Quantum Imaginary Time Evolution

Winter school: QC-4C – Quantum Computers for Chemistry

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Chalmers University of Technology

Helsinki, October 31, 2023

My Background and Learning Goals

PostDoc at Chalmers University (Oct.2021)
Development of **quantum algorithms** to enable accurate and efficient **quantum chemistry** calculations on current and near-term quantum computers

CHALMERS
UNIVERSITY OF TECHNOLOGY

Gothenburg

MARIE CURIE ACTIONS

WACQT Wallenberg Centre for Quantum Technology

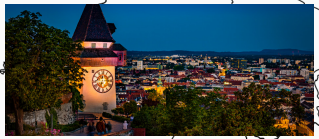
140M EUR Research effort for Sweden's Quantum Computing Stack
≈30 PIs, 20 PostDocs and 40 PhDs

IBM Academic Network

NordIQuEst:
HPC-QC ecosystem in the Nordics + Estonia

MAX PLANCK INSTITUTE
FOR SOLID STATE RESEARCH

Stuttgart



Graz

TU Graz

St. Lorenzen im Paltental

PhD in **theoretical quantum chemistry** at MPI Stuttgart and University of Stuttgart
Method Development for Quantum Chemistry.
Development of Quantum Monte Carlo methods for strongly correlated electron systems

BSc/MSc Studies in **physics** at TU Graz
Specialization: **Computational/Solid State Physics**.

Take-home messages

- How can quantum computing help quantum chemistry?
- What are some problems of the state-of-the-art VQE algorithm?
- What is the quantum imaginary time evolution (QITE) algorithm?
- What are the benefits and drawbacks of QITE?

Outline

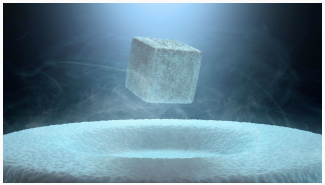
- Motivation – Quantum Chemistry
- “Conventional” Imaginary Time Evolution
- Quantum Imaginary Time Evolution
- Recap: Quantum Imaginary Time Evolution
- Applications
- Conclusions

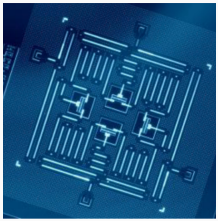
Motivation – Quantum Chemistry

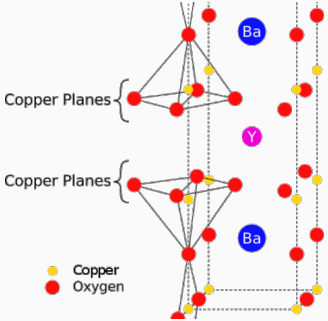
Surprisingly small systems at the center of fascinating physical and chemical effects

High-temperature superconductivity

Zero electrical resistivity





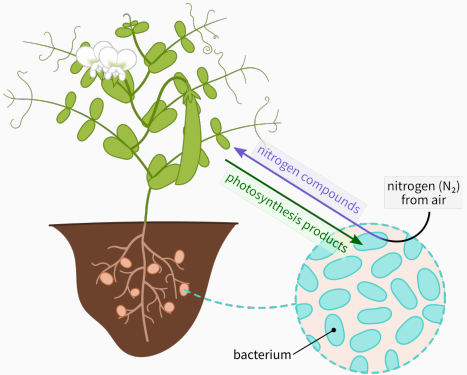


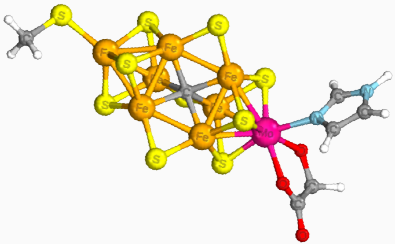
YBCO

shutterstock; CERN; Tokamak; Wikimedia

Nitrogen fixation

Haber-Bosch process: 1-2% global energy consumption, huge CO_2 emission



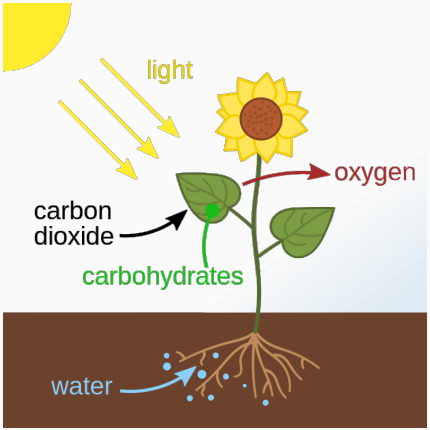


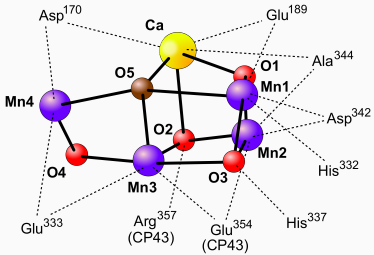
Iron-sulfur clusters

$\Rightarrow$ Cheaper and cleaner ammonia production for fertilizers

Wikimedia

Photosynthesis



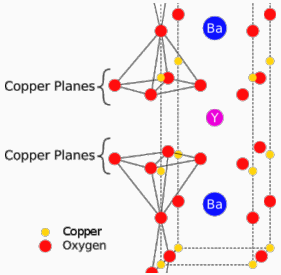


Manganese-Cadmium-Oxygen Clusters

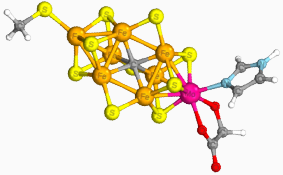
Artificial photosynthesis: Carbon capture and hydrogen and oxygen for fuel cell

Wikimedia; Wikimedia

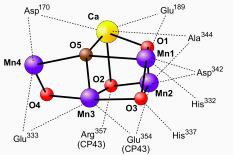
Ab Initio Quantum Chemistry – Electronic Structure Theory



YBCO: Unconventional high-T_c superconductivity



FeMoCo: primary cofactor of nitrogenase



Manganese-Cadmium-Oxygen Clusters: Oxygen evolving clusters

Surprisingly small systems responsible for interesting physical/chemical properties!

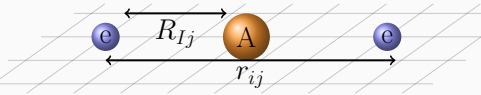
Strongly correlated ⇒ challenging systems for computational approaches!

Accurate theoretical understanding at nano-scale for bottom-up materials design!

Ab Initio Quantum Chemistry – Electronic Structure Theory

All necessary information of a quantum system contained in electronic **molecular Hamiltonian** (Born-Oppenheimer approx., atomic units and first quantization)

$$\hat{H} = \underbrace{-\sum_i \nabla^2_{\mathbf{r}_i}}_{\text{kinetic energy of e}^-} \underbrace{-\sum_{I,j} \frac{Z_I}{|\mathbf{R}_I - \mathbf{r}_j|}}_{\text{Attr. potential}} + \underbrace{\frac{1}{2}\sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}}_{\text{e}^- - \text{e}^- \text{ repulsion}}$$



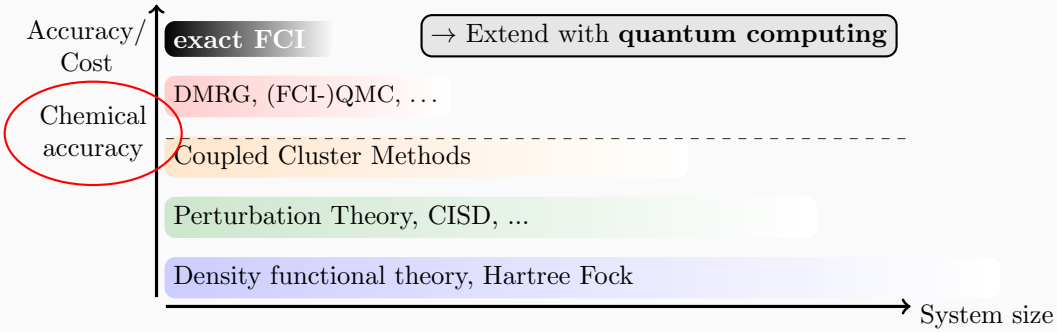
Electronic properties: Ground- and low-lying excited state properties, energy differences, polarization, response functions, ...

