Quantum Dynamics of Molecules in Space:
How Can Quantum AI Help Reduce Complexity?

Dr. Taha Selim

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Co-founder and General Manager MolKet SAS, and Founder iQafé Academy
Amsterdam University of Applied Sciences

Feb 1st, 2026
King Abdullah University of Science and Technology (KAUST) Graduate Course Talk

About Me

- Researcher in **quantum information** and **quantum machine learning**, at the intersection of quantum mechanics, quantum chemistry, and machine learning
- Ph.D., Radboud University; M.Sc., University of Burgundy; B.Sc., American University in Cairo
- Lecturer and Researcher at the **Amsterdam University of Applied Sciences** of Quantum Information, Algorithms, and Quantum Theoretical Chemistry
- General Manager of **MolKet SAS**, an AI-driven consultancy and software startup
- Expertise in quantum algorithms for chemistry and machine learning
- Invited and peer-reviewed speaker at international conferences
- Founder of **iQafé**, an online education platform for quantum computing and AI
- Technology-focused YouTuber sharing content in **English and Arabic**

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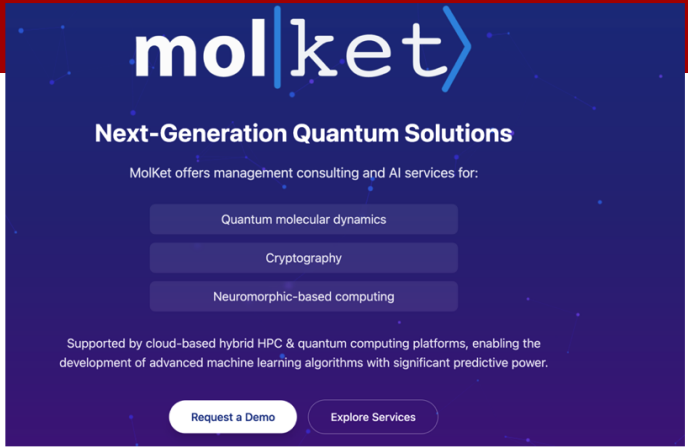
- GitHub: https://github.com/tahaselim/
- YouTube (English): https://www.youtube.com/@DrTahaSelim
- YouTube (Arabic): https://www.youtube.com/@Dr-Taha-Selim
- iQafé YouTube Channel: https://www.youtube.com/@iQafe

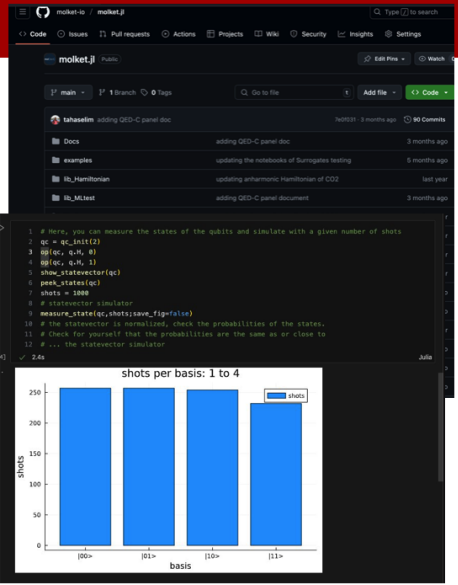
MolKet



The company also offers consulting services for training AI on datasets from fields such as chemistry, biology, materials science, and cosmology. These services are supported by physics-based kernels (e.g., quantum-mechanical kernels), enabling the development of advanced machine learning algorithms with significant predictive power.

Example projects

- Develop quantum algorithms and software for chemistry- and physics-inspired use cases across various quantum platforms, and we provide benchmarking services
- Train Smart AI-assistants for chemistry and physics simulations and design
- Automate Hamiltonian constructions with AI



contact: business@molket.io

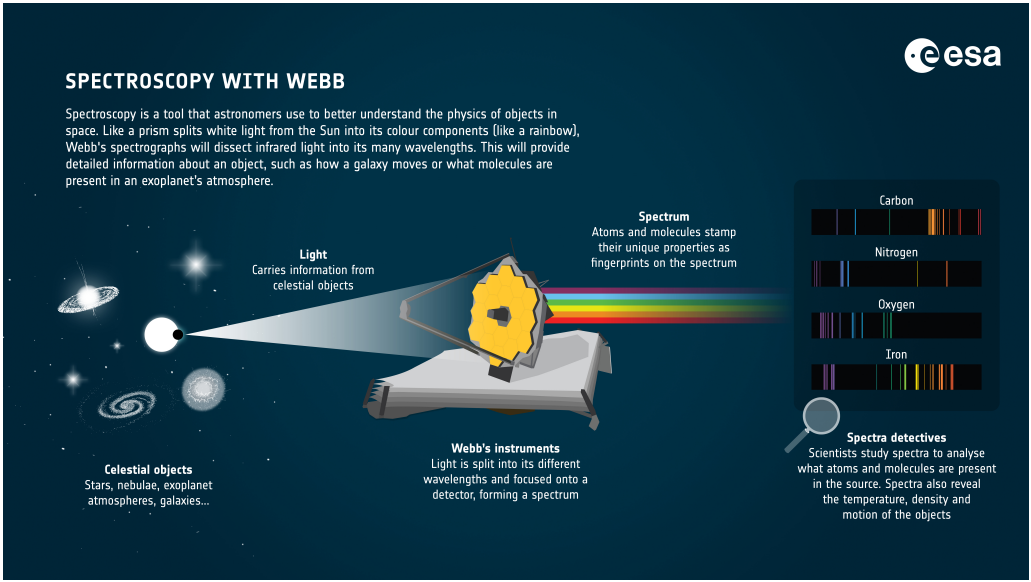
MolKet's cloud: www.molket.io

GitHub: molket-io/molket.jl

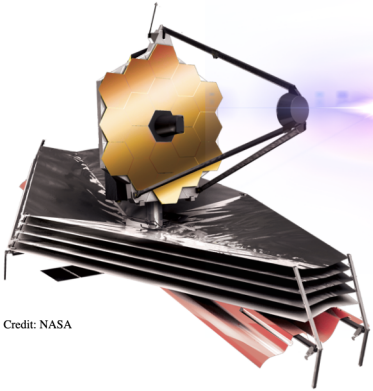
Outline

Story of Quantum simulations:

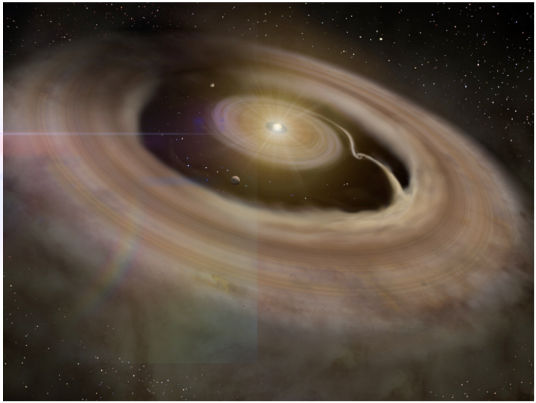
- PhD Work on Infrared Molecular Spectroscopy and Modelling
- X-ray Astronomy Simulations and Black Hole Spin Measurements
- Quantum Computing for Atomic Data Calculations
- Quantum Computing architectures and roadmap


esa
SPECTROSCOPY WITH WEBB
Spectroscopy is a tool that astronomers use to better understand the physics of objects in space. Like a prism splits white light from the Sun into its colour components (like a rainbow), Webb's spectrographs will dissect infrared light into its many wavelengths. This will provide detailed information about an object, such as how a galaxy moves or what molecules are present in an exoplanet's atmosphere.
Light
Carries information from celestial objects
Spectrum
Atoms and molecules stamp their unique properties as fingerprints on the spectrum
Carbon
Nitrogen
Oxygen
Iron
Celestial objects
Stars, nebulae, exoplanet atmospheres, galaxies...
Webb's instruments
Light is split into its different wavelengths and focused onto a detector, forming a spectrum
Spectra detectives
Scientists study spectra to analyse what atoms and molecules are present in the source. Spectra also reveal the temperature, density and motion of the objects

