Quantum Computing Meets Quantum Chemistry:

A Potential New Era of Simulation and Study

Werner Dobrautz

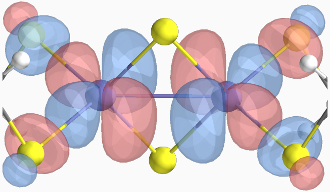
Chalmers University of Technology

QuantumBW Colloquium

September 26, 2024

Wallenberg Centre for
Quantum Technology

Take-home messages – Big picture



- **What is quantum chemistry?**
  Why is it worthwhile?

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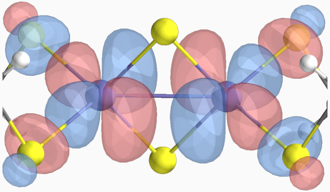

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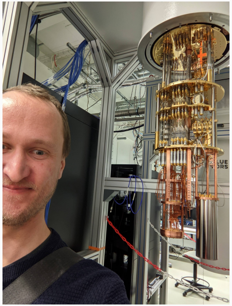


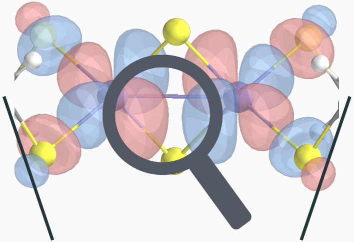
- **What is quantum computing?**
  What are the potential advantages?

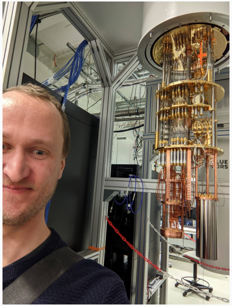
Take-home messages – Big picture

- What is quantum chemistry?
  Why is it worthwhile?

- What is quantum computing?
  What are the potential advantages?

- How can it help quantum chemistry?
  – What are state-of-the-art approaches?





Werner Dobrautz

PostDoc at Chalmers University

Quantum algorithms for accurate **quantum chemistry** on current and near-term quantum computers

CHALMERS
UNIVERSITY OF TECHNOLOGY

WACQT Wallenberg Centre for Quantum Technology

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

MARIE CURIE ACTIONS

IBM

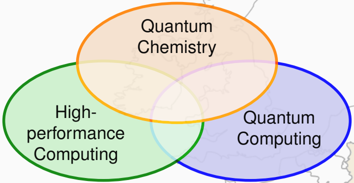
Academic Network

NordIQuEst

HPC+QC ecosystem in the Nordics + Estonia
Lumi HPC + QAL9000 and Helmi QCs

OpenSuperQPlus

28 EU partners aiming to build a 1,000 qubit QC
Including a focus on HPC+QC integration



MAX PLANCK INSTITUTE
FOR SOLID STATE RESEARCH

PhD in **Theoretical Quantum Chemistry**

Quantum Monte Carlo methods
for strongly correlated electron problems in HPC environments

TU Graz

BSc/MSc Studies in **Physics** at TU Graz

Computational/Solid State Physics

Outline

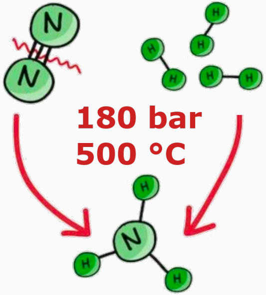
- Quantum Chemistry and Electronic Structure Theory
- The Case for Quantum Computing
- Quantum Computing for Quantum Chemistry
- Conclusion and Outlook

Quantum Chemistry and Electronic Structure Theory

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

Motivation: Haber-Bosch process and biological nitrogen fixation

Haber-Bosch Process



- Crucial for fertilizer production
- 2% of world's energy consumption
- 3% of global carbon emissions
- 5% of natural gas consumption

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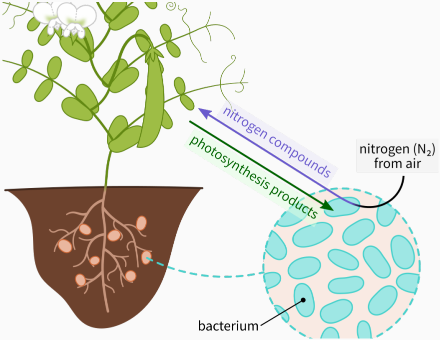
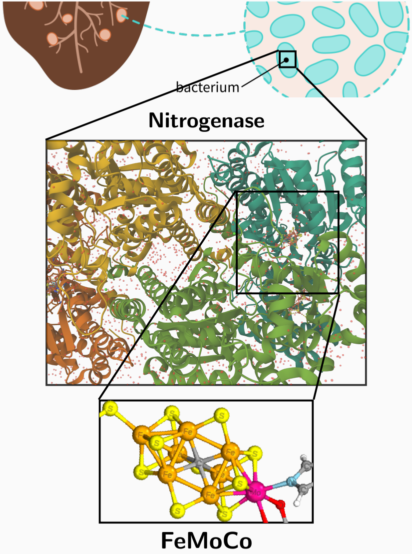
Biological nitrogen fixation



- Ambient pressure and temperatures
- Process not yet understood → Bio-catalysts for more **efficient** and **greener** ammonia production

Problem: Strongly correlated quantum systems

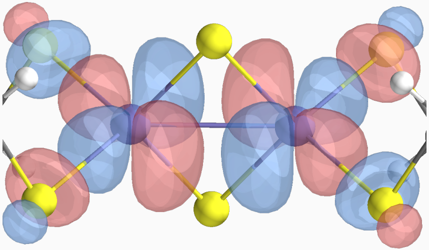
- Small molecular systems act as catalysts: Iron-Molybdenum cofactor (FeMoCo)
- **Experimental study very difficult!**

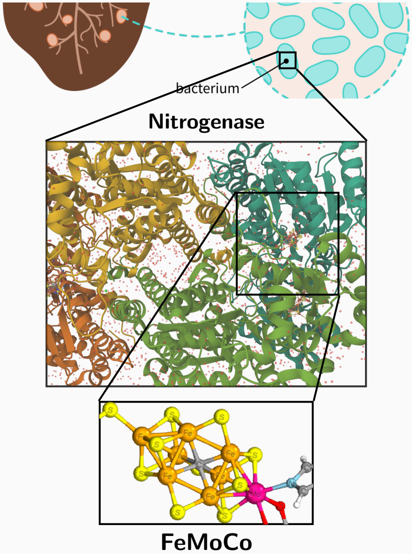


Problem: Strongly correlated quantum systems

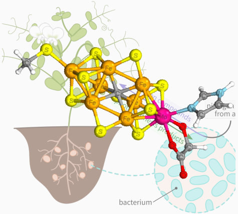
- Small molecular systems act as catalysts: Iron-Molybdenum cofactor (FeMoCo)
- **Experimental study very difficult!**

→ Numerical studies of relevant **electronic** quantum phenomena necessary!

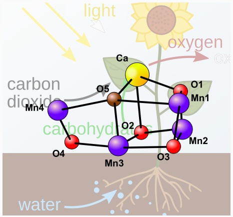




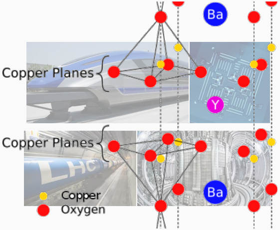
Quantum Chemistry – Applications



Nitrogen fixation



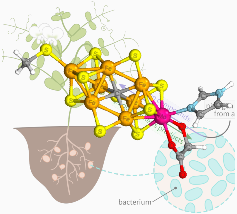
Artificial photosynthesis

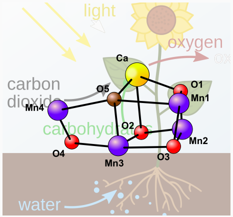


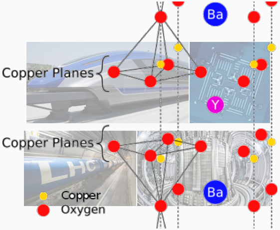
High-T$_c$ superconductivity

- Drug discovery
- Materials design
- Battery development
- ...

Quantum Chemistry – Applications







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Nitrogen fixation **Artificial photosynthesis** **High-T$_c$ superconductivity**

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

$\approx$ 30% of high-performance computing resources for chemistry-related problems

Quantum Chemistry – Electronic Structure Theory

Insight on **physical** and **chemical properties** (ground- and excited state energies, chemical reactions, ...) of quantum systems by **solving the Schrödinger equation:**

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

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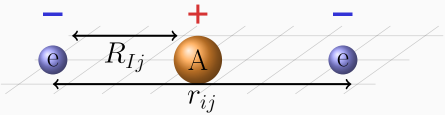
All information of a quantum system contained in **electronic Hamiltonian:**

$$\hat{H} = \hat{T}_{\text{Kin.}}(\mathbf{r}) + \hat{V}_{\text{Attr.}}(\mathbf{r}, \mathbf{R}) + \hat{V}_{\text{Rep.}}(\mathbf{r}, \mathbf{r}')$$



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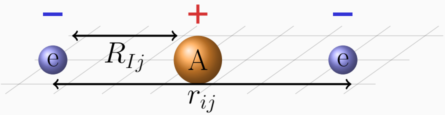
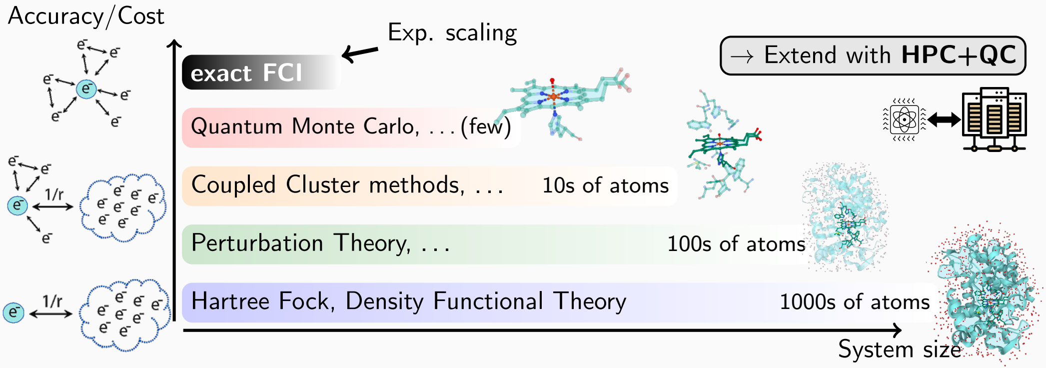