Task: Solve the Schrödinger equation derived from first principles

$$\hat{H}\,|\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_n)\rangle = E\,|\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_n)\rangle$$

Target: High / chemical accuracy to ensure predictability, interpretability and comparison with experimental results.

Hierarchy of methods

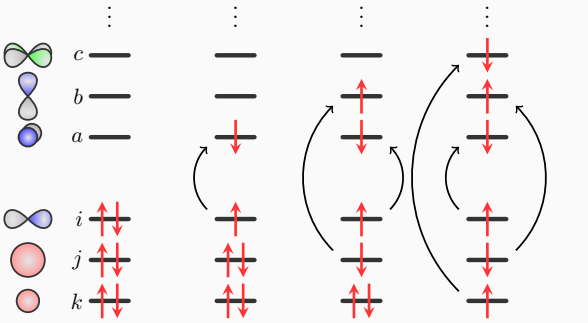


Highly accurate methods only applicable to **very small** system sizes

Exponential scaling of Full Configuration Interaction

FCI $\Rightarrow$ exact solution in a given basis: linear combination of determinants

$$|\Psi\rangle = |\Phi_{HF}\rangle + \sum_i c_i |\Phi_i\rangle$$

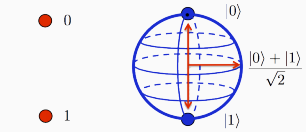


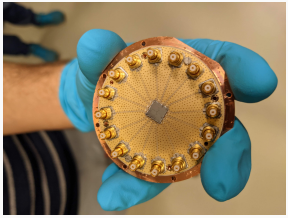
All possible excitations from HF determinant

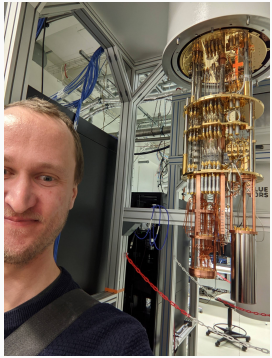
Number of possible states for given number of electrons, N, and orbitals, n, $\sim \binom{N}{n}$

Mol.	#orbitals	#electrons	#states
H_2	2	2	4
LiH	4	4	36
Be_2	8	8	4900
H_2O	12	12	$\sim 8 \cdot 10^5$
C_2H_4	16	16	$\sim 16 \cdot 10^6$
F_2	18	18	$\sim 2 \cdot 10^9$

The case for quantum computing







@ Chalmers

n qubits can encode $\sim 2^n$ states. Quantum algorithms use **entanglement, superposition** and **interference** to find solution

$$\overbrace{(|0\rangle_1 + |1\rangle_1)}^{\text{qubit1}} \otimes \overbrace{(|0\rangle_2 + |1\rangle_2)}^{\text{qubit2}} = |00\rangle + |01\rangle + |10\rangle + |11\rangle$$

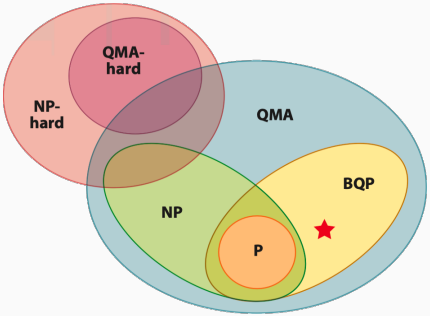
$$|q_1\rangle \otimes |q_2\rangle \otimes |q_3\rangle = \\ = |000\rangle + |001\rangle + |010\rangle + |100\rangle \\ + |011\rangle + |101\rangle + |110\rangle + |111\rangle$$

Benioff, J. Stat. Phys. **22** (5), 563 (1980); Feynman, Int. J. Theo. Phys. **21** (6/7), 467 (1982); Preskill, Quantum **2**, 79 (2018);

The case for quantum computing

Quantum chemistry potential use-case / killer-application of noisy intermediate-scale quantum (NISQ) devices and "quantum advantage" for relevant systems

- Efficient encoding of exponentially scaling wavefunction
- Effective measurement of Hamiltonian expectation values
- A system with > 60 qubits cannot be simulated with a classical computer
- A moderately-sized quantum processor (≈ 100 qubits) could outperform supercomputers for accurate solutions
- But how do we representand solve the problem on quantum hardware? **Ansätze** and **algorithms**



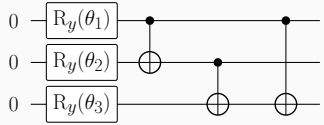
Kassal *et al.*, Annu. Rev. Phys. Chem. 2011. 62:185 (2010)

Ansatz for the quantum chemistry wavefunction:s $|\Psi(\boldsymbol{\theta})\rangle = \hat{U}(\boldsymbol{\theta})\,|\mathbf{0}\rangle$

Hardware efficient Ansätze:

- Gates directly tailored for the specific quantum device
- Spans a very large portion of the Fock space (inefficient)
- Large number of parameters, hard to optimize, "barren plateaus"

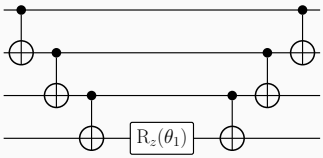
$$|\Psi(\boldsymbol{\theta})\rangle = \prod_{i}^{d} \left[\hat{U}_{ent}\hat{U}_{\mathrm{rot}}(\{\boldsymbol{\theta}_i\})\right] |\psi_{\mathrm{init}}\rangle$$



Chemically/Physically motivated:

- Chemistry-inspired exponential Ansatz: *Unitary coupled cluster Ansatz*
- Encode excitations of electrons between different orbitals, $|1100\rangle \rightarrow |0011\rangle$
- Not hardware efficient, deep circuits
- Less parameters, easier to optimize

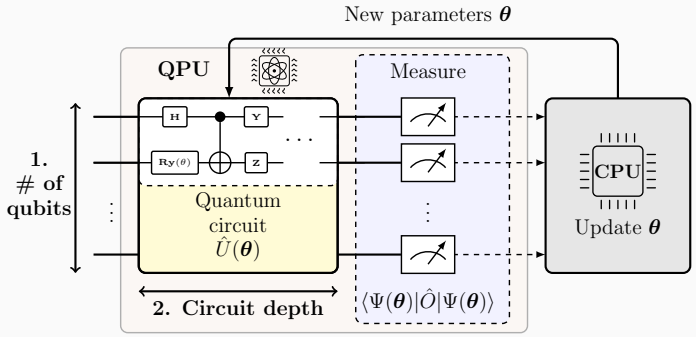
$$|\Psi(\boldsymbol{\theta})\rangle = \mathrm{e}^{\hat{T}(\boldsymbol{\theta}) - \hat{T}^{\dagger}(\boldsymbol{\theta})}\,|\psi_{HF}\rangle$$



Quantum Chemistry on Quantum Computers

Current quantum hardware has many problems still: **noise, decoherence and limited number of qubits** – noisy intermediate-scale quantum (NISQ) era

Hybrid quantum-classical approach:



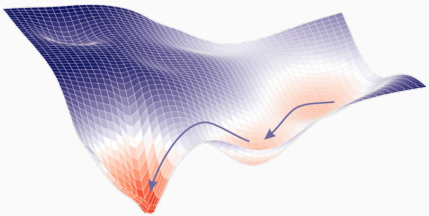
1. Prepare state with Ansatz $|\Psi(\boldsymbol{\theta})\rangle = \hat{U}(\boldsymbol{\theta})\,|\mathbf{0}\rangle$
2. Measure observable $\langle\Psi(\boldsymbol{\theta})|\,\hat{O}\,|\Psi(\boldsymbol{\theta})\rangle$ on QPU
3. Update parameters $\boldsymbol{\theta}$ on CPU and iterate until convergence

Use pros of both classical and quantum hardware

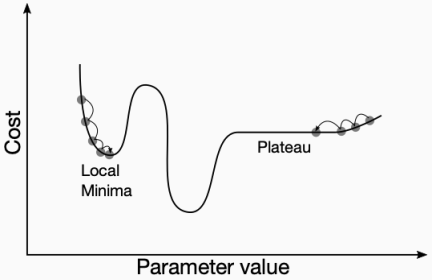
QPE: Kitaev, arXiv:quant-ph/9511026 (1995), Nielsen and Chuang, *Quantum computation and quantum information* (2001); **VQE:** Peruzzo *et al.*, Nature Comm., **5**, 4213, (2014), McClean, *et al.*, New J. Phys. **18**, 023023 (2016);

Variational Quantum Eigensolver – VQE

Main hybrid quantum-classical approach, many advantages (see other talks).



