Reducing necessary quantum hardware resources with explicitly correlated methods

QC-4C: Quantum Computers for Chemistry

Werner Dobrautz

Chalmers University of Technology

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CHALMERS
UNIVERSITY OF TECHNOLOGY

MARIE CURIE ACTIONS

Take-home messages

Take-home messages

- Why do we need to use large basis sets?

- What is a explicitly correlated Ansatz?

- What is the transcorrelated method?

- Why do we need quantum imaginary time evolution?

- What are the advantages of the TC method on quantum hardware?

Outline
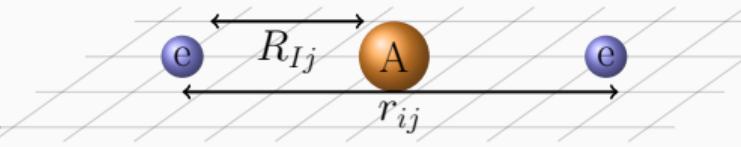
- Recap – Quantum Chemistry

- Correlated Ansatz to reduce the computational footprint on quantum hardware

- Applications: Circuit depth – Hubbard model

- Applications: Circuit width – *Ab initio* problems

- Conclusions and Outlook

Recap – Quantum Chemistry

Ab Initio Quantum Chemistry – Electronic Structure Theory

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

$$\hat{H} = \underbrace{-\sum_i \nabla^2_{\mathbf{r}_i}}_{\text{kinetic energy of e}^-} \underbrace{-\sum_{I,j} \frac{Z_I}{|\mathbf{R}_I - \mathbf{r}_j|}}_{\text{Attr. potential}} + \underbrace{\frac{1}{2}\sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}}_{\text{e}^- - \text{e}^- \text{ repulsion}}$$
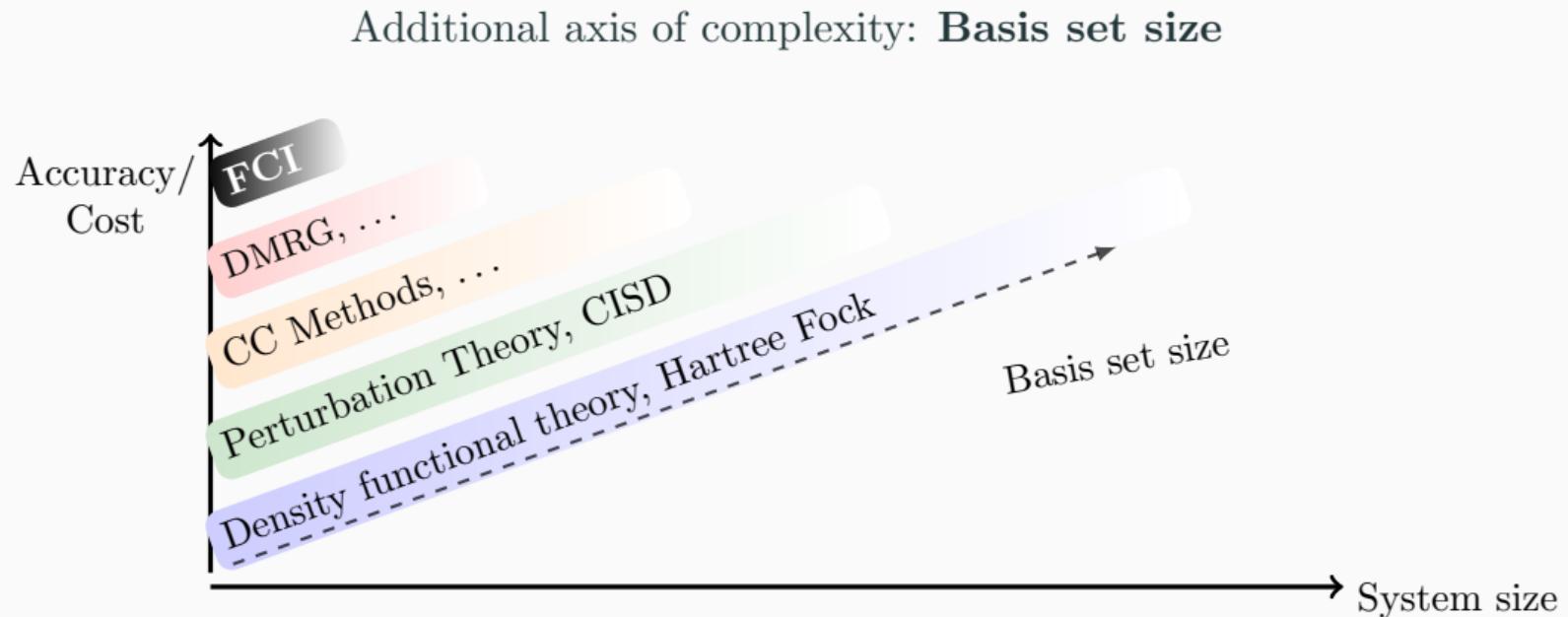
Electronic properties: Ground- and low-lying excited state properties, energy
differences, polarization, response functions, ...

Task: Solve the Schrödinger equation derived from first principles

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

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

Additional axis of complexity: **Basis set size**
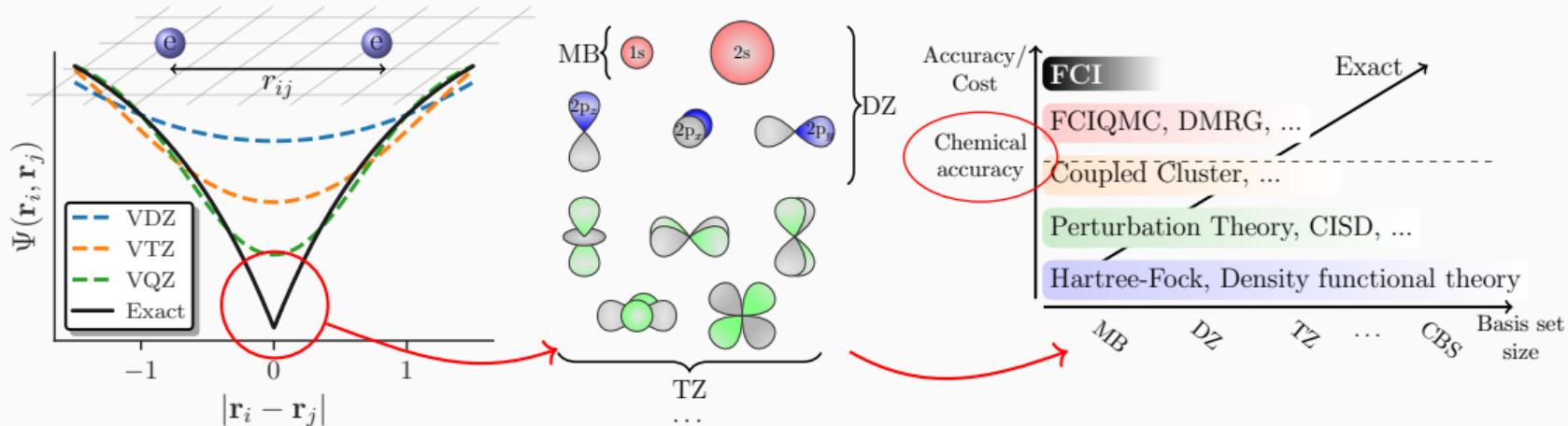
Current quantum computing calculations/experiments use small/**minimal basis sets** far from experimental results, due to **limited number of qubits**

Problems for accurate description: Cusp condition

Cusp condition: Singularity of Coulomb potential, $\frac{1}{r_{ij}}$, for $r_{ij} = 0 \rightarrow$ sharp cusp of exact wavefunction $\Psi(\{\mathbf{r}\})$ at electron coalescence ($r_{ij} = 0$)
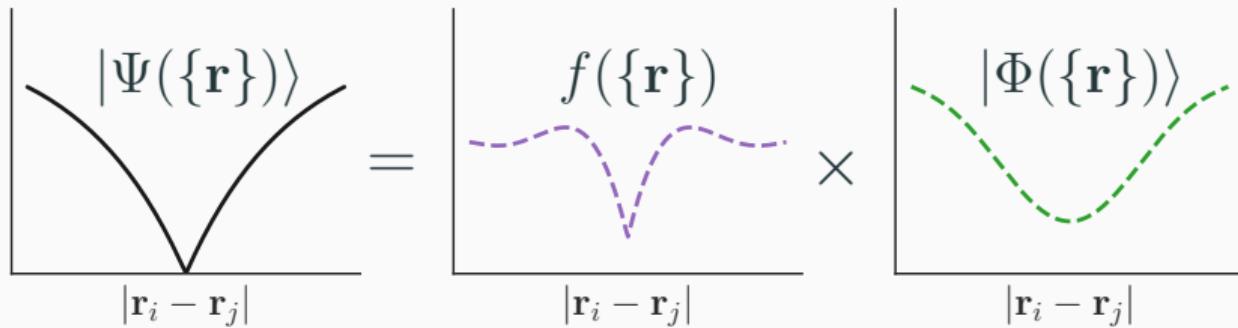
$$\hat{H} = -\sum_i \nabla_{\mathbf{r}_i}^2 - \sum_{I,j} \frac{Z_I}{|\mathbf{R}_I - \mathbf{r}_j|} + \frac{1}{2} \sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}, \quad \hat{H} |\Psi(\{\mathbf{r}\})\rangle = E_0 |\Psi(\{\mathbf{r}\})\rangle$$