Coulomb repulsion correlates all electrons of a system → analytic solution too complex → **approximations and computational approaches**

Quantum Chemistry – Accuracy and cost

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



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

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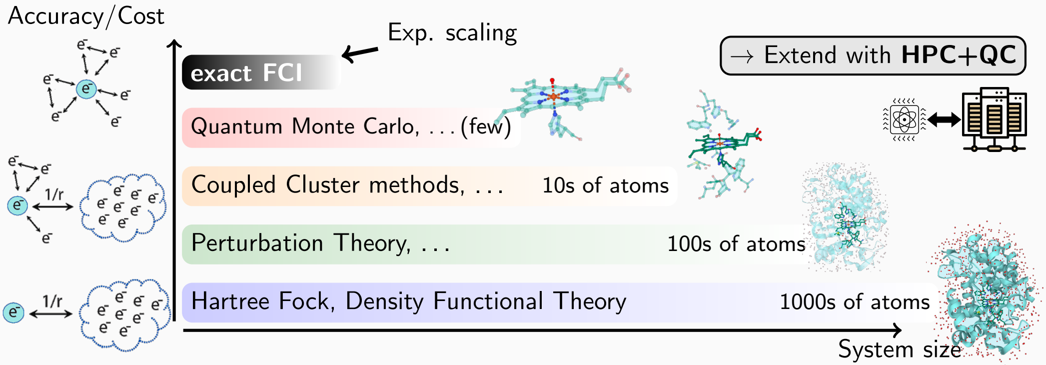
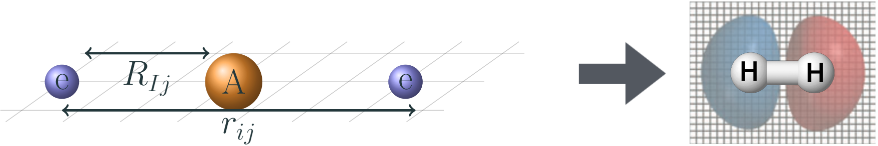
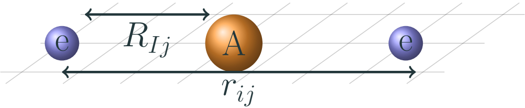


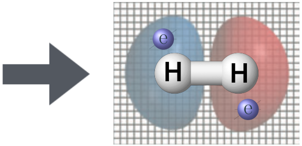
Need **highly-accurate** methods to describe **strongly correlated** problems

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

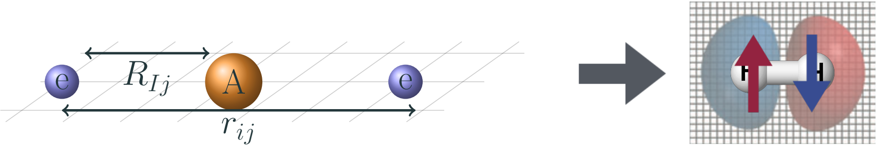
Exponential scaling of the exact solution




e
R_{Ij}
A
e
r_{ij}


e
H
H
e

Exponential scaling of the exact solution



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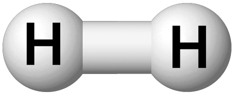
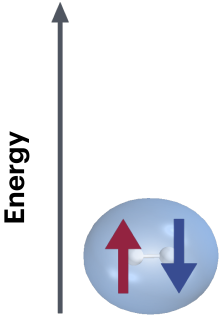
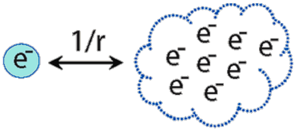




Hartree-Fock



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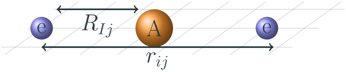
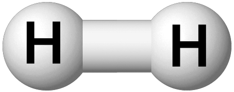
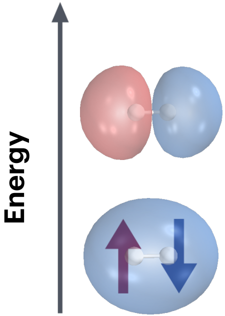


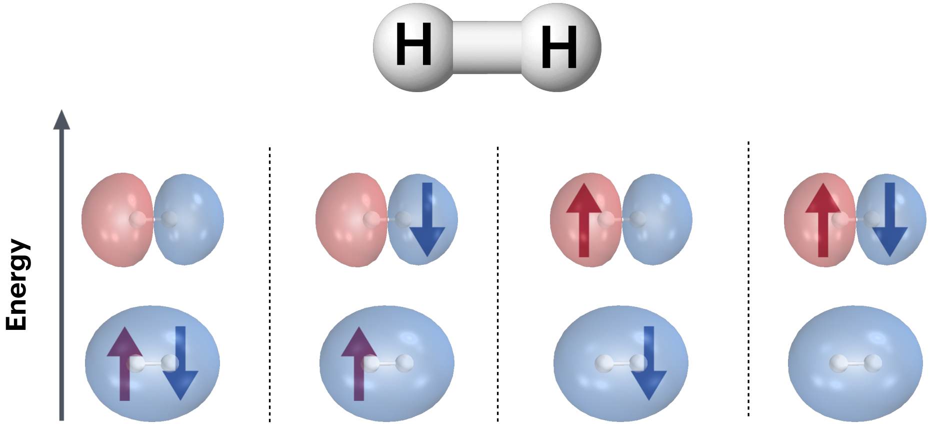




Hartree-Fock

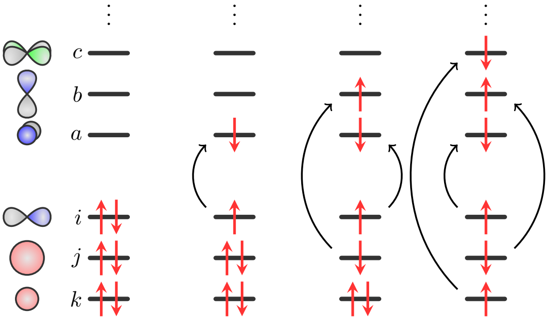
1100

Exponential scaling of the exact solution



Hartree-Fock	Single excitations		Double excitations
1100	1001	0110	0011

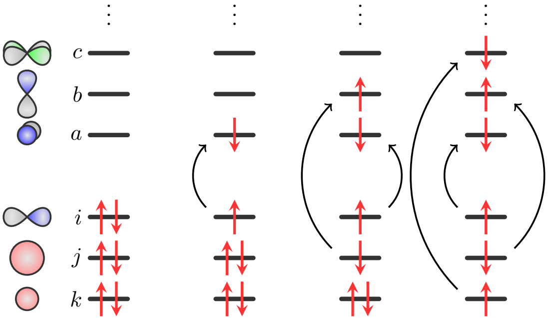
Exponential scaling of the exact solution



$$|\Phi_{HF}\rangle \quad + \quad |\Phi_i^a\rangle \quad + \quad |\Phi_{ij}^{ab}\rangle \quad + \quad |\Phi_{ijk}^{abc}\rangle + \cdots$$

All possible excitations from HF state

Exponential scaling of the exact solution



$$|\Phi_{HF}\rangle + |\Phi_i^a\rangle + |\Phi_{ij}^{ab}\rangle + |\Phi_{ijk}^{abc}\rangle + \cdots$$

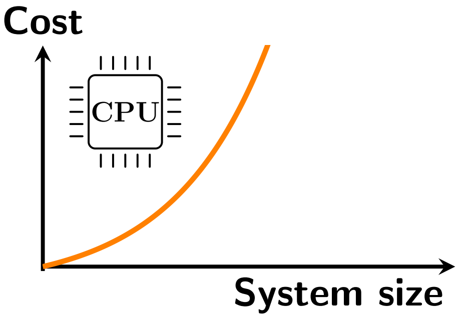
All possible excitations from HF state

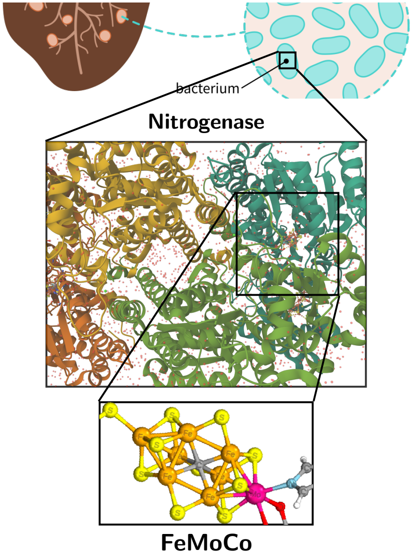
Number of possible states for given number of electrons and orbitals

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	$\sim 2 \cdot 10^9$

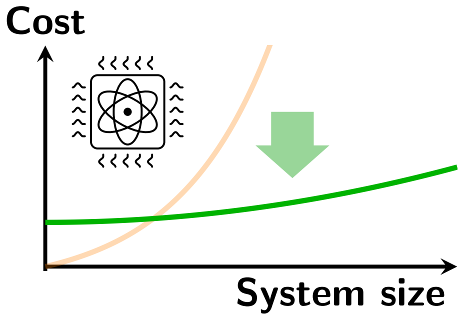
$\approx$ 256 GB to store wavefunction

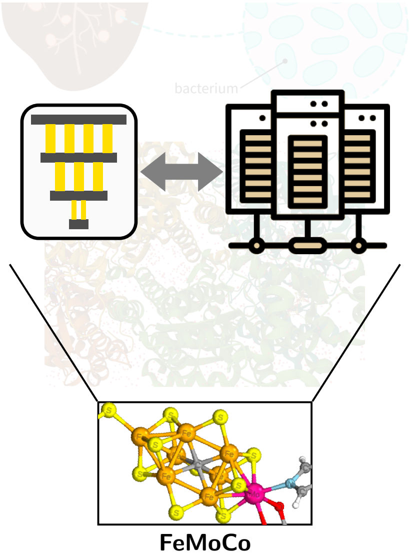
We have the equations at hand, but **exponentially costly** on classical computers!