James Webb Space Telescope (JWST)



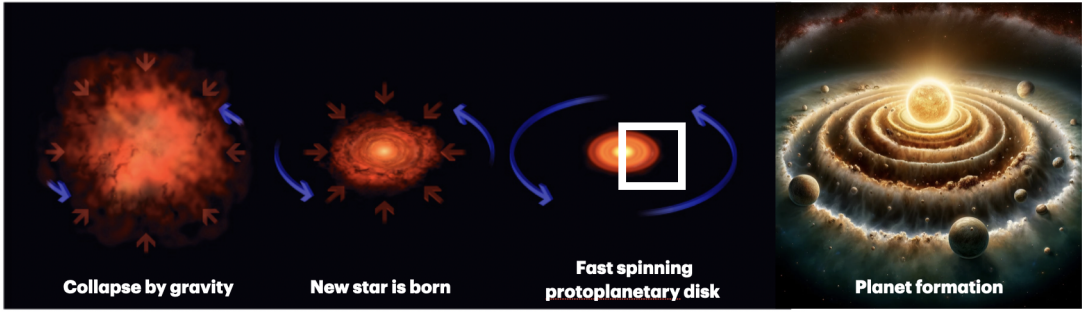
Credit: NASA



Credit: The Graduate University for Advanced Studies/NAOJ

Powerful near and mid-infrared observational capabilities

Protoplanetary disks and molecular spectroscopy



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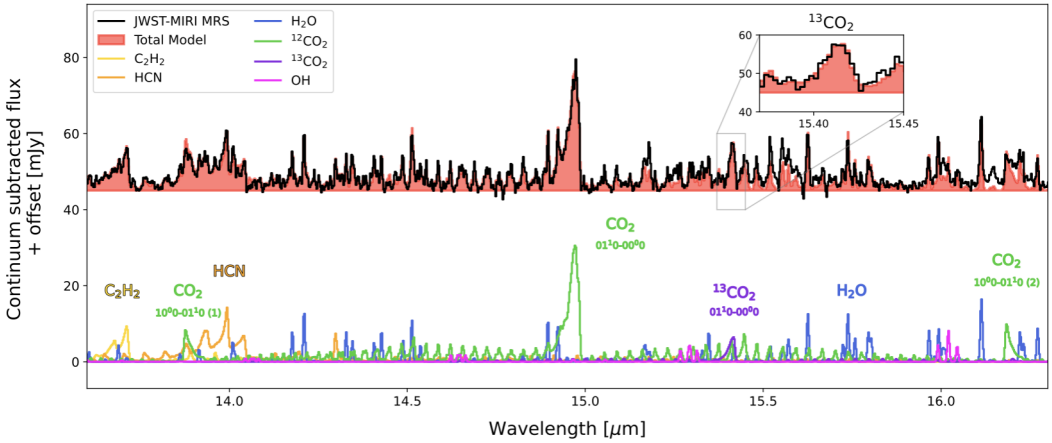
Conceptual illustration

Key molecules CO CO_2 HCN H_2O C_2H_2 CH_4

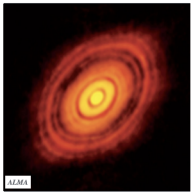
Modelling recorded spectra



Sierra L. Grant, Ewine F. van Dishoeck, et al. 2023 ApJL 947 L6

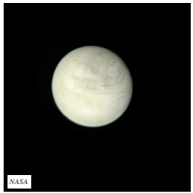
CO_2 is a key molecule in interstellar media

CO_2 was found in interstellar media and (exo-)planets



Protoplanetary disk T Tauri Star

Venus

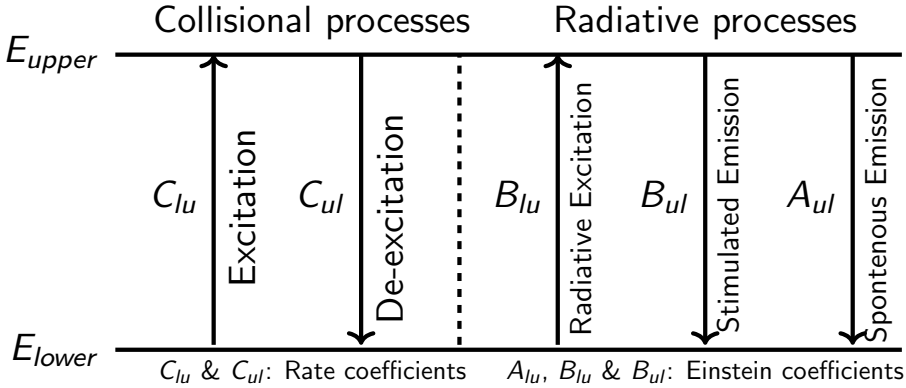


Jupiter's moon Europa

Exoplanet K2-18 b

Modeling the observed spectra requires:

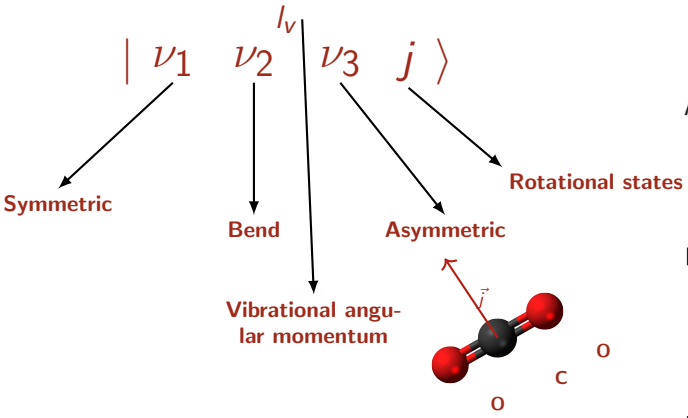
Not in Thermodynamic Equilibrium (Non-LTE) environment modeling

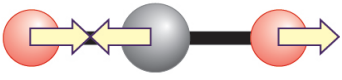


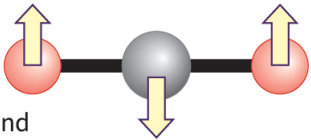
CO_2 Rotational-vibrational states

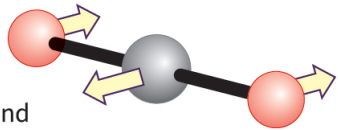
CO_2 three vibrational modes - two modes are infrared active **Labeling the rovibrational**

quantum state: 5 quantum numbers









Recipe for simulating CO_2 + He inelastic collisions

An example for a rotational-vibrational transition of CO_2 induced by the collision with **He**.

Vibrational relaxation

→ Via couplings - energy dissipated.