Kato, Communications on Pure and Applied Mathematics **10** (2), 151 (1957)

Correlated Ansatz to reduce the computational footprint on quantum hardware

## Cusp Condition – Explicitly Correlated Ansatz
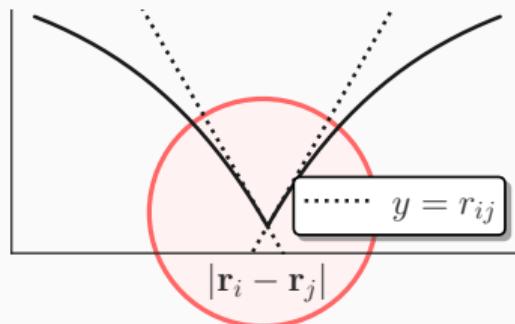
Short range behavior $\rightarrow$ **dynamic correlation**. Important for accurate results $\rightarrow$ Necessitates **large basis set expansion**.

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

$$|\Psi(\{\mathbf{r}\})\rangle = f(\{\mathbf{r}\}) |\Phi(\{\mathbf{r}\})\rangle$$

Hylleras, Z. Phys. 54, 347 (1929)

Linear behavior in electron-electron distance $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ for small r_{ij}!
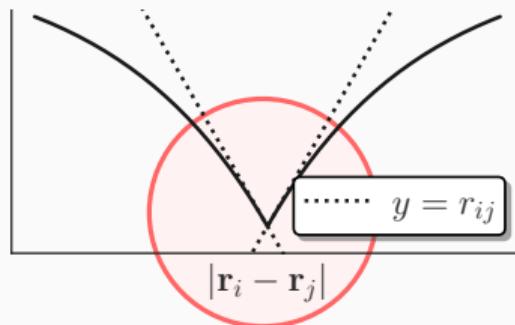
R12 methods[*]: $\quad |\Psi\rangle = r_{ij} |\Phi\rangle$

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

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

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

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

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

Variational Quantum Monte Carlo to optimize Jastrow factors

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

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

- The choice of trial wavefunction is critical in VMC calculations $\rightarrow$ accuracy limited by $|\Phi_T\rangle = e^{\hat{\tau}} |\Phi_0\rangle$!
- 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**

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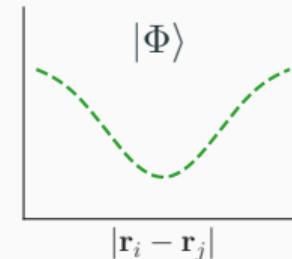
Similarity Transformation – Transcorrelated (TC) Method

Describe the cusp condition and/or capture part of correlation with a correlated wavefunction Ansatz → incorporate into Hamiltonian!

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

$$\hat{H}\,|\Psi\rangle = E\,|\Psi\rangle, \quad \text{with} \quad |\Psi\rangle = \mathrm{e}^{\hat{\tau}}\,|\Phi\rangle$$

$$\mathrm{e}^{-\hat{\tau}} \rightarrow | \quad \hat{H}\,\mathrm{e}^{\hat{\tau}}\,|\Phi\rangle = E\,\mathrm{e}^{\hat{\tau}}\,|\Phi\rangle, \qquad (\hat{\tau}^{\dagger} = \hat{\tau})$$

$$\left(\mathrm{e}^{-\hat{\tau}}\,\hat{H}\,\mathrm{e}^{\hat{\tau}}\right)|\Phi\rangle = E\,\mathrm{e}^{-\hat{\tau}}\,\mathrm{e}^{\hat{\tau}}\,|\Phi\rangle = E\,|\Phi\rangle$$

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

$$\bar{H} = \mathrm{e}^{-\hat{\tau}}\,\hat{H}\,\mathrm{e}^{\hat{\tau}} = \hat{H} + [\,\hat{H},\hat{\tau}\,] + \frac{1}{2}\,[\,[\,\hat{H},\hat{\tau}\,],\hat{\tau}\,] + \dots$$

For the molecular Hamiltonian the BCH exp. terminates at 2nd order, as only kinetic energy operators in $\hat{H}$ do not commute with $\hat{\tau}$!

Hirschfelder, JCP, **39**, 3145 (1963); Boys and Handy, Proc. R. Soc. A (**1969**); **WD**, Luo, Alavi, PRB **99** (7), 075119 (2019); Cohen, Luo, Guther, **WD**, Tew, Alavi, JCP **151** (6), 061101 (2019); **WD**, Cohen, Alavi, Giner, JCP **156** (23), 234108 (2022)

The Similarity Transformed TC Hamiltonian

Consequences:

- Sim. transf. $\bar{H}$ is non-Hermitian ($[\hat{H}, \hat{\tau}], \dots$)
  $\rightarrow$ loss of variational principle
- 3-body interactions (and possibly higher order)
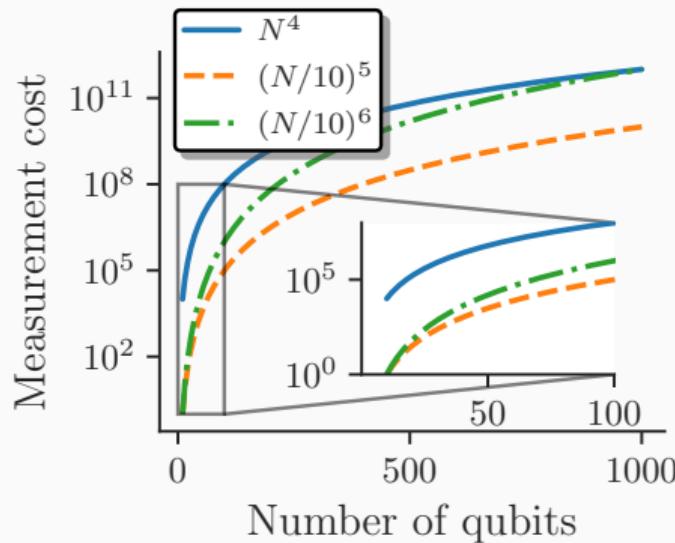
$$\bar{H} = \hat{H} - \sum_i \left(\frac{1}{2} \nabla_i^2 \hat{\tau} + (\nabla_i \hat{\tau}) \nabla_i + \frac{1}{2} (\nabla_i \hat{\tau})^2 \right)$$

$$= \hat{H} - \sum_{i<j} \hat{K}(\mathbf{r}_i, \mathbf{r}_j) - \sum_{i<j<k} \hat{L}(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k)$$

Rapid basis set convergence and more compact (right) eigenvector!

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

Scaling of TC – Measurement Cost
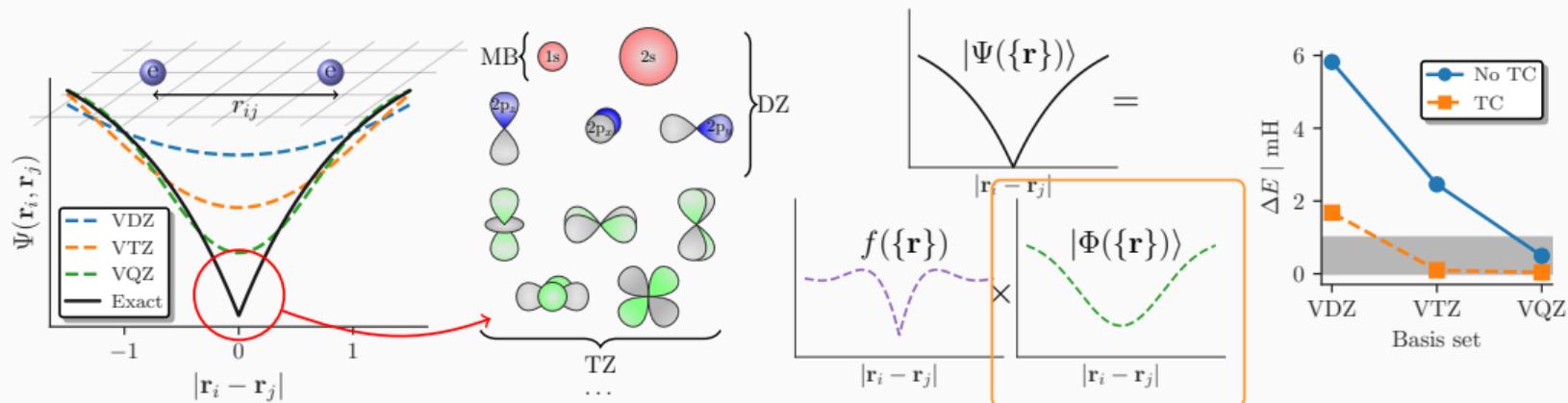
$$\bar{H} = \sum_{pq,\sigma} h_q^p a_{p,\sigma}^\dagger a_{q,\sigma} + \frac{1}{2} \sum_{pqrs,\sigma\tau} \bar{V}_{rs}^{pq} a_{p,\sigma}^\dagger a_{q,\tau}^\dagger a_{s,\tau} a_{r,\sigma} - \frac{1}{6} \sum_{pqrstu,\sigma\tau\lambda} L_{stu}^{pqr} a_{p,\sigma}^\dagger a_{q,\tau}^\dagger a_{r,\lambda}^\dagger a_{u,\lambda} a_{t,\tau} a_{s,\sigma}$$

- 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!