Quantum computers could provide a potential **speedup!**





The Case for Quantum Computing

Classical bit

0 1

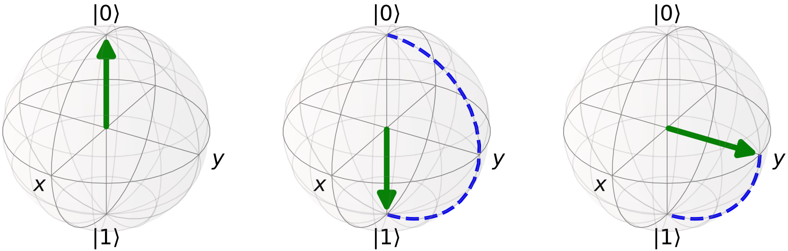
Quantum bit = qubit

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

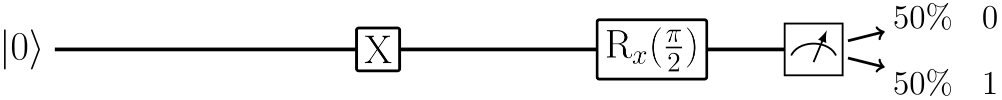
Quantum bit = qubit

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

Qubits – Bloch Sphere



$$\frac{|1\rangle - i|0\rangle}{\sqrt{2}}$$



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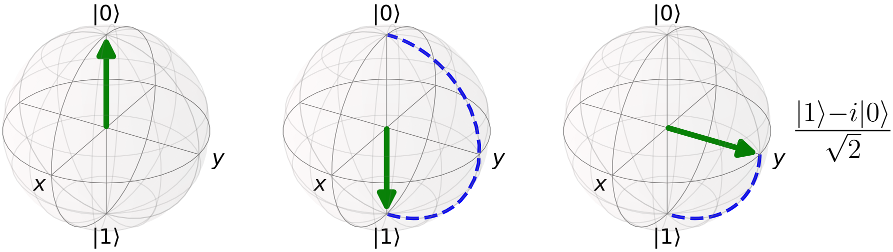

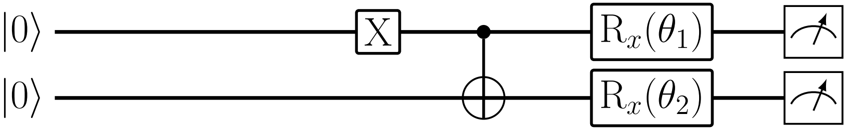

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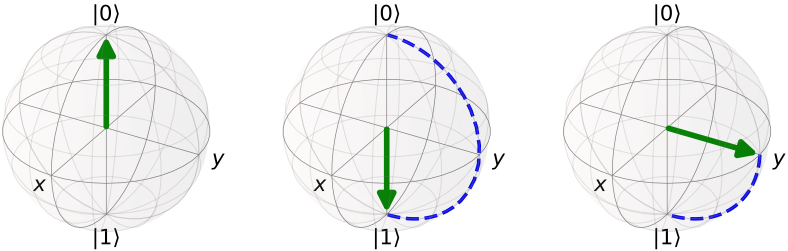

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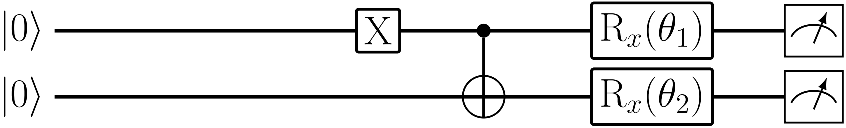

$$|\Psi\rangle \approx \hat{U}(\boldsymbol{\theta})\,|\mathbf{0}\rangle$$

Multiple Qubits – Entanglement

Bringing **two** qubits together:

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

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Three qubits:

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

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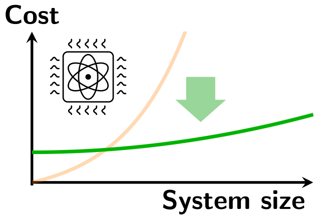
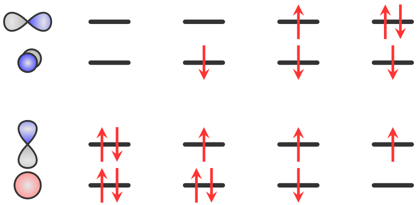
N qubits can encode exponentially many (2^N) states.
40 qubits enough to encode the $\sim 2 \cdot 10^9$ states of F_2!
$\rightarrow$ Need new **quantum algorithms** to
use this potential advantage!



Quantum Computing for Quantum Chemistry

How can Quantum Computing help Quantum Chemistry?

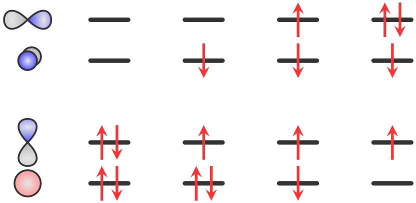
2^N states



$$|\Phi_{\mathrm{HF}}\rangle = |1100\rangle \, , |\Phi_i^a\rangle = |1010\rangle \, , \ldots$$

Fermion to qubit mapping

2^N states ⟶ N qubits



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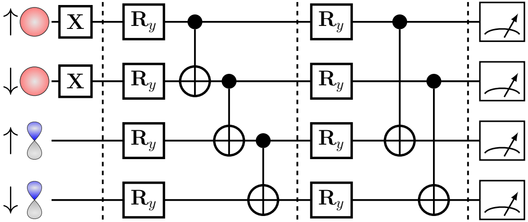

- Map our problem (Hamiltonian/basis functions) onto quantum hardware/qubits
  - Qubits encode occupation of spin-orbitals $\in [0, 1]$

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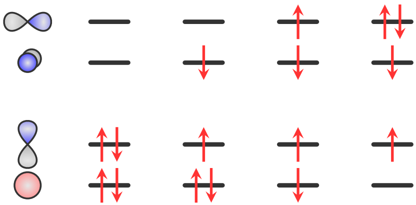
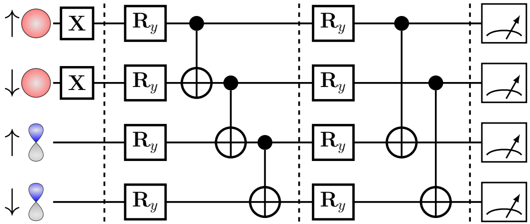


$|\Phi_{\mathrm{HF}}\rangle = |1100\rangle\,, |\Phi_i^a\rangle = |1010\rangle\,, \ldots$



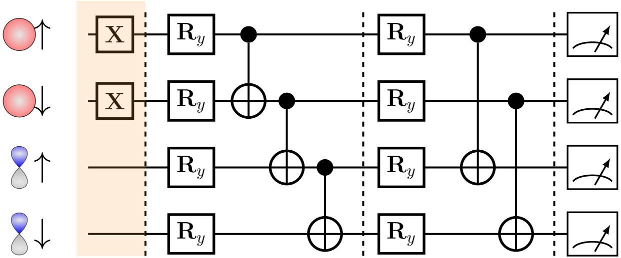
- Map our problem (Hamiltonian/basis functions) onto quantum hardware/qubits
  - Qubits encode occupation of spin-orbitals $\in [0, 1]$

→ Use quantum algorithms for ground-, excited states, dynamics, ...

Quantum Chemistry on Quantum Hardware

1) Prepare an initial state $|\Phi_0\rangle$:

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



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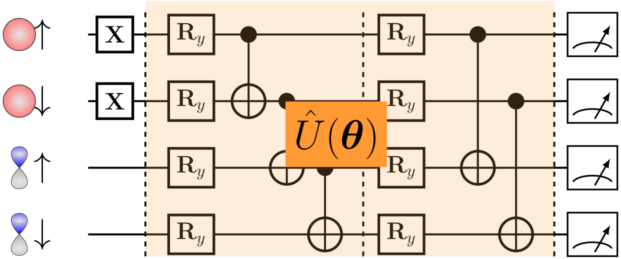

2) Perform **unitary** operations of chosen quantum algorithm:

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

Quantum Chemistry on Quantum Hardware

1) Prepare an initial state $|\Phi_0\rangle$:

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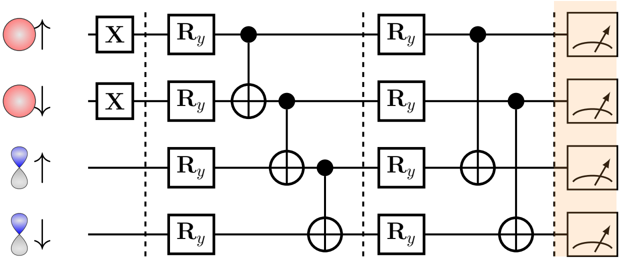
3) Measure observable $\langle \hat{O} \rangle$



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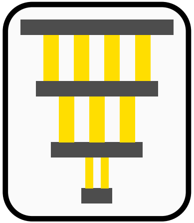
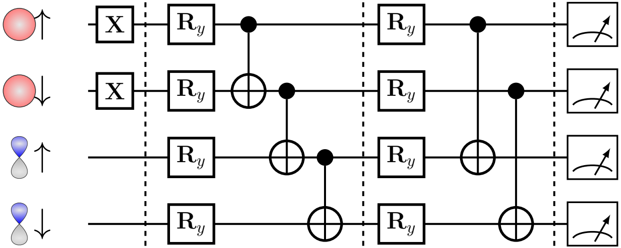
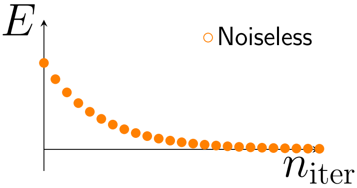
Quantum Chemistry on Quantum Hardware

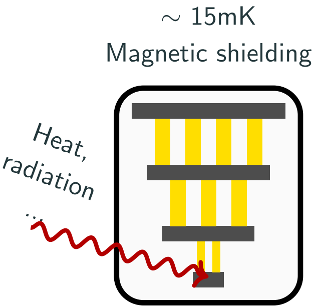
$\sim$ 15mK

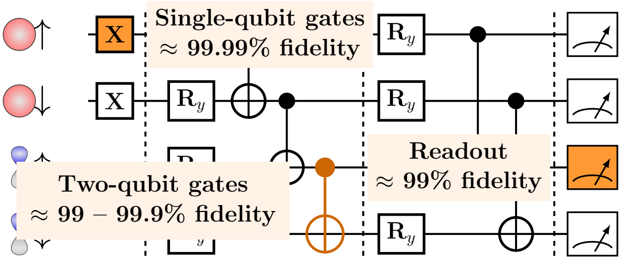
Magnetic shielding





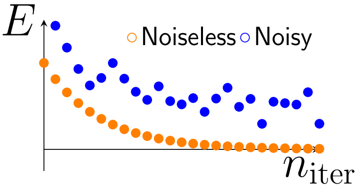




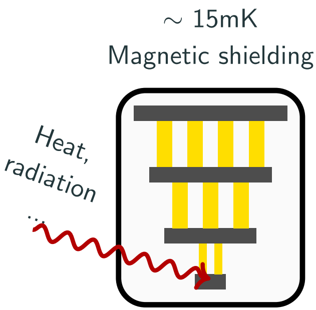


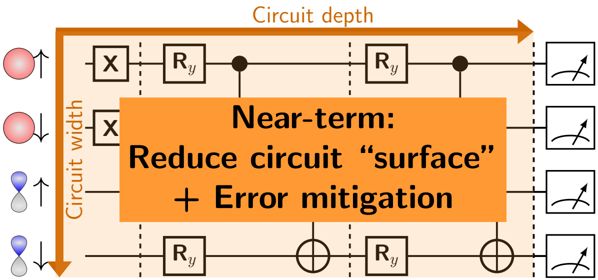
Effect of noise:

- Bit flip: $|0\rangle \leftrightarrow |1\rangle$
- Phase flip: $|0\rangle \leftrightarrow -|0\rangle$
- Decoherence: $|0\rangle + |1\rangle \rightarrow |0\rangle + e^{i?}|1\rangle$
- ...



