Variational Hybrid Quantum Algorithms

with Applications to Quantum Chemistry Problems

OsloMet – Autumn School on Quantum Computing

Werner Dobrautz

Chalmers University of Technology

Oslo, November 7, 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

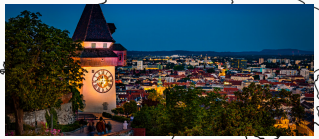
140M EUR Research effort for Sweden's Quantum Computing Stack
≈30 PIs, 20 PostDocs and 40 PhDs

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

- What is quantum chemistry concerned with?
- How can quantum computing help quantum chemistry?
- What are hybrid quantum-classical algorithms?
- How can we simulate chemistry on quantum hardware?
- What is the Variational Quantum Eigensolver (VQE)?

Outline

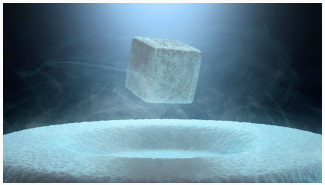
- Motivation – Quantum Chemistry and Electronic Structure Theory
- The Case for Quantum Computing
  - Gate-based Quantum Computing and the Quantum Circuit Model
- How to do quantum chemistry on quantum hardware?
- Quantum Circuit Ansätze and the Variational Quantum Eigensolver
- Applications and Outlook

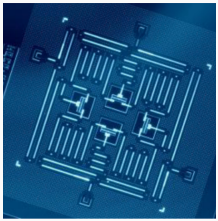
Motivation – Quantum Chemistry and Electronic Structure Theory

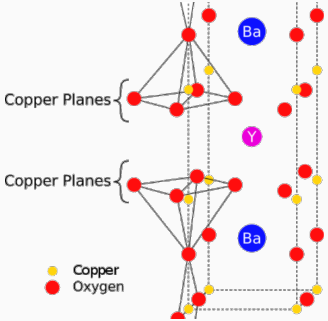
Surprisingly small systems at the center of fascinating physical and chemical effects

High-temperature superconductivity

Zero electrical resistivity





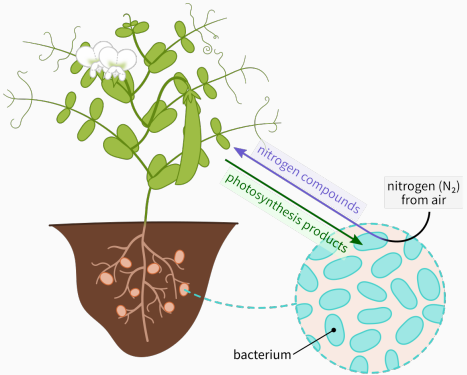


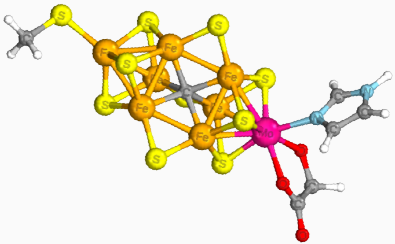
YBCO

shutterstock; CERN; Tokamak; Wikimedia

Nitrogen fixation

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



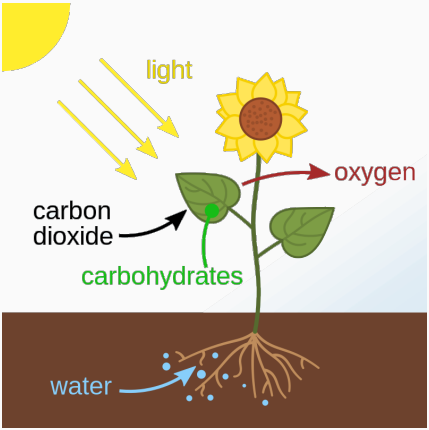


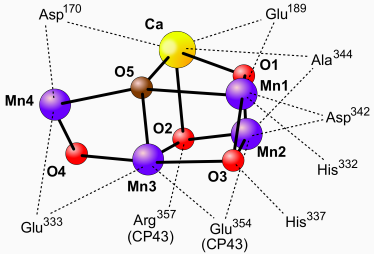
Iron-sulfur clusters

$\Rightarrow$ Cheaper and cleaner ammonia production for fertilizers

Wikimedia

Photosynthesis



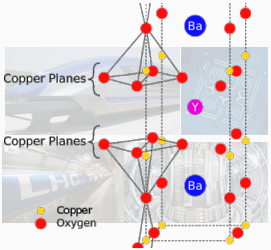


Manganese-Calcium-Oxygen Clusters

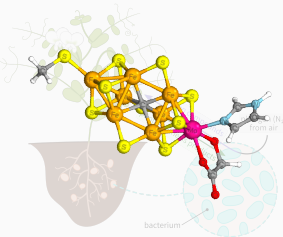
Artificial photosynthesis: Carbon capture and hydrogen and oxygen for fuel cell

Wikimedia; Wikimedia

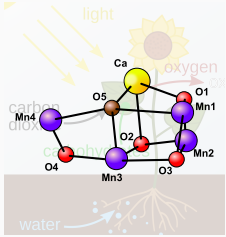
Applications of Quantum Algorithms: *Ab Initio* Quantum Chemistry



YBCO: Unconventional high-T_c superconductivity



FeMoCo: primary cofactor of nitrogenase → nitrogen fixation



Manganese-Calcium-Oxygen Clusters: Oxygen evolving clusters in photosystem II

Surprisingly small systems responsible for interesting physical/chemical properties!

Strong electron correlation ⇒ challenging systems for computational approaches!