Parameter landscape

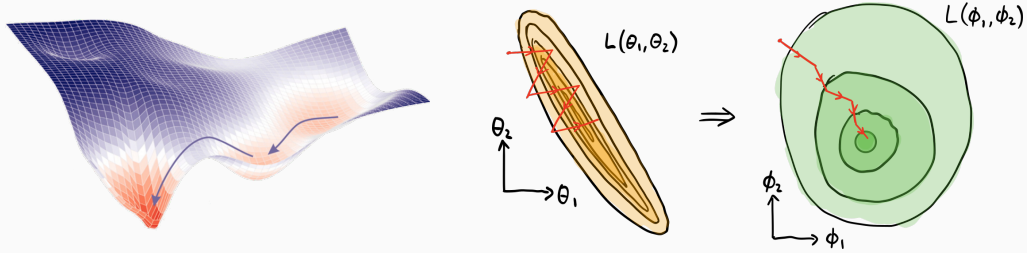


Problems, e.g. difficult classical optimizations of parameters $\boldsymbol{\theta}$ (**local minima, barren plateaus**) and relies on variational principle: $E_0 \leq \min_{\boldsymbol{\theta}} E(\boldsymbol{\theta}) = \langle \Psi(\boldsymbol{\theta}) | \hat{H} | \Psi(\boldsymbol{\theta}) \rangle$
$\rightarrow$ not applicable to open quantum system and transport problems (non-Hermitian Hamiltonians)

McClean *et al.*, Nature Communications **9**, 4812 (2018); winder.ai; primo.ai

Motivation – Imaginary Time Evolution

What if we can take the geometry/curvature of parameter space into account?



Quantum Imaginary time evolution: 2^{nd}-order method (gradient + Hessian)
$\rightarrow$ smoother convergence and guaranteed monotonic decrease in energy, see (6)

– Related to (quantum) **natural gradient***

primo.ai; pennylane.ai; *Stokes *et al.*, Quantum 4, 269 (2020);

“Conventional” Imaginary Time Evolution

Real Time Evolution

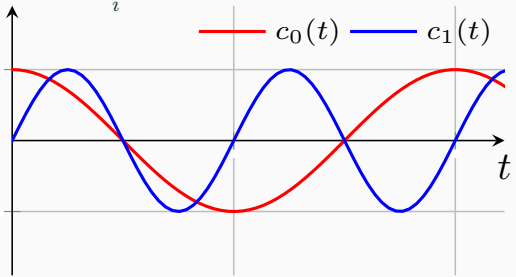
Schrödinger equation: unitary (real) time evolution, reversible and norm conserving

$$\frac{\partial\,|\Psi(t)\rangle}{\partial t} = -i\hat{H}\,|\Psi(t)\rangle \rightarrow \quad |\Psi(t)\rangle = \mathrm{e}^{-i\hat{H}t}\,|\Psi(t=0)\rangle\,, \quad \text{with} \quad \hat{U} = \mathrm{e}^{-i\hat{H}t}, \quad \hat{U}^{\dagger}\hat{U} = 1$$

Expansion of $|\Psi(t)\rangle$ in eigenfunctions of $\hat{H}\,|\Phi_i\rangle = E_i\,|\Phi_i\rangle$:

$$|\Psi(t)\rangle = \sum_i c_i(t)\,|\Phi_i\rangle \quad \rightarrow \quad |\Psi(t)\rangle = \sum_i \mathrm{e}^{-iE_it}\,c_i(0)\,|\Phi_i\rangle$$

Oscillating coefficients $c_i(t) = \mathrm{e}^{-iE_it}\,c_i(0)$
with frequency determined by energy E_i



Imaginary Time

. . . the words ***real*** *and* ***imaginary*** *are picturesque relics of an age when the nature of* ***complex numbers*** *was not properly understood.*

- H.S.M. Coxeter

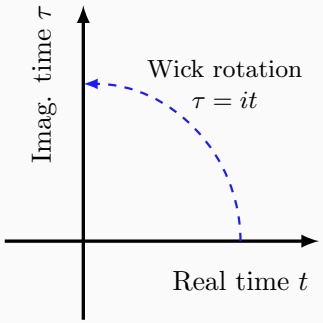
Stephen Hawking – YouTube

Minkowski space-time (special relativity)

$$d^2 = x^2 + y^2 + z^2 + (it)^2$$

Schrödinger equation:

$$\frac{\partial \left|\Psi(t)\right\rangle}{\partial t} = -i\hat{H}\left|\Psi(t)\right\rangle$$



“Classical” Imaginary Time Evolution (ITE)

Use “imaginary” time, $\tau = it$, to transform Schrödinger equation:

$$\frac{\partial \left|\Psi(t)\right\rangle}{\partial t} = -i\hat{H}\left|\Psi(t)\right\rangle \quad \overset{\tau=it}{\Rightarrow} \quad \frac{\partial \left|\Psi(\tau)\right\rangle}{\partial \tau} = -\hat{H}\left|\Psi(\tau)\right\rangle,$$

which has the solution:

$$\left|\Psi(\tau)\right\rangle = N(\tau)\,\mathrm{e}^{-\hat{H}\tau}\left|\Psi(\tau=0)\right\rangle, \quad \text{with} \quad N(\tau) = \sqrt{\frac{1}{\langle\Psi(0)|\mathrm{e}^{-2\hat{H}\tau}|\Psi(0)\rangle}}$$

with a **non-unitary** operator $\mathrm{e}^{-\hat{H}\tau}$. Imaginary time evolution enables to obtain the ground state, $|\Psi_0\rangle$, of $\hat{H}$ in the long-time limit*, if the overlap $\langle\Psi(0)\,|\,\Psi_0\rangle \neq 0$

$$\lim_{\tau\to\infty}\left|\Psi(\tau)\right\rangle = N(\tau)\,\mathrm{e}^{-\hat{H}\tau}\left|\Psi(0)\right\rangle \to \left|\Psi_0\right\rangle$$

* for $\tau > 1/\Delta$, with $\Delta = E_1 - E_0$ being the many-body spectral gap, Beach *et al.*, Phys. Rev. B 100, 094434 (2019)