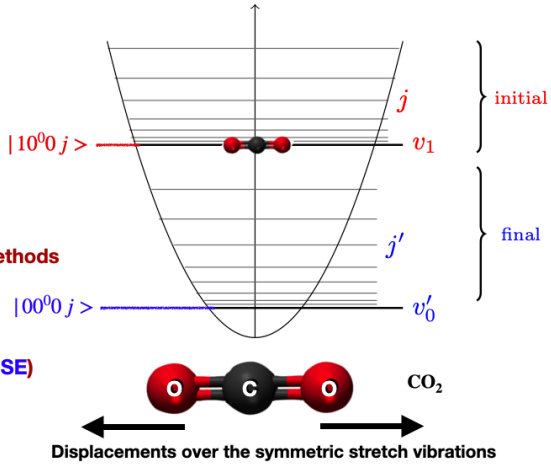
→ $CO_2(1\ 0^0\ 0) + He \xrightarrow[\text{collision}]{\text{Inelastic}} CO_2(0\ 0^0\ 0) + He$

Most accurate simulations: Quantum mechanical (QM) methods

Most accurate QM method: Coupled-Channels (CC)

CC method:

Solving the time-independent Schrödinger's equation (TISE)



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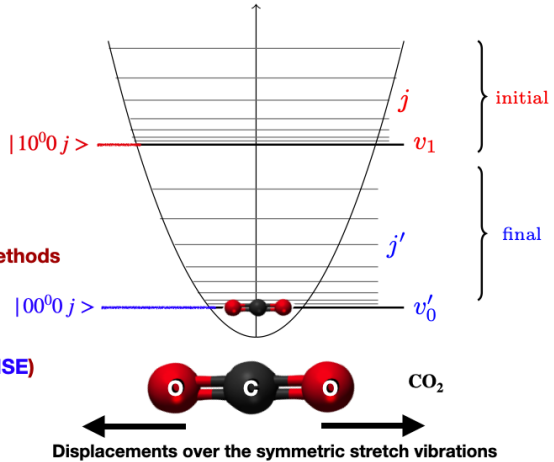


Recipe for simulating CO_2 + He inelastic collisions

First, we construct the 1D Hamiltonian $\hat{H}_{CO_2}$ to obtain the rotational-vibrational wavefunctions and energy eigenvalues of CO_2 ($v\ 0^0\ 0\ j$):

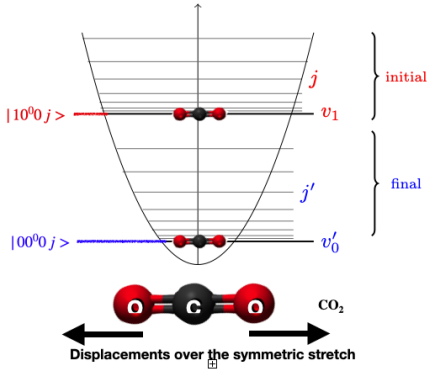
$$\hat{H}_{CO_2}(Q) = -\underbrace{\frac{\hbar^2}{2\mu_{CO_2}(Q)}\frac{\partial^2}{\partial Q^2}}_{\text{Nuclear motion}} + \underbrace{\frac{\hat{j}^2}{2I(Q)}}_{\substack{CO_2 \text{ angular} \\ \text{Momentum}}} + \underbrace{V_{CO_2}(Q)}_{\text{1D potential}}$$

CO_2 computational basis/space:

$$|\, v\ 0^0\ 0\ j >$$

CO_2 rotational vibrational wave functions:

$$|\, v\ j > = \chi_{vj}(Q)\ Y_{j0}(\theta,0)$$



Simulating CO_2 + He inelastic collisions

Second, we construct the 3D Hamiltonian of the dimer $\hat{H}_{HeCO_2}$ to obtain the scattering wavefunctions and channel basis:

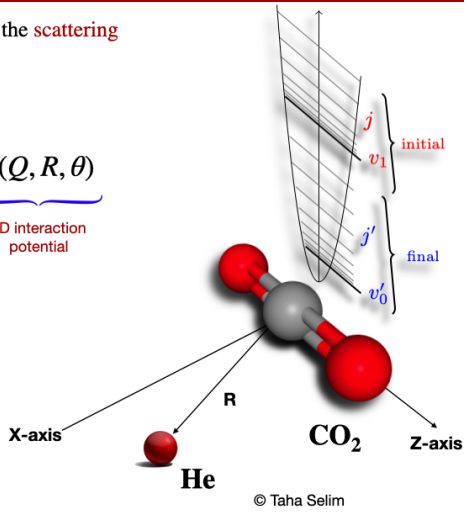
$$\hat{H}_{HeCO_2} = \underbrace{-\frac{1}{2\mu R}\frac{\partial^2}{\partial R^2}R}_{\text{Kinetic energy of the dimer}} + \underbrace{\hat{H}_{CO_2}}_{CO_2\text{ Hamiltonian}} + \underbrace{\frac{\hat{L}^2}{2\mu R^2}}_{\text{Angular kinetic energy of the dimer}} + \underbrace{V(Q,R,\theta)}_{\text{3D interaction potential}}$$

dimer: refers to both $He+CO_2$

$HeCO_2$ computational basis/space, used for solution:

Space-fixed (SF): $|v\ j\ L|JM_J>$

Body-fixed (BF): $|v\ j\ \Omega|JM_J>$



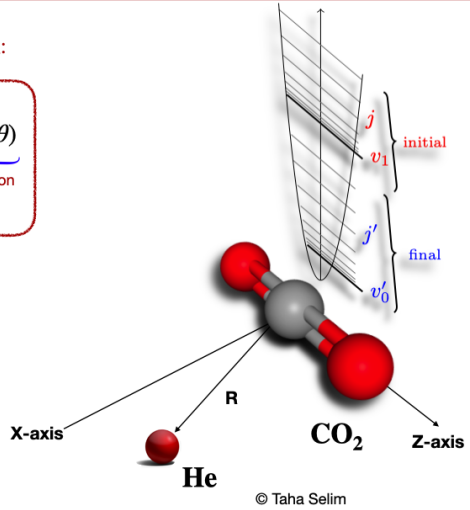
Quantum Chemistry: computing the potential energy surface

Computing 3D interaction potential energy surface of the dimer He-CO_2:

$$\hat{H}_{\mathbf{HeCO_2}} = \underbrace{-\frac{1}{2\mu R}\frac{\partial^2}{\partial R^2}R}_{\text{Kinetic energy of the dimer}} + \underbrace{\hat{H}_{\mathbf{CO_2}}}_{CO_2\ \text{Hamiltonian}} + \underbrace{\frac{\hat{L}^2}{2\mu R^2}}_{\text{Angular kinetic energy of the dimer}} + \underbrace{V(Q,R,\theta)}_{\text{3D interaction potential}}$$

The potential: **CCSD(T)** level of theory.

CCSD(T): **C**oupled-**C**luster with **S**ingle and **D**ouble and Perturbative **T**riple excitations.



Quantum Chemistry: computing the potential energy surface

Computing 3D interaction potential energy surface of the dimer He-CO_2:

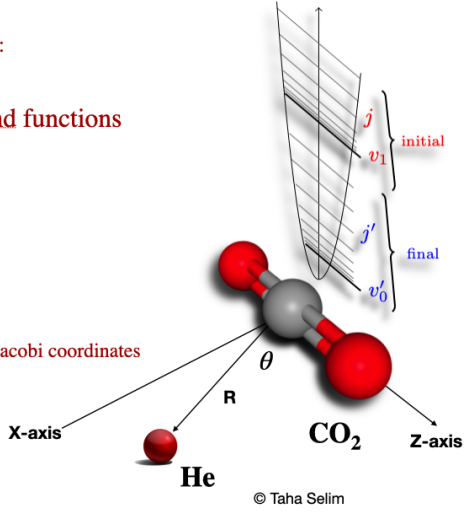
$\underbrace{V(Q,R,\theta)}_{\text{3D interaction potential}}$ CCSD(T)

- $HeCO_2$ basis set: aug-cc-pVTZ + midbond functions
- CO_2 basis set: aug-cc-pVQZ
- Grid: Q, R, and the polar angle θ