Quantum Chemistry on Quantum Hardware





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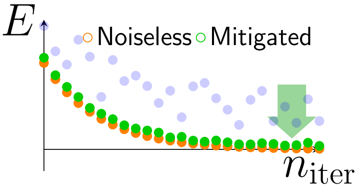
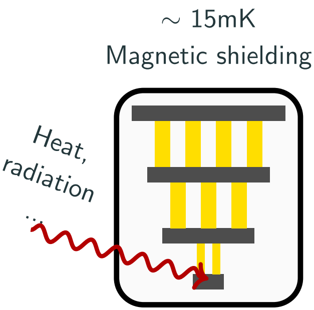
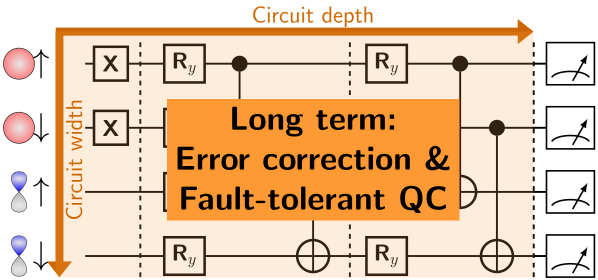


Quantum Chemistry on Quantum Hardware

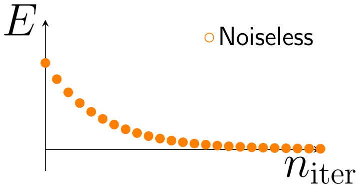




Use many physical qubits to encode a logical qubit:

$11111 \to 1$ $\quad\quad$ $11\mathbf{0}11 \to 1$

$00000 \to 0$ $\quad\quad$ $0\mathbf{1}000 \to 0$



Possible Quantum Advantage – Quantum Phase Estimation

Unitary op. Phase

$$\hat{U}|\Psi\rangle = e^{i\theta}|\Psi\rangle$$

Eigenstate

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Schrödinger eq.

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

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$$\downarrow$$

$$\mathrm{e}^{-i\hat{H}t}|\Psi\rangle = \mathrm{e}^{-iEt}|\Psi\rangle$$

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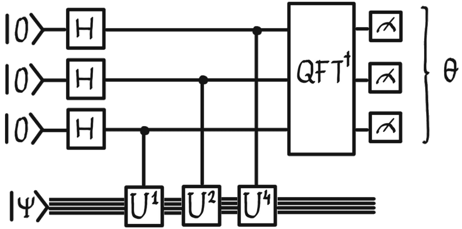

No matrix diagonalization!

Subroutine of Shor's algorithm

Schrödinger eq.

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

$$\downarrow$$

$$e^{-i\hat{H}t}|\Psi\rangle = e^{-iEt}|\Psi\rangle$$

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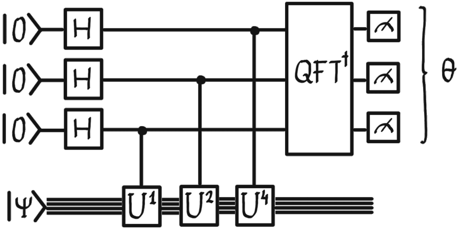

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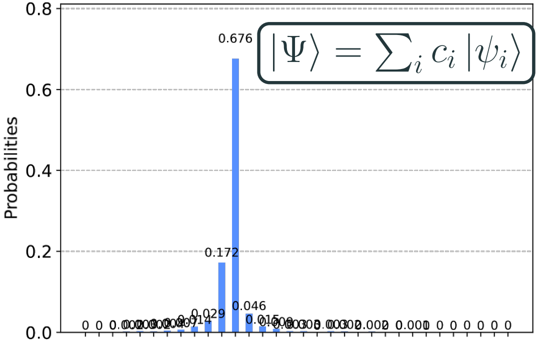

$$|\Psi\rangle = \sum_i c_i\,|\psi_i\rangle$$

Possible Quantum Advantage – Quantum Phase Estimation

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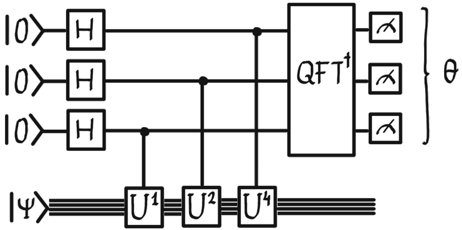
Eigenstate



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Schrödinger eq.

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

$$\downarrow$$

$$e^{-i\hat{H}t}|\Psi\rangle = e^{-iEt}|\Psi\rangle$$

- Many qubits, deep circuits → requires error corrected quantum devices
- State preparation: how to get good approximations of $|\Psi\rangle$?

Transition toward fault-tolerance

NISQ:

- Noisy and small quantum devices
- Limited utility
- Hybrid approaches

Fault-tolerant QC:
Quantum advantage

- Shor's algorithm
- Quantum phase estimation

Transition toward fault-tolerance

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Continuous transition to fault-tolerant QC:

- Develop intuition on quantum algorithm development
- Transferability of developed algorithms to FT regime
- Feedback for experimentalists to improve devices

– Near-term utility and relevant applications
– No need for 'quantum for everything'

Fault-tolerant QC:

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Fault-tolerant QC:

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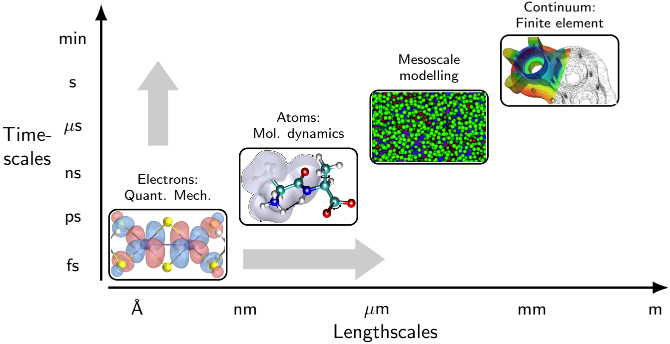
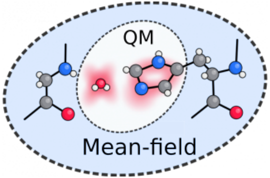
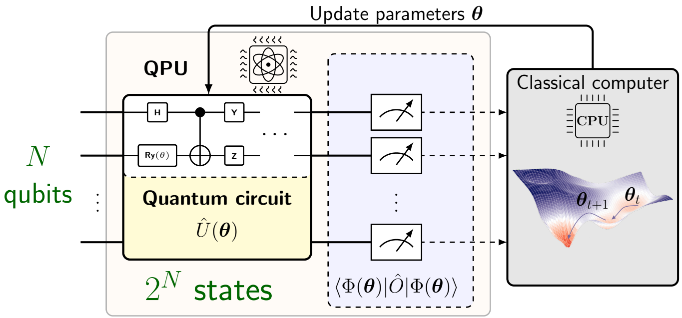




Near-term approaches and our work

NISQ Era – Hybrid Quantum-Classical Approach

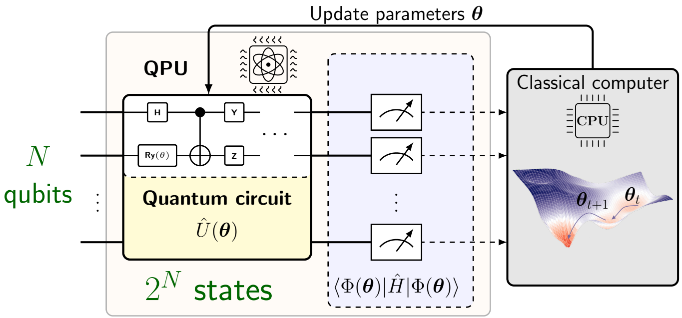
Use benefits of both quantum and classical resources



- Use short-depth quantum circuits that fit current hardware
- Improve on classical estimates by non-classical states
- Store quantum state with exponentially fewer resources

NISQ Era – Hybrid Quantum-Classical Approach

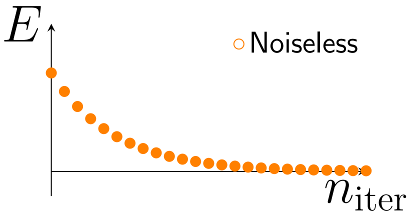
Use benefits of both quantum and classical resources