Imaginary Time Evolution (ITE) – Details

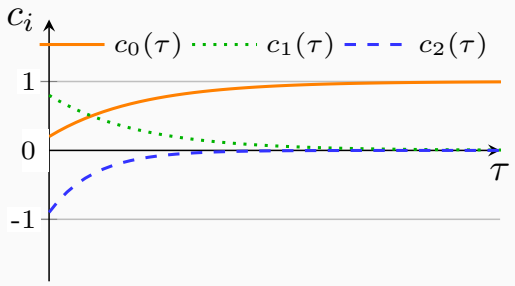
With $|\Psi(0)\rangle$ expanded in eigenfunctions of $\hat{H}$: $\hat{H}\,|\Phi_i\rangle = E_i\,|\Phi_i\rangle$, with $E_0 < E_i, \forall i$ and introducing an adaptive diagonal energy shift, $\hat{H} \to \hat{H} - \mathbb{1}S_\tau$:

$$|\Psi(0)\rangle = \sum_i c_i(0)\,|\Phi_i\rangle \quad \to \quad |\Psi(\tau)\rangle = \mathrm{e}^{-\tau(\hat{H}-S_\tau)} \sum_i c_i(0)\,|\Phi_i\rangle = \sum_i c_i(0)\,\mathrm{e}^{-\tau(E_i-S_\tau)}\,|\Phi_i\rangle$$

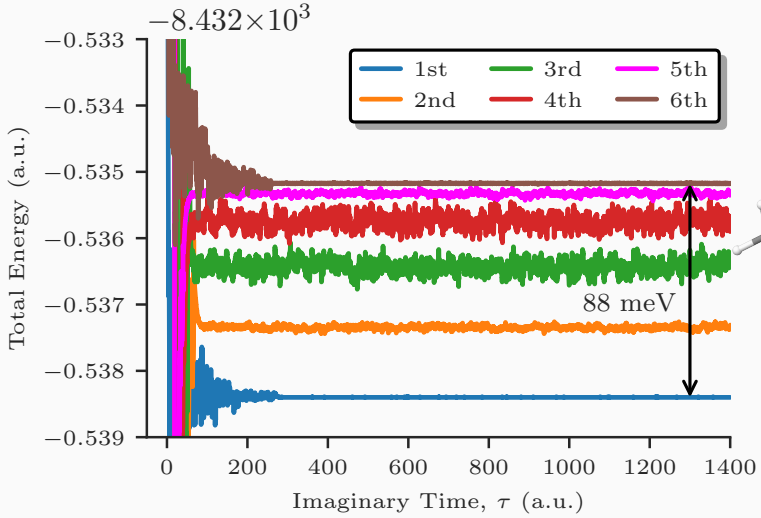
$c_i(\tau) = c_i(0)\,\mathrm{e}^{-\tau(E_i-S_\tau)}$:

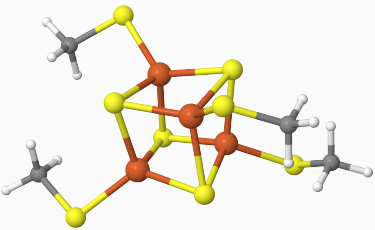
- $E_i - S_\tau > 0 \to c_i$ decays exponentially
- $E_i - S_\tau < 0 \to c_i$ increases exponentially
- $E_i - S_\tau = 0 \to c_i$ stays constant

Normalization, $\langle\Psi(\tau)|\Psi(\tau)\rangle = 1$, ensures convergence to groundstate. For free on quantum computer, due to unitary evolution, see (4).



Imaginary Time Evolution – Quantum Monte Carlo Example





6 Singlet states of Fe_4S_4 system

Li Manni, **WD**, Bogdanov, Guther, Alavi, JPC A, 125, 22, 4724 (2021); https://github.com/ghb24/NECI_STABLE; Guther *et al.*, J. Chem. Phys. 153, 034107 (2020)

Quantum Imaginary Time Evolution

Quantum Imaginary Time Evolution – Flavour 1

nature physics

ARTICLES

https://doi.org/10.1038/s41567-019-0704-4

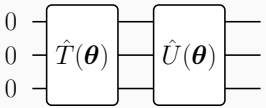
Determining eigenstates and thermal states on a quantum computer using quantum imaginary time evolution

Mario Motta[1*], Chong Sun[1], Adrian T. K. Tan[2], Matthew J. O'Rourke[1], Erika Ye[2], Austin J. Minnich[2], Fernando G. S. L. Brandão[3] and Garnet Kin-Lic Chan[1*]

*Motta *et al.*, Nature Physics, 16, 205 (2020)

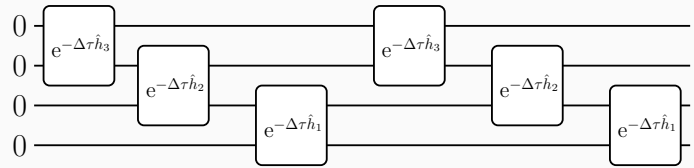
Trotterization

Hamiltonian $\hat{H} = \sum_i \hat{h}_i$. How could we represent $\exp(-\tau \sum_i \hat{h}_i)$, , where each term acts on at most k qubits, on a quantum computer? Product of operators, $\hat{U}\hat{T}\,|\mathbf{0}\rangle$:



Trotter decomposition (Trotterization): if $\left[\hat{h}_i, \hat{h}_j\right] \neq 0$:

$$\mathrm{e}^{-\tau \hat{H}} = \mathrm{e}^{\sum_i \hat{h}_i} = \left(\mathrm{e}^{-\Delta\tau \hat{h}_i}\, \mathrm{e}^{-\Delta\tau \hat{h}_2} \dots\right)^n + \mathcal{O}(\Delta\tau); \quad n = \frac{\tau}{\Delta\tau}$$

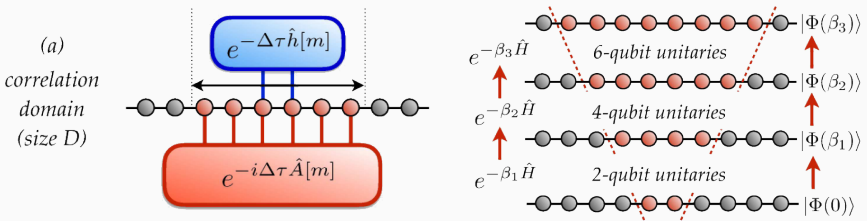


*Motta *et al.*, Nature Physics, 16, 205 (2020); Cao *et al.*, Nature Comm. Physics, 5, 57 (2022); Gomes *et al.*, JCTC, 16, 10, 6256 (2020); Yeter-Aydeniz *et al.*, PRA, 105, 012412 (2022); †A. Uhlmann, Rep. Math. Phys. 9, 273 (1976)

Quantum Imaginary Time Evolution (QITE) – Flavour 1

BUT $e^{-\Delta\tau\hat{h}_i}$ is **not** unitary! Operations on a quantum computer **must be** unitary! After a single Trotter step: $|\Psi'\rangle = e^{-\Delta\tau\hat{h}_i}|\Psi\rangle$.

Idea is to approximate the action of the **non-unitary** $e^{-\Delta\tau h_i}$ by action of **unitary** operator $e^{-i\Delta\tau A_i}$ acting on a neighborhood of the qubits acted on by $\hat{h}_i \Rightarrow$ minimize: $||\Psi' - (1 - i\Delta\tau A_i)\Psi||^2$ (Uhlmanns theorem†)



No Ansatz needed, but exponentially scaling in the number *entangled* qubits

*Motta *et al.*, Nature Physics, 16, 205 (2020); Cao *et al.*, Nature Comm. Physics, 5, 57 (2022); †A. Uhlmann, Rep. Math. Phys. 9, 273 (1976)

Variational Ansatz-based QITE – Flavour 2

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ARTICLE OPEN

Variational ansatz-based quantum simulation of imaginary time evolution

Sam McArdle[1], Tyson Jones[1], Suguru Endo[1], Ying Li[2], Simon C. Benjamin[1] and Xiao Yuan[1]