Fitting and expansion

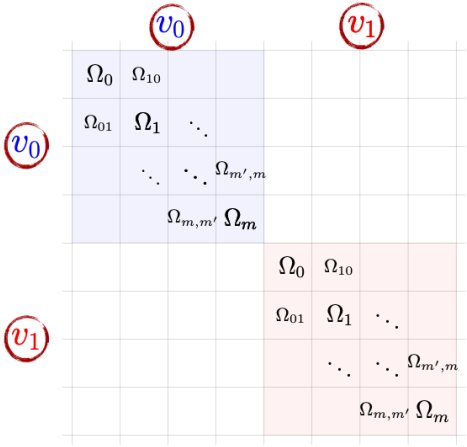
$$V(Q,R,\theta) = \sum_{\lambda} \sum_{p=0}^{2} \underbrace{c_{p,\lambda}(R)}_{\text{Expansion coefficients}} \underbrace{P_{\lambda}(\cos\theta)}_{\text{Gauss-Legendre polynomials}}$$

2nd degree polynomial expansion of Q



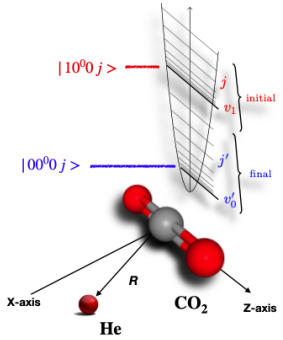
The Coupled-channels (CC) matrix: a close look!

For a two energy level system in the symmetric stretch, the CC matrix looks like this on the computer:



Ω

eigenvalue of both $\hat{j}_z$ and $\hat{j}_z$.



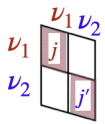
Huge matrices

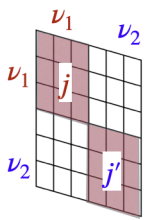
Computational complexity of rovibrational of transition rates

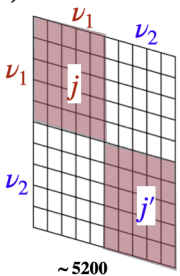
Two main challenges, considering CO_2:

- Theoretical formalism and codes to enable the calculations
- Efficient procedures to reduce the computational complexity

Time $\propto$ (Number of coupled equations)^3

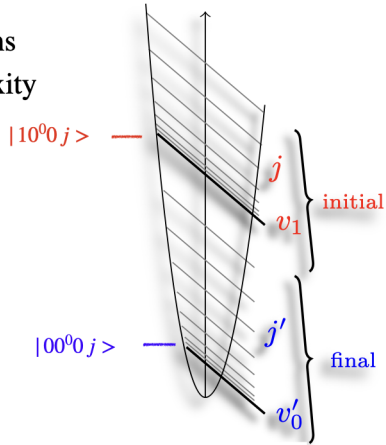






Single calculation

Number of coupled equations:	**~100**	**~300**	**~5200**
Time (seconds):	**~0.5 s**	**~4.15 s**	**~6600 s**



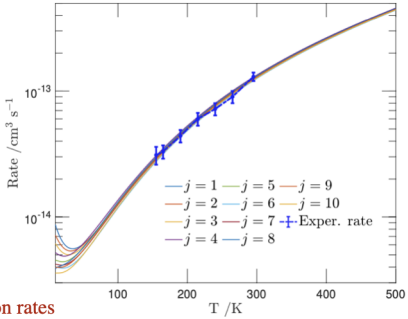
Example: symmetric stretch

PhD work results

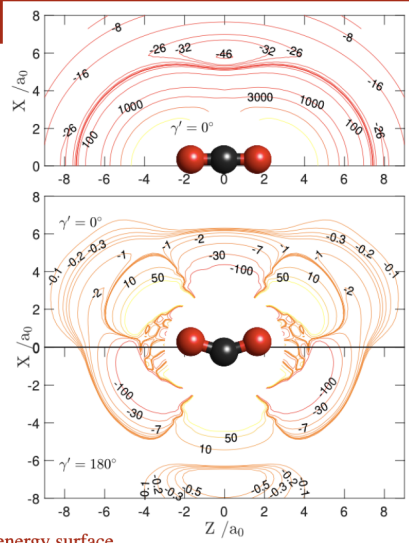
PhD work

Develop theoretical formalisms and codes to calculate rates of collision-induced rovibrational transitions of $\mathbf{CO_2}$ with **He** atoms.

Calculations: Symmetric, asymmetric, and bend modes



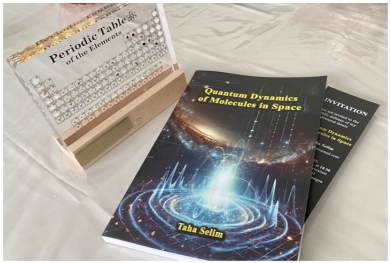
Example,
bend collision rates



Example,
bend potential energy surface

PhD Research Overview

- Taha Selim. (2024). *Quantum dynamics of molecules in space: Theoretical studies and efficient computational methods for collision-induced rovibrational transition rates in molecules*. [Doctoral dissertation, Radboud University].
- Taha Selim, Arthur Christianen, Ad van der Avoird, & Gerrit C. Groenenboom. (2021). Multi-channel distorted-wave Born approximation for rovibrational transition rates in molecular collisions. *The Journal of Chemical Physics*, 155(3), 034105.
- Taha Selim, Ad van der Avoird, & Gerrit C. Groenenboom. (2022). Efficient computational methods for rovibrational transition rates in molecular collisions. *The Journal of Chemical Physics*, 157(6), 064105.
- Taha Selim, Ad van der Avoird, & Gerrit C. Groenenboom. (2023). State-to-state rovibrational transition rates for C_3 in the bend mode in collisions with He atoms. *The Journal of Chemical Physics*, 159(16), 164310.



PhD Thesis Cover Page,
Taha Selim, 2024

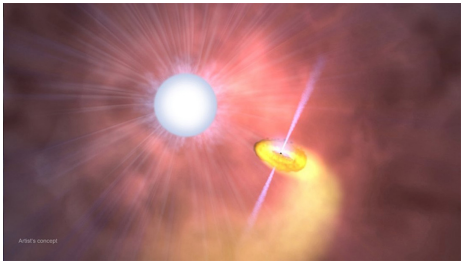
Computational complexity of molecular modelling and simulations

- Molecular systems are inherently quantum mechanical, requiring accurate quantum descriptions for properties and dynamics.
- Atomic transitions also cost extensive computational resources to model accurately.
- Multi-electron calculations scale exponentially with the number of electrons.
- Classical computers struggle with simulating quantum systems due to this exponential scaling.
- Quantum computers can potentially simulate quantum systems more efficiently by leveraging qubits and quantum algorithms

X-ray astronomy simulations and black hole spin measurements

X-ray astronomy simulations help in studying underlying physics of the accretion of massive black holes, testing general relativity predictions in strong gravity fields, and measuring black hole spin rates through high-resolution spectroscopy.