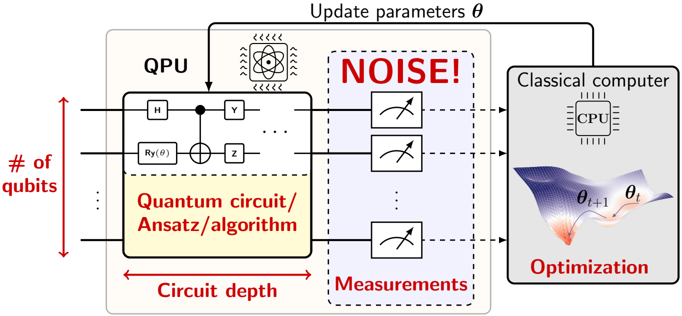
Variational Quantum Eigensolver

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

Quantum Imaginary Time Evolution



Use benefits of both quantum and classical resources



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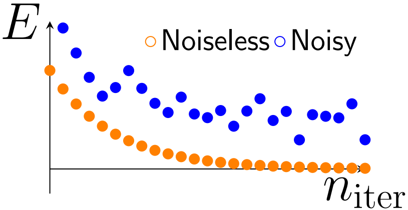
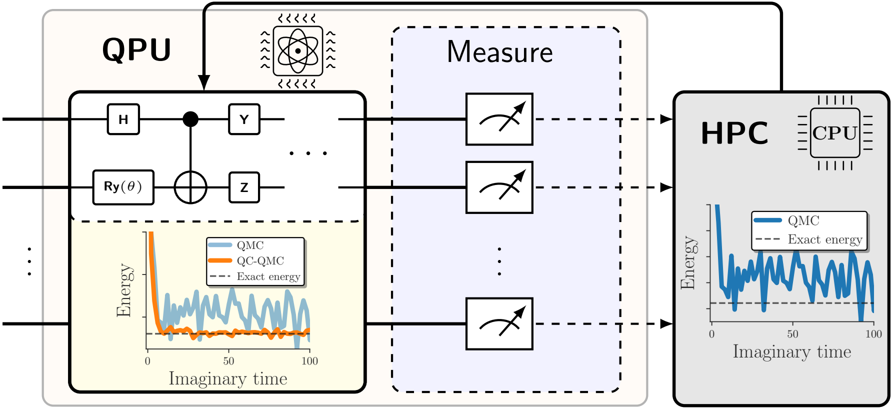


State-of-the-art

Quantum-enhanced QMC methods:

– Use the QPU to alleviate **computational bottlenecks** of conventional QMC methods

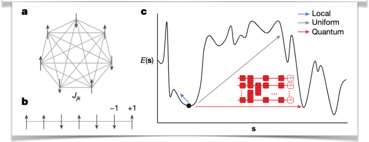


State-of-the-art – Quantum Computing Quantum Monte Carlo

Quantum-enhanced Markov chain Monte Carlo

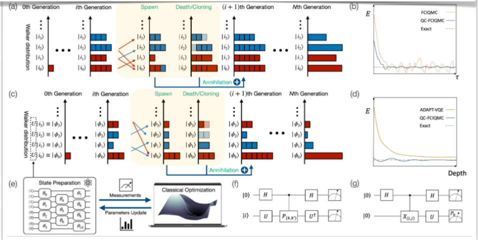
David Layden, Guglielmo Mazzola, Ryan V. Mishmash, Mario Motta, Pawel Wocjan, Jin-Sung Kim & Sarah Sheldon

Nature 619, 282–287 (2023) | Cite this article



Quantum Computing Quantum Monte Carlo

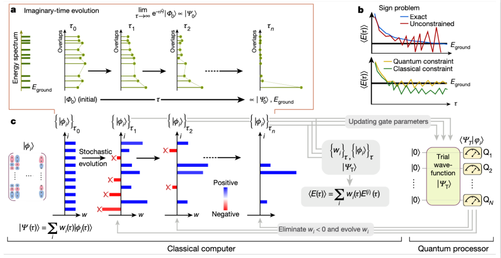
Yukun Zhang,[1,2,*] Yifei Huang,[3,*] Jinzhao Sun,[4,5] Dingshun Lv,[3] and Xiao Yuan[1,2,†]
[1] Center on Frontiers of Computing Studies, Peking University, Beijing 100871, China
[2] School of Computer Science, Peking University, Beijing 100871, China
[3] ByteDance Research, Zhonghang Plaza, No. 43, North 3rd Ring West Road, Haidian District, Beijing, China
[4] Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU, United Kingdom
[5] Quantum Advantage Research, Beijing 100080, China



Unbiasing fermionic quantum Monte Carlo with a quantum computer

William J. Huggins, Bryan A. O'Gorman, Nicholas C. Rubin, David R. Reichman, Ryan Babbush & Joonho Lee

Nature 603, 416–420 (2022) | Cite this article



Classical and quantum trial wave functions in auxiliary-field quantum Monte Carlo applied to oxygen allotropes and a $CuBr_2$ model system

Maximilian Amsler; Peter Deglmann; Matthias Degroote; Michael P. Kaicher; Matthew Kiser; Michael Kühn; Chandan Kumar; Andreas Maier; Georgy Samsonidze; Anna Schroeder; Michael Streif; Davide Vodola; Christopher Wever; QUTAC Material Science Working Group

State-of-the-art – Subspace Expansion Methods

$$\hat{H}|\Psi\rangle = E|\Psi\rangle \qquad \longrightarrow \qquad \mathsf{span}\{|\psi\rangle, \hat{H}|\psi\rangle, \hat{H}^2|\psi\rangle, \dots\}$$

State-of-the-art – Subspace Expansion Methods

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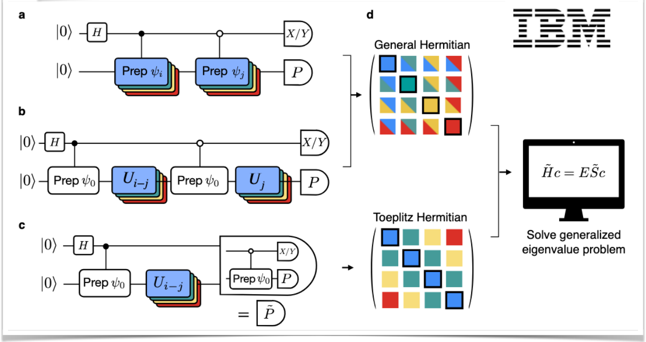
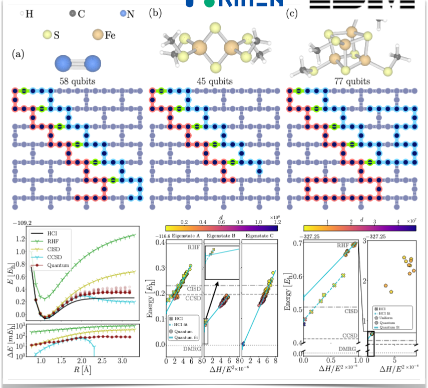
Diagonalization of large many-body Hamiltonians on a quantum processor

Nobuyuki Yoshioka*,[1,†] Mirko Amico*,[2,‡] William Kirby*,[3,§] Petar Jurcevic,[2] Arkopal Dutt,[3] Bryce Fuller,[2] Shelly Garion,[4] Holger Haas,[2] Ikko Hamamura**,[5] Alexander Ivrii,[4] Ritajit Majumdar,[6] Zlatko Minev,[2] Mario Motta,[2] Bibek Pokharel,[7] Pedro Rivero,[2] Kunal Sharma,[2] Christopher J. Wood,[2] Ali Javadi-Abhari,[2] and Antonio Mezzacapo[2]



Chemistry Beyond Exact Solutions on a Quantum-Centric Supercomputer

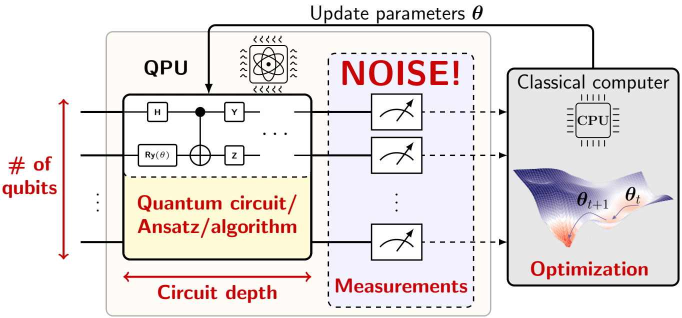
Javier Robledo-Moreno,[1,*] Mario Motta,[1,†] Holger Haas,[1] Ali Javadi-Abhari,[1] Petar Jurcevic,[1] William Kirby,[2] Simon Martiel,[3] Kunal Sharma,[1] Sandeep Sharma,[4] Tomonori Shirakawa,[5,6,7] Iskandar Sitdikov,[1] Rong-Yang Sun,[5,6,7] Kevin J. Sung,[1] Maika Takita,[1] Minh C. Tran,[2] Seiji Yunoki,[5,6,7,8] and Antonio Mezzacapo[1,‡]



Our work

Hybrid Quantum-Classical Approach

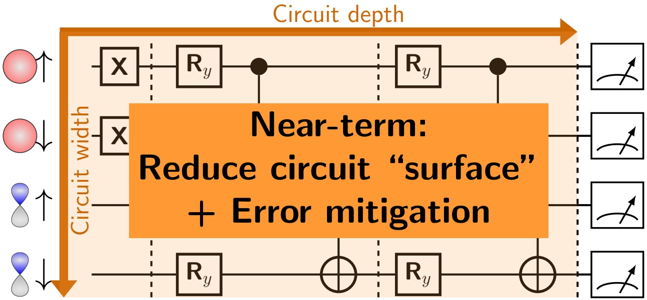
Use benefits of both quantum and classical resources



- Algorithms:
  Quantum imaginary time evolution (QITE)
- Classical optimization
- Resource reduction:
  Qubits and circuit depth
- Error mitigation

Hybrid Quantum-Classical Approach

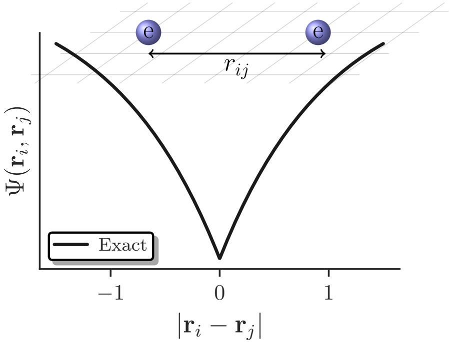
Use benefits of both quantum and classical resources



- Algorithms:
  Quantum imaginary time evolution (QITE)
- Classical optimization
- **Resource reduction: Qubits and circuit depth**
- **Error mitigation**

Resource Reduction: Qubits and circuit depth

Cusp condition: Singularity of Coulomb potential ($\sim \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$)
$\rightarrow$ sharp cusp of exact wavefunction $\Psi(\{\mathbf{r}\})$ at electron coalescence ($|\mathbf{r}_i - \mathbf{r}_j| = 0$)