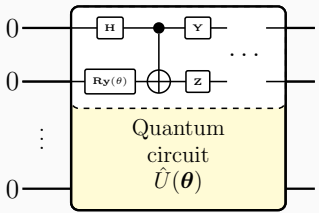
Variational Ansatz-based QITE – VarQITE

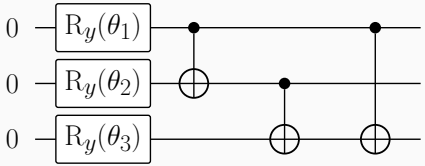
(Normalized) imaginary-time Schrödinger equation:

$$\frac{\partial\,|\Psi(\tau)\rangle}{\partial\tau} = -(\hat{H} - S_\tau)\,|\Psi(\tau)\rangle \quad \rightarrow \quad |\Psi(\tau)\rangle = \mathrm{e}^{-\tau(\hat{H}-S_\tau)}\,|\Psi(0)\rangle$$

would yield the ground state, but **non-unitary** $\mathrm{e}^{-\tau(\hat{H}-S_\tau)}$ not possible on a quantum computer! Approximate $|\Psi(\tau)\rangle$ with an Ansatz with parametrized unitary gates:

$$|\Psi(\tau)\rangle \approx |\Phi(\boldsymbol{\theta}(\tau))\rangle\,, \quad \text{with} \quad |\Phi(\boldsymbol{\theta}(\tau))\rangle = \hat{U}_n(\theta_n(\tau)) \cdots \hat{U}_1(\theta_1(\tau))\,|\mathbf{0}\rangle = \hat{U}(\boldsymbol{\theta}(\tau))\,|\mathbf{0}\rangle$$





State preparation $|\Psi(\boldsymbol{\theta})\rangle = \hat{U}(\boldsymbol{\theta})\,|\mathbf{0}\rangle$

McArdle *et al.*, npj Quantum, 5, 75 (2019); Yuan *et al.* Quantum 3, 191 (2019); Beach *et al.* PRB 100, 094434 (2019); Zoufal *et al.*, arXiv:2108.00022 (2021); McArdle *et al.* arXiv:2006.11181 (2019); Sokolov, **WD**, Luo, Alavi, Tavernelli, arXiv:2201.03049 (2022)

VarQITE

Three ingredients:

1. Evolution of $|\Phi(\boldsymbol{\theta}(\tau))\rangle$ according to imaginary time Schrödinger equation, $|\Psi(\tau)\rangle = \mathrm{e}^{-\tau(\hat{H}-S_\tau)}\,|\Psi(0)\rangle$ for small $\delta\tau$: $\mathrm{e}^{-\delta\tau(\hat{H}-S_\tau)} \approx (1-\delta\tau(\hat{H}-S_\tau))$

$$|\Phi(\boldsymbol{\theta}(\tau+\delta\tau))\rangle \approx \Big[1-\delta\tau(\hat{H}-S_\tau)\Big]\,|\Phi(\boldsymbol{\theta}(\tau))\rangle \tag{1}$$

2. Variation of $|\Phi(\boldsymbol{\theta}(\tau))\rangle$ w.r.t. to parameters $\partial\theta$:

$$|\Phi(\boldsymbol{\theta}(\tau+\delta\tau))\rangle \approx |\Phi(\boldsymbol{\theta}(\tau))\rangle + \sum_j \frac{\partial\,|\Phi(\boldsymbol{\theta}(\tau))\rangle}{\partial\theta_j}\frac{\partial\theta_j}{\partial\tau}\delta\tau \tag{2}$$

Equate r.h.s. of Eqs. (1) and (2) $\Rightarrow$

McLachlan's variational principle

$$\implies \sum_j \frac{\partial \left|\Phi(\boldsymbol{\theta}(\tau))\right\rangle}{\partial \theta_j}\dot{\theta}_j \approx -(\hat{H} - S_\tau)\left|\Phi(\boldsymbol{\theta}(\tau))\right\rangle, \quad \text{with} \quad \dot{\theta}_j = \frac{\partial \theta_j}{\partial \tau} \tag{3}$$

3. McLachlan's variational principle to minimize the distance between l.h.s and r.h.s. of (3)

$$\delta \left|\left|\left(\frac{\partial}{\partial \tau} + \hat{H} - S_\tau\right)\left|\Phi(\boldsymbol{\theta}(\tau))\right\rangle\right|\right| = 0, \quad \text{with} \quad \left|\left|\left|\Phi\right\rangle\right|\right| = \sqrt{\langle\Phi\,|\,\Phi\rangle}.$$

After some calculations, see Appendix (5), we find a formula to update the parameters $\boldsymbol{\theta}$ to emulate imaginary time evolution on quantum computers

McLachlan, Molecular Physics, 8(1),39 (1964)

Connection to natural gradient

Equation for change in parameters $\boldsymbol{\theta}$ due to McLachlan's variational principle to enable Ansatz-based quantum imaginary time evolution:

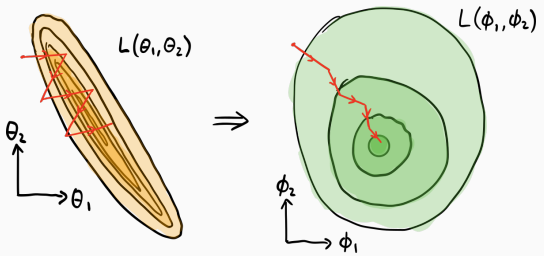
$$\sum_j A_{ij}\dot{\theta}_j = C_i, \quad \Longrightarrow \dot{\boldsymbol{\theta}} = \mathbf{A}^{-1}\boldsymbol{C}$$

with the metric:

$$A_{ij} = \frac{\partial \langle\Phi|}{\partial\theta_i}\frac{\partial |\Phi\rangle}{\partial\theta_j}$$

and energy gradient:

$$C_i = -\frac{\partial \langle\Phi|}{\partial\theta_i}\hat{H}|\Phi\rangle$$



*Motta *et al.*, Nature Physics, 16, 205 (2020); pennylane.ai

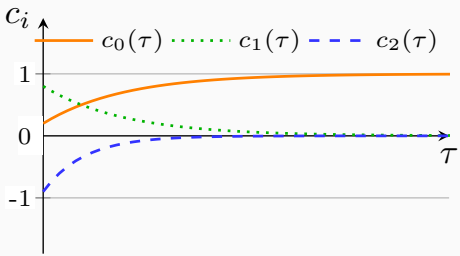
Recap: Quantum Imaginary Time Evolution

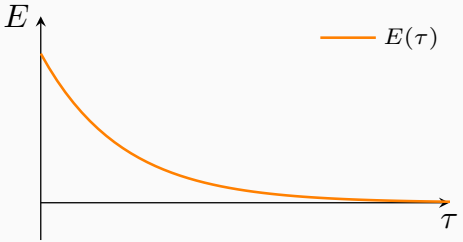
Quantum Imaginary Time Evolution – QITE

→ Solve for the **right** eigenvector of operator $\hat{H}$ by (quantum) imaginary-time evolution (QITE)

$$i\frac{\partial|\Psi\rangle}{\partial t} = \hat{H}|\Psi\rangle \quad \overset{\tau=it}{\rightarrow} \quad \frac{\partial|\Psi\rangle}{\partial\tau} = -\hat{H}|\Psi\rangle \quad \rightarrow \quad |\Psi(\tau)\rangle = N(\tau)\,\mathrm{e}^{-\hat{H}\tau}|\Psi(0)\rangle$$

$$|\Psi(0)\rangle = \sum_i c_i(0)|\psi_i\rangle \quad \rightarrow \quad |\Psi(\tau)\rangle = \mathrm{e}^{-\tau(\hat{H}-S_\tau)}\sum_i c_i(0)|\psi_i\rangle = \sum_i c_i(0)\,\mathrm{e}^{-\tau(E_i-S_\tau)}|\psi_i\rangle$$





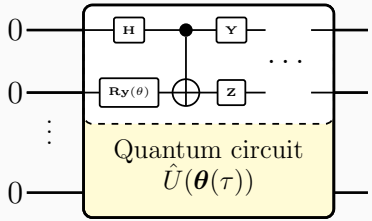
Motta *et al.*, Nature Physics **16**, 205, 2020; *McArdle, *et al.*, npj Quantum Information **5**, 75, 2019;