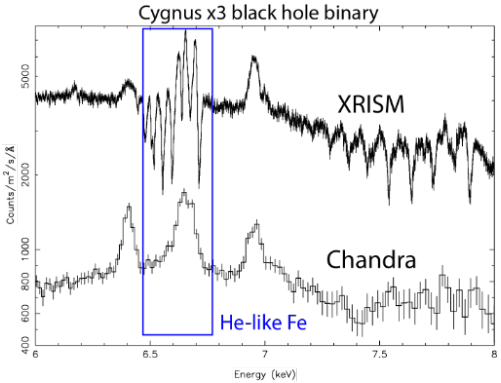
- Investigating the extreme physics of black hole accretion to test predictions of General Relativity in strong gravity fields.
- Identifying the last stable orbit of matter around black holes, known as the Innermost Stable Circular Orbit (ISCO), before falling into the event horizon.
- The ISCO location directly correlates to spin. Rapidly spinning (*Kerr*) black holes pull the ISCO closer to the event horizon than static (*Schwarzschild*) ones.
- XRISM resolves fine spectral features (like Iron lines) distorted by extreme gravity and velocity, allowing precise calculation of spin rates for black holes of all sizes.
- This mission serves as a pathfinder for the upcoming *Athena* telescope (10x sensitivity) and complements future gravitational wave data from *LISA*.



Artist impression of Cygnus X-3. The image illustrates a black hole candidate traversing the dense stellar winds of a Wolf-Rayet companion star. This environment is believed to sustain an accretion disk and launch powerful jets from the black hole.Photo: NASA

Computational complexity of x-ray astronomy simulations

- Significant improvement provided by XRISM comparing to Chandra Groundbreaking capabilities in x-ray spectroscopy similar to JWST in infrared and optical wavelengths.
- XRISM significantly outperforms Chandra in spectral resolution for black hole observations, particularly within the He-like Iron band.
- Both spectra are normalized to ensure a direct and accurate comparison.
- The spectra provides quantum level of details aiding the modeling process of the chemical composition of of matter around black holes for the first time.
- Athena mission is expected to further enhance the spectra by 10x compared to XRISM.



Comparison of Chandra and XRISM resolution capabilities. Reference:

Atomic transition rates and level populations

the demand for larger and accurate atomic data to model high-resolution spectra from XRISM and Athena missions.

- Atomic transition rates and level populations are crucial for modeling X-ray spectra from astrophysical sources.
- Computational complexity: Calculating accurate atomic data involves solving complex quantum mechanical equations, which can be computationally intensive.
- Large datasets: High-resolution spectra require extensive atomic databases, leading to increased storage and retrieval challenges.
- Focus on speeding up spectral modeling codes like SPEX by optimizing atomic data calculations using quantum computing techniques.

Reference: [1]

Why do we need quantum computing?

Classical computing vs. quantum computing

Classical bits:

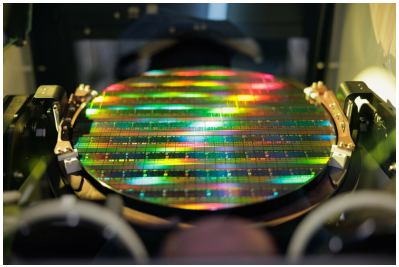
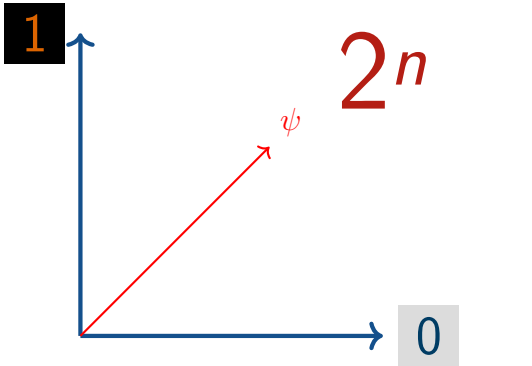


Illustration of a wafer. Photo: ASML

Quantum bits (qubits):



Bit 0 1

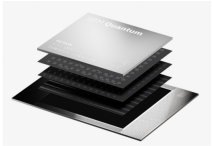
Qubit $= a\,0 + b\,1$

Current quantum computing technologies and architectures

IBM quantum computer >

A sequence of gates applied to a given quantum register of qubits:

IBM Q



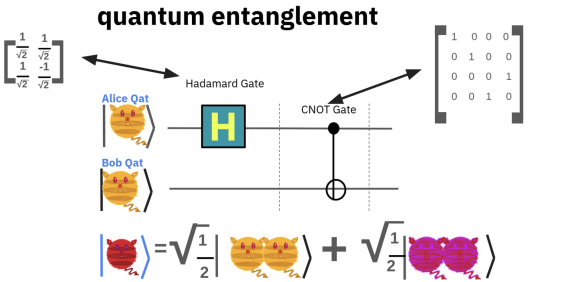


Image credit: Alberto Maldonado Romo

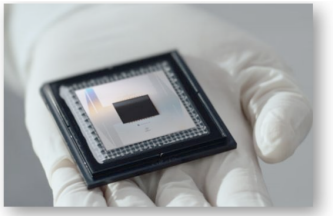
Time

Current quantum computing technologies and architectures

Different types of quantum computing, each has its own mechanism.

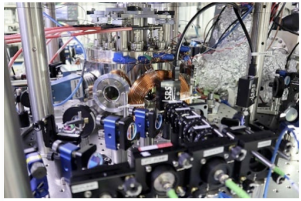
QuiX - https://www.quixquantum.com/

Photonic quantum processor



Google, new Willow chip

Superconducting quantum processor

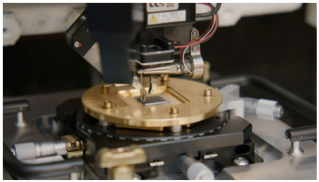


Kenji Ohmori group at the Institute for Molecular Science. Courtesy of Takafumi Tomita.

Ultracold neutral atoms quantum processor

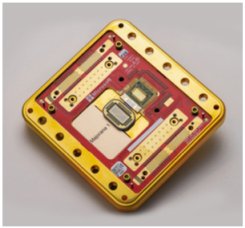
Hardware for quantum computing >

Different types of quantum computing, each has its own mechanism.



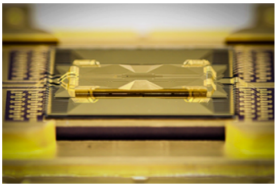
AWS- New 'Ocelot' chip

Cat qubits



Microsoft, Majorana 1

Topological qubits



IonQ

IonQ's trapped ion technology

Manufacturers of the same type have their own technologies as well.

Available quantum computers, portable technologies >

Different types of quantum computing, each has its own mechanism.

SpinQ

Nuclear Magnetic Resonance (MRI)

~ 2 qubits

- hard to scale

Raspberry pi

Quantum circuit emulator

~ 100 euros

NVIDIA Jetson Orin Nano Super Developer Kit

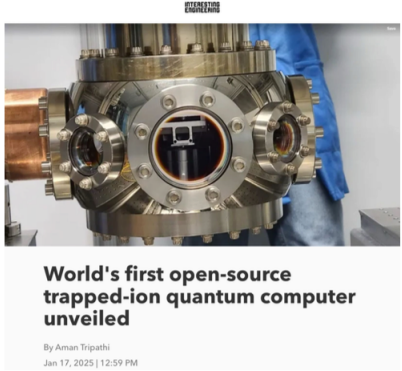
Quantum circuit emulator +

AI applications

~ 250 euros

Available quantum computers, portable technologies >

Open Quantum Design (OQD), a non-profit based in Waterloo, is breaking down barriers to quantum computing with the release of the world's first open-source, full-stack trapped-ion quantum computer. This initiative grants free access to both hardware and software, empowering researchers, developers, and institutions globally to explore and contribute to the field.