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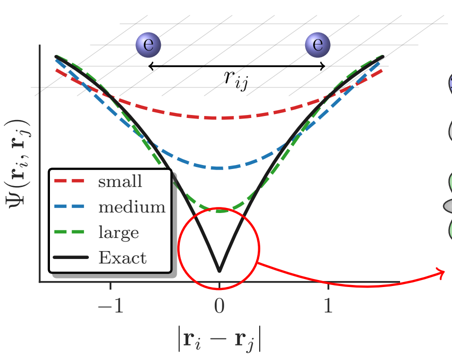

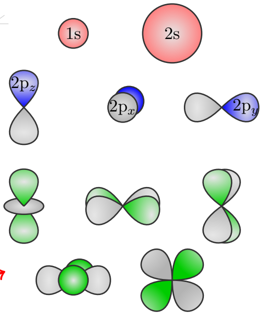

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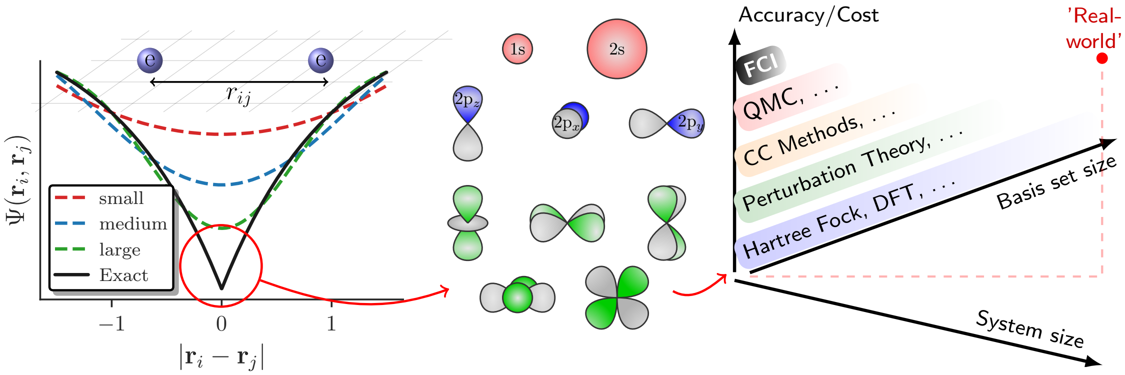

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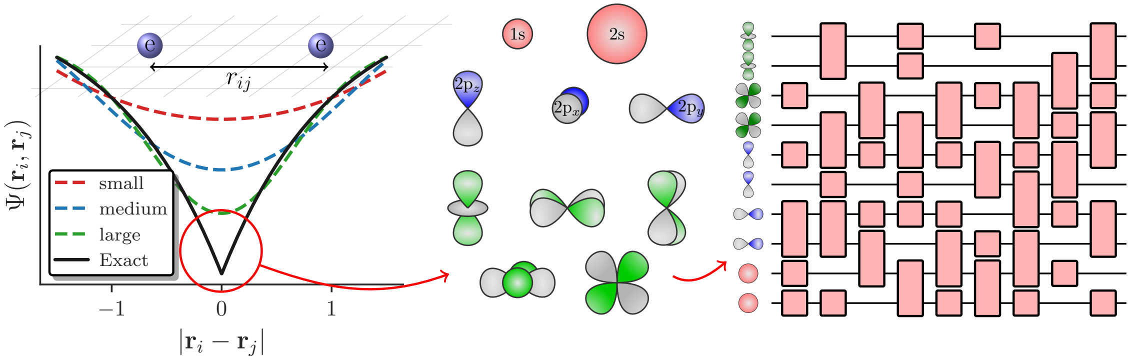
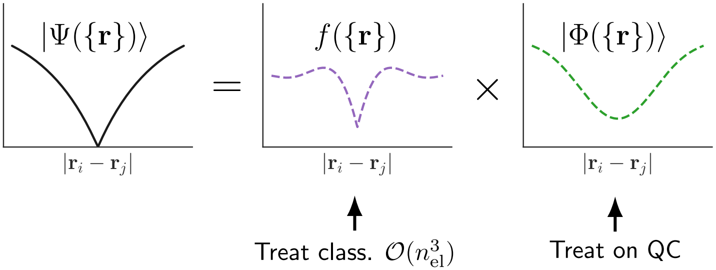


Resource Reduction: Transcorrelation (TC)



WD, Luo, Alavi, PRB **99** (7), 075119 (2019); Cohen, Luo, Guther, **WD**, Tew, Alavi, JCP **151** (6), 061101 (2019);

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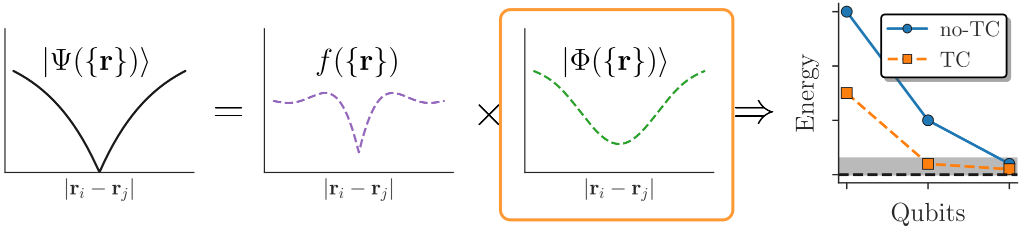

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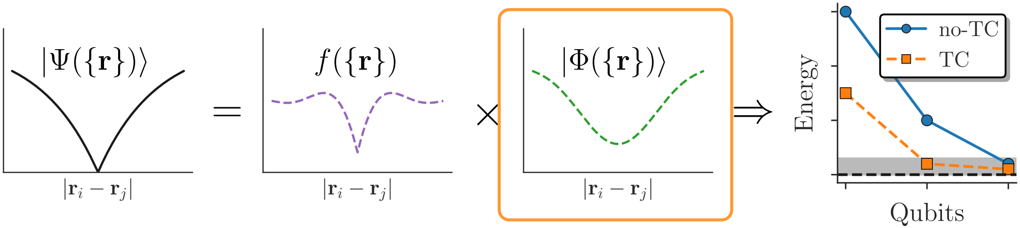
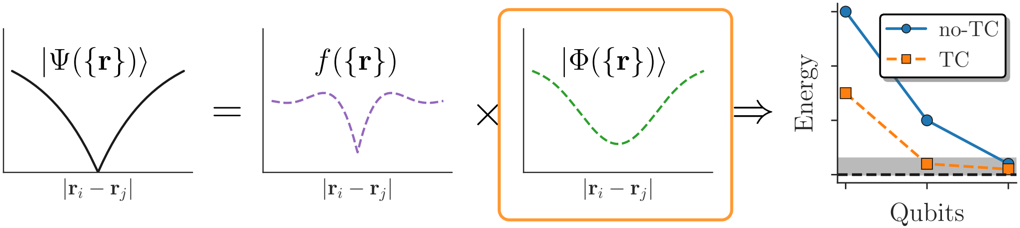


$$\hat{H}|\Psi\rangle = E|\Psi\rangle \quad \rightarrow \quad |\Psi\rangle = f|\Phi\rangle \quad \rightarrow \quad \overbrace{f^{-1}\hat{H}f}^{\hat{H}_{\mathrm{TC}}}|\Phi\rangle = E|\Phi\rangle$$

WD, Luo, Alavi, PRB **99** (7), 075119 (2019); Cohen, Luo, Guther, **WD**, Tew, Alavi, JCP **151** (6), 061101 (2019);

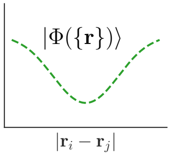
Resource Reduction: Transcorrelation (TC)



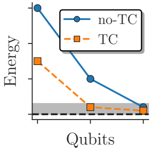
$$\hat{H}\,|\Psi\rangle = E\,|\Psi\rangle \quad \rightarrow \quad |\Psi\rangle = f\,|\Phi\rangle \quad \rightarrow \quad \overbrace{f^{-1}\hat{H}f}^{\hat{H}_{\text{TC}}}\,|\Phi\rangle = E\,|\Phi\rangle$$

$|\Phi\rangle$ easier to represent with less basis functions/qubits $\rightarrow$ immense resource reduction

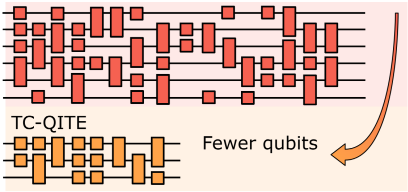
WD, Luo, Alavi, PRB **99** (7), 075119 (2019); Cohen, Luo, Guther, **WD**, Tew, Alavi, JCP **151** (6), 061101 (2019);



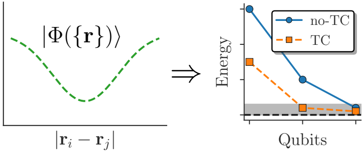
$\Rightarrow$



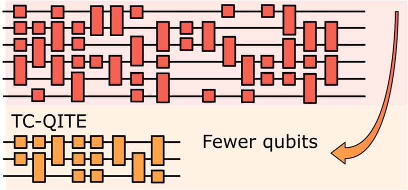
Smaller basis $\rightarrow$ fewer qubits



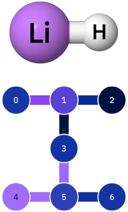
Quantum Computing – Resource Reduction – Transcorrelation

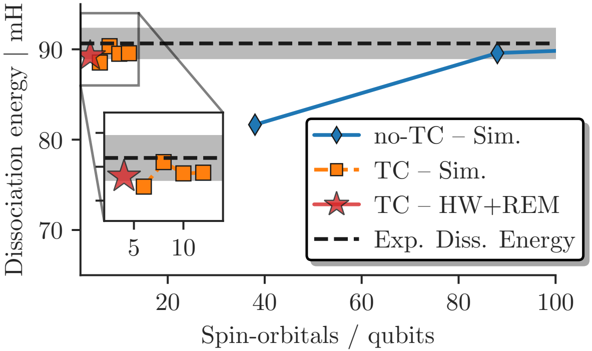


Smaller basis → fewer qubits

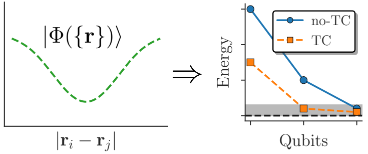


Towards real chemical accuracy on current quantum hardware through the transcorrelated method, J. Chem. Theory Comput. **20**, 10, 4146 (2024)
W. Dobrautz, I. O. Sokolov, K. Liao, P. Lopez Rios, M. Rahm, A. Alavi, I. Tavernelli