Ansatz-based QITE

$e^{-\hat{H}\tau}$ is **not** unitary! However, **Ansatz-based QITE**[*] allows to formulate non-unitary time evolution, as a minimization:

$$\frac{\partial\,|\Psi(\tau)\rangle}{\partial\tau} = -(\hat{H} - E(\tau))\,|\Psi(\tau)\rangle\,, \quad \text{with} \quad E(\tau) = \langle\Psi(\tau)|\hat{H}|\Psi(\tau)\rangle,$$

1) Use an Ansatz for the target wavefunction $|\Psi(\tau)\rangle \approx |\Phi(\boldsymbol{\theta}(\tau))\rangle$



[*]McArdle, *et al.*, npj Quantum Information **5**, 75, 2019; Motta *et al.*, Nature Physics **16**, 205, 2020; Sokolov, **WD**, Luo, Alavi, Tavernelli, arXiv:2201.03049; Zoufal *et al.*, arXiv:2108.00022 (2021);

Ansatz-based QITE

2) Use McLachlan's variational principle with Ansatz: $|\Psi(\tau)\rangle \approx |\Phi(\boldsymbol{\theta}(\tau))\rangle$

$$\delta || \frac{\partial}{\partial \tau} + \hat{H} - E(\tau) \, |\Phi(\boldsymbol{\theta}(\tau))\rangle \, || \stackrel{!}{=} 0$$

to obtain equation for change in parameters $\dot{\boldsymbol{\theta}}$:

$$\sum_j A_{ij} \dot{\theta}_j = C_i, \quad \Longrightarrow \dot{\boldsymbol{\theta}} = \mathbf{A}^{-1} \boldsymbol{C}$$

with the **metric A** and **gradient C**:

$$A_{ij} = \frac{\partial \, \langle \Phi(\tau)|}{\partial \theta_i} \frac{\partial \, |\Phi(\tau)\rangle}{\partial \theta_j} \quad \text{and} \quad C_i = -\frac{\partial \, \langle \Phi(\tau)|}{\partial \theta_i} \hat{H} \, |\Phi(\tau)\rangle$$

*McArdle, *et al.*, npj Quantum Information **5**, 75, 2019; Motta *et al.*, Nature Physics **16**, 205, 2020; Sokolov, **WD**, Luo, Alavi, Tavernelli, arXiv:2201.03049; Zoufal *et al.*, arXiv:2108.00022 (2021);

Update in parameters

- No need for optimization $\rightarrow$ solution to linear system of equations
- Change in parameters with e.g. Euler method with timestep $\Delta\tau$

$$\boldsymbol{\theta}(\tau + \Delta\tau) \approx \boldsymbol{\theta}(\tau) + \dot{\boldsymbol{\theta}}\Delta\tau = \boldsymbol{\theta}(\tau) + \mathbf{A}^{-1}\boldsymbol{C}\Delta\tau$$

- Repeating this $N_\tau = \frac{\tau_{tot}}{\Delta\tau}$ times, allows to simulate imaginary time evolution for a total time τ_{tot}.
- To perform VarQITE $\mathbf{A}$ and $\mathbf{C}$ must be measured on a quantum computer $\rightarrow$ need to measure derivatives w.r.t. θ_i

Evaluation A and C with Quantum Circuits

How do we measure the metric, $\mathbf{A}$, and the gradient, $\mathbf{C}$ on quantum hardware.

$$A_{ij} = \frac{\partial \langle \Phi |}{\partial \theta_i} \frac{\partial |\Phi\rangle}{\partial \theta_j}, \qquad C_i = -\frac{\partial \langle \Phi |}{\partial \theta_i} \hat{H} |\Phi\rangle$$

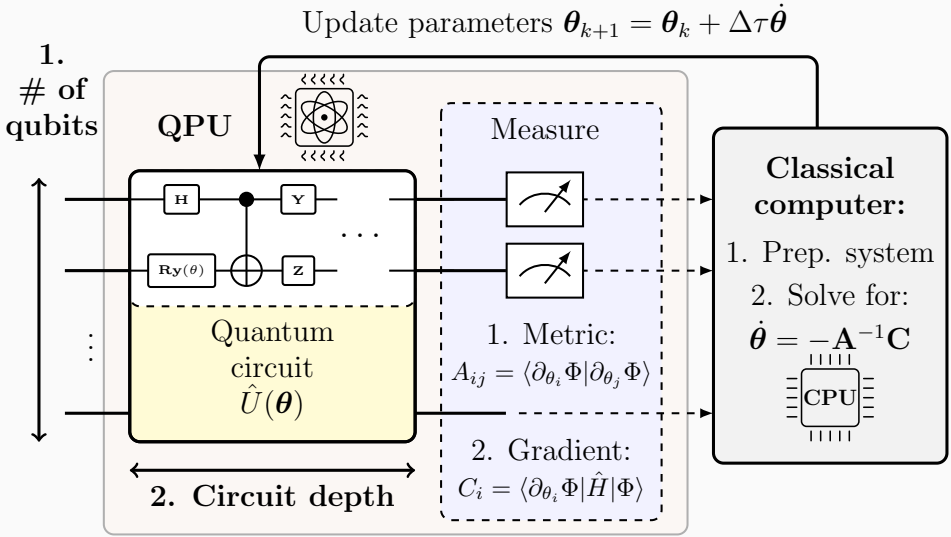
$|\Phi(\boldsymbol{\theta}(\tau))\rangle$ encoded by unitary gates acting on initial state: Ansatz $\hat{U}(\boldsymbol{\theta}(\tau))$

$$|\Phi(\boldsymbol{\theta}(\tau))\rangle = \hat{U}_n(\theta_n(\tau)) \cdots \hat{U}_i(\theta_i(\tau)) \cdots \hat{U}_1(\theta_1(\tau)) |\mathbf{0}\rangle = \hat{U}(\boldsymbol{\theta}(\tau)) |\mathbf{0}\rangle$$

- Numerical differentiation/approximation: $\frac{\partial \hat{U}_i(\theta_i)}{\partial \theta_i} \approx \frac{\hat{U}_i(\theta_i + \Delta\theta_i) - \hat{U}_i(\theta_i)}{\Delta \theta_i}$
- Parameter-shift rule* (for single qubit gates):
  $R_z(\theta_i) = \mathrm{e}^{-i\theta_i \sigma_z} \rightarrow \frac{\partial U_i(\theta_i)}{\partial \theta_i} = -i\sigma_z R_Z(\theta_i)$
- Linear combination of unitaries* (for general gates), see (7)ff for details
- Automatic differentiation (talk by Davide Castaldo yesterday)

*Schuld *et al.*, Phys. Rev. A 99, 032331 (2019); Romero *et al.*, Quantum Science and Technology, 4, 1 (2019)l; Li and Benjamin, Phys. Rev. X 7, 021050 (2017);

QITE Workflow



VarQITE – Pros and Cons

Pros:

- No classical optimization
- Convergence robust against noise
- Energy measurement only at end*
- Applicable to open/transport problems (non Hermitian)

Cons:

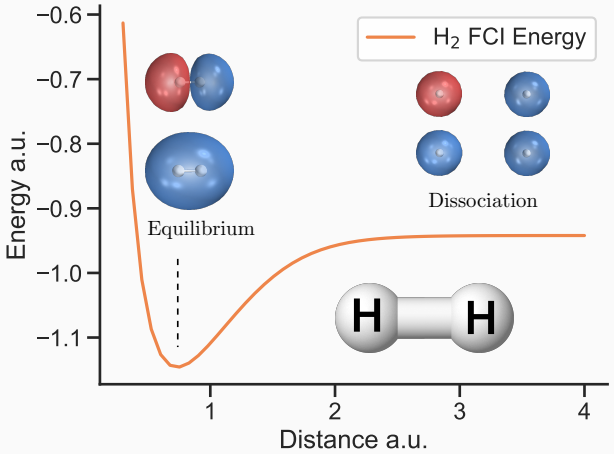
- 2^{nd} order method – costly $\rightarrow$ metric $\mathbf{A}$ needs to be measured – n^2 scaling with n parameters
- $\mathbf{A}$ can be singular $\rightarrow$ inversion $\mathbf{A}^{-1}$ can problematic†

*Norm of $\mathbf{A}$ and $\mathbf{C}$ usable to detect convergence!