Quantum computing workflow

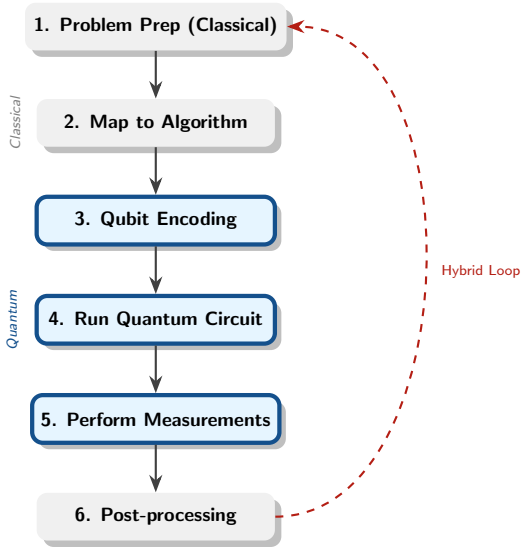
Typical steps in a quantum computing workflow:

- Problem preparation with a classical algorithm
- Map the problem into a quantum algorithm or a hybrid classical-quantum workflow
- Initial data loading on the quantum register (qubit encoding)
- Translate the quantum algorithm into a quantum circuit and run it
- Perform measurements
- Post-processing

Quantum Computing Workflow

Quantum computing workflow diagram

- **Problem Preparation:**
  Define Hamiltonian using classical algorithm.
- **Mapping:**
  Convert problem to quantum compatible format (Hybrid workflow).
- **Data Loading:**
  Initial state encoding on quantum register (Qubit encoding).
- **Execution:**
  Translate algorithm to circuit and run on QPU.
- **Measurement:**
  Collapse state and read classical bits.
- **Post-processing:**
  Classical analysis of measurement results.



Traditional qubits:

- Most quantum computers utilize qubits as two-energy level systems.
- They can be achieved with Fermonic particles like electrons, not neccessarily using Fermonic properties directly.

Fermionic qubits:

- Leverage the Fermionic properties directly.
- Important to simulate Fermionic systems in quantum chemistry and materials science.
- Natural simulations of Fermonic systems: sing Fermionic qubits can allow for more natural simulations of Fermionic systems, because the quantum computer itself is using the same rules as the simulated system.
- Encoding Fermionic information into standard qubits is challenging. Encoding Fermionic information into Fermionic qubits is more natural and efficient.

Bosonic qubits:

- Leverage the Bosonic properties directly.
- Utilize bosonic systems directly such as photons or modes of a harmonic oscillator.
- Information is encoding in the infinite-dimensional Hilbert space of the boson rather than in two-level systems.
- Offer potential advatenge regarding error correction and fault tolerance.
- Use infinite number of quantum states, available to a boson, to encode information in a more robust way.

Mapping problem Hamiltonian to qubit Hamiltonian

Several transformations can be used to map the problem Hamiltonian to a qubit Hamiltonian.

- Jordan-Wigner transformation.
- Bravyi-Kitaev transformation.
- Parity transformation.
- Fermionic-to-qubit mapping.
- Bosonic-to-qubit mapping.

Examples of qubit mappers

Common qubit mappers:

- Jordan-Wigner transformation [**?**]. Implemented in Qiskit.
- Bravyi-Kitaev transformation [**?**]. Implemented in Qiskit.
- Parity transformation [**?**]

Example: Ground state of a hydrogen H_2 molecule with VQE

Jordan-Wigner transformation [?]: formalism

- First, map the problem to Fermionic operators/Fermionic Hamiltonian. Example: Molecular Hamiltonian.

$$\hat{H} = \sum_{p,q} h_{pq} \hat{a}_p^\dagger \hat{a}_q + \frac{1}{2} \sum_{p,q,r,s} h_{pqrs} \hat{a}_p^\dagger \hat{a}^\dagger \hat{a}_r \hat{a}_s + h_0$$

where $\hat{a}_p^\dagger$ and $\hat{a}_p$ are the creation and annihilation operators of the Fermionic mode p, and h_{pq} and h_{pqrs} are the one- and two-electron integrals, respectively. Also, h_0 is a correction constant term.

- Then, map the Fermionic operators to qubit operators:

$$a_n^\dagger \mapsto \frac{1}{2} \left[\prod_{j=0}^{n-1} -Z_j \right] (X_n - iY_n) \qquad a_n \mapsto \frac{1}{2} \left[\prod_{j=0}^{n-1} -Z_j \right] (X_n + iY_n)$$

where X_n, Y_n, and Z_n are the Pauli matrices acting on the n-th qubit.

- The Final Hamiltonian to be executed on a quantum computer is:

$$\hat{H} = -\frac{1}{2}(\hat{I} \otimes \hat{I} + \hat{X} \otimes \hat{X} + \hat{Y} \otimes \hat{Y} + \hat{Z} \otimes \hat{Z}) + d(\hat{Z} \otimes \hat{I} + \hat{I} \otimes \hat{Z}),$$

where $\hat{I}$, $\hat{X}$, $\hat{Y}$, and $\hat{Z}$ are the identity, Pauli-X, Pauli-Y, and Pauli-Z operators, respectively.

Example: Ground state of a hydrogen H_2 molecule with VQE

Jordan-Wigner transformation [?]: executing with qiskit

- Formulate the problem.
- Obtain the operators of the Hamiltonian in a second quantized form with `second_q_ops`:
  `hamiltonian = problem.second_q_ops()[0]`. [1].
- Mapping: Transform the molecular Hamiltonian operators to qubit operators with:

```
mapper = JordanWignerMapper()
converter = QubitConverter(mapper, two_qubit_reduction=False)
qubit_op = converter.convert(hamiltonian)
```

- After processing, the final Hamiltonian is obtained in Pauli operators (Pauli-strings) form:

$$
\begin{aligned}
H = & -0.807184 I \otimes I \otimes I \otimes I + 0.175106 Z \otimes I \otimes Z \otimes I + 0.169404 I \otimes Z \otimes I \otimes Z \\
& - 0.230474 (I \otimes I \otimes Z \otimes I + Z \otimes I \otimes I \otimes I) + 0.173740 (I \otimes I \otimes I \otimes Z + I \otimes Z \otimes I \otimes I) \\
& + 0.045094 (Y \otimes Y \otimes Y \otimes Y + X \otimes X \otimes Y \otimes Y) + 0.045094 (Y \otimes Y \otimes X \otimes X + X \otimes X \otimes X \otimes X) \\
& + 0.166582 (X \otimes I \otimes I \otimes Z + I \otimes Z \otimes Z \otimes I) + 0.121488 (Z \otimes Z \otimes I \otimes I + I \otimes I \otimes Z \otimes Z)
\end{aligned}
$$

[1] Actual implementation might vary depending on the version of qiskit

Computational complexity of quantum algorithms

Estimating Computational complexity of quantum algorithms requires [?]:

- Estimating the number of qubits and gates required to execute the quantum algorithm.
- Example: Hubbard model with VQE: $n = 2N$, where N is number of energy-levels in the model. Error correction needs: $O(n)$ The computational complexity of the Hubbard model with VQE is $O(n^2)$, where n is the number of qubits.
- Example: single-particle Hamiltonian has $\approx O(n^2)$ qubits.
- Example: two-particle Hamiltonian has $\approx O(n^4)$ qubits.

Estimating Computational complexity of Mappers [?]:

- Jordan-Wigner transformation: requires $O(N)$ qubit operations to simulate one electronic operation.
- Bravyi-Kitaev transformation: requires $O(\log N)$ qubit operations to simulate one electronic operation.

Nots:

- Bravyi-Kitaev transformation was found to be more efficient than the Jordan-Wigner transformation in some quantum chemistry calculations [**?**].

Methods to reduce the computational complexity: optimization

On algorithmic level:

- Trotterization: Decomposing the Hamiltonian into a sum of Pauli operators [?].
- Optimization of the on the level of second quantized operators [?].
- Simplifying the Hamiltonian by reducing the number of terms in the Hamiltonian. Example: the work of Simplified projection on total spin zero for state preparation on quantum computers [?].
- Algorithmic optimization. Example: Discovering optimal fermion—qubit mappings through algorithmic enumeration [?].