Quantum Computing – Resource Reduction – Transcorrelation



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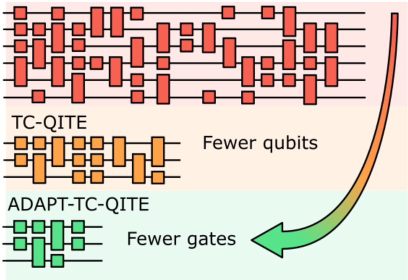

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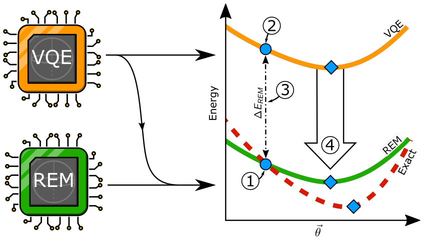
Reducing quantum circuit depth for noise-resilient quantum chemistry, E. Magnusson, A. Fitzpatrick, S. Knecht, M. Rahm, **W. Dobrautz**, **Faraday Discussions** on *Correlated Electronic Structure* (2024)

Quantum Computing – Reference-state Error Mitigation (REM)

Reference-State Error Mitigation: A Strategy for High Accuracy Quantum Computation of Chemistry, *J. Chem. Theory Comput.*, **19**, 3, 783 (2023)

P. Lolur, M. Skogh, **W. Dobrautz**, C. Warren, J. Biznárová, A. Osman, G. Wendin, J. Bylander, M. Rahm



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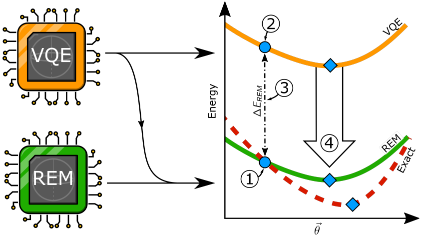

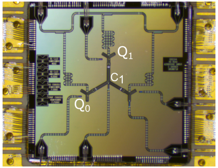

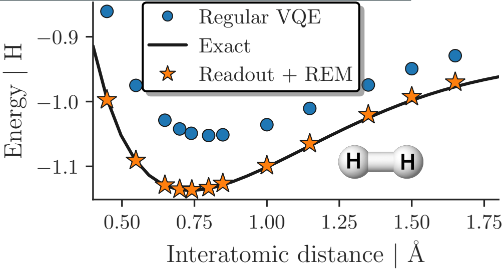

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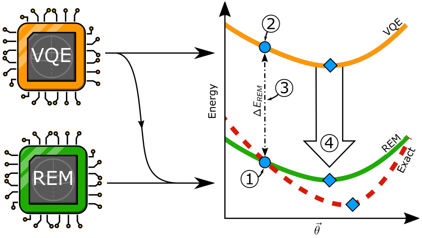
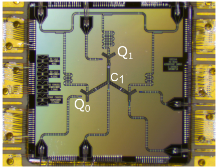
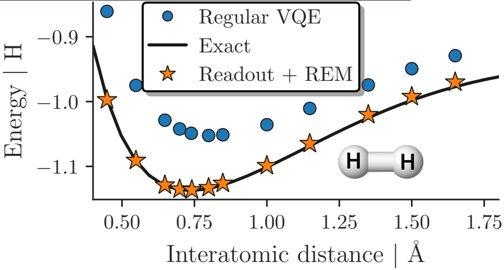
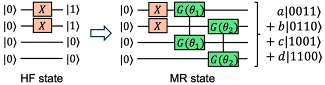






— **Multireference-state error mitigation for strong correlation**,

H. Zou, E. Magnusson, H. Brunander, M. Rahm, **W. Dobrautz**, *to be submitted*



Quantum Computing – Reference-state Error Mitigation (REM)

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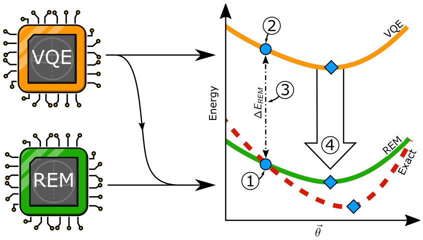

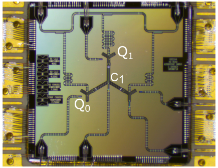

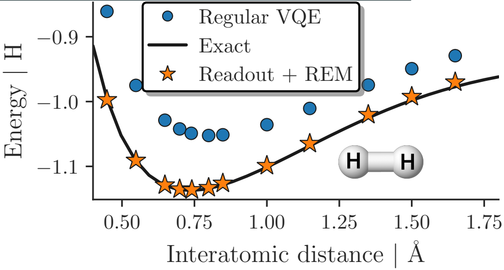

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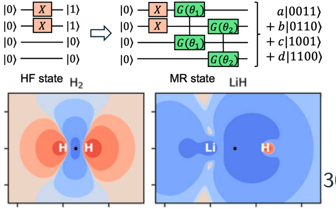


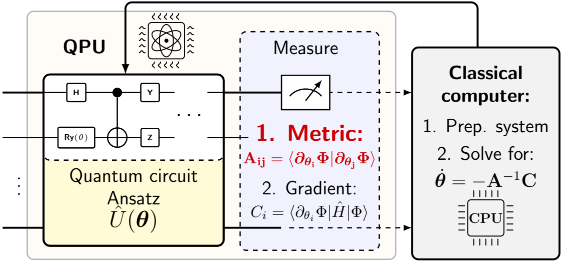
— **Electron density**: M. Skogh, P. Lolur, **W. Dobrautz**, C. Warren, J. Biznárová, A. Osman, G. Tancredi, J. Bylander, M. Rahm, Chemical Science **15**, 2257 (2024)

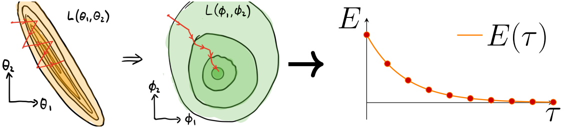
Quantum Computing – Algorithms and Classical Optimization

Orders of magnitude increased accuracy for quantum many-body problems on quantum computers via an exact transcorrelated method, *Phys. Rev. Research* **5**, 023174 (2023), I. O. Sokolov*, **W. Dobrautz***, H. Luo, A. Alavi, I. Tavernelli

Variational Quantum Imaginary Time Evolution:

Update parameters $\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k + \Delta\tau\dot{\boldsymbol{\theta}}$





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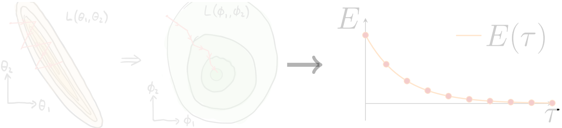

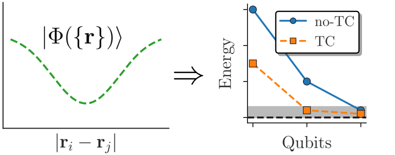

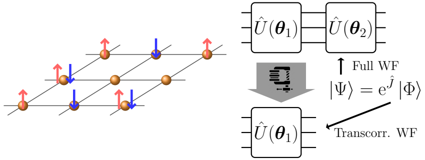

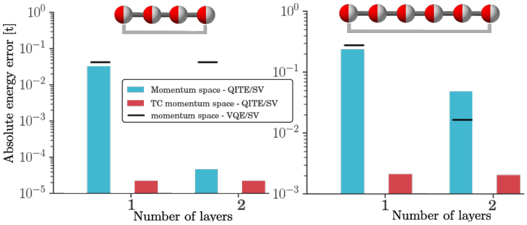

Quantum Computing – Algorithms and Classical Optimization

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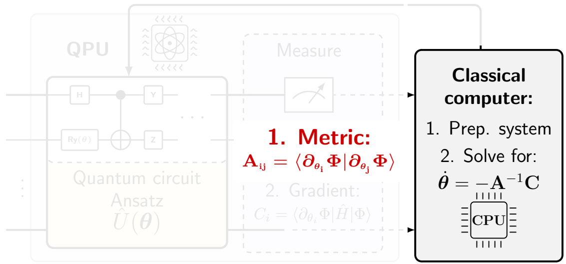
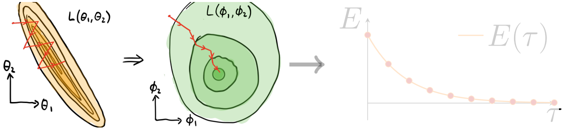
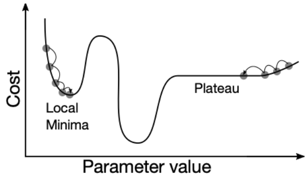
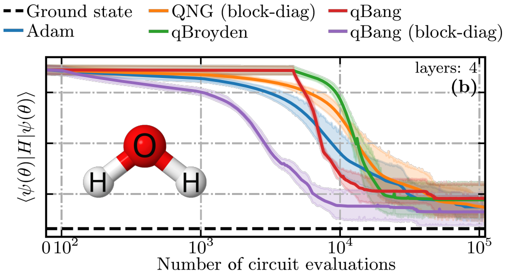




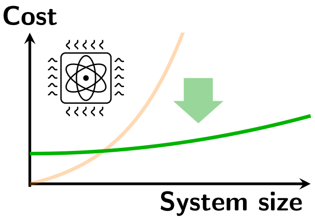
Optimizing Variational Quantum Algorithms with qBang: Efficiently Interweaving Metric and Momentum to Tackle Flat Energy Landscapes, D. Fitzek, R. S. Jonsson, **W. Dobrautz**, C Schäfer, Quantum **8**, 1313 (2024)