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

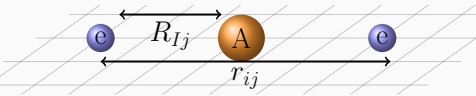
Ab Initio Quantum Chemistry – Electronic Structure Theory

To obtain insight on the **physical** and **chemical properties** (ground- and excited state energies, energy differences, response functions, ...) of quantum systems we need to **solve the Schrödinger equation:**

$$\hat{H}\,|\Psi\rangle = E\,|\Psi\rangle\,,$$

where all necessary information of a quantum system contained in electronic **molecular Hamiltonian:**

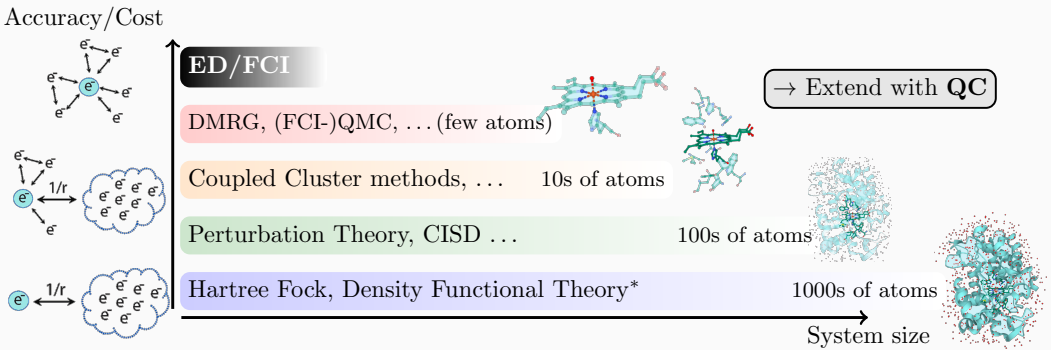
$$\hat{H} = \underbrace{-\frac{1}{2}\sum_i \nabla^2_{\mathbf{r}_i}}_{\text{kinetic energy of e}^-} \underbrace{-\sum_{I,j}\frac{Z_I}{|\mathbf{R}_I - \mathbf{r}_j|}}_{\text{Attr. potential}} + \underbrace{\frac{1}{2}\sum_{i\neq j}\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}}_{\text{e}^- - \text{e}^- \text{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



Coulomb repulsion correlates all electrons of a system → analytic solution too complex
→ **approximations and computational approaches**

Accuracy and cost – scaling and hierarchy of methods

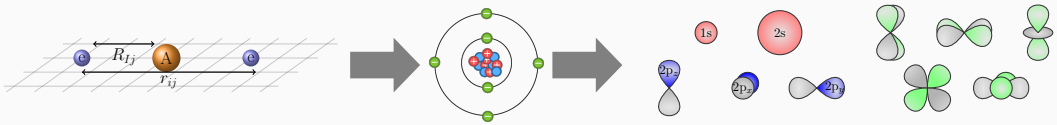
Depending how accurately we treat correlation: various methods and **levels of theory** to solve the Schrödinger equation



Need **highly-accurate** methods to describe **strongly correlated** problems

Cytochrome c: enzyme that eliminates toxic radicals produced by cells. From Santagati *et al.*, arXiv:2301.04114

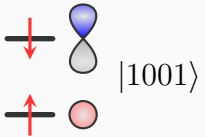
We have to choose a **basis/orbitals** we perform our calculations in! In quantum chemistry: starting orbitals are most often "atomic-like" orbitals (for each atom):



Second quantized form of molecular Hamiltonian:

$$\hat{H} = \underbrace{\sum_{i,j} t_{ij} \sum_{\sigma=\uparrow,\downarrow} a^\dagger_{i,\sigma} a_{j,\sigma}}_{\text{kinetic/hopping term}} + \underbrace{\sum_{i,j,k,l} V_{ijkl} \sum_{\sigma,\tau=\uparrow\downarrow} a^\dagger_{i,\sigma} a^\dagger_{j,\tau} a_{l,\tau} a_{k,\sigma}}_{\text{e}^-\text{-e}^- \text{ interaction term}}$$

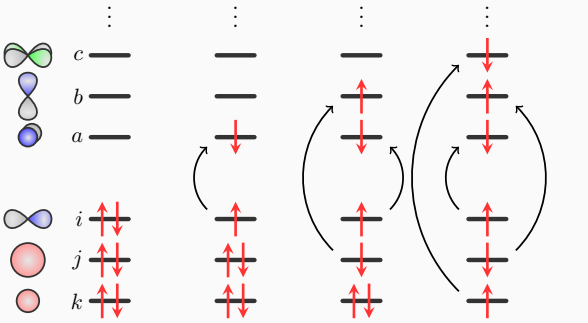
$a^{(\dagger)}_{i,\sigma}$ annihilates(creates) an electron with spin $\sigma = \{\uparrow, \downarrow\}$ in orbital i. e.g. for 2 electrons in 2 orbitals (=4 spin-orbitals): $a^\dagger_{1,\uparrow} a^\dagger_{2,\downarrow} |\text{vac}\rangle = |1001\rangle$:



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

Classical bit

0 1

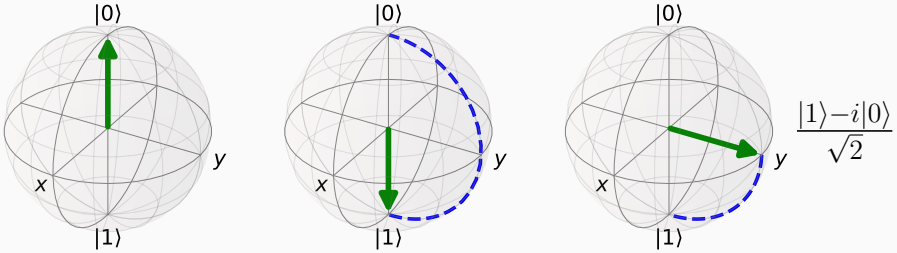
Quantum bit = qubit

$$a\,|0\rangle \quad + \quad b\,|1\rangle$$

Quantum bit = qubit

$$a\,|0\rangle \quad + \quad b\,|1\rangle$$
$$|a|^2 + |b|^2 = 1$$

Qubits – Bloch Sphere



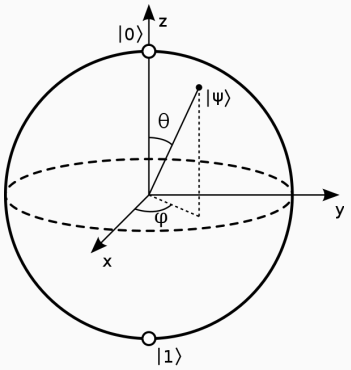
Parametrized gates

For flexibility, we need **parametrized** gates, e.g. rotation around axis:

$$R_X(\theta) = \exp(-i\frac{\theta}{2}\hat{X}) = \begin{pmatrix} \cos(\theta/2) & -i\sin(\theta/2) \\ -i\sin(\theta/2) & \cos(\theta/2) \end{pmatrix}$$

$$R_Y(\theta) = \exp(-i\frac{\theta}{2}\hat{Y}) = \begin{pmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(\theta/2) \end{pmatrix}$$

$$R_Z(\varphi) = \exp(-i\frac{\varphi}{2}\hat{Z}) = \begin{pmatrix} \exp(-i\varphi/2) & 0 \\ 0 & \exp(i\varphi/2) \end{pmatrix}$$



with the Pauli matrices: $\hat{X} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\hat{Y} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\hat{Z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

Multiple Qubits

Bringing **two** qubits together:

$$|\Psi\rangle = \overbrace{(|0\rangle + |1\rangle)}^{\text{qubit 1}} \otimes \overbrace{(|0\rangle + |1\rangle)}^{\text{qubit 2}} = |00\rangle + |01\rangle + |10\rangle + |11\rangle \qquad \text{4 states}$$

Three qubits:

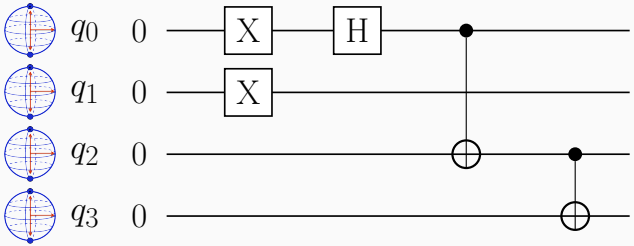
$$\begin{aligned} |\Psi\rangle &= \overbrace{(|0\rangle + |1\rangle)}^{\text{qubit 1}} \otimes \overbrace{(|0\rangle + |1\rangle)}^{\text{qubit 2}} \otimes \overbrace{(|0\rangle + |1\rangle)}^{\text{qubit 3}} \\ &= |000\rangle + |001\rangle + |010\rangle + |100\rangle + |011\rangle + |101\rangle + |110\rangle + |111\rangle \qquad \text{8 states} \end{aligned}$$

n qubits can encode exponentially many (2^n) states.
$\rightarrow$ Need new **quantum algorithms** to use this potential advantage!

$\approx$ 40 qubits enough to encode the $\sim 2 \cdot 10^9$ states of F_2!

Quantum circuit model

Circuit model: Lines represent qubits and similar to classical circuits (AND, OR, ...) we can act with **operations/gates** on one (rotations) or **multiple qubits** (CNOT, ...)



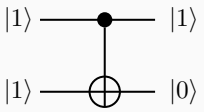
Hadamard gate (H):

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

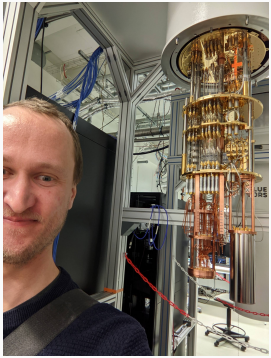
Controlled NOT (CNOT):
target qubit ($\bigoplus$) is inverted if control qubit ($\cdot$) is in $|1\rangle$ state

Exercise: *what is the state $|\Phi\rangle$ at the end of the above circuit?*

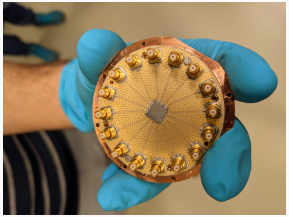
Parametrized gates ($\mathrm{R}_x(\theta)$, ...) and multi-qubit gates allow us to prepare flexible **entangled** (non-classical) states, $|\Psi(\boldsymbol{\theta})\rangle = \hat{U}(\boldsymbol{\theta})\,|0\rangle$.



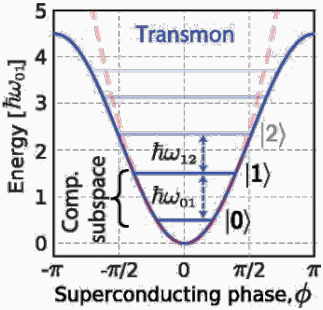
Noisy intermediate-scale quantum - NISQ



@ Chalmers



3 qubit device @Chalmers

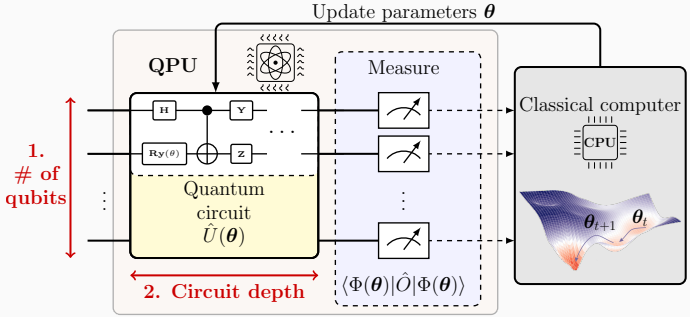


Qubits rely on quantum effects → very fragile, easily influenced by environmental effects/noise. Need to isolate and cool them close to absolute zero! Only few of them...