On circuit level[?]:

- Optimize the usage of quantum gates. Example, reduce the number of CNOT gates.
- Optimization by Gate Cancellation Rule.
- Optimization by Gate Commutation Rule.
- Optimization by Hadamard Gate Reduction.
- Merging Rz Gates Using Phase Polynomial Estimation: When a circuit comprises only `CNOT`, `NOT`, and R_z gates, R_z gates can be merged if they produce the same phase pattern, effectively reducing both circuit depth and gate count.
- Depth Reduction: example, rearranging the order of gates while preserving correctness can minimize the number of computations and reduce depth.

Methods to reduce the computational complexity: optimization

On circuit level: using machine learning, reinforcement learning, and generative AI

- Reinforcement Learning (RL): RL agents can learn to apply sequences of circuit transformations, to reduce gate counts and circuit depths.
- Example 1: Reducing the number of two-qubit gates in quantum circuits using reinforcement learning [**?**].
- Example 2: Reducing then number of iterations in VQE by using a generative model to produce quantum circuits with desired properties or good ansatz for the ground state of a Hamiltonian [**?**].
- Example 3: Optimizing the number of T gates of quantum algorithms with AlphaTensor [**?**].
- More examples: A Study on Optimization Techniques for Variational Quantum Circuits in Reinforcement Learning [**?**].

On Encoding level: Efficient and approximate encoding of quantum states

- Example 1: Approximate encoding of quantum states using shallow circuits [**?**].
- Example 2: Efficient Circuit Depth Reductions by Approximate Encoding for Quantum Machine Learning [**?**].
-

HHL algorithm overview

HHL algorithm is a quantum algorithm designed to solve linear systems of equations. It computes:

$$|\mathbf{b}\rangle \xrightarrow{\text{HHL}} |A^{-1}\mathbf{b}\rangle.$$

where the solution vector $|\mathbf{x}\rangle$ is represented as:

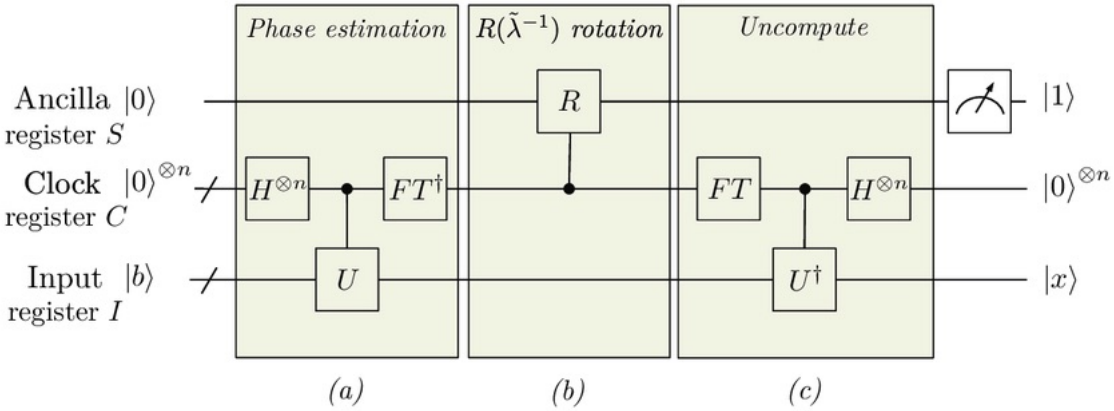
$$|\mathbf{x}\rangle = \frac{\sum_i x_i |i\rangle}{\sqrt{\sum_i |x_i|^2}}, \quad |\mathbf{b}\rangle = \frac{\sum_i b_i |i\rangle}{\sqrt{\sum_i |b_i|^2}},$$

where x_i and b_i are the components of the solution and input vectors, respectively, and $|i\rangle$ denotes the computational basis states corresponding to the binary representation of the index i. For example, $|5\rangle = |0 \ldots 0101\rangle$ [2]. A is a Hermitian matrix, and $|\mathbf{b}\rangle$ is the input state vector.

Key points about HHL's computational complexity:

- Representing a vector of size N requires $\log_2(N)$ qubits.
- Computational complexity of HHL scales as $\mathcal{O}(\text{polylog}(N))$ or about $\mathcal{O}((\log N))$ polynomially, depending on the condition number κ of matrix A.
- HHL is most efficient for large, sparse matrices with low condition numbers.

HHL algorithm steps



Typically, we need to convert a non-Hermitian matrix equation into a Hermitian one to apply HHL. This can be done by constructing an augmented matrix:

$$\tilde{A} = \begin{pmatrix} O & A \\ A^\dagger & O \end{pmatrix}, \tilde{\mathbf{b}} = \begin{pmatrix} \mathbf{b} \\ \mathbf{0} \end{pmatrix}$$

Quantum computing approach

First quantization

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$$

$$a^\dagger \Psi_n(x) = \sqrt{n+1}\Psi_{n+1}(x)$$
$$a\Psi_n(x) = \sqrt{n}\Psi_{n-1}(x)$$
$$a^\dagger a\Psi_n(x) = n\Psi_n(x)$$

where $\Psi_n(x)$ are the wavefunctions.

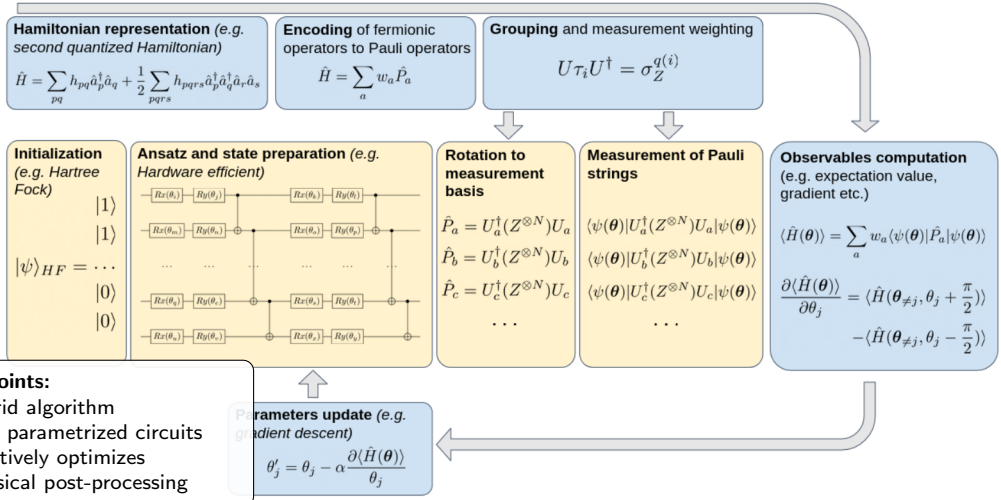
Second Quantization

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$$

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}x - i\frac{1}{\sqrt{2m\hbar\omega}}\frac{d}{dx}$$
$$a = \sqrt{\frac{m\omega}{2\hbar}}x + i\frac{1}{\sqrt{2m\hbar\omega}}\frac{d}{dx}$$

$E_n = (n + \frac{1}{2})\hbar\omega$ are the energy levels
$n = 0, 1, 2, \ldots$ is the quantum number.

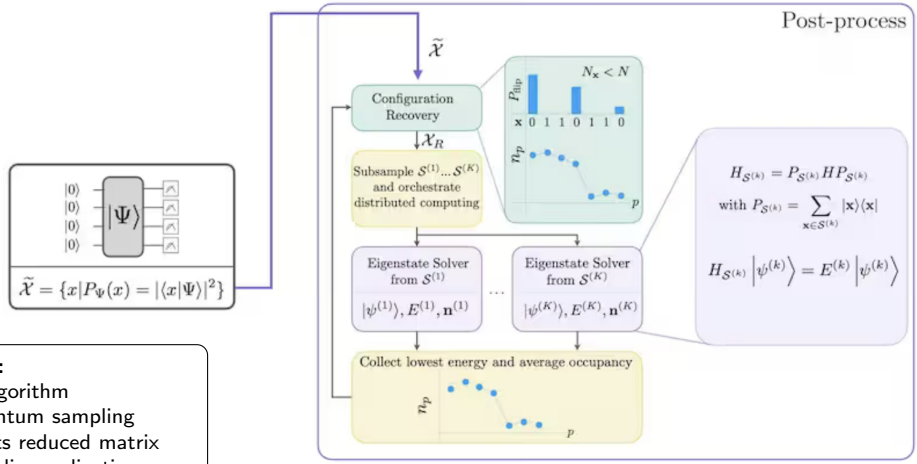
Variational Quantum Eigensolver (VQE) approach



Key Points:
- Hybrid algorithm
- Uses parametrized circuits
- Iteratively optimizes
- Classical post-processing

VQE algorithm workflow diagram. It is a hybrid quantum-classical algorithm used to find the ground state energy of a quantum system. Goal: Compute transition probability in He-like Iron in plasma state.

Sample-based Quantum Diagonalization (SQD) approach



Key Points:
- Hybrid algorithm
- Uses quantum sampling
- Constructs reduced matrix
- Classical diagonalization

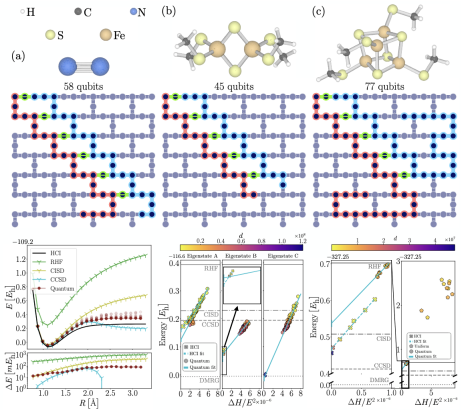
VQE algorithm workflow diagram. It is a hybrid quantum-classical algorithm used to find the ground state energy of a quantum system. Goal: Compute transition probability in He-like Iron in plasma state.

Use case I: IBM quantum-centric supercomputing architecture

IBM uses quantum-centric supercomputing architecture to tackle complex quantum chemistry problems: With HPC as Fugaku and QPU as Heron.

Recent IBM work using SQD to use chemistry on large basis set and compute:

- N_2 triple bond dissociation energy: well-known test of the accuracy of electronic structure methods in the presence of static electronic correlation.
- Ground states of Iron-Sulfur (FeS) clusters: The [2 Fe−2 S] cluster and [4 Fe−4 S] cluster, challenging systems for classical methods due to their complex electronic structure and strong electron correlation effects.

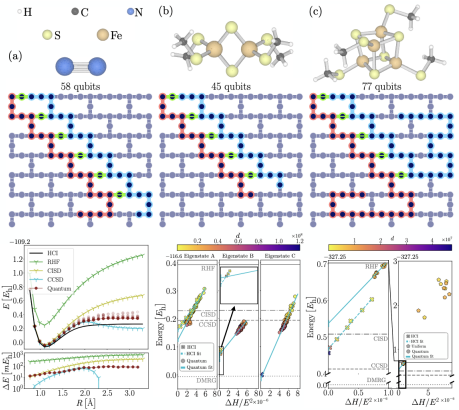


SQD use cases by IBM research team. Reference: [3]

Use case I: IBM quantum-centric supercomputing architecture

Nitrogen Molecule (N_2) Dissociation (6-31G basis)

Metric	Details
Qubits Used	**36 total qubits** used, with **32** for the Jordan-Wigner (JW) encoding.
Quantum Gates	**762 CNOT gates**. **1,408 total gates**. Circuit depth $d = 148$.
HPC Usage (Classical)	Subspace diagonalization was performed on classical nodes using the **PySCF** library. A subspace dimension of $d = 4\mathrm{M}$ was used for wavefunction visualization analysis.

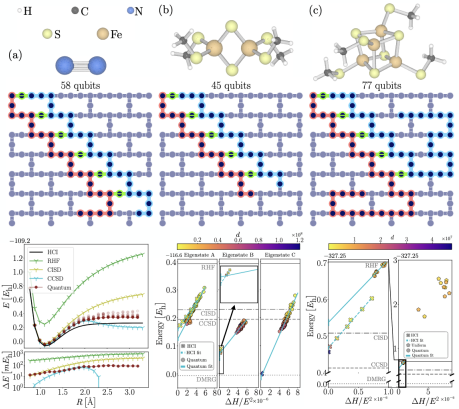


SQD use cases by IBM research team. Reference: [3]

Use case I: IBM quantum-centric supercomputing architecture

Nitrogen Molecule (N_2) Dissociation (cc-pVDZ basis)

Metric	Details
Qubits Used	**58 total qubits** used, with **52** for the Jordan-Wigner (JW) encoding.
Quantum Gates	**1,792 CNOT gates**. **3,412 total gates**. Circuit depth $d = 223$. The circuit size reached approximately **1–1.5K two-qubit gates**.
HPC Usage (Classical)	Used $d = 16 \cdot 10^6$ (16M) configurations for projection and diagonalization. The combined quantum runtime for all points in the dissociation curve was approximately **45 minutes**. Classical diagonalization used the **PySCF** library on a single node.

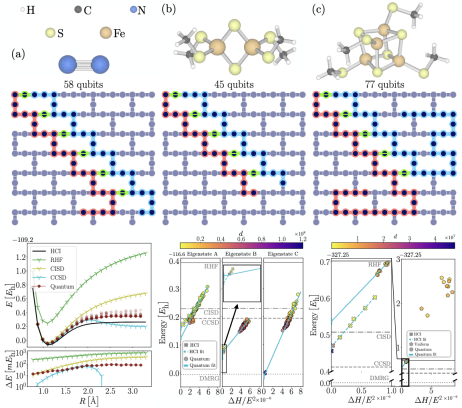


SQD use cases by IBM research team. Reference: [3]

Use case I: IBM quantum-centric supercomputing architecture

[2 Fe−2 S] Cluster Simulation

Metric	Details
Qubits Used	**45 total qubits** used, with **40** for the Jordan-Wigner (JW) encoding.
Quantum Gates	**1,100 CNOT gates**. **2,070 total gates**. Circuit depth $d = 173$. Circuit sizes reached approximately **1–1.5K two-qubit gates**.
HPC Usage (Classical)	Quantum runtime was approximately **45 minutes**. Classical diagonalization used the **PySCF** library on a single node. Vertical scaling analysis showed the optimal configuration for this system required **30+ CPUs per node** for the eigenstate solver.



SQD use cases by IBM research team. Reference: [3]

Current projects and future work

Several ongoing projects and future directions aim to further explore and enhance the application of quantum computing in astrophysical simulations:

- optimize computing atomic transition rates and level populations using quantum algorithms to improve the accuracy and efficiency of spectral modeling codes like SPEX.
- Explore leveraging hybrid quantum-classical algorithms to speed up the computation of radiative transfer simulations in astrophysical contexts.
- Investigate the potential of quantum computing to run accurate simulations and provide accurate atomic data for high-resolution X-ray spectra analysis.

References/extra reading

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