

Chemistry Meets Quantum Computing: A New Era of Simulation and Study

SmallTalks [about Nanoscience]

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Chemistry and Chemical Engineering,
Chalmers University of Technology

Gothenburg, June 1, 2023



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- **Part I:** Motivation – take-home messages
 - Computational chemistry
 - The case for quantum computing
- **Part II:** Motivation: Quantum chemistry
 - Reducing hardware requirements with the **transcorrelated** method
 - Applications: Reducing the number of qubits for chemistry
 - Conclusions and outlook

Learning goals:

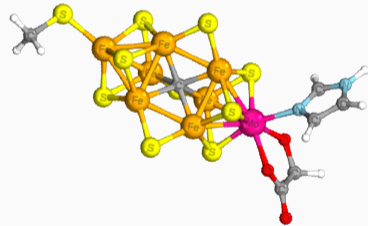
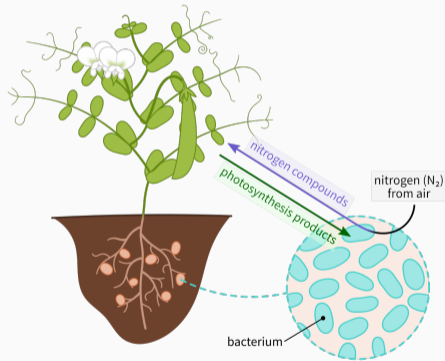
- What is **computational chemistry**?
- Why is it worthwhile?
- Why do we need computers for chemistry?
- Why and how could **quantum computing** help?

Why is it worthwhile?

Surprisingly small molecules responsible for fascinating
physical and chemical effects

Nitrogen fixation

Conversion of molecular nitrogen, N_2 , to ammonia, NH_3 , → important for fertilizers
Haber-Bosch process: **1-2% of global energy consumption**, huge CO_2 emission

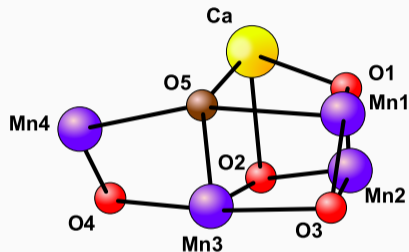
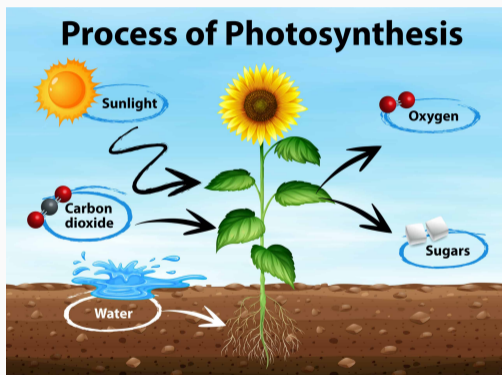


Iron-sulfur clusters

Artificial nitrogen fixation for cheaper and cleaner ammonia production for fertilizers

Photosynthesis

Conversion of solar energy into chemical energy



Manganese-Calcium-Oxygen Clusters

Artificial photosynthesis for carbon capture and hydrogen and oxygen for fuel cells

Scientific method

- We want a **theoretical understanding** of these phenomena and explain the physical and chemical behavior of these systems
- We want to derive a mathematical description/model
- We want to test the validity of these models and compare with experiments
- We want to predict properties of new materials based on our models

✓ Mathematical description possible! Schrödinger equation

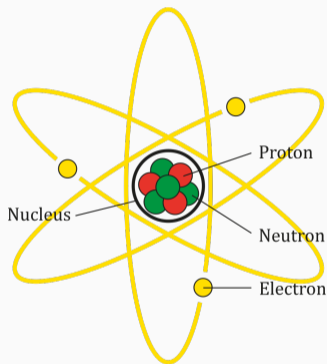
⚡ Too complex and impossible to solve exactly/analytically! Need computers to **approximately** solve the equations! → computational chemistry.

~**30%** of **high-performance computing** used for chemistry-related problems

Computational chemistry

How do we describe these phenomena?

Atoms – the building blocks of nature

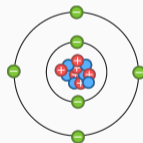
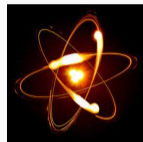


- If we knew the **position** and **motion** of all electrons and nuclei **at all times** we could describe the systems behavior and properties.
- Due to the size of the particles → **quantum effects**. We **can not** know the position and motion/momentum exactly at the same time. Heisenberg uncertainty relation/particle-wave duality.
- We can use **quantum mechanics** and write down an equation to describe the behavior of the system!

Ingredients – what do we need?

We want an equation to describe the behavior of our system. How it evolves with time.

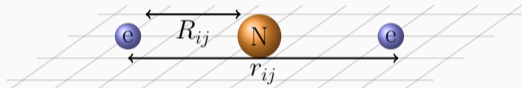
1. Nuclei **much heavier** than electrons (1000 fold) → assume nuclei fixed!
2. Motion of electrons → **kinetic energy**
3. Negative charged electrons attracted to positive charged nuclei
4. Negative charged electrons repel each other! ⚡
→ movement and position of all electrons depend on each other! It is a **correlated problem!**



Schrödinger equation

Ingredients to describe the behavior of the electrons of our system

$$\hat{H} = T_{\text{Kinetic}}(\mathbf{r}) + V_{\text{Attraction}}(\mathbf{r}, \mathbf{R}) + V_{\text{Repulsion}}(\mathbf{r}, \mathbf{r}')$$



Current state of all the electrons at time t described by the so-called wavefunction:

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_n; t)$$

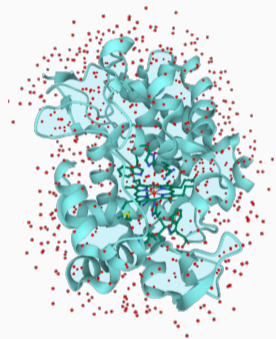
Schrödinger equation describes the change of the system with time t :

$$i \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = \hat{H} \Psi(\mathbf{r}, t)$$

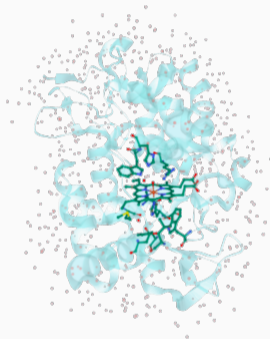
The case for quantum computing

Problem: Nature is very complex

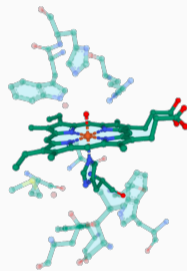
Cytochrome c: enzyme that eliminates toxic radicals (O_2^- , H_2O_2) produced by cells



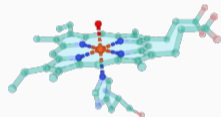
Cytochrome c in solution



Binding site



Heme group

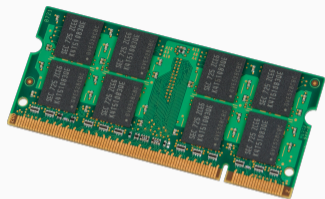


Iron cluster

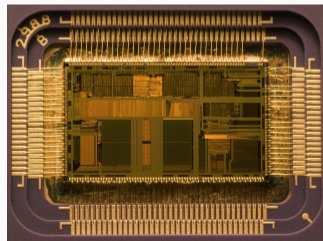
Exact solution scales **exponential!** > 20 electrons $> \sim 100$ GB information!

→ can not even store wavefunction in computer memory

How is information stored and handled on a computer?



RAM



CPU

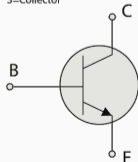
- Modern electronics are based on **transistors**, which can be seen as electronic switches that are either “off” or “on”; **0** or **1**.
- A logical state with **two** possible values: **a bit**.
- These **bits** of information can either store data (RAM/harddrive) or control operations (CPU)

Transistor



1 2 3

1=Emitter
2=Base
3=Collector



0011

0101

0110

1001

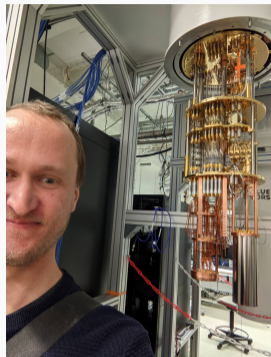
1010

1100

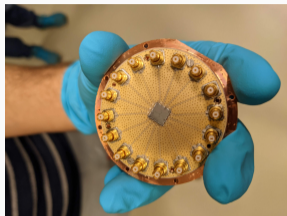
...

} # of states

Quantum Bits – Qubits

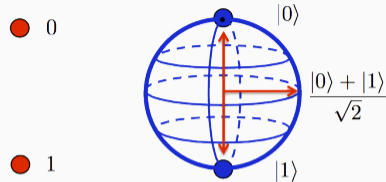


@ Chalmers



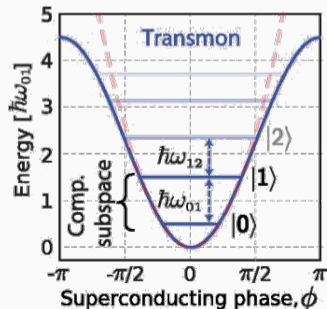
3 qubit device @Chalmers

Qubits can be both $|0\rangle$ and $|1\rangle$.



Classical Bit

Qubit



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

Quantum bits (qubits) can be in a **superposition** of both $|0\rangle$ and $|1\rangle$

Bringing together **two** qubits:

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

Three qubits:

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

n qubits can encode exponentially many (2^n) states.

→ Need new **quantum algorithms** to use this potential advantage!

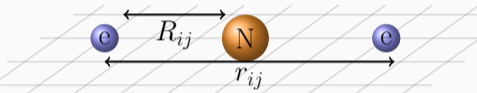
Part II

- **Part I:** Motivation – take-home messages
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Ab Initio Quantum Chemistry – Electronic Structure Theory

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

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



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

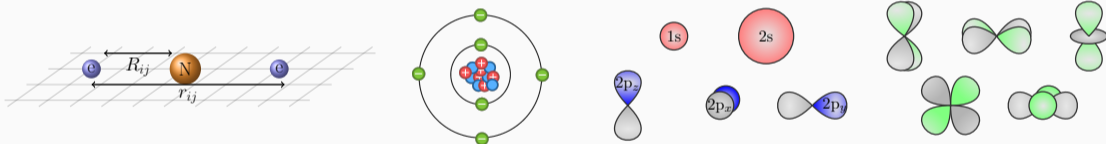
Target: High / “chemical accuracy” to ensure predictability, interpretability and comparison with experimental results

Task: Solve the Schrödinger equation derived from first principles:

$$\hat{H} |\Psi(\mathbf{r}_1, \dots, \mathbf{r}_n)\rangle = E_0 |\Psi(\mathbf{r}_1, \dots, \mathbf{r}_n)\rangle$$

Ab Initio Quantum Chemistry – Electronic Structure Theory

We have to choose a numerical **basis/orbitals** to perform our calculations in! In comp. chemistry: orbitals are smooth, “atomic-like” orbitals (for each atom):

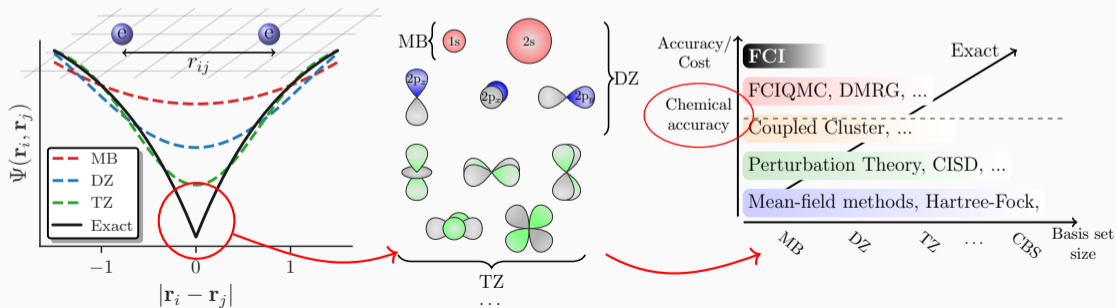


For accurate results we need **dozens to hundreds** of orbitals per atom!

Problems for accurate description: Cusp condition

Cusp condition: Singularity of Coulomb potential, $\frac{1}{r_{ij}}$, for $r_{ij} = 0$
 → sharp cusp of exact wavefunction $\Psi(\{\mathbf{r}\})$ at electron coalescence ($r_{ij} = 0$)

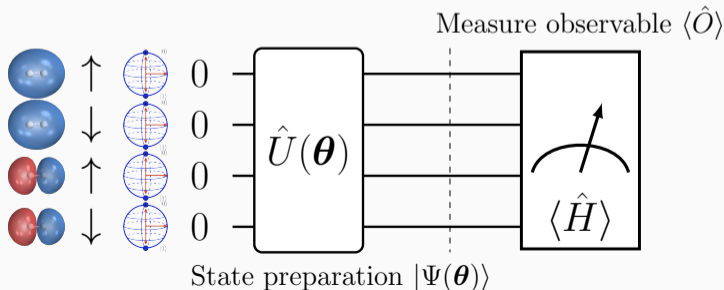
$$\hat{H} = -\sum_{I,j} \frac{Z_I}{|\mathbf{R}_I - \mathbf{r}_j|} - \frac{1}{2} \sum_i \nabla_{\mathbf{r}_i}^2 + \frac{1}{2} \sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}, \quad \hat{H} |\Psi(\{\mathbf{r}\})\rangle = E_0 |\Psi(\{\mathbf{r}\})\rangle$$





Digital Quantum Simulation/Computation

1. Map fermionic Hamiltonian onto quantum hardware/qubits
2. Use quantum algorithms to solve the problem at hand

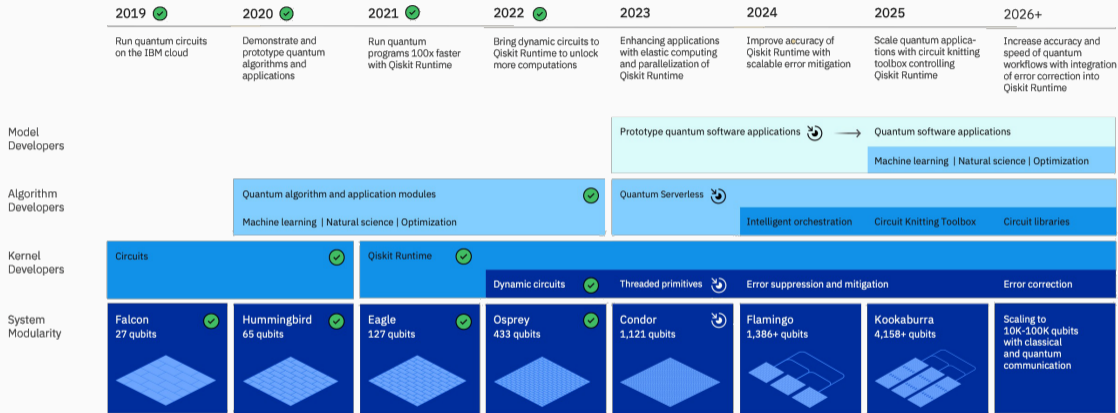
Circuit model: Lines/wires represent qubits encoding the **occupation** (0-1) of the associated spin-orbital. Similar to classical circuits (AND, OR, ...) we can act with **operations/gates** on one or more qubits. For quantum computers have to be **reversible/unitary operations** $\hat{U}(\theta) \rightarrow$ prepare **entangled** target state $|\Psi(\theta)\rangle$.



Development Roadmap

Executed by IBM 
On target 

IBM Quantum



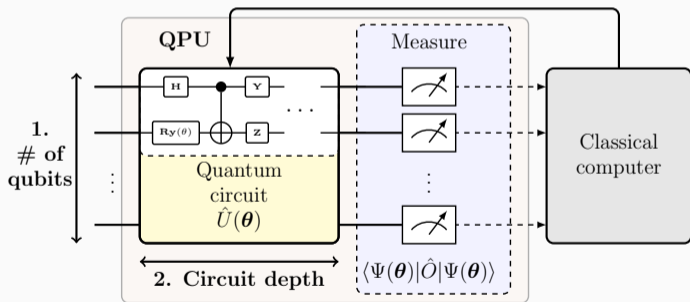
Chalmers next-gen chip: 25 qubits, compared to **billions** of transistors in current CPUs! Only small problems currently tractable on quantum devices

Overview: 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:

Update parameters θ

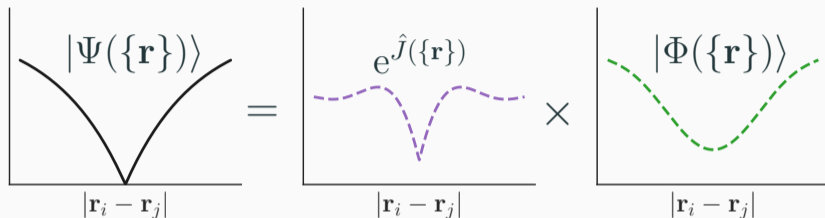


- Use pros of both classical and quantum hardware
- Use **short-depth quantum circuits** that fit current hardware
- Can **improve on classical estimates** by non-classical states
- Store quantum state with **exponentially fewer resources**

Need two qubits per orbital \rightarrow only very small, inaccurate chemistry calculations possible!

Reducing hardware requirements with the
transcorrelated method

Cusp Condition – Explicitly Correlated Ansatz



Describe the cusp exactly and capture part of correlation with a **correlated (Jastrow) wavefunction Ansatz**

$$|\Psi(\{\mathbf{r}\})\rangle = e^{\hat{J}} |\Phi(\{\mathbf{r}\})\rangle, \quad \text{with} \quad \hat{J}(\{\mathbf{r}\}) = \sum_{i < j} J_{ij} u(\mathbf{r}_i, \mathbf{r}_j),$$

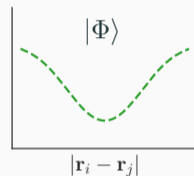
where J_{ij} are optimizable parameters and $u(\mathbf{r}_i, \mathbf{r}_j)$ polynomials dependent on the electron positions. J_{ij} optimizable with, e.g. Variational Monte Carlo (VMC)

Similarity Transformation – Transcorrelated (TC) Method

Incorporate the Ansatz into the Hamiltonian:

Instead of $\hat{H} |\Psi\rangle = E |\Psi\rangle$ solve the similarity transformed/transcorrelated (TC) problem

$$\begin{aligned} \hat{H} |\Psi\rangle &= E |\Psi\rangle, \quad \text{with } |\Psi\rangle = e^{\hat{J}} |\Phi\rangle \\ e^{-\hat{J}} \rightarrow | \hat{H} e^{\hat{J}} |\Phi\rangle &= E e^{\hat{J}} |\Phi\rangle, \quad (\hat{J}^\dagger = \hat{J}) \\ (e^{-\hat{J}} \hat{H} e^{\hat{J}}) |\Phi\rangle &= E e^{-\hat{J}} e^{\hat{J}} |\Phi\rangle = E |\Phi\rangle \end{aligned}$$



Baker-Campbell-Hausdorff (BCH) exp. to obtain TC Hamiltonian:

$$\bar{H} = e^{-\hat{J}} \hat{H} e^{\hat{J}} = \hat{H} + [\hat{H}, \hat{J}] + \frac{1}{2!} [[\hat{H}, \hat{J}], \hat{J}] + \dots \rightarrow 0$$

For the **molecular Hamiltonian** the BCH exp. **terminates at 2nd order**

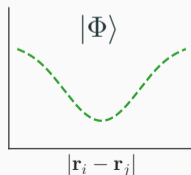
The Similarity Transformed TC Hamiltonian

Consequences:

- Transcorrelated \bar{H} is not Hermitian! \rightarrow loss of variational principle
 - Additional 3-body terms in \bar{H}
- \rightarrow Ansatz-based **quantum imaginary time evolution**[†] can handle both drawbacks on quantum hardware

Benefits:

More accurate results with smaller basis sets/less qubits!

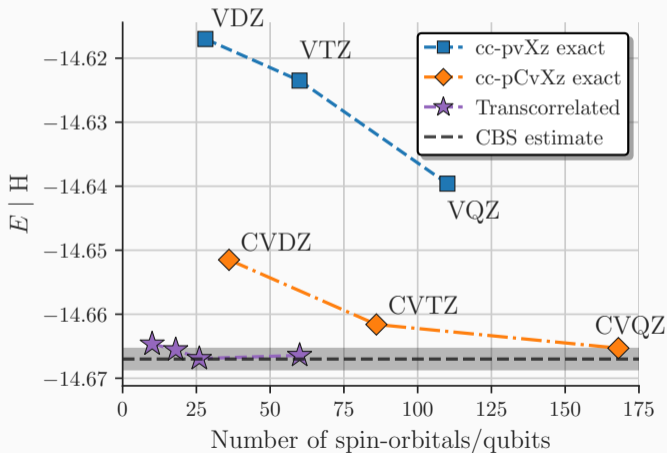


Applications: Reducing the number of qubits for
chemistry

Beryllium atom

Beryllium atom – exact simulation of a quantum device (no noise)

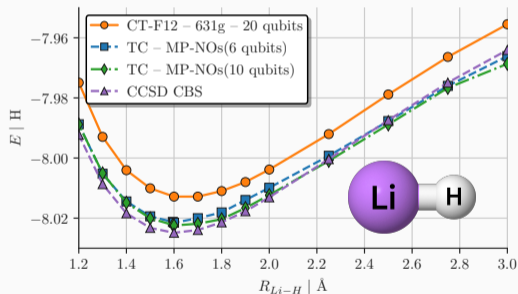
Goal: complete basis set (CBS) limit \rightarrow full description to compare with experiment



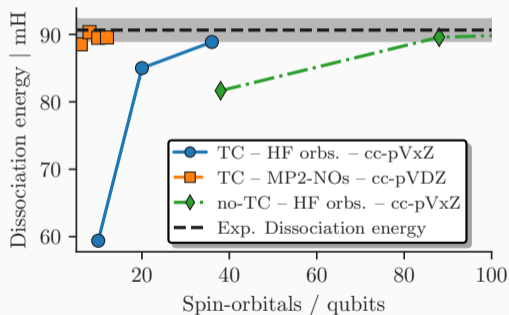
Lithium hydride – LiH

Lithium hydride – exact, noiseless simulation of quantum device

“Standard basis sets” not optimized for the TC method → use pre-optimized orbitals, e.g. natural orbitals from perturbation theory calculation (MP2-NOs)



Error wrt. CBS result vs bond distance



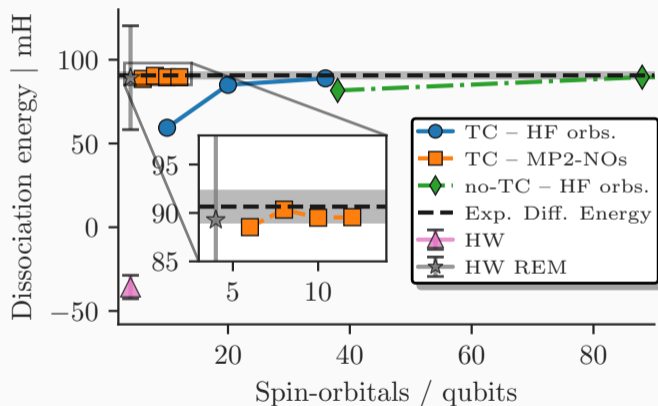
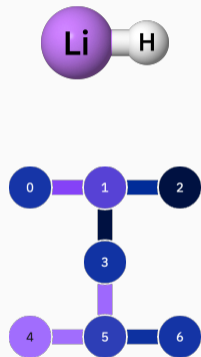
Experimental[†] dissociation energy

Order of magnitude less qubits!

*CT-F12: Motta *et al.*, Phys. Chem. Chem. Phys. **22**, 24270, 2020; [†]Haeffler *et al.*, Phys. Rev. A, 1996, 53, 6, 4127 (1996); **WD**, Sokolov, Liao, Lopez Rios, Rahm, Alavi, Tavernelli, [arXiv:2303.02007](https://arxiv.org/abs/2303.02007) 2023

LiH – Experiment on IBM Quantum devices

Hardware (HW) experiment: **lithium hydride** dissociation energy on `ibm_lagos`

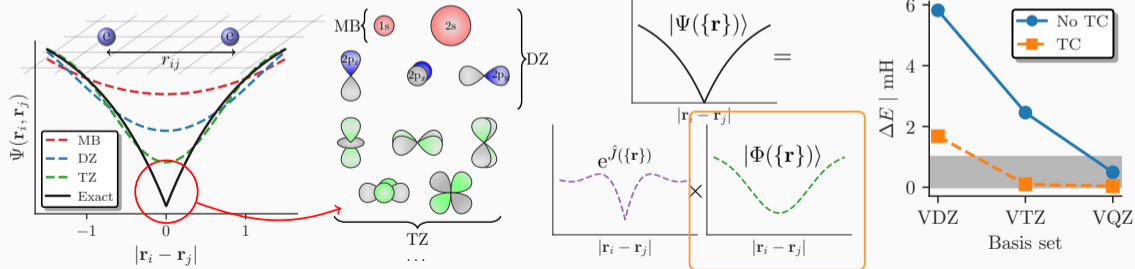


Large effect of noise! Error mitigation techniques* to reduce effect of noise.

Conclusions and outlook

Conclusion – Transcorrelated Approach on Quantum Hardware

- The **TC method** partially transfers electronic correlations from the wavefunction into the Hamiltonian, **capturing the cusp condition**.
- **Reduce qubit requirements and circuit depth**, due to accurate results with a small basis sets.
- **Extends applicability of current and near-term quantum devices** to more relevant quantum chemistry problems.



Workshop – Frontiers of near-term quantum computing



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The workshop aims to bring together researchers from the fields of **computer science, quantum information and chemistry**: <https://tinyurl.com/frontiers-of-qc>.
29th August – 1st September, 2023, Gothenburg, Sweden

Confirmed speakers:

- Ivano Tavernelli
- Sophia Economou
- Sevag Gharibian
- Richard Kueng
- Xiao Yuan
- Christian Gogolin
- Zoë Holmes
- Stefan Knecht
- Jakob Kottmann
- Panagiotis Barkoutsos
- Ashley Montanaro
- Anand Natarajan
- Pauline Ollitrault
- Benjamin Brown
- Francesco Tacchino
- Juani Bermejo-Vega
- David Muñoz Ramo
- Tony Metger

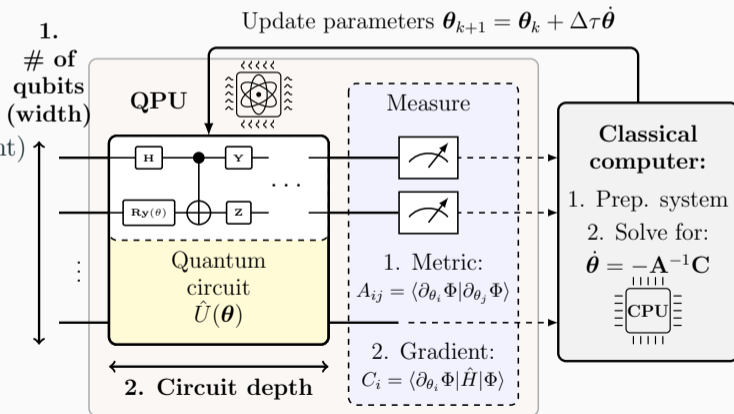
Thank you for your attention!

How to solve non-Hermitian problems on quantum hardware

Since the TC Hamiltonian is **non Hermitian**, VQE not applicable!

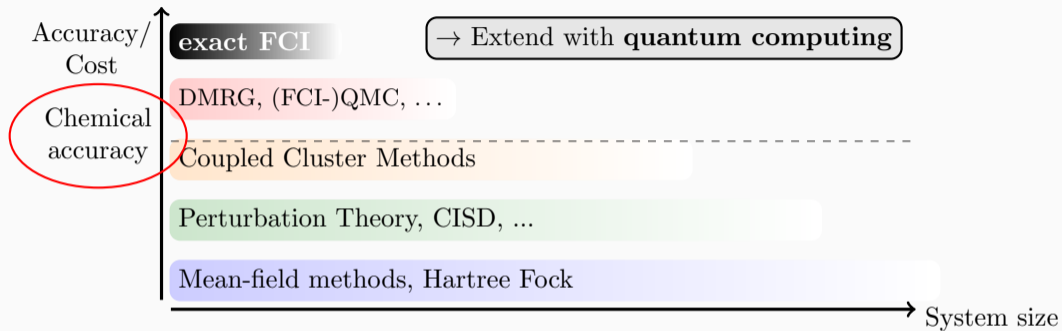
→ Use Ansatz-based Variational **Quantum Imaginary Time Evolution***

- Based on imaginary-time Schrödinger equation
- Projector method to obtain (right) eigenvector
- Allows to formulate non-unitary time evolution as minimization
- Applicable to non-Hermitian problems



*McArdle, et al., npj Quantum Information 5, 75, 2019; Sokolov, WD, Luo, Alavi, Tavernelli, arXiv:2201.03049 (2022);

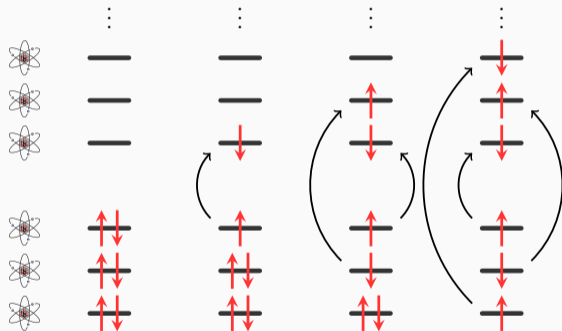
Hierarchy of methods



Highly accurate methods only applicable to **very small** system sizes.
Current quantum computing calculations/experiments use small/**minimal**
basis sets far from experimental results, due to **limited number of qubits**

Exponential scaling of Full Configuration Interaction

There is a long history and wide variety of computational approaches in chemistry



Mol.	#electrons	#states
H ₂	2	4
LiH	4	36
Be ₂	8	4900
H ₂ O	12	$\sim 8 \cdot 10^5$
C ₂ H ₄	16	$\sim 16 \cdot 10^6$
F ₂	18	$\sim 2 \cdot 10^9$

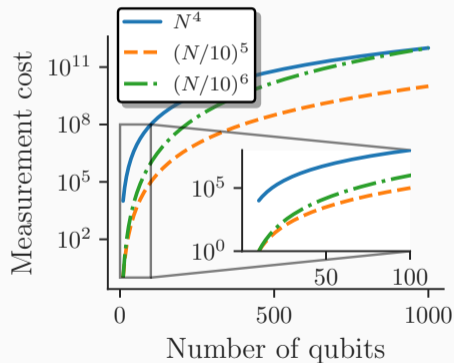
> 20 electrons >~ 100 GB information!

→ can not even store wavefunction in computer memory

Scaling of TC – Measurement Cost

$$\bar{H} = \sum_{pq,\sigma} h_q^p a_{p,\sigma}^\dagger a_{q,\sigma} + \frac{1}{2} \sum_{pqrs,\sigma\tau} \bar{V}_{rs}^{pq} a_{p,\sigma}^\dagger a_{q,\tau}^\dagger a_{s,\tau} a_{r,\sigma} - \frac{1}{6} \sum_{pqrst,\sigma\tau\lambda} L_{st\lambda}^{pqr} a_{p,\sigma}^\dagger a_{q,\tau}^\dagger a_{r,\lambda}^\dagger a_{u,\lambda} a_{t,\tau} a_{s,\sigma}$$

- Measurement formally scaling as N^6 , with N being the number of orbitals
- Recently shown that N^6 -scaling terms can be neglected to good accuracy*
- Current work on N^4 -scaling approximation
- Order of magnitude less orbitals: since also no core functions needed in basis set†
- Shorter circuit depth, due to more compact ground state!



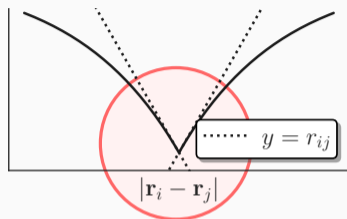
Variational Quantum Monte Carlo to optimize Jastrow factors

Minimize variational energy, by optimizing trial wavefunction parameters J_{ij} :

$$E_{VMC} = \min_{\hat{J}(J_{ij})} \frac{\langle \Phi_0 | e^{\hat{J}} \hat{H} e^{\hat{J}} | \Phi_0 \rangle}{\langle \Phi_0 | e^{2\hat{J}} | \Phi_0 \rangle}, \quad |\Phi_T\rangle = e^{\hat{J}} |\Phi_0\rangle$$

- The choice of trial wavefunction is critical in VMC calculations \rightarrow accuracy limited by $|\Phi_T\rangle = e^{\hat{J}} |\Phi_0\rangle!$
- Hartree-Fock state usually first starting point for $|\Phi_0\rangle$, but more elaborate/accurate states possible...
- Polynomial scaling $\sim N^3$
- Such a VMC calculations to optimize J_{ij} with a HF state $|\Phi_0\rangle = |\Phi_{HF}\rangle$ our **starting point** for the **transcorrelated method**

Explicitly Correlated methods



Linear behavior in electron-electron distance $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ for small r_{ij} !

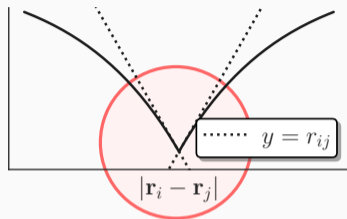
R12 methods*: $|\Psi\rangle = r_{ij} |\Phi\rangle$

F12 methods[†]: $|\Psi\rangle = f(r_{ij}) |\Phi\rangle$, $f(r_{ij}) = \frac{1 - \exp(-\gamma r_{ij})}{\gamma}$

Jastrow Ansatz[‡]: $|\Psi\rangle = e^{\hat{J}} |\Phi\rangle$, $\hat{J} = \sum_{ij} J_{ij} g(\tilde{r}_{ij})$

* Kutzelnigg, Theoretica chimica acta 68, 445 (1985); [†] Ten-no, J. Chem. Phys. 121, 117 (2004); [‡] Jastrow, Phys. Rev. **98**, 1479 (1955);

Explicitly Correlated methods



Linear behavior in electron-electron distance $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ for small r_{ij} !

$$\mathbf{R12} \text{ methods}^*: \quad |\Psi\rangle = r_{ij} |\Phi\rangle$$

$$\mathbf{F12} \text{ methods}^\dagger: \quad |\Psi\rangle = f(r_{ij}) |\Phi\rangle, \quad f(r_{ij}) = \frac{1 - \exp(-\gamma r_{ij})}{\gamma}$$

$$\mathbf{Jastrow} \text{ Ansatz}^\ddagger: \quad |\Psi\rangle = e^{\hat{J}} |\Phi\rangle, \quad \hat{J} = \sum_{ij} J_{ij} g(\tilde{r}_{ij})$$

$$\exp(-x) \approx 1 - x + \mathcal{O}(x^2), \quad \tilde{r}_{ij} = \frac{r_{ij}}{1 + r_{ij}}, \quad \lim_{r_{ij} \rightarrow 0} \tilde{r}_{ij} \rightarrow 0, \quad \lim_{r_{ij} \rightarrow \infty} \tilde{r}_{ij} \rightarrow 1$$

* Kutzelnigg, Theoretica chimica acta 68, 445 (1985); [†] Ten-no, J. Chem. Phys. 121, 117 (2004); [‡] Jastrow, Phys. Rev. **98**, 1479 (1955);

Non-Hermitian Hamiltonian – Problem for VQE

Since TC Hamiltonian is **non Hermitian**, variational algorithms like VQE not applicable

$$E_{\text{VQE}} = \min_{\boldsymbol{\theta}} \langle \Psi(\boldsymbol{\theta}) | \hat{H} | \Psi(\boldsymbol{\theta}) \rangle$$

Our Approach:

Solve for the **right** eigenvector of non-Hermitian \bar{H} by **projection** with QITE:

$$|\Phi_0^R\rangle \propto \lim_{t \rightarrow \infty} e^{-t\bar{H}} |\phi^R\rangle, \quad \text{with} \quad \bar{H} |\Phi_0^R\rangle = E |\Phi_0^R\rangle,$$

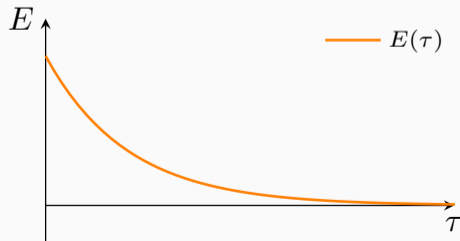
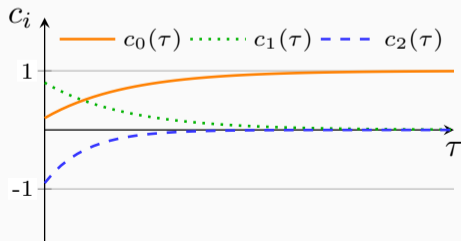
where $|\Phi^R\rangle$ is a full expansion in SDs $|\Phi^R\rangle = \sum_i c_i |D_i\rangle$

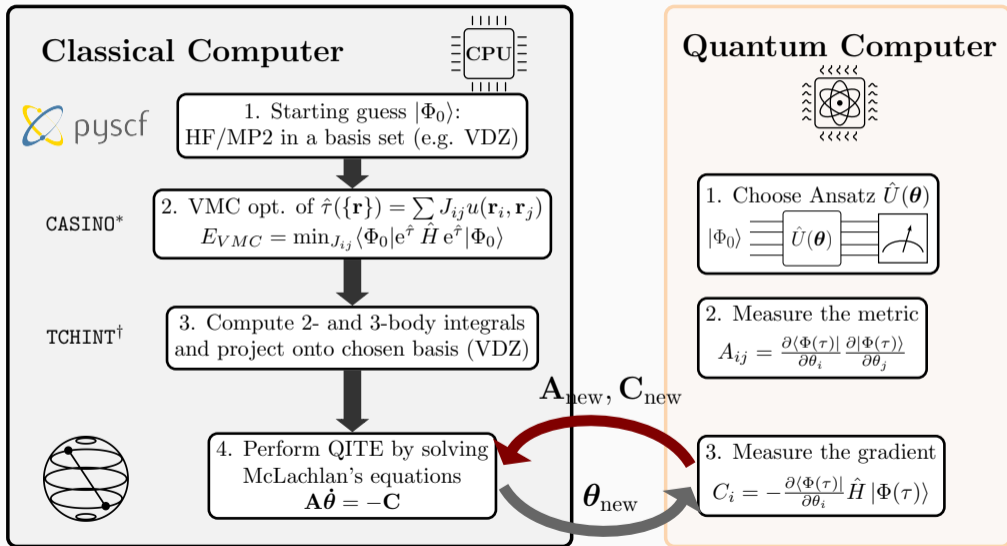
Quantum Imaginary Time Evolution – QITE

→ Solve for the **right** eigenvector of non-Hermitian \bar{H} by (quantum) imaginary-time evolution (QITE)

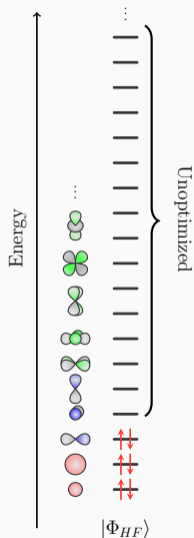
$$i \frac{\partial |\Psi\rangle}{\partial t} = \hat{H} |\Psi\rangle \quad \tau \xrightarrow{=it} \quad \frac{\partial |\Psi\rangle}{\partial \tau} = -\hat{H} |\Psi\rangle \quad \rightarrow \quad |\Psi(\tau)\rangle = N(\tau) e^{-\hat{H}\tau} |\Psi(0)\rangle$$

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

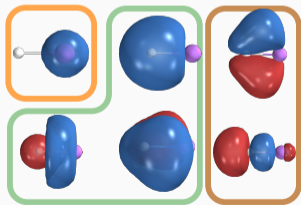
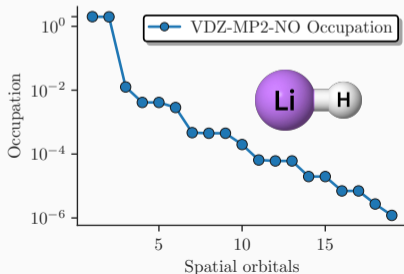




(Virtual) orbital optimization



- “Standard basis sets” not optimized for the TC method
- include effect of virtuals through orbital optimization / downfolding
- e.g. natural orbitals (NO) from a “cheap” perturbation theory (MP2) calculation

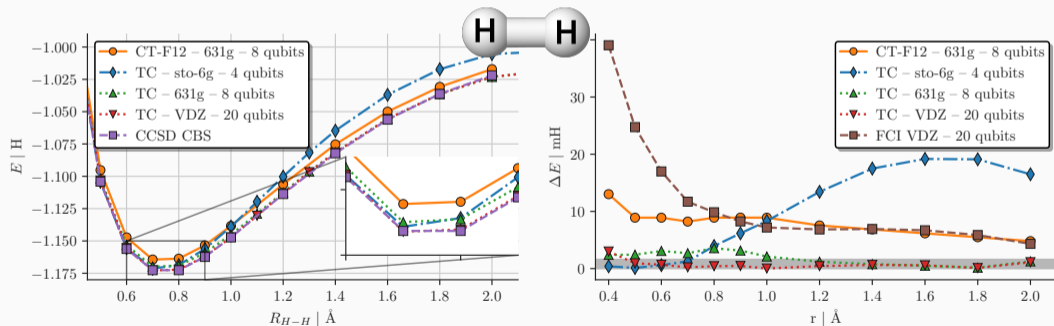


Hydrogen molecule

Favorite quantum chemistry test case: Hydrogen molecule – H_2

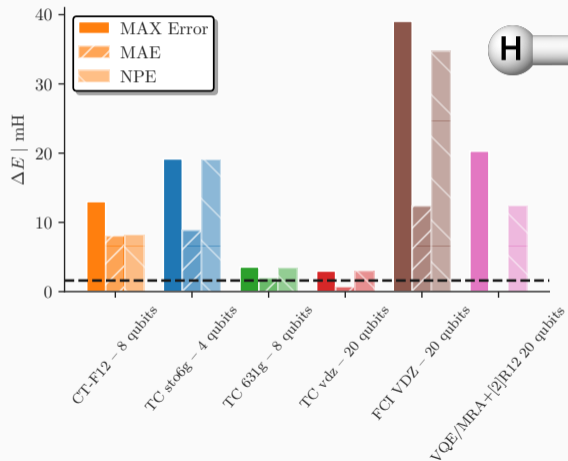
CT-F12 approximated explicitly correlated method, by Motta *et al.**

Exact statevector simulation – UCCSD Ansatz

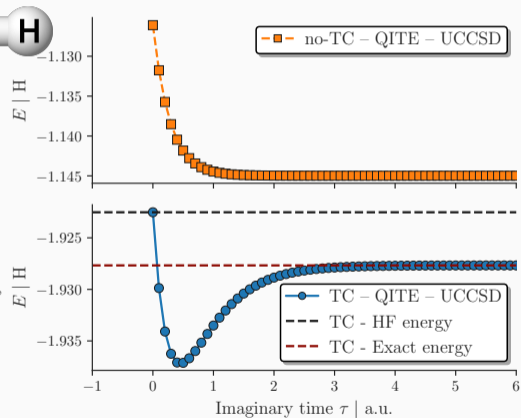


*CT-F12: Motta *et al.*, Phys. Chem. Chem. Phys. **22**, 24270, 2020

H₂ cont



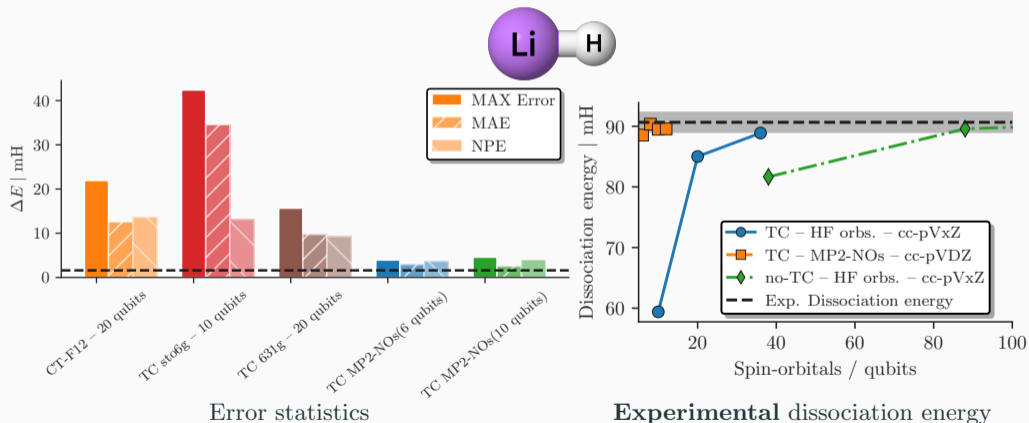
Error statistics



Imaginary time evolution - STO-6G - 0.7Å

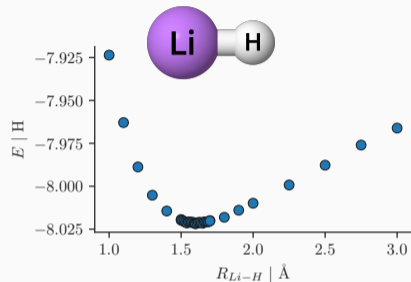
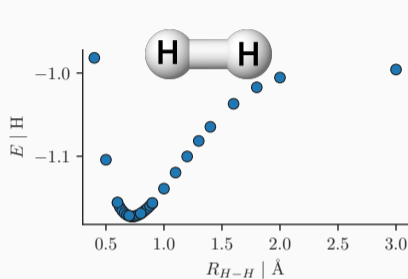
LiH – Dissociation energy

Error statistics and comparison to **experimental*** dissociation energy



*Haeffler *et al.*, Phys. Rev. A, 1996, 53, 6, 4127 (1996)

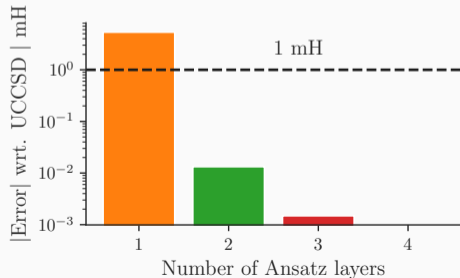
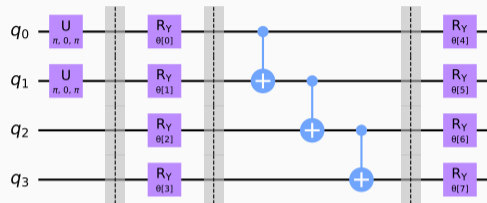
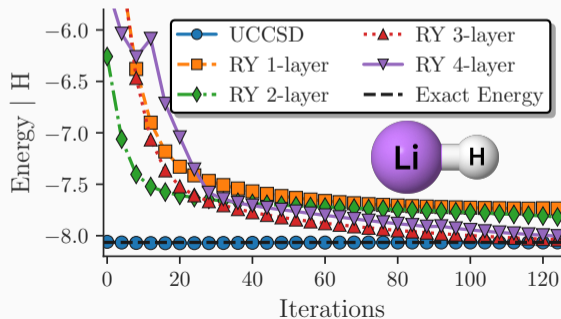
Spectroscopic Constants



	H ₂				LiH			
	qubits	$R_e(\text{\AA})$	$D_0(\text{eV})$	$\omega_e(\text{cm}^{-1})$	qubits	$R_e(\text{\AA})$	$D_0(\text{eV})$	$\omega_e(\text{cm}^{-1})$
no-TC	4	0.73	3.67	4954	12	1.54	2.66	1690
	8	0.75	3.87	4297	22	1.67	1.80	1283
	20	0.76	4.19	4353	38	1.62	2.17	1360
TC	4	0.74	4.69	4435	6	1.60	2.42	1377
Exp.		0.74	4.52	4401		1.60	2.47	1406

LiH – Hardware-efficient Ansatz

- LiH at equilibrium bond distance with 3 MP2 NOs.
- Hardware efficient RY Ansatz with linear entangling layer and parity encoding.
- Statevector simulation



LiH – Hardware-efficient Ansatz – QASM Simulations

- Reference-state error mitigation (REM)* (see Poster session I today – G00/292) or zero-noise extrapolation