Benioff, J. Stat. Phys. **22** (5), 563 (1980); Feynman, Int. J. Theo. Phys. **21** (6/7), 467 (1982); Preskill, Quantum **2**, 79 (2018); Kantz *et al.*, Applied Physics Reviews 6, 021318

Hybrid quantum-classical approach

Current quantum hardware has many flaws: **noise, decoherence and limited number of qubits** → **Hybrid quantum-classical approach**



Use pros of both CPUs and QPUs:

- Use **short-depth quantum circuits** that fit current hardware
- Can **improve on classical estimates** by non-classical states
- Store quantum state with **exponentially fewer resources**
- Use CPU to i.e. optimize gate parameters, $\boldsymbol{\theta}$

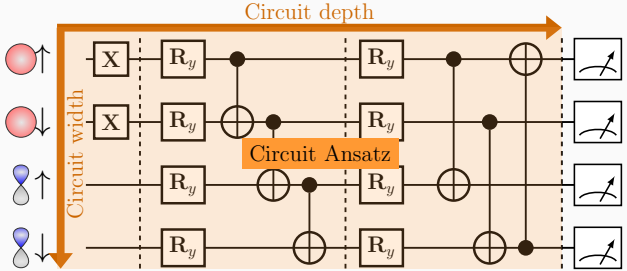
How to do quantum chemistry on quantum hardware?

Quantum Chemistry on Quantum Computers

1. Map fermionic Hamiltonian/basis functions onto quantum hardware/qubits*
2. Choose an 'Ansatz'
3. Use quantum algorithms for ground-, excited states, dynamics, ...

a) Prepare an initial state

$$|\Phi_0\rangle = \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$



b) Perform **unitary** operations of the quantum algorithm on the qubits

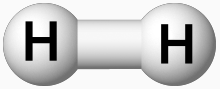
c) Measure observables of interest, ($\langle \hat{H} \rangle$)

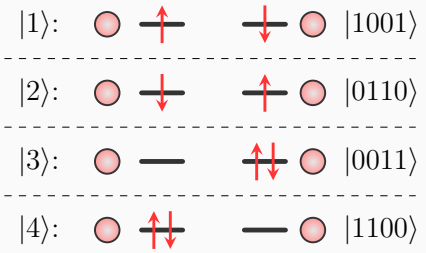
$$|\Phi\rangle = \hat{U}\,|\Phi_0\rangle = a_1 \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} + a_2 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \cdots + a_{2^N} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

*Jordan-Wigner, Bravyi-Kitaev, (Ann. Phys. **298**, 210 (2002)), Parity encoding ...

Example: Classic solution of hydrogen molecule – H_2

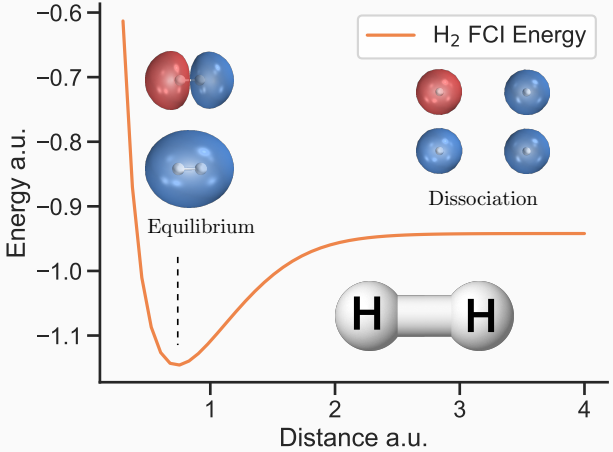
Hydrogen molecule in a "minimal" basis set: 1s orbital for each hydrogen.
4-dimensional Hilbert space for two electrons in two orbitals (4 spin-orbitals).





Solution: Construct matrix representation of quantum chemistry Hamiltonian in this basis, $H_{ij} = \langle i | \hat{H} | j \rangle$, $\rightarrow$ diagonalize $\rightarrow$ exact solution in given basis

Example: Hydrogen molecule – H_2 – PES



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

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

Encoding the problem on a quantum computer

Qubits can quite naturally store the occupation of an spin-orbital:
$|0\rangle$-state/$\binom{1}{0}$: empty, $|1\rangle$-state/$\binom{0}{1}$: occupied

Also: action of creation and annihilation operators representable by Pauli matrices:

$$\hat{a}^\dagger |0\rangle = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hat{X} - i\hat{Y}}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle$$

$$\hat{a} |1\rangle = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{\hat{X} + i\hat{Y}}{2} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle ,$$

with the Pauli matrices

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

(Anti-)Symmetric wave functions – Pauli exclusion principle

However:

- For Fermions, the Pauli exclusion principle requires the wavefunction to be **anti-symmetric** under the exchange of two particles:

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_i, \ldots, \mathbf{r}_j, \ldots, \mathbf{r}_N) = -\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_j, \ldots, \mathbf{r}_i, \ldots, \mathbf{r}_N)$$

- While Bosonic wave functions are **symmetric** under the exchange of particles

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_i, \ldots, \mathbf{r}_j, \ldots, \mathbf{r}_N) = +\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_j, \ldots, \mathbf{r}_i, \ldots, \mathbf{r}_N)$$

Anti-symmetry/Anti-commutation relations

Electrons are **indistinguishable Fermions**, with anti-symmetric wavefunction and anti-commuting creation/annihilation operators:

$$\left\{a_i^\dagger, a_j^\dagger\right\} = 0, \qquad a_i^\dagger a_j^\dagger = -a_j^\dagger a_i^\dagger$$

Unlike **individually addressable** qubits, with Pauli operators:

$$\left(\frac{X_i - iY_i}{2}\right)\left(\frac{X_j - iY_j}{2}\right) = +\left(\frac{X_j - iY_j}{2}\right)\left(\frac{X_i - iY_i}{2}\right)$$