† Good approximations to $\mathbf{A}$ and $\mathbf{A}^{-1}$ exist!

Applications

Example: Hydrogen molecule – H_2 – minimal basis – PES



Groundstate wavefunction at dissociation: $|\Psi_0\rangle = \frac{1}{\sqrt{2}}(|1100\rangle - |0011\rangle)$

Groundstate wavefunction at equilibrium: $|\Psi_0\rangle \approx 0.995\,|1100\rangle - 0.105\,|0011\rangle$

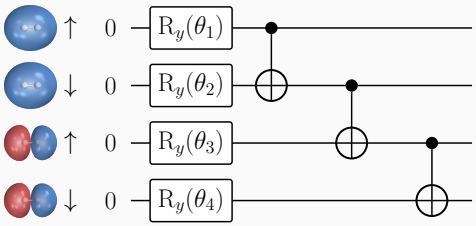
H_2 – Hardware efficient Ansatz

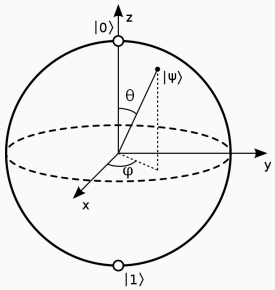
H_2 groundstate wavefunction at equilibrium:

$$|\Psi_0\rangle = 0.995\,|1100\rangle - 0.105\,|0011\rangle + 0\cdot|1001\rangle + 0\cdot|0110\rangle$$

Need a general "Ansatz", $\hat{U}(\boldsymbol{\theta})\,|\mathbf{0}\rangle$:

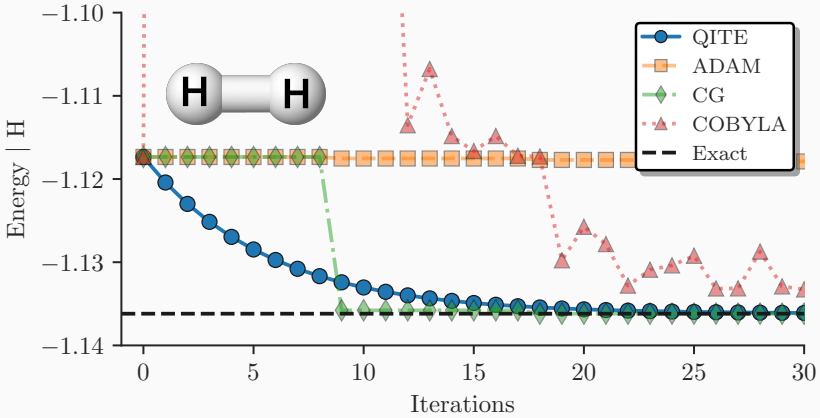
$$|\Psi(\boldsymbol{\theta})\rangle = \hat{U}(\boldsymbol{\theta})\,|0000\rangle \stackrel{!}{=} c_1\,|1100\rangle + c_2\,|0011\rangle + c_3\,|1001\rangle + c_4\,|0110\rangle$$





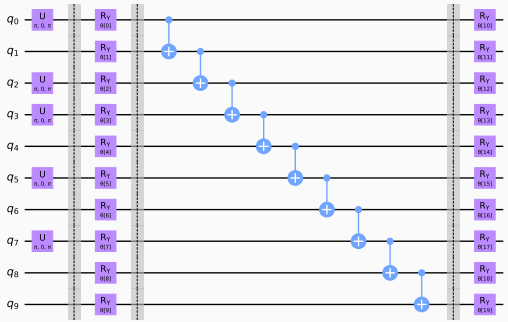
H_2 QITE/VQE Statevector simulation

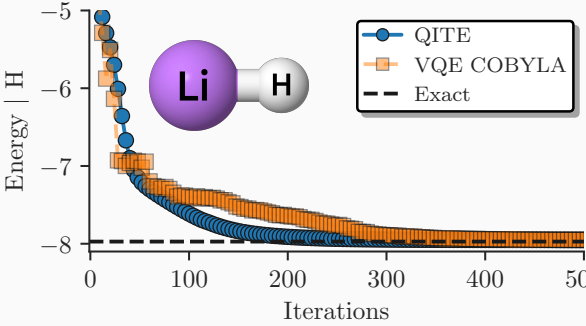
H_2 at 0.7 Å in a STO-6G basis using 4 qubits: Default `Qiskit` VQE settings.
QITE $\Delta\tau = 0.05$



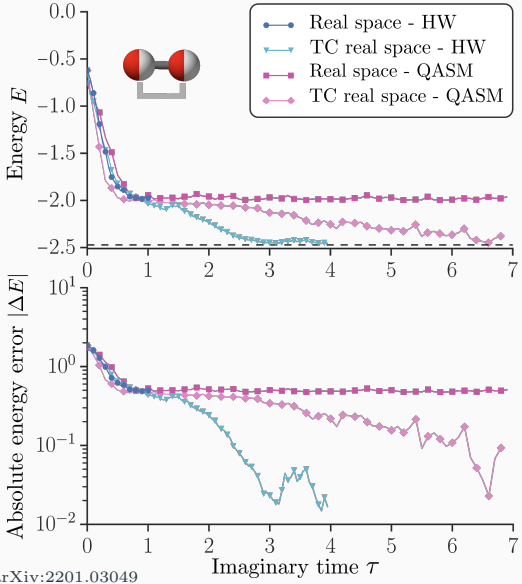
LiH Statevector

LiH – minimal basis – 1.6Å– parity mapping – HEA Ansatz





Actual experimental results for the Hubbard model on ibmq_lima



Sokolov, **WD**, Luo, Alavi, Tavernelli, arXiv:2201.03049

Conclusions

Conclusion

- VQE can have problems with **classical optimization** (barren plateaus, local minima)
- Imaginary time evolution yields groundstate of operator $\hat{H}$ even for non-Hermitian Hamiltonians
- Non-unitary dynamics not straightforward to implement on quantum computers
- Two versions in the quantum computing setting: Focus on Ansatz-based QITE
- (Imaginary) time evolution of Ansatz parameters $\dot{\boldsymbol{\theta}}$ obtained by solving linear system: $\dot{\boldsymbol{\theta}} = \mathbf{A}^{-1}\boldsymbol{C}$, following McLachlan's variational principle
- Metric $\mathbf{A}$ and gradient $\boldsymbol{C}$ obtained by measuring on a quantum device

Thank you for your attention!