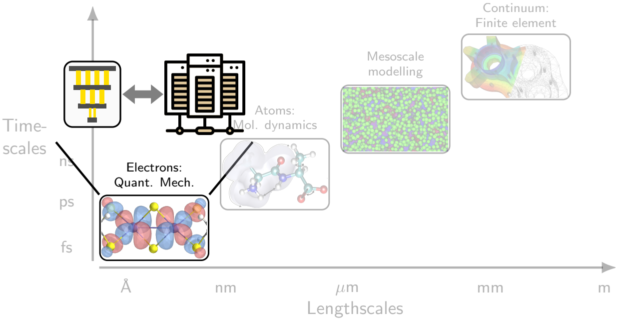


Conclusion and Outlook

Conclusion

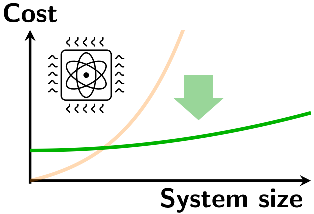


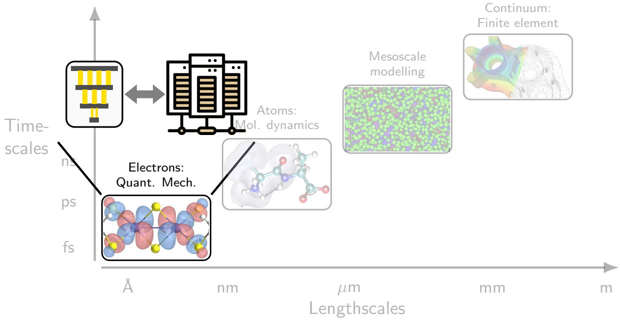
Cost
System size

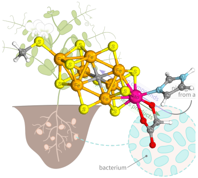


Continuum:
Finite element
Mesoscale
modelling
Atoms:
Mol. dynamics
Electrons:
Quant. Mech.
Time-
scales
ns
ps
fs
Å
nm
μm
mm
m
Lengthscales

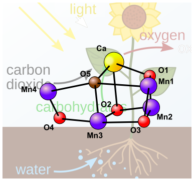
Conclusion



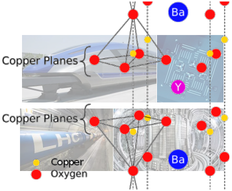




Nitrogen fixation



Artificial photosynthesis



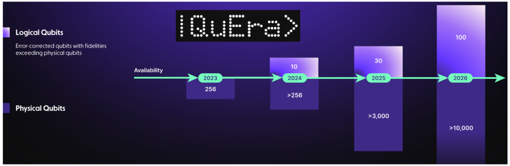
High-T$_c$ superconductivity

- Drug discovery
- Materials design
- Battery development
- ...

Quantum Hardware Roadmaps

IBM

Heron (5K)	Flamingo (5K)	Flamingo (7.5K)	Flamingo (10K)	Flamingo (15K)	Starling (100M)
Error Mitigation	Error Mitigation	Error Mitigation	Error Mitigation	Error Mitigation	Error correction
5k gates 133 qubits	5k gates 156 qubits	7.5k gates 156 qubits	10k gates 156 qubits	15k gates 156 qubits	100M gates 200 qubits
Classical modular	Quantum modular	Quantum modular	Quantum modular	Quantum modular	Error corrected modularity
133x3 = 399 qubits	156x7 = 1092 qubits	156x7 = 1092 qubits	156x7 = 1092 qubits	156x7 = 1092 qubits	

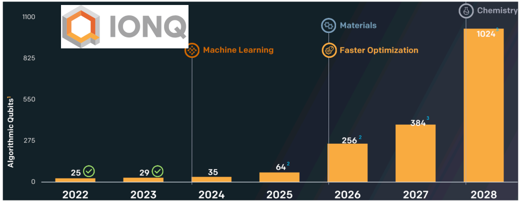


PASQAL

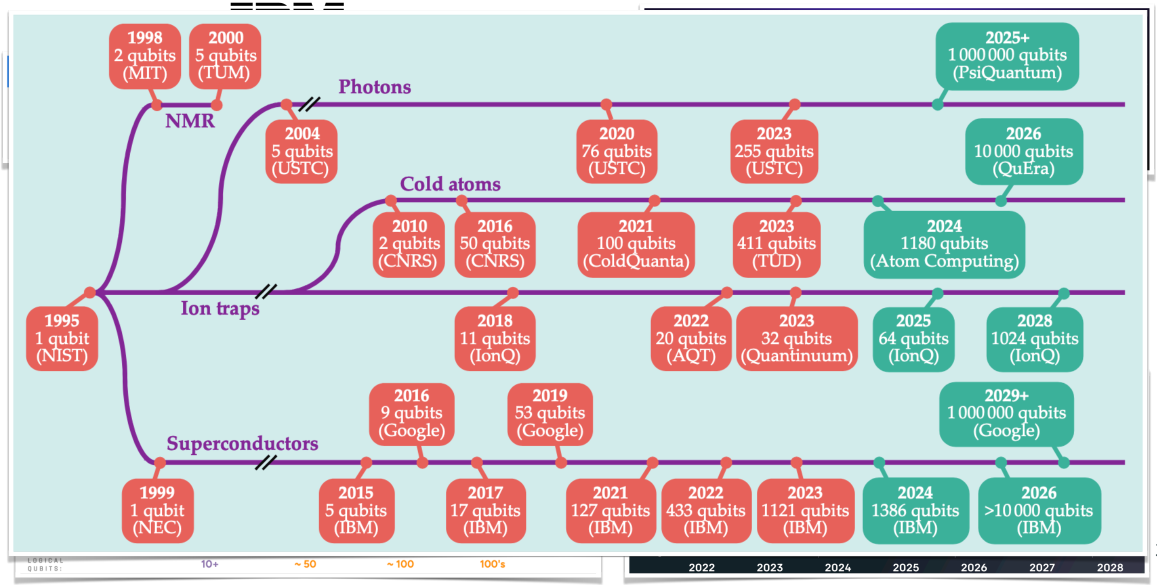
HARDWARE PLATFORM	2022 - 2023	2024 - 2025	2026 - 2027
Max qubits	200	1,000	10,000
Addressability	Z add	Z+X add	Addressable 1Q and 2Q gates
Base repetition rate	1 Hz	3 Hz	10 Hz

QUANTINUUM

	2020	2023	2025	2027	2029
SYSTEMS:	H1	H2	HELIOS	SOL	APOLLO
PHYSICAL QUBITS:	20	56	96	192	1000's
PHYSICAL 2-QUBIT GATE ERROR:	1×10^{-3}	1×10^{-3}	$< 5 \times 10^{-4}$	$< 2 \times 10^{-4}$	1×10^{-4}
LOGICAL QUBITS:		10+	~ 50	~ 100	100's



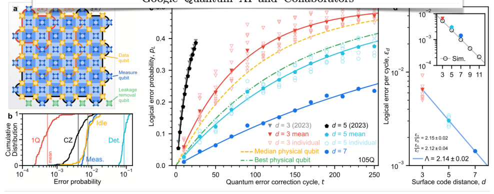
Quantum Hardware Roadmaps



Quantum Error Correction

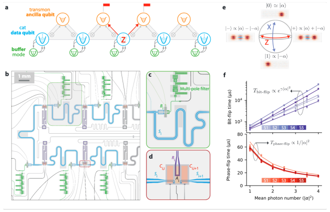
Quantum error correction below the surface code threshold

Google Quantum AI and Collaborators



Hardware-efficient quantum error correction using concatenated bosonic qubits

amazon | science

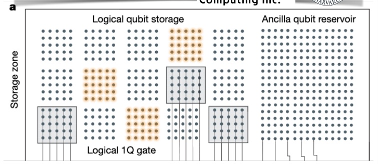


Logical quantum processor based on reconfigurable atom arrays

Dolev Bluvstein, Simon J. Evered, Alexandra A. Geim, Sophie H. Li, Hengyun Zhou, Tom Manovitz, Sepehr Ebadi, Madelyn Cain, Marcin Kalinowski, Dominik Hangleiter, J. Pablo Bonilla Ataides, Nishad Maskara, Iris Cong, Xun Gao, Pedro Sales Rodriguez, Thomas Karolyshyn, Giulia Semeghini, Michael J. Gullans, Markus Greiner, Vladan Vuletić & Mikhail D. Lukin

Nature 626, 58–65 (2024) | Cite this article

QuEra Computing Inc.



High-fidelity teleportation of a logical qubit using transversal gates and lattice surgery

C. RYAN-ANDERSON, N. C. BROWN, C. H. BALDWIN, J. M. DREILING, C. FOLTZ, J. P. GAEBLER, T. M. GATTERMAN, N. HEWITT, C. HOLLIMAN, [...] AND D. HAYES +14 authors Authors Info & Affiliations

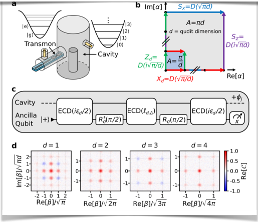
SCIENCE • 19 Sep 2024 • Vol 385, Issue 6715 • pp. 1327-1331 • DOI: 10.1126/science.adp6016

QUANTINUUM

Quantum Error Correction of Qudits Beyond Break-even

Benjamin L. Brock,* Shraddha Singh, Alec Eickbusch,† Volodymyr V. Sivak,† Andy Z. Ding, Luigi Frunzio, Steven M. Girvin, and Michel H. Devoret‡

Departments of Applied Physics and Physics, Yale University, New Haven, CT, USA
Yale Quantum Institute, Yale University, New Haven, CT, USA



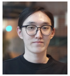
Acknowledgments

algorithmiq

S. Knecht
Adaptive QITE
IC-POVMs

WACQT OpenSuperQPlus



M. Rahm, E. Magnusson, M. Skogh, H. Zou,
P. Lolur,, C. Schäfer, J. Bylander . . .
TC+QC for Chemistry, Error mitigation, experiments

VOLVO D. Fitzek, Class. Opt.

SORBONNE UNIVERSITÉ

E. Giner
efficient TC,
Paris

PASQAL

I. Sokolov,
TC and QITE

MAX PLANCK INSTITUTE
FOR SOLID STATE RESEARCH



A. Alavi, G. Li Manni, P. Lopez Rios, . . .
QMC on HPCs, TC, TM clusters

IBM Research | Zurich


I. Tavernelli, M. Rossmannek,
TC for QC

Funding:

CHALMERS
UNIVERSITY OF TECHNOLOGY

MARIE CURIE ACTIONS

Wallenberg Centre for Quantum Technology

IBM
Academic Network

Thank you for your attention!