Task: We need to map the **fermionic** Hamiltonian to a **qubit** Hamiltonian in terms of Pauli operators:

$$\hat{H}_f = \sum V_{ijkl} a_{i,\sigma}^\dagger a_{j,\tau}^\dagger a_{l,\tau} a_{k,\sigma} \quad \Rightarrow \quad \hat{H}_q = \sum_i c_i \hat{P}_i$$

Jordan Wigner Mapping

Note that the following Pauli operators anti-commute:

$$\hat{Z}\hat{X} = -\hat{X}\hat{Z}, \qquad \hat{Z}\hat{Y} = -\hat{Y}\hat{Z}$$

Exercise: *convince yourself of equation above*

Jordan-Wigner encoding:

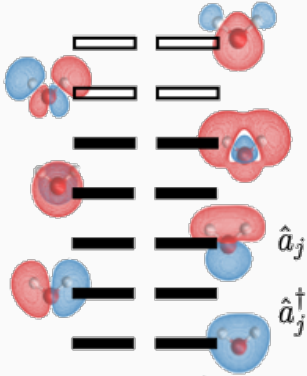
$$\begin{aligned}
a_1^\dagger &= \frac{X_1 - iY_1}{2} \\
a_2^\dagger &= Z_1 \left(\frac{X_2 - iY_2}{2} \right) \\
a_3^\dagger &= Z_1 Z_2 \left(\frac{X_3 - iY_3}{2} \right) \\
a_i^\dagger &= \bigotimes_{j=1}^{i-1} Z_j \left(\frac{X_i - iY_i}{2} \right)
\end{aligned}$$

- Fix anti-symmetry by tracking parity/phase before each creation/annihilation operator with $\hat{Z}_i$
- **Exercise:** Demonstrate anti-symmetry of JW-encoded $a_3^\dagger a_2^\dagger = -a_2^\dagger a_3^\dagger$!

JW Mapping – Recap

Fermions

$$\{a_i, a_i\} = 0,\ \{a_i^\dagger, a_i^\dagger\} = 0, \{a_i, a_i^\dagger\} = \delta_{i,j}$$



mapping

Jordan-Wigner

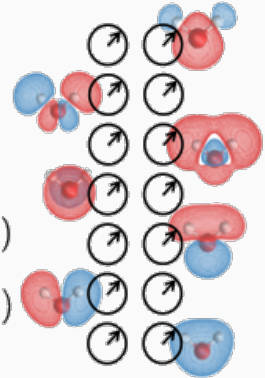
$$\hat{a}_j = \bigotimes_{i=1}^{j-1} \hat{\sigma}_i^z \otimes (\hat{\sigma}_j^x + i\hat{\sigma}_j^y)$$

$$\hat{a}_j^\dagger = \bigotimes_{i=1}^{j-1} \hat{\sigma}_i^z \otimes (\hat{\sigma}_j^x - i\hat{\sigma}_j^y)$$

$$\hat{H}_{elec} = \sum_{pq} h_{pq} \hat{a}_p^\dagger \hat{a}_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s$$

Spins

$$[\sigma_i, \sigma_i] = 0,\ [\sigma_i^\dagger, \sigma_i^\dagger] = 0, [\sigma_i, \sigma_j^\dagger] = \delta_{i,j}$$

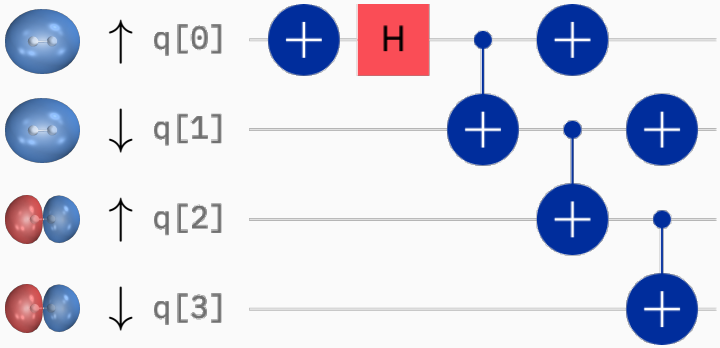


$$\hat{H}_{elec} = \sum_i c_i \hat{P}_i$$

https://qiskit.org/documentation/nature/tutorials/01_electronic_structure.html

Re: H_2 at dissociation

What is the state of this quantum circuit?



Try: IBM Quantum Composer

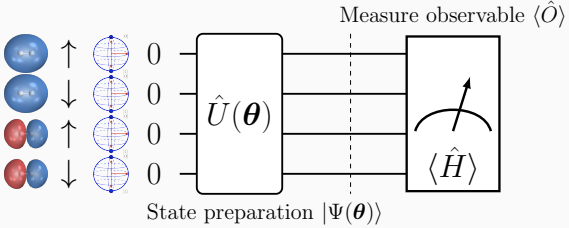
More general quantum circuits – Ansätze

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

$$\begin{aligned} |\Psi(\boldsymbol{\theta})\rangle &= \hat{U}(\boldsymbol{\theta})\,|0000\rangle \\ &\overset{!}{=} c_1\,|1100\rangle + c_2\,|0011\rangle \\ &\quad + c_3\,|1001\rangle + c_4\,|0110\rangle \end{aligned}$$



Given a general quantum Ansatz $\hat{U}(\boldsymbol{\theta})$: We need algorithms to find the optimal gate parameters $\boldsymbol{\theta}$! The variational quantum eigensolver (VQE) can find the **most optimal** parameters/angles $\boldsymbol{\theta}$ to minimize the energy expectation value:

$$E(\boldsymbol{\theta}) = \min_{\boldsymbol{\theta}} \langle \mathbf{0}|\, \hat{U}^\dagger(\boldsymbol{\theta}) \hat{H} \hat{U}(\boldsymbol{\theta})\, |\mathbf{0}\rangle$$

Quantum Circuit Ansätze and the Variational Quantum Eigensolver

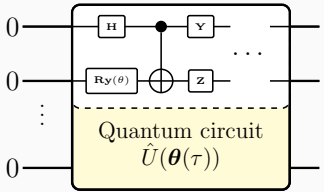
Ansatz for the quantum chemistry wavefunction

In general: an **Ansatz** is a quantum circuit with parametrized gates

Desired in Ansätze:

- Expressive – spans large and correct portion of Hilbert space
- Small number of qubits
- Short-depth

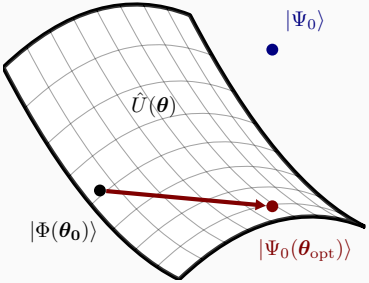
→ **Hardware efficient**



State prep. $|\Phi(\boldsymbol{\theta}(\tau))\rangle$

Consideration due to noise and coherence times:

- Circuit depth
- Circuit connectivity
- Number of parameters
- Number of 2-qubit gates
- Gate types (Native to hardware?)

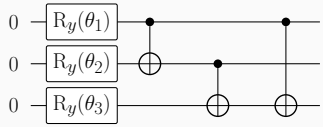


Ansatz for the quantum chemistry wavefunction:s $|\Psi(\boldsymbol{\theta})\rangle = \hat{U}(\boldsymbol{\theta})\,|0\rangle$

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"

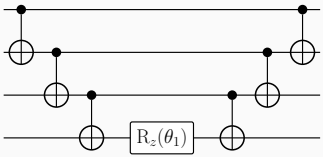
$$|\Psi(\boldsymbol{\theta})\rangle = \prod_{i}^{d} \left[\hat{U}_{ent}\hat{U}_{\mathrm{rot}}(\{\boldsymbol{\theta}_i\})\right] |\psi_{\mathrm{init}}\rangle$$



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

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



$\Rightarrow$ **Adaptive Ansätze***

Lun *et al.*, PRX Quantum 2, 020310; Grimsley *et al.*, Nat Commun 10, 3007

Variational Quantum Eigensolver – VQE

Ground state, $|\Psi_0\rangle$, is fundamental in quantum chemistry and electronic structure theory $\rightarrow$ used to calculate all sort of properties, like reaction rates and reaction pathways

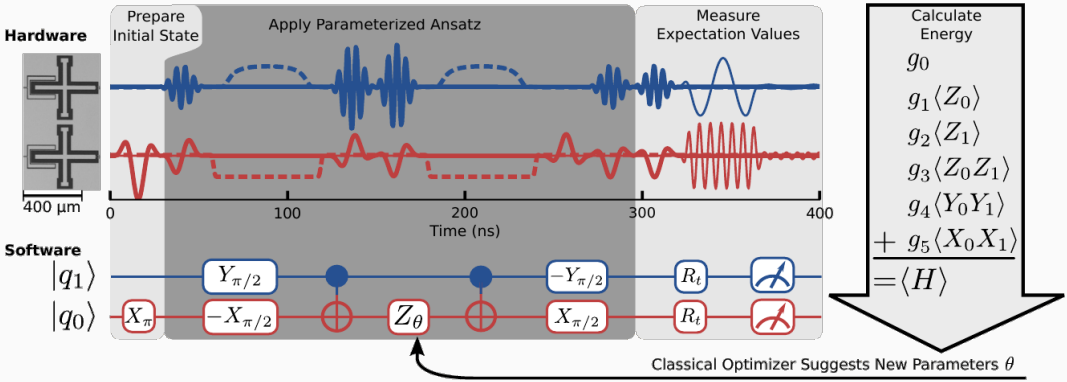
Our goal is to estimate: $\hat{H}\,|\Psi_0\rangle = E_0\,|\Psi_0\rangle \quad \Rightarrow \langle\Psi_0|\,\hat{H}\,|\Psi_0\rangle = E_0$

Variational principle: an arbitrary state, $|\Psi(\boldsymbol{\theta})\rangle$, the expectation value of $\hat{H}$, will be an upper bound to E_0

$$\langle\Psi(\boldsymbol{\theta})|\,\hat{H}\,|\Psi(\boldsymbol{\theta})\rangle = E(\boldsymbol{\theta}) \geq E_0$$

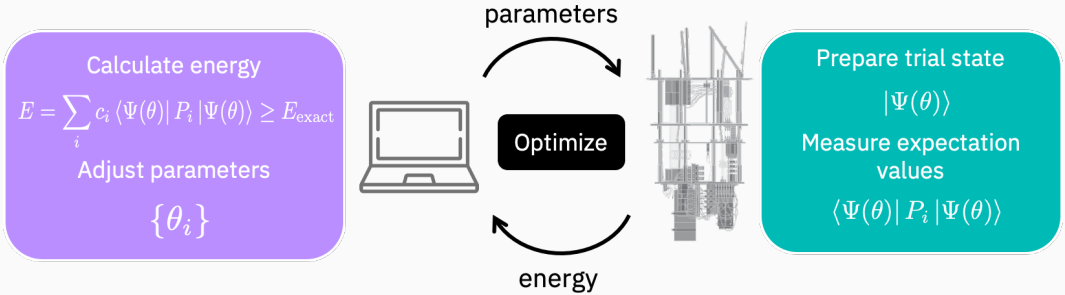
Variational Quantum Eigensolver

Leverage pros of both classical and quantum computers:



Variational Quantum Eigensolver

VQE: Efficiently prepare and encode $|\Psi(\boldsymbol{\theta})\rangle$ with a suitable *Ansatz*, $\hat{U}(\boldsymbol{\theta})$, on **quantum hardware** and measure the expectation values of "Pauli strings", $\hat{P}_i$. Reconstruct the energy and update the parameters (with some optimizer) on a **classical computer**. Repeat until convergence of $E(\boldsymbol{\theta}) = \langle\Psi(\boldsymbol{\theta})|\,\hat{H}\,|\Psi(\boldsymbol{\theta})\rangle$



Qiskit Tutorial

Applications and Outlook

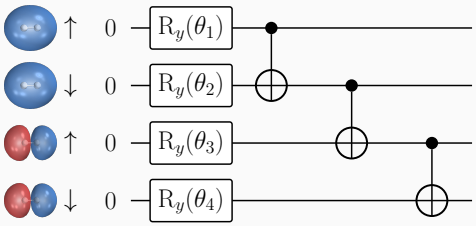
H_2 – Hardware efficient Ansatz

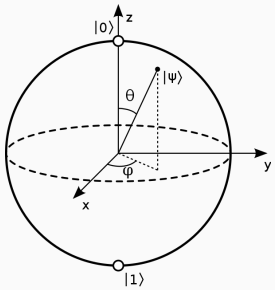
H_2 groundstate wavefunction at equilibrium:

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

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

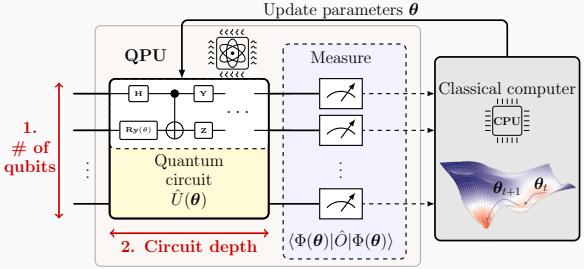
$$|\Psi(\boldsymbol{\theta})\rangle = \hat{U}(\boldsymbol{\theta})\,|0000\rangle \stackrel{!}{=} c_1(\boldsymbol{\theta})\,|1100\rangle + c_2(\boldsymbol{\theta})\,|0011\rangle + c_3(\boldsymbol{\theta})\,|1001\rangle + c_4(\boldsymbol{\theta})\,|0110\rangle$$

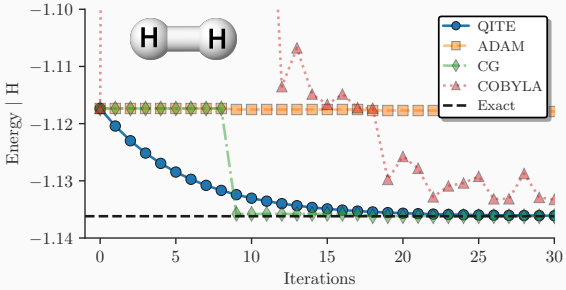




H_2 VQE Statevector simulation

H_2 at 0.7 Å in a STO-6G basis using 4 qubits: Default `Qiskit` VQE settings for different types of optimizers, no noise!

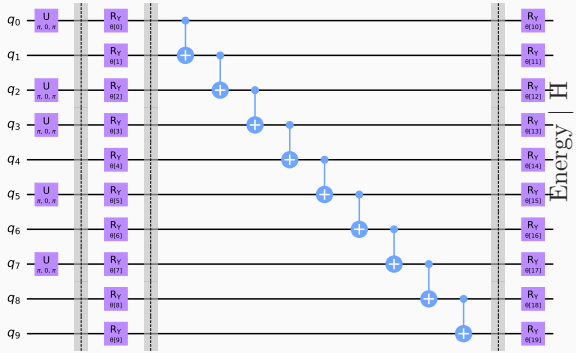


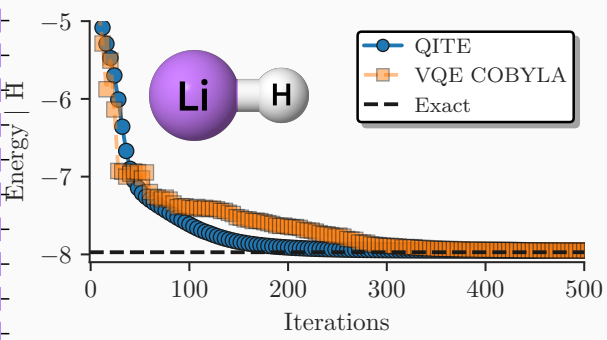


Jupyter Notebook Example

LiH Statevector

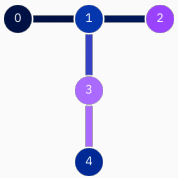
LiH – minimal basis – 1.6Å– parity mapping – HEA Ansatz

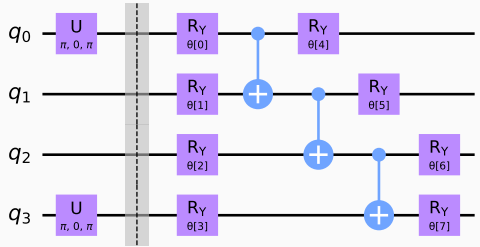




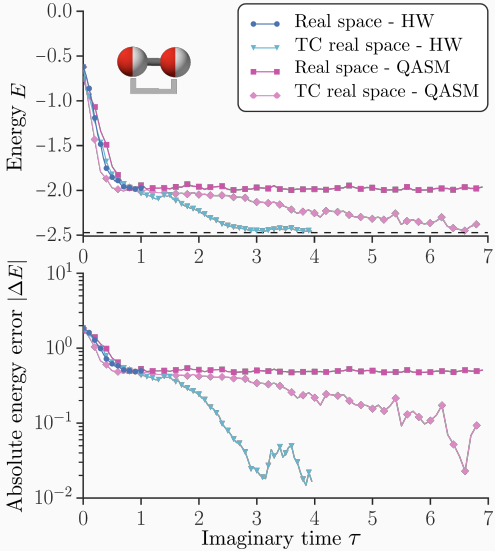
Actual experimental results for the Hubbard model on ibmq_lima

- 2-site Hubbard model
- On ibmq_lima





Hardware-efficient RY Ansatz



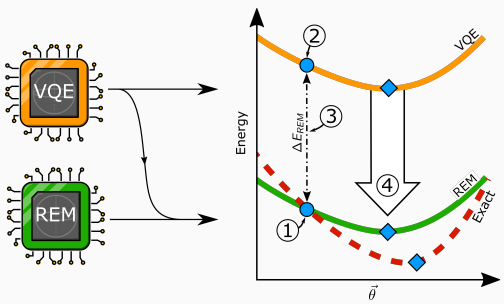
Reference-state Error Mitigation

JCTC Journal of Chemical Theory and Computation
pubs.acs.org/JCTC Article

Reference-State Error Mitigation: A Strategy for High Accuracy Quantum Computation of Chemistry

Phalgun Lolur,[‖] Mårten Skogh,[‖] Werner Dobrautz, Christopher Warren, Janka Biznárová, Amr Osman, Giovanna Tancredi, Göran Wendin, Jonas Bylander, and Martin Rahm[*]

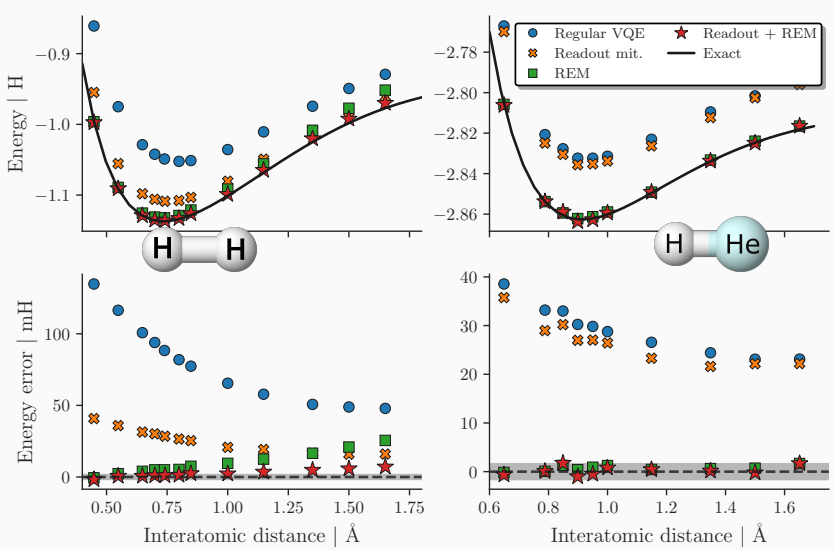
Cite This: *J. Chem. Theory Comput.* 2023, 19, 783−789

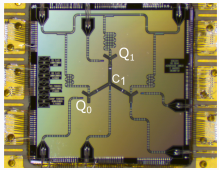


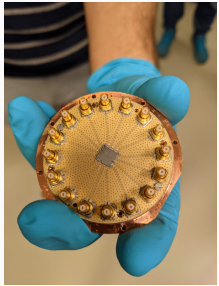
1. Classically compute exact reference energy (i.e. Hartree-Fock), $E(\boldsymbol{\theta}_{\text{ref}})$
2. Measure reference energy on noisy device $\mathcal{E}(\boldsymbol{\theta}_{\text{ref}})$, with reference parameters $\boldsymbol{\theta}_{\text{ref}}$
3. Calculate REM correction: $\Delta E_{\text{REM}} = \mathcal{E}(\boldsymbol{\theta}_{\text{ref}}) - E(\boldsymbol{\theta}_{\text{ref}})$
4. Correct final VQE energy with REM correction

[*] Lolur, Skogh, **WD**, Warren, Biznárová, Osman, Tancredi, Wendin, Bylander, and Rahm, J. Chem. Theory Comput. 2023, **19**, 3, 783

Reference-state Error Mitigation







*Lolur, Skogh, **WD**, Warren, Biznárová, Osman, Tancredi, Wendin, Bylander, and Rahm, J. Chem. Theory Comput. 2023, **19**, 3, 783

Further Topics

- Noise!
- Scaling up!
- Calculations on real-hardware over the cloud
- Error mitigation: Reference-State Error Mitigation: A Strategy for High Accuracy Quantum Computation of Chemistry, with calculations/experiments on Chalmers devices
- Resource reduction: Phys. Rev. Research 5, 023174, arXiv:2303.02007
- Many more...

Algorithms on quantum hardware

On near-term intermediate-scale quantum (NISQ) hardware (low number of qubits and short circuits): **hybrid quantum-classical algorithms**

- Quantum Approximate Optimization algorithm (QAOA)
- Quantum (Imaginary) Time Evolution
- **Variational Quantum Eigensolver (VQE)**
- ...

There is a variety of quantum algorithms for different kind of problems, most are for future **fault-tolerant** quantum hardware with many qubits and deep circuits.

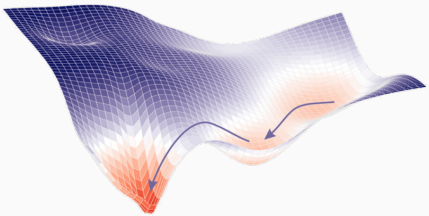
- Shor's algorithm – Encryption
- Grover's algorithm – Database search
- Quantum Fourier Transformation
- **Quantum Phase Estimation**

QPE: Kitaev, arXiv:quant-ph/9511026 (1995), Nielsen and Chuang, *Quantum computation and quantum information* (2001);

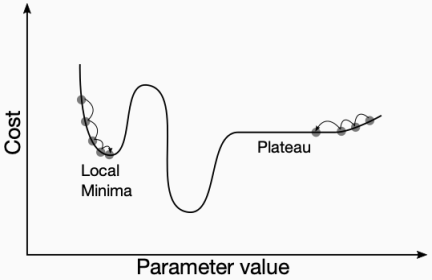
Thank you for your attention!

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