Imaginary Time Evolution (ITE) – Normalization

$E_0 - S_\tau = 0$ would require knowledge of ground state. Alternative, and also to ensure proper normalization:
For small time-steps $\Delta\tau$ approximate exponential by first-order Taylor approximation* and obtain iterative solution:

$$\mathrm{e}^{-\Delta\tau(\hat{H}-S_\tau)} \approx 1 - \Delta\tau(\hat{H} - S_\tau) + \mathcal{O}(\Delta\tau^2) \quad \rightarrow \quad |\Psi(\tau+\Delta\tau)\rangle = \Big[1 - \Delta\tau(\hat{H} - S_\tau)\Big]\,|\Psi(\tau)\rangle \tag{4}$$

Assuming $\langle\Psi(\tau)\,|\,\Psi(\tau)\rangle = 1$:

$$\begin{aligned}\langle\Psi(\tau+\Delta\tau)\,|\,\Psi(\tau+\Delta\tau)\rangle &= \langle\Psi(\tau)|\Big[1 - \Delta\tau(\hat{H} - S_\tau)\Big]^2|\Psi(\tau)\rangle \stackrel{!}{=} 1 \\ &= \underbrace{\langle\Psi(\tau)\,|\,\Psi(\tau)\rangle}_{=1} - 2\Delta\tau \underbrace{\Big(\langle\Psi(\tau)|\hat{H}|\Psi(\tau)\rangle - S_\tau\Big)}_{\stackrel{!}{=}0} + \mathcal{O}(\Delta\tau^2)\end{aligned}$$

$\Longrightarrow S_\tau = \langle\Psi(\tau)|\hat{H}|\Psi(\tau)\rangle$ ensures normalization of $|\Psi(\tau)\rangle$ and allows ITE to converge to the groundstate

* for $\Delta\tau < 1/E_W$, with $E_W = E_{max} - E_0$ being the many-body spectral width, Trivedi and Ceperley, Phys. Rev. B, 41, 4552 (1990)

$$\langle\Phi|\Big(\partial/\partial\tau+\hat{H}-S_\tau\Big)^\dagger\Big(\partial/\partial\tau+\hat{H}-S_\tau\Big)|\Phi\rangle=\sum_{ij}\frac{\partial\langle\Phi|}{\partial\theta_i}\frac{\partial|\Phi\rangle}{\partial\theta_j}\dot{\theta}_i\dot{\theta}_j+\sum_i\frac{\partial\langle\Phi|}{\partial\theta_i}(\hat{H}-S_\tau)|\Phi\rangle\,\dot{\theta}_i$$

$$+\sum_i\langle\Phi|(\hat{H}-S_\tau)\frac{\partial|\Phi\rangle}{\partial\theta_i}\dot{\theta}_i+\langle\Phi|(\hat{H}-S_\tau)^2|\Phi\rangle \tag{5}$$

Variations in $\dot{\theta}_i \Longrightarrow$ and focusing on one term in $\dot{\theta}_i$:

$$\frac{\partial||(\partial/\partial\tau+\hat{H}-S_\tau)|\Phi\rangle||}{\partial\dot{\theta}_i}=\sum_j\left(\frac{\partial\langle\Phi|}{\partial\theta_i}\frac{\partial|\Phi\rangle}{\partial\theta_j}+\frac{\partial\langle\Phi|}{\partial\theta_j}\frac{\partial|\Phi\rangle}{\partial\theta_i}\right)\dot{\theta}_j$$

$$+\frac{\partial\langle\Phi|}{\partial\theta_i}\hat{H}|\Phi\rangle+\langle\Phi|\hat{H}\frac{\partial|\Phi\rangle}{\partial\theta_i}-S_\tau\left(\frac{\partial\langle\Phi|}{\partial\theta_i}|\Phi\rangle+\langle\Phi|\frac{\partial|\Phi\rangle}{\partial\theta_i}\right)$$

with

$$\langle\Phi\,|\,\Phi\rangle=1,\quad\rightarrow\quad\frac{\partial\langle\Phi\,|\,\Phi\rangle}{\partial\theta_i}=\frac{\partial\langle\Phi|}{\partial\theta_i}|\Phi\rangle+\langle\Phi|\frac{\partial|\Phi\rangle}{\partial\theta_i}=0$$

$$\Longrightarrow\frac{\partial||(\partial/\partial\tau+\hat{H}-S_\tau)|\Phi\rangle||}{\partial\dot{\theta}_i}=\sum_j A_{ij}\dot{\theta}_j-C_i\stackrel{!}{=}0$$

Monotonic energy convergence

$$\frac{dE(\tau)}{d\tau} = \langle\Phi(\tau)|\,\hat{H}\,\frac{d\,|\Phi(\tau)\rangle}{d\tau} = \sum_i \langle\Phi(\tau)|\,\hat{H}\,\frac{\partial\,|\Phi(\tau)\rangle}{\partial\theta_i}\dot{\theta}_i \tag{6}$$
$$= -\sum_i C_i\dot{\theta}_i = -\sum_i C_i A_{ij}^{-1} C_j \leq 0,$$

if $\mathbf{A}^{-1}$ is positive. For arbitrary $\mathbf{x} = (x_1, x_2, \ldots, x_N)^T$:

$$\mathbf{x}^\dagger \cdot \mathbf{A} \cdot \mathbf{x} = \sum_{ij} x_i^* A_{ij} x_j = \sum_{ij} x_i^* \left(\frac{\partial\,\langle\Phi(\tau)|}{\partial\theta_i}\frac{\partial\,|\Phi(\tau)\rangle}{\partial\theta_j} \right) x_j$$

with a general $|\zeta\rangle = \sum_i x_i \frac{\partial|\Phi(\tau)\rangle}{\partial\theta_i}$:

$$\sum_{ij} x_i^* \left(\frac{\partial\,\langle\Phi(\tau)|}{\partial\theta_i}\frac{\partial\,|\Phi(\tau)\rangle}{\partial\theta_j} \right) x_j = \langle\zeta|\zeta\rangle \geq 0.$$

And we only consider non-zero eigenvalues in case $\mathbf{A}^{-1}$ is singular

Linear combination of unitaries

Assuming: each unitary gate depends only on one parameter θ_i and each U_i is a rotation or controlled rotation gate.

$$\frac{\partial U_i(\theta_i)}{\partial \theta_i} = \sum_k f_{k,i} U_i(\theta_i) u_{k,i}, \quad \rightarrow \quad \frac{\partial \left|\Phi(\tau)\right\rangle}{\partial \theta_i} = \sum_k f_{k,i} V'_{k,i} \left|\mathbf{0}\right\rangle \tag{7}$$

with a unitary operator $u_{k,i}$, scalar parameter $f_{k,i}$ and:

$$V'_{k,i} = U_n(\theta_n) \dots U_i(\theta_i) u_{k,i} \dots U_1(\theta_1)$$

Derivative Example

- $U_i(\theta_i)$ is a single qubit rotation: $R_Z(\theta_i) = \mathrm{e}^{-i\theta_i\sigma_z}$:

$$\frac{\partial U_i(\theta_i)}{\partial \theta_i} = -\frac{i}{2}\sigma_z R_Z(\theta_i)$$

  $\rightarrow$ add an extra σ_z gate with factor $-i/2$

- $U_i(\theta_i)$ a controlled rotation: $|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes R_Z(\theta_i)$:

$$\frac{\partial U_i(\theta_i)}{\partial \theta_i} = |1\rangle\langle 1| \otimes \partial R_Z(\theta_i)/\partial\theta_i = -\frac{i}{2}|1\rangle\langle 1| \otimes \sigma_z R_Z(\theta_i)$$

  $\rightarrow$ realized with

$$u_{1,i} = I \otimes \sigma_z, f_{1,i} = -i/4,$$
$$u_{2,i} = \sigma_z \otimes \sigma_z, f_{2,i} = i/4$$

  in $\sum_k f_{k,i} U_i(\theta_i) u_{k,i}$ from previous slide

Evaluation A and C with Quantum Circuits – cont.

$$A_{ij} = \sum_{k,l} f^*_{k,i} f_{l,j} \langle \mathbf{0} | V'^{\dagger}_{k,i} V'_{l,j} | \mathbf{0} \rangle, \qquad C_i = \sum_{k,l} f^*_{k,l} \lambda_l \langle \mathbf{0} | V'^{\dagger} h_l \hat{V} | \mathbf{0} \rangle \tag{8}$$

with $\hat{H} = \sum_l \lambda_l h_l$. Both $\mathbf{A}$ and $\boldsymbol{C}$ are of the form $a \cdot \mathrm{e}^{i\phi} \langle \mathbf{0} | \hat{U} | \mathbf{0} \rangle$ and can be evaluated on a quantum circuit.