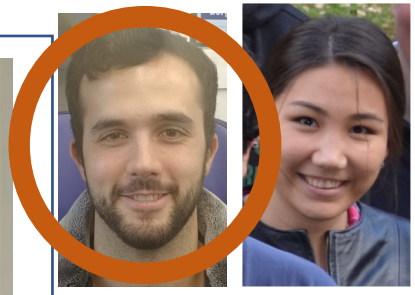
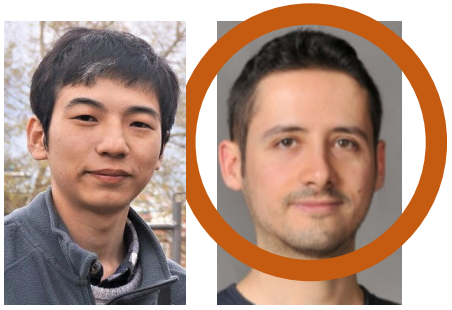
IBM-Research
Zurich





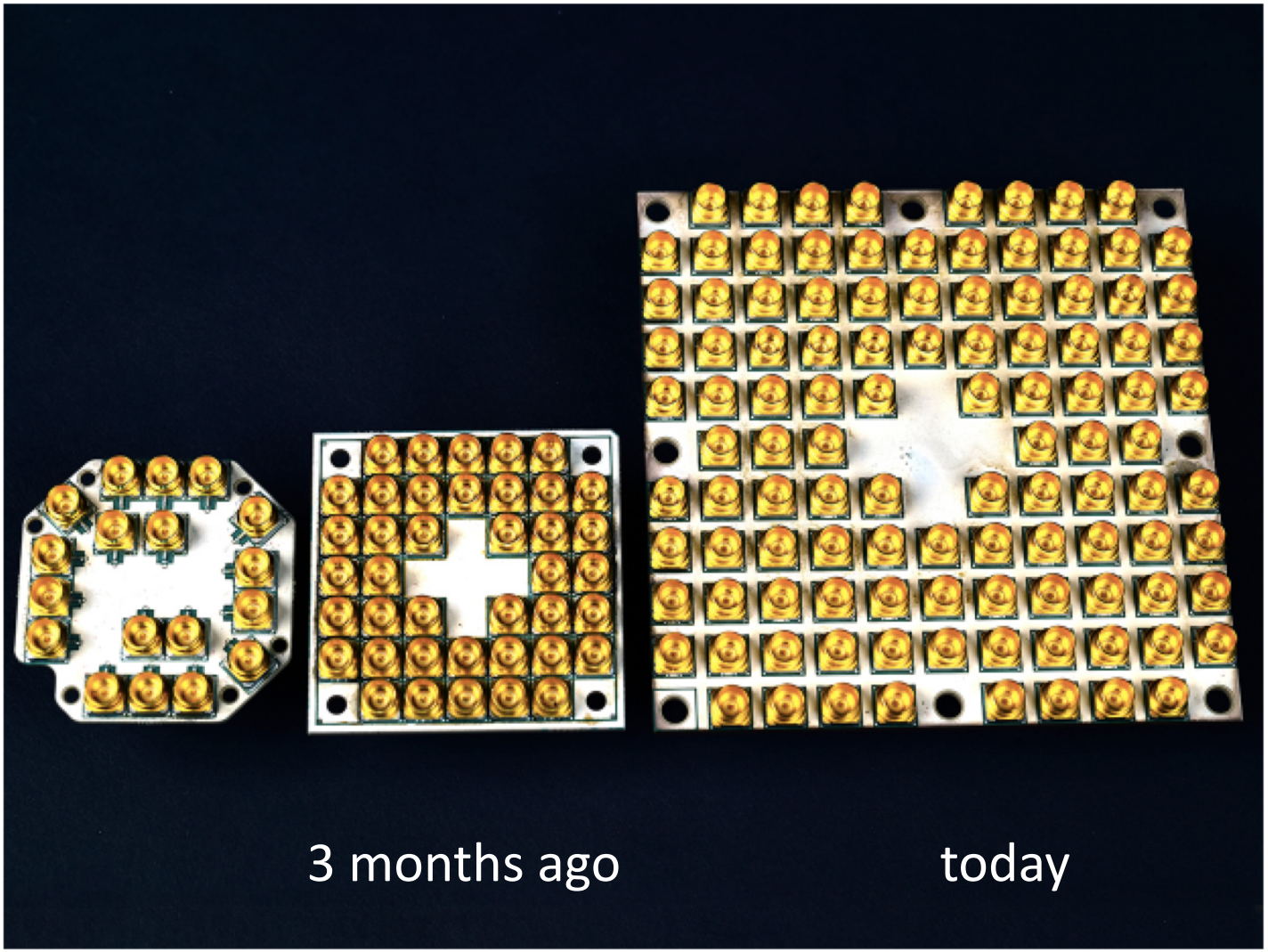



Photo: Intel

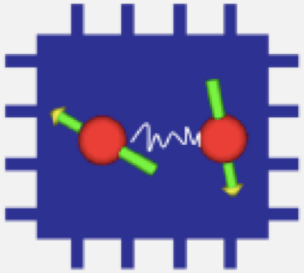
Shown here are Intel's 7-qubit, 17-qubit, and 49-qubit chips.

Spin-Qubit promise good miniaturization and scale up

# Quantum Computing: present and future applications

## QTRL

Quantum Technology Readiness Levels describing the maturity of Quantum Computing Technology



| | |
|---|---|
| QTRL9 | QCs (QAs) exceed power of classical computers |
| QTRL8 | Scalable version of QC (QA) completed and qualified in test |
| QTRL7 | Prototype QC (QA) built solving small but user-relevant problems |
| QTRL6 | Components integrated in small quantum processor w/ error correction |
| QTRL5 | Components integrated in small quantum processor w/o error correction |
| QTRL4 | Multi-qubit system fabricated; classical devices for qubit manipulation developed |
| QTRL3 | Imperfect physical qubits fabricated |
| QTRL2 | Applications / technologically relevant algorithms formulated |
| QTRL1 | Theoretical framework for quantum computation (annealing) formulated |

D-Wave quantum annealer

IBM
Google
Rigetti
Computing

Experimental qubit devices

- **Linear Algebra**

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# Quantum Algorithm Providing Exponential Speed Increase for Finding Eigenvalues and Eigenvectors

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(Received 27 July 1998)

We describe a new polynomial time quantum algorithm that uses the quantum fast Fourier transform to find eigenvalues and eigenvectors of a local Hamiltonian, and that can be applied in cases (commonly found in *ab initio* physics and chemistry problems) for which all known classical algorithms require exponential time. Applications of the algorithm to specific problems are considered, and we find that classically intractable and interesting problems from atomic physics may be solved with between 50 and 100 quantum bits.