[*]**WD** *et al.*, Journal of Chemical Physics 156 (23), 234108 (2022); [†]Cohen, Luo, Guther, **WD**, Tew, Alavi, JCP **151** (6), 061101 (2019);

Sharp cusp $\rightarrow$ necessitates **large basis set expansion**

Every spin-orbital needs a qubit $\rightarrow$ Minimal basis far from CBS results!

Transcorrelation (TC) enables **more accurate results with less spin-orbitals/qubits**

Non-Hermitian Hamiltonian – Problem for VQE

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

$$E_{\mathrm{VQE}} = \min_{\boldsymbol{\theta}} \langle \Psi(\boldsymbol{\theta})| \hat{H} |\Psi(\boldsymbol{\theta})\rangle$$
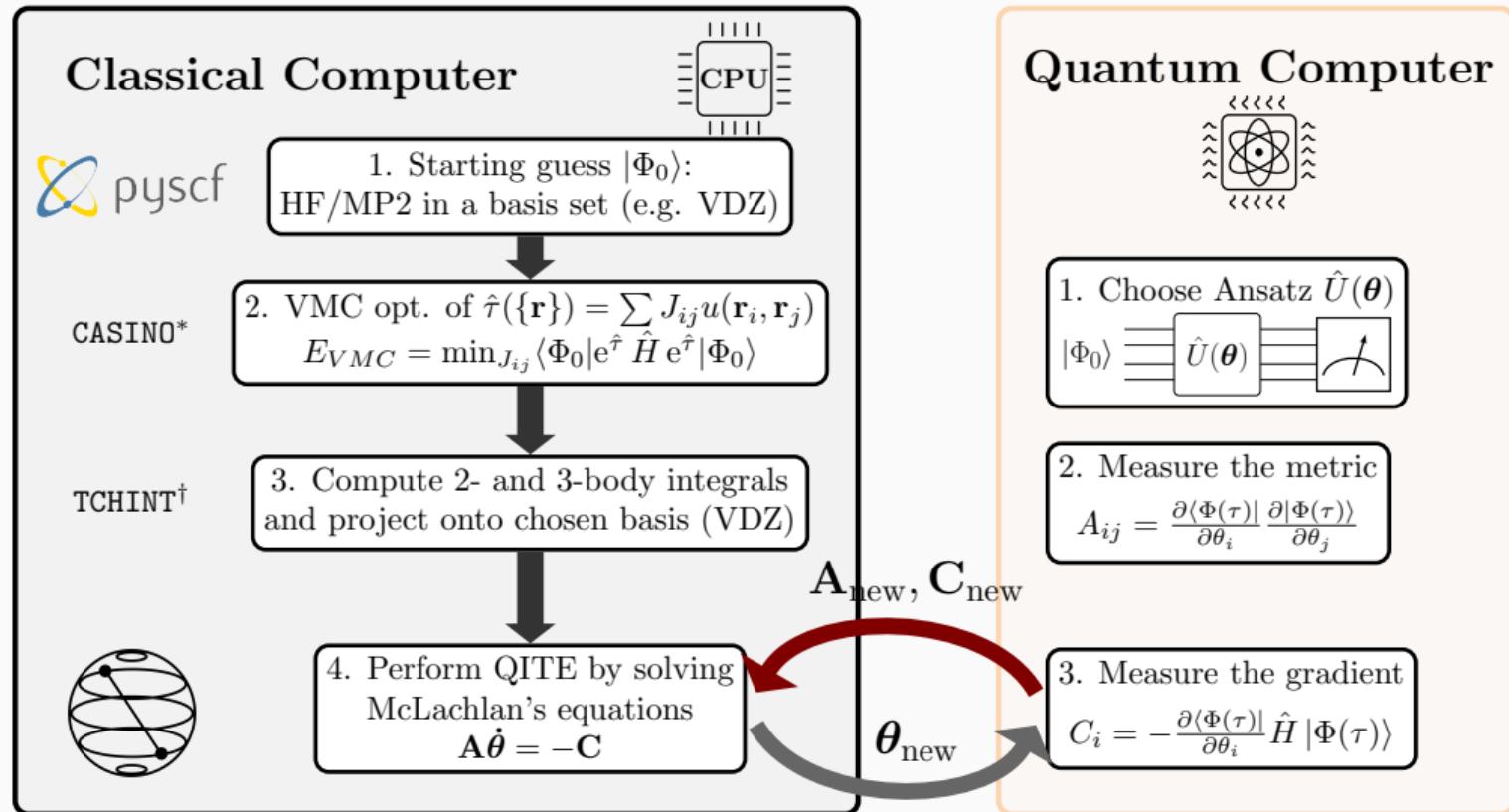
Our Approach:

Solve for the **right** eigenvector of non-Hermitian $\bar{H}$ py **projection** with QITE:
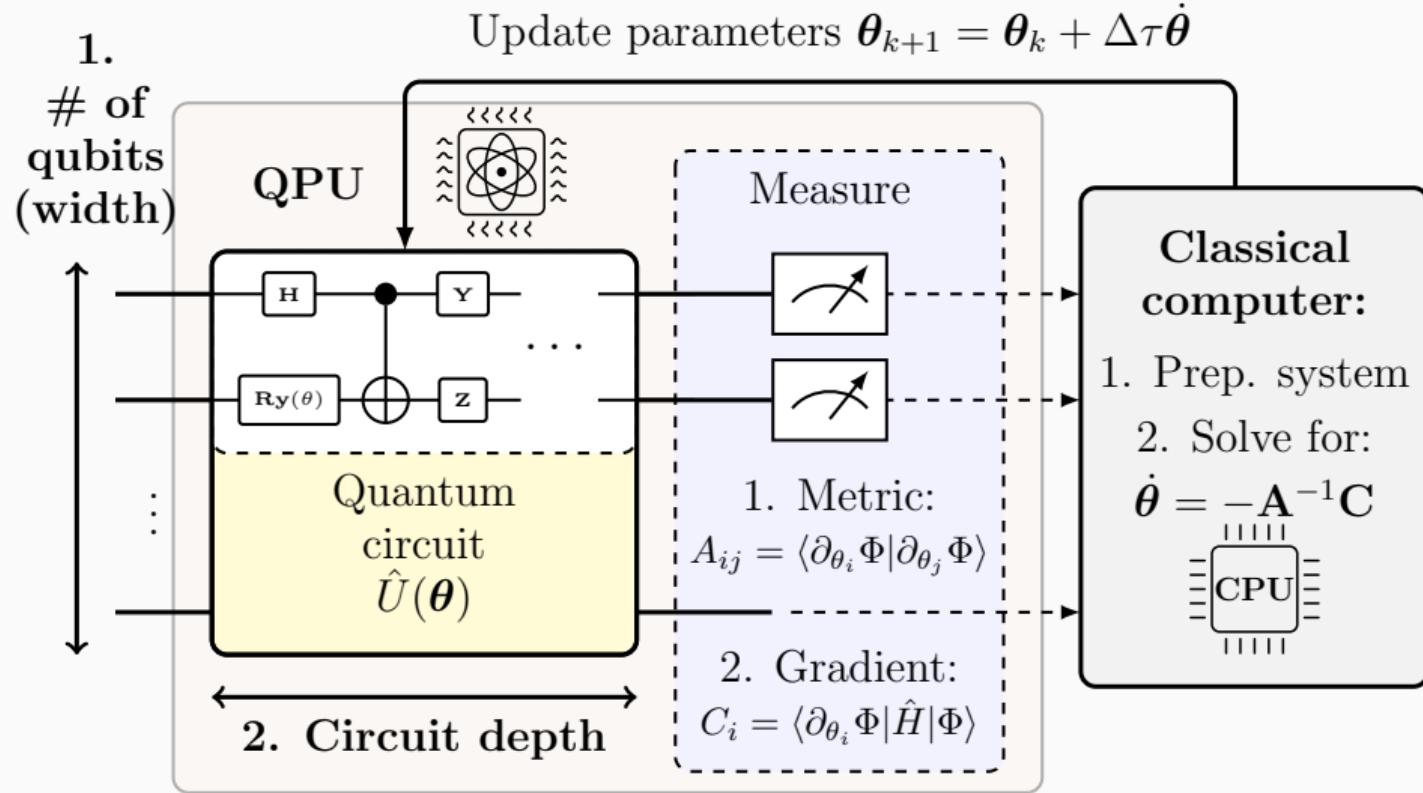
$$|\Phi_0^R\rangle \propto \lim_{t \to \infty} \mathrm{e}^{-t\bar{H}} |\phi^R\rangle, \quad \text{with} \quad \bar{H} |\Phi_0^R\rangle = E |\Phi_0^R\rangle,$$

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

Classical Computer | CPU

1. Starting guess $|\Phi_0\rangle$:
HF/MP2 in a basis set (e.g. VDZ)

2. VMC opt. of $\hat{\tau}(\{\mathbf{r}\}) = \sum J_{ij} u(\mathbf{r}_i, \mathbf{r}_j)$
$E_{VMC} = \min_{J_{ij}} \langle \Phi_0 | e^{\hat{\tau}} \hat{H} e^{\hat{\tau}} | \Phi_0 \rangle$

CASINO*

3. Compute 2- and 3-body integrals
and project onto chosen basis (VDZ)

TCHINT†

4. Perform QITE by solving
McLachlan's equations
$\mathbf{A}\dot{\boldsymbol{\theta}} = -\mathbf{C}$

Quantum Computer

1. Choose Ansatz $\hat{U}(\boldsymbol{\theta})$

$|\Phi_0\rangle$ — $\hat{U}(\boldsymbol{\theta})$

2. Measure the metric
$A_{ij} = \frac{\partial \langle \Phi(\tau) |}{\partial \theta_i} \frac{\partial | \Phi(\tau) \rangle}{\partial \theta_j}$

3. Measure the gradient
$C_i = -\frac{\partial \langle \Phi(\tau) |}{\partial \theta_i} \hat{H} | \Phi(\tau) \rangle$

$\mathbf{A}_{\text{new}}, \mathbf{C}_{\text{new}}$

$\boldsymbol{\theta}_{\text{new}}$

1.
# of qubits (width)

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

QPU

Measure

Classical computer:

H   Y

Ry(θ)   Z

. . .

Quantum circuit $\hat{U}(\boldsymbol{\theta})$

2. Circuit depth

1. Metric:
$A_{ij} = \langle \partial_{\theta_i}\Phi | \partial_{\theta_j}\Phi \rangle$

2. Gradient:
$C_i = \langle \partial_{\theta_i}\Phi | \hat{H} | \Phi \rangle$

1. Prep. system
2. Solve for:
$\dot{\boldsymbol{\theta}} = -\mathbf{A}^{-1}\mathbf{C}$

CPU

Applications: Circuit depth – Hubbard model

High-T$_C$ Superconductors and the Hubbard Model

YBCO

Mapping to an effective lattice model:

The Hubbard Hamiltonian

$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} \left(c_{i,\sigma}^{\dagger} c_{j,\sigma} + h.c. \right) + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$
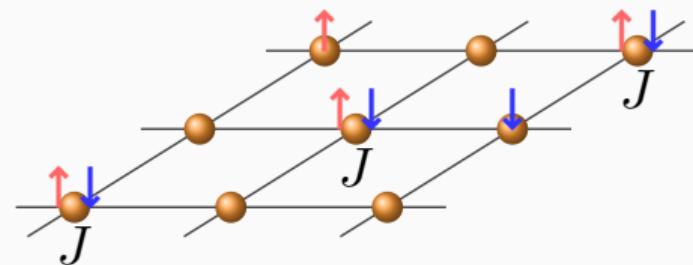
Strong interaction $\Rightarrow$ highly multiconfigurational

Hubbard, 1963; Kanamori, 1963; Gutzwiller; 1963; Anderson, 1987; Emery, 1987; Zhang and Rice, 1988; Bednorz and Müller, 1986

Similarity Transformation based on the Gutzwiller Ansatz

Reduce circuit depth with transcorrelated Ansatz

- Suppress energetically unfavourable double occupancies via the *Gutzwiller* Ansatz:

$$|\Psi\rangle = \mathrm{e}^{\hat{\tau}}\,|\Phi\rangle\,, \quad \hat{\tau} = J\sum_i n_{i\uparrow}n_{i\downarrow}$$
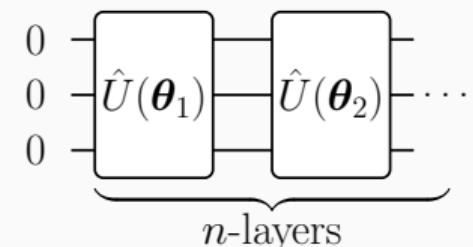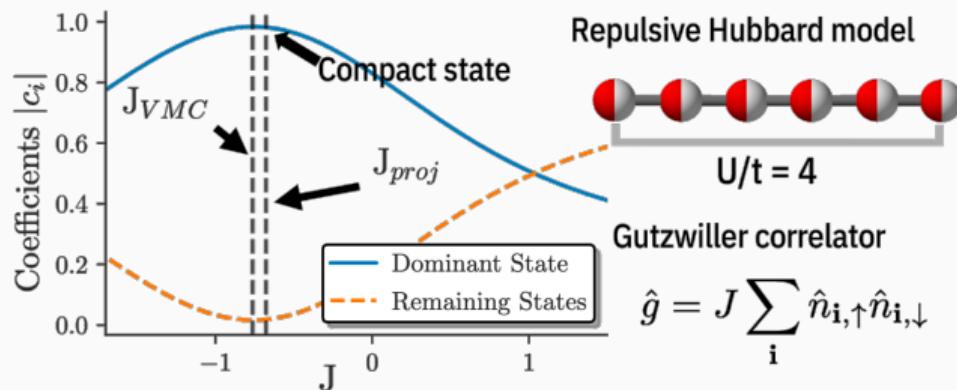
- Perform an exact *similarity transformation* (ST) of the Hubbard Hamiltonian $\hat{H}$:

$$\mathrm{e}^{-\hat{\tau}}\,\hat{H}\,\mathrm{e}^{\hat{\tau}} = \bar{H}\,|\Phi\rangle = \left(-t\sum_{\langle i,j\rangle,\sigma}\mathrm{e}^{-\hat{\tau}}a_{i\sigma}^{\dagger}a_{j\sigma}\mathrm{e}^{\hat{\tau}} + U\sum_i n_{i\uparrow}n_{i\downarrow}\right)|\Phi\rangle = E\,|\Phi\rangle$$

Gutzwiller, PRL 10, **159** (1963); Tsuneyuki, Prog. Theor. Phys. Supp., **176**, 134 (2008); Scuseria et al., PRB, **91**, 041114 (2015); **WD**, Luo, Alavi, PRB, **99**, 075119 (2019);

Increased compactness of right eigenvector

- Leads to a **non-Hermitian** operator with **3-body interactions** in a momentum space representation
- **Increased compactness** of the right EV, due to downfolding of correlations into Hamiltonian

Repulsive Hubbard model

$U/t = 4$

Gutzwiller correlator

$$\hat{g} = J \sum_{\mathbf{i}} \hat{n}_{\mathbf{i},\uparrow} \hat{n}_{\mathbf{i},\downarrow}$$
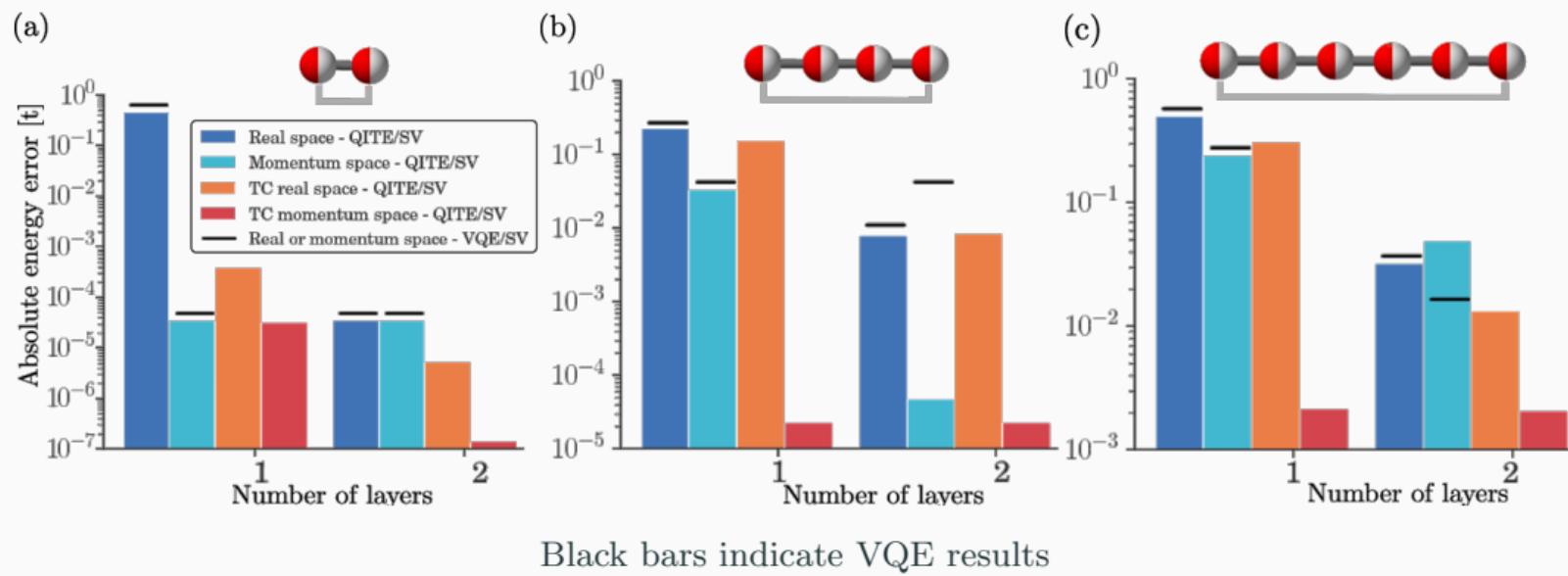
$\Rightarrow$ Does the increased compactness/more single reference character have an impact on the necessary Ansatz (depth)?

WD, Luo, Alavi, PRB, **99**, 075119 (2019); Sokolov, **WD**, Luo, Alavi, Tavernelli, arXiv:2201.03049

Results – Hubbard model
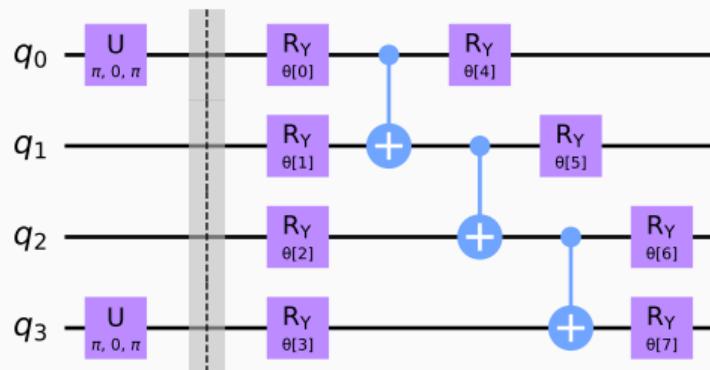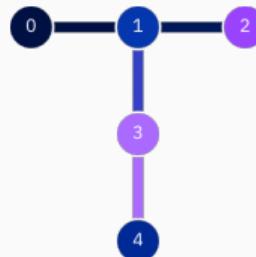
Increased compactness $\Rightarrow$ less expressive Ansatz on quantum hardware necessary $\Rightarrow$ **shorter quantum circuit**/less layers $\Rightarrow$ cheaper and more resilient to noise

Statevector simulation – n-layer UCCSD Ansatz – $U/t = 4$

Black bars indicate VQE results

Sokolov, **WD**, Luo, Alavi, Tavernelli, arXiv:2201.03049
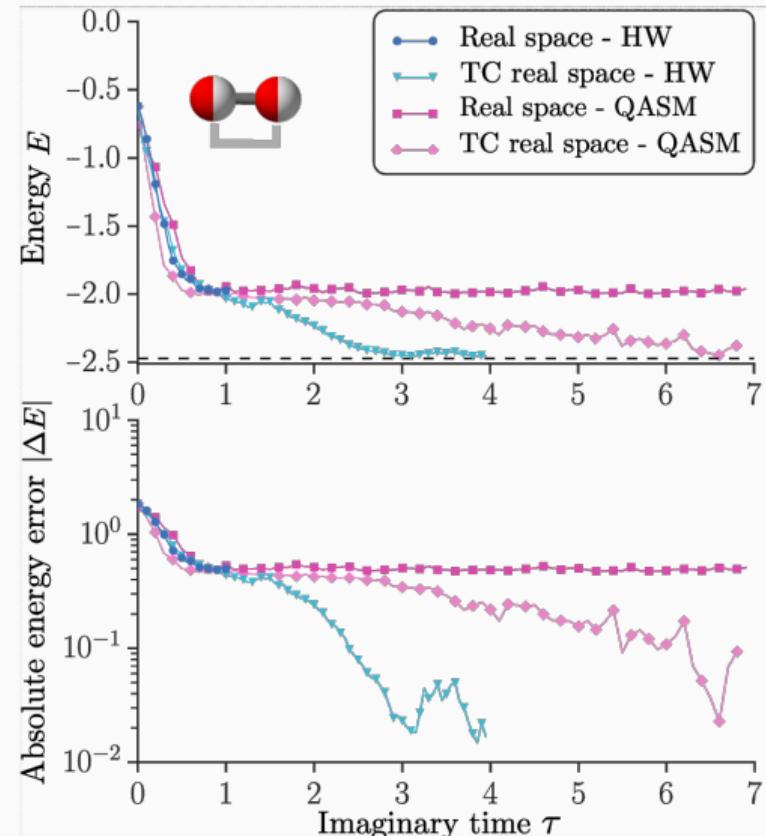
- 2-site Hubbard model

Hardware-efficient RY Ansatz

Sokolov, **WD**, Luo, Alavi, Tavernelli, arXiv:2201.03049
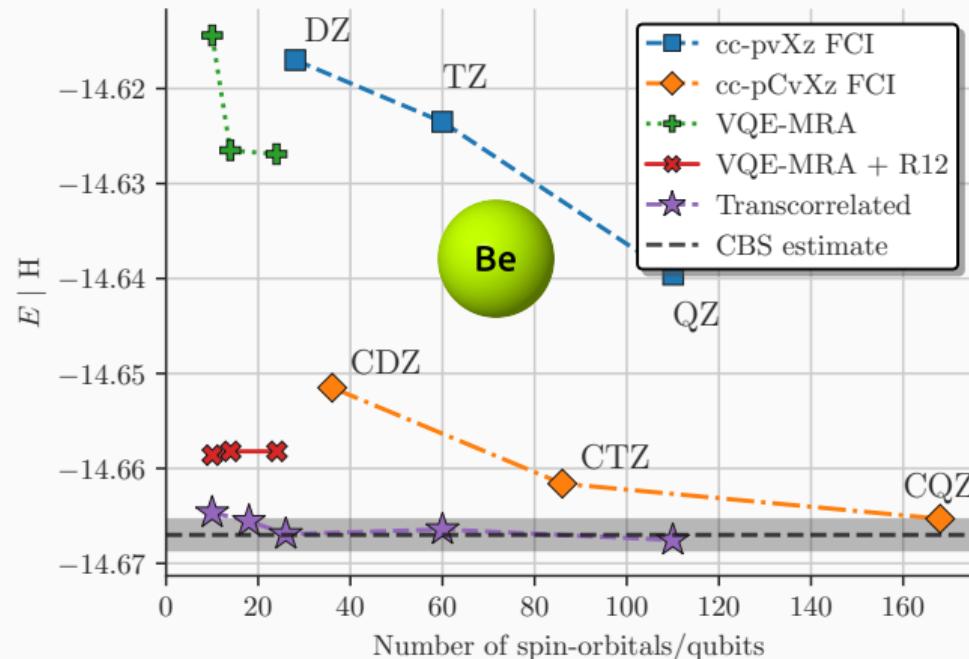
Applications: Circuit width – *Ab initio* problems

Can we reduce the number of necessary qubits (width)?

Beryllium atom – exact statevector simulations

VQE+MRA (+R12): (approx.) explicitly correlated method by Schleich *et al.*[*]
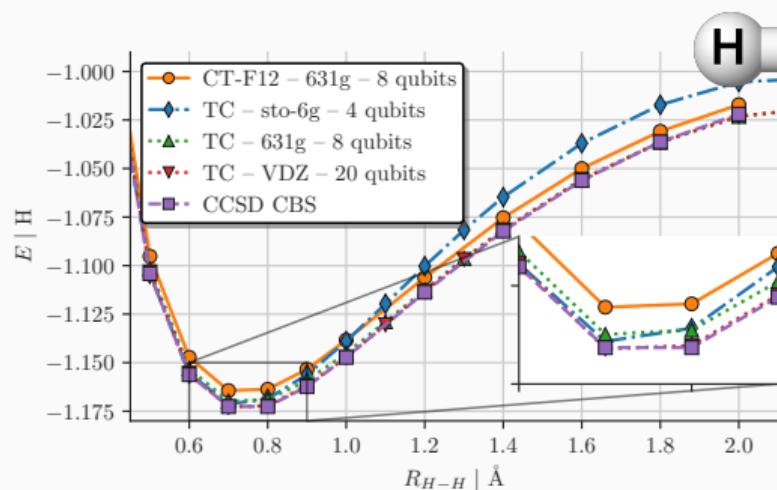
Favorite quantum chemistry test case: Hydrogen molecule – H_2

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

Exact statevector simulation – UCCSD Ansatz
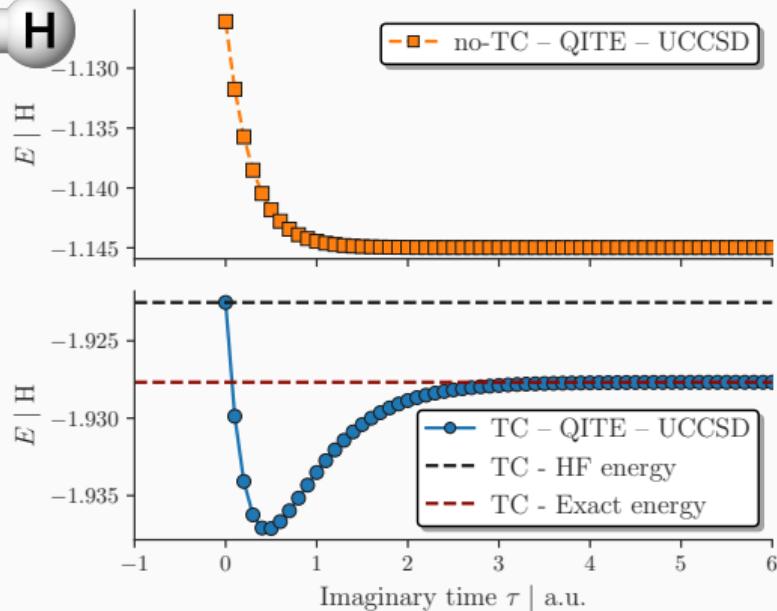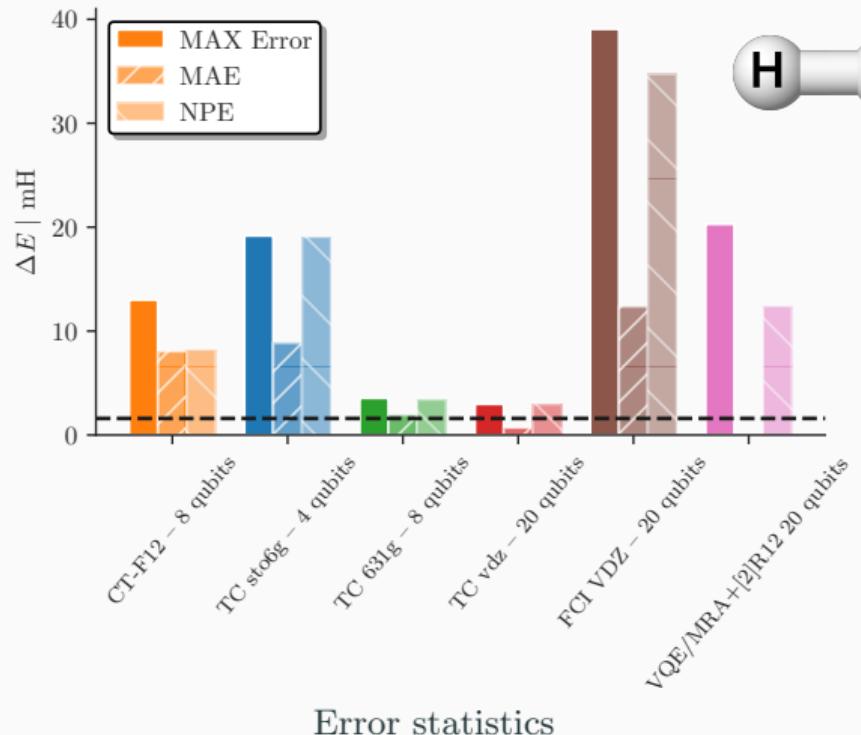
Energy vs. bond distance

Error wrt. CBS result vs. bond distance

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

Error statistics
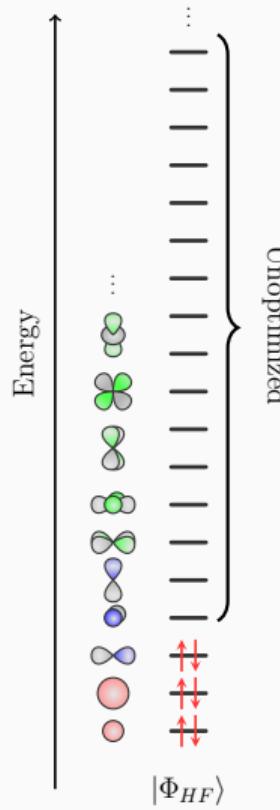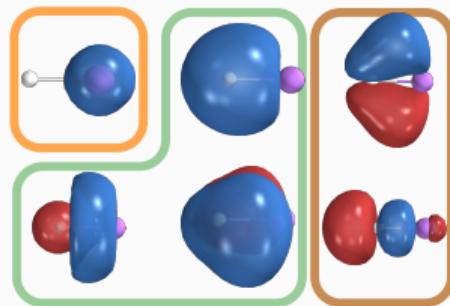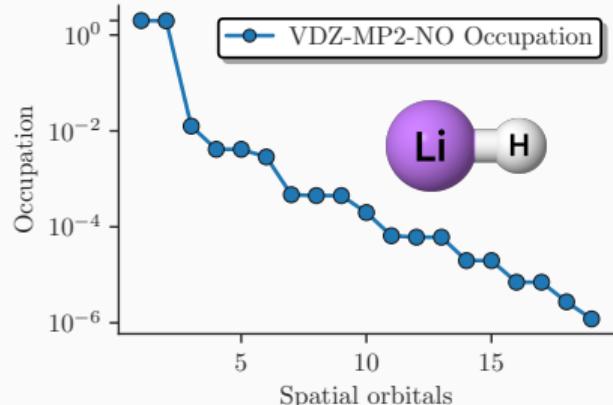
Imaginary time evolution – STO-6G – 0.7Å

CT-F12: Motta *et al.*, Phys. Chem. Chem. Phys. **22**, 24270, 2020 VQE/MRA+[2]R12: Schleich *et al.*, arXiv:2110.06812, 2021

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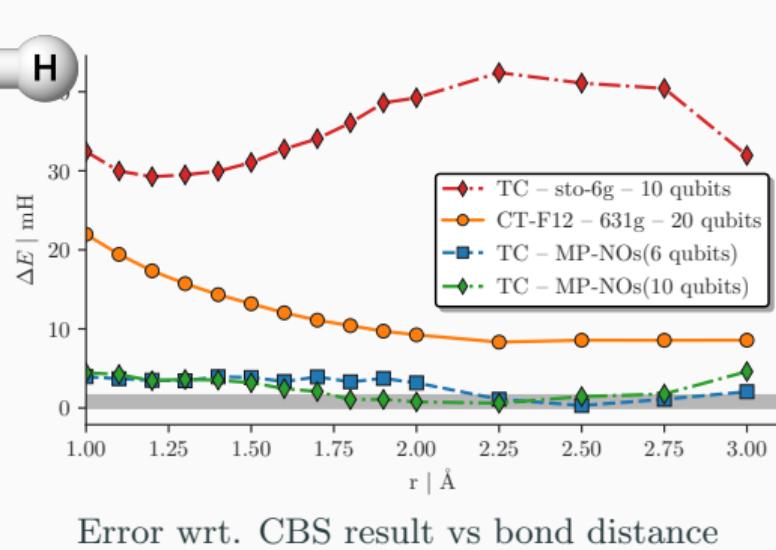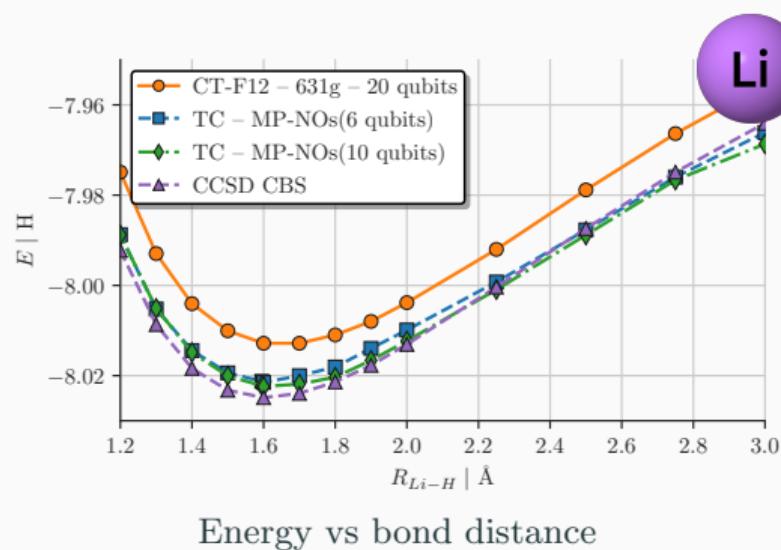
- "Standard basis sets" not optimized for the TC method
- → include effect of virtuals through orbital optimization / downfolding
- → e.g. natural orbitals (NO) from a "cheap" perturbation theory (MP2) calculation

FNO: Sosa *et al.*, Chem. Phys. Lett. **159** (2-3) 148 (1989); Taube and Bartlett Collect. Czech. Chem. Commun. **70**, 837 (2005); **NISQ:** Gonthier *et al.* arXiv:2012.04001; (2020); Verma *et al.* JCP **155**, 034110 (2021)
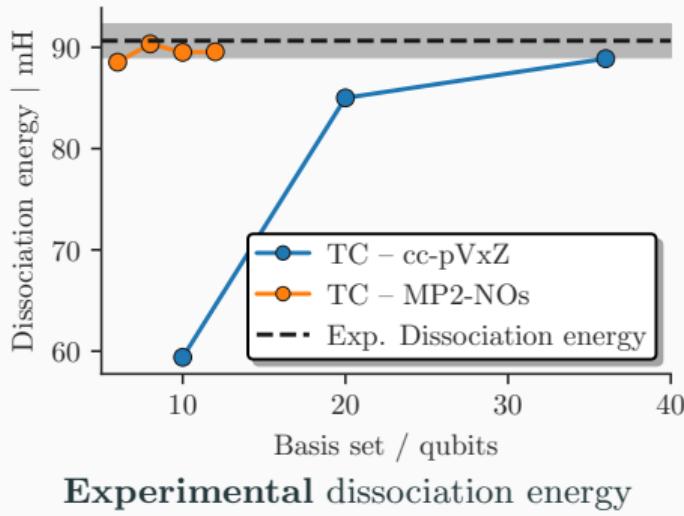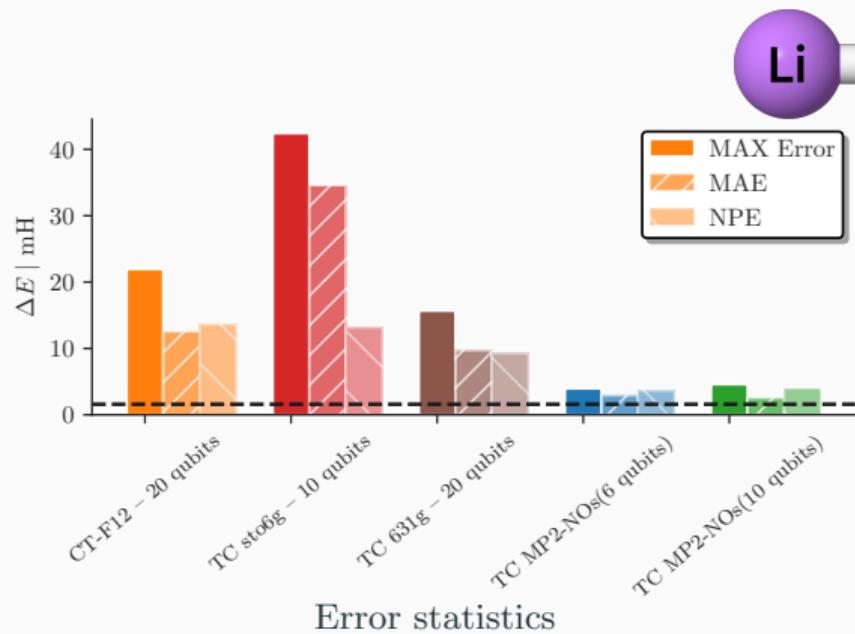
Lithium hydride – exact statevector simulation – UCCSD Ansatz – Li 1s frozen

Energy vs bond distance

Error wrt. CBS result vs bond distance

26
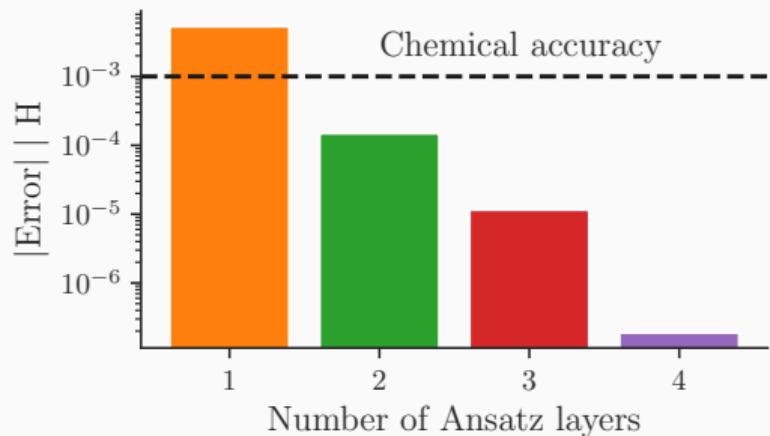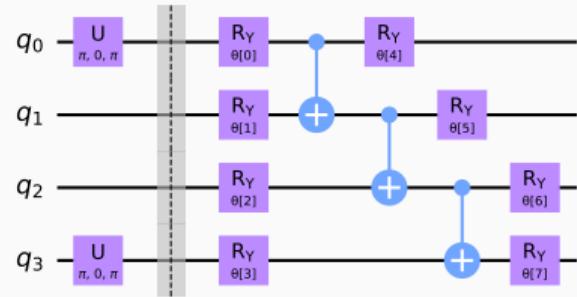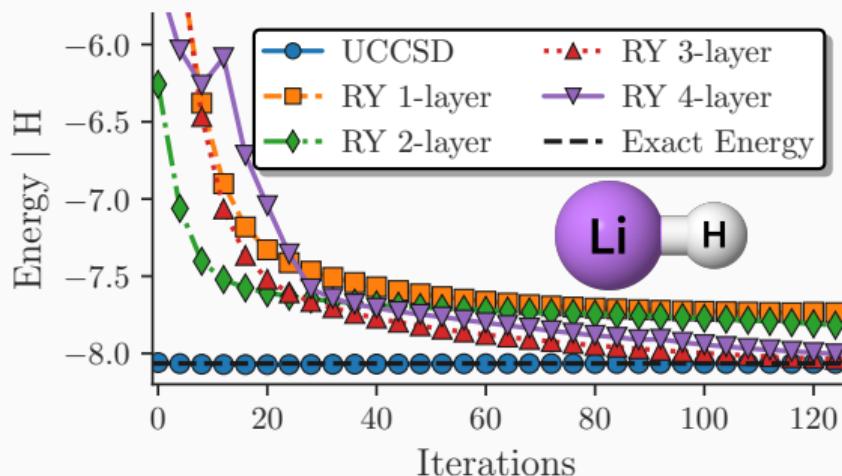
Error statistics and comparison to **experimental**[*] dissociation energy

Error statistics

Experimental dissociation energy

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

LiH – Hardware-efficient Ansatz
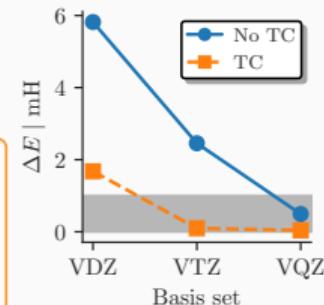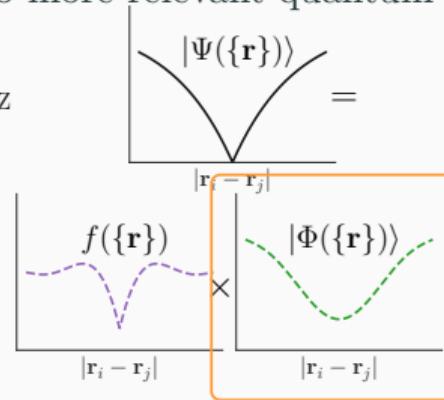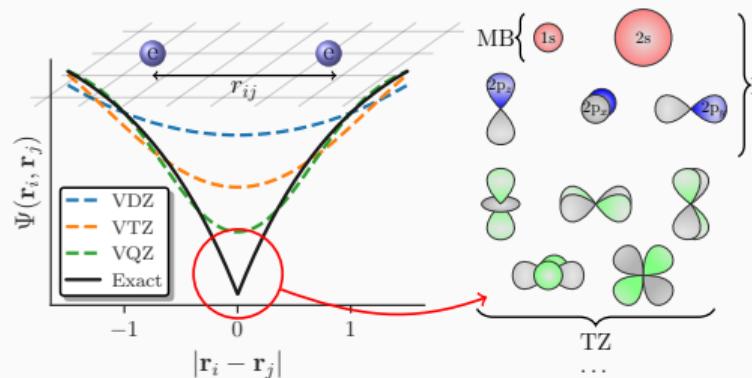
- LiH at equilibrium bond distance with 3 MP2 NOs.