- **Optimization problems**

## Quantum speedup in solving the maximal-clique problem

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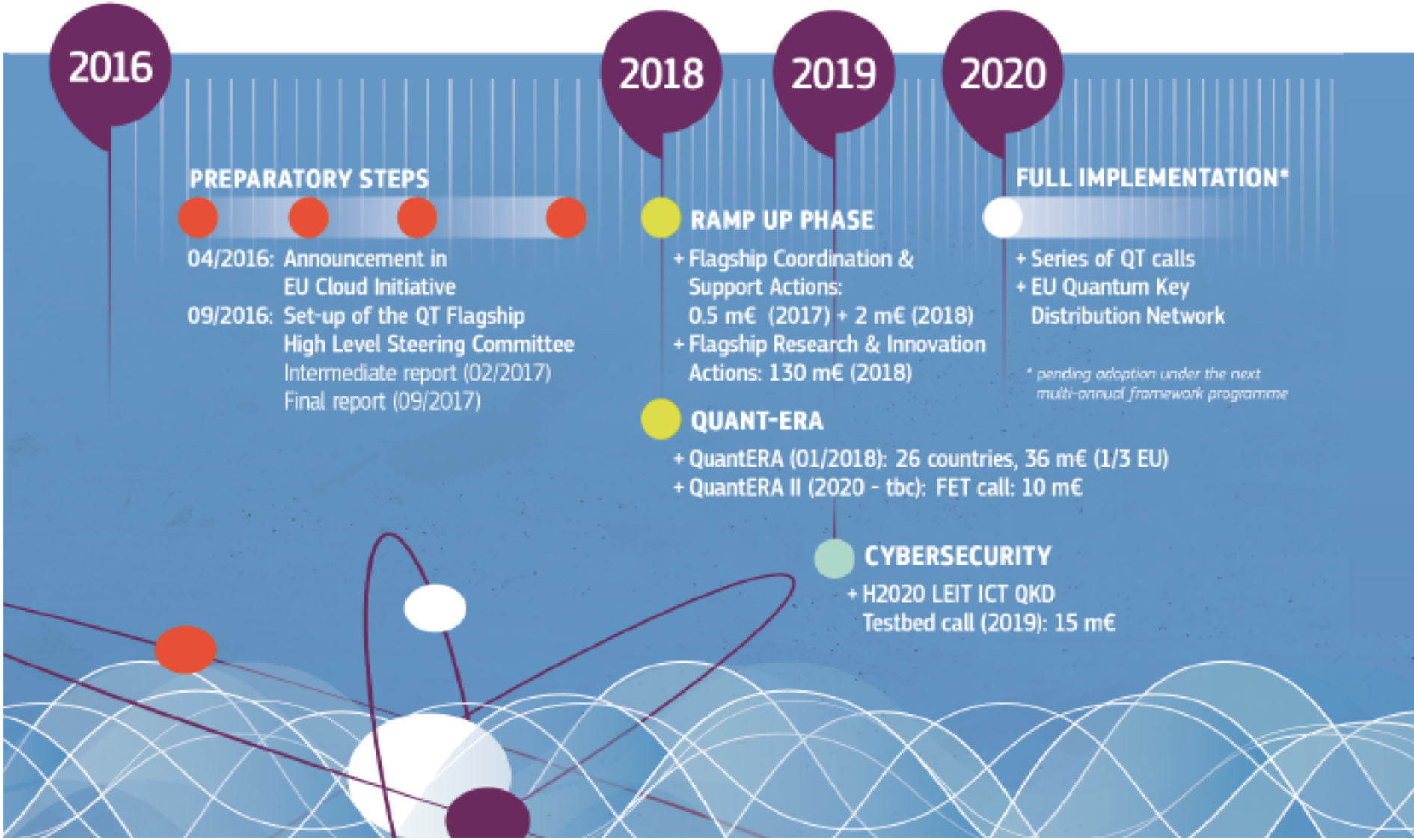
The maximal-clique problem, to find the maximally sized clique in a given graph, is classically an NP-complete computational problem, which has potential applications ranging from electrical engineering, computational chemistry, and bioinformatics to social networks. Here we develop a quantum algorithm to solve the maximal-clique problem for any graph $G$ with $n$ vertices with quadratic speedup over its classical counterparts, where the time and spatial complexities are reduced to, respectively, $O(\sqrt{2^n})$ and $O(n^2)$. With respect to oracle-related quantum algorithms for the NP-complete problems, we identify our algorithm as optimal. To justify the feasibility of the proposed quantum algorithm, we successfully solve a typical clique problem for a graph $G$ with two vertices and one edge by carrying out a nuclear magnetic resonance experiment involving four qubits.

# EU Quantum Technology Flagship 1.3 billions euros up to 2028



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| Entanglement Partners_ >
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## Enabling Technologies

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quantum computing hardware
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## New Funding Strategies

Qubit Protocol
QuantumX
CREATIVE DESTRUCTION LAB
The Quantum Revolution Fund
Quantum Valley INVESTMENTS

Representative list of players. A very active ecosystem!

QUANTUM WORLD ASSOCIATION