- Hardware efficient RY Ansatz with linear entangling layer and parity encoding.

- Statevector simulation

Conclusions and Outlook
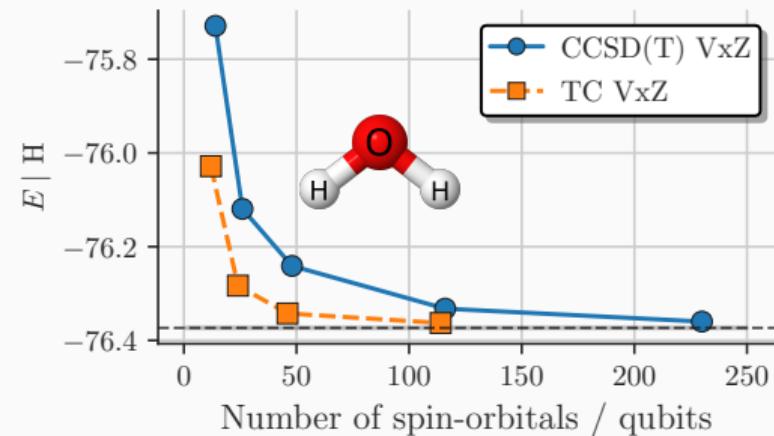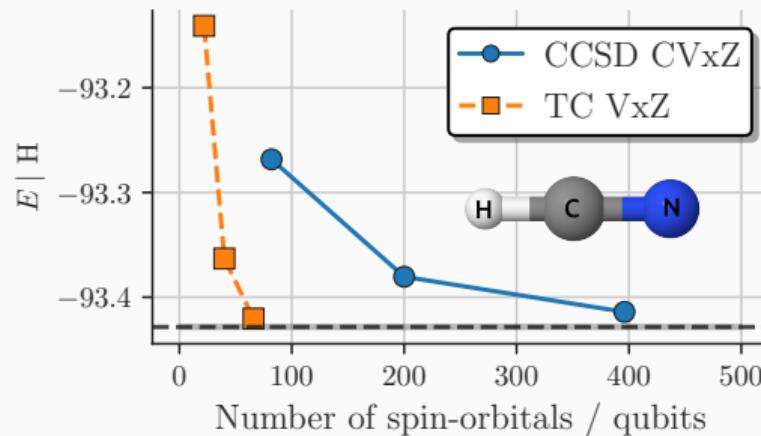
Conclusion – Transcorrelated Approach on Quantum Hardware

- Partially transferring electronic correlations from the wavefunction into the Hamiltonian, exactly capturing the cusp condition.

- Non-Hermitian Hamiltonian requires quantum imaginary time evolution, instead of standard VQE.

- Reduce qubit requirements and circuit depth, due to accurate results with a small basis sets.

- Extends applicability of NISQ devices to more relevant quantum chemistry problems.

Scaling to larger systems

Open questions: **Noise**, approximations to metric **A**, which Ansatz to use? ...

Postdoc in Chemical Bonding Analysis on Quantum Computers

Link. Supervisor: Martin Rahm, rahmlab.com

Thank you for your attention!

Jastrow s.t. Hamiltonian in 2nd quantised form

$$\bar{H} = \sum_{pq,\sigma} h_q^p a_{p,\sigma}^\dagger a_{q,\sigma} + \frac{1}{2} \sum_{pqrs} (V_{rs}^{pq} - K_{rs}^{pq}) \sum_{\sigma,\tau} a_{p,\sigma}^\dagger a_{q,\tau}^\dagger a_{s,\tau} a_{r,\sigma}$$

$$- \frac{1}{6} \sum_{pqrstu} L_{stu}^{pqr} \sum_{\sigma\tau\lambda} a_{p,\sigma}^\dagger a_{q,\tau}^\dagger a_{r,\lambda}^\dagger a_{u,\lambda} a_{t,\tau} a_{s,\sigma}$$

with

$$K_{rs}^{pq} = \langle \phi_p \phi_q | \hat{K} | \phi_r \phi_s \rangle$$
$$L_{stu}^{pqr} = \langle \phi_p \phi_q \phi_r | \hat{L} | \phi_s \phi_t \phi_u \rangle \quad \text{(48-fold symmetry in } L \text{ for real orbitals)}$$

Both integrals K and L are computed numerically using standard DFT grids over gaussian orbitals. The main problem is the storage of L. Current limit ≈ 80 orbitals

Other work

Mario Motta,†*[a] Tanvi P. Gujarati,†*[a] Julia E. Rice, †*[a] Ashutosh Kumar,[b] Conner Masteran,[b] Joseph A. Latone,[a] Eunseok Lee,[c] Edward F. Valeev[b] and Tyler Y. Takeshita†*[c]

2 Methods

2.1 Canonical transcorrelated F12 Hamiltonian

In the CT-F12 method, two main approximations are employed in addition to the approximate BCH expansion of eqn (2): (a) the expansion is truncated to only include up to double commutators and (b) in the double commutator term, the full Hamiltonian $\hat{H}$ is replaced by its effective 1-body constituent, the Fock operator $\hat{F}$,

$$\hat{H}' \approx \hat{H} + [\hat{H}, \hat{A}]_{1,2} + \frac{1}{2}\Big[[\hat{F}, \hat{A}]_{1,2}, \hat{A}\Big]_{1,2}. \qquad (3)$$

Hydrogen Fluoride

Motta *et al.*, Phys. Chem. Chem. Phys. **22**, 24270, 2020

Ab initio systems – other work

On the contrary, we opt to use an *a posteriori* correction based on a perturbative *explicitly correlated* method, namely the spin-free variant of [2]$_{R12}$ [18–20]. This approach is to be contrasted with other post-corrections in form of the family of quantum subspace expansion techniques [8, 9, 21]; and an application of VQE together with the transcorrelated approach, [2]$_{R12}$ or a so called "CABS singles" correction [22] has yet to be suggested in [23]. Brief comments on the distinction of our approach with this one will follow.

(b) Ro... E..... 14.667 [06]

Other work

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

Quantum Simulation of Molecular Electronic States with a Transcorrelated Hamiltonian: Higher Accuracy with Fewer Qubits

Ashutosh Kumar,* Ayush Asthana, Conner Masteran, Edward F. Valeev,* Yu Zhang,* Lukasz Cincio, Sergei Tretiak, and Pavel A. Dub*

$$\hat{\bar{H}} \approx \hat{H} + [\hat{H}, \hat{A}]_{1,2} + \frac{1}{2}[[\hat{F}, \hat{A}]_{1,2}, \hat{A}]_{1,2}$$
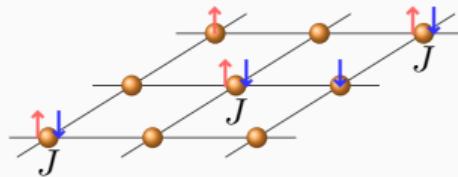
Improving the accuracy of quantum computational chemistry using the transcorrelated method

Sam McArdle[1],* and David P. Tew[2]
[1] Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom
[2] Physical and Theoretical Chemical Laboratory, University of Oxford, South Parks Road, Oxford OX1 3QZ, United Kingdom
(Dated: June 22, 2020)
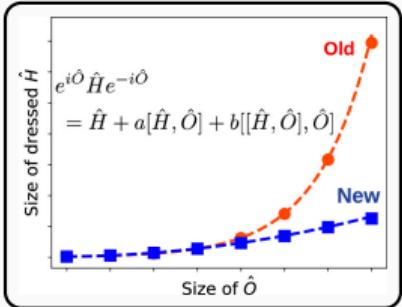
JCTC — Journal of Chemical Theory and Computation
pubs.acs.org/JCTC — Article

Unitary Transformation of the Electronic Hamiltonian with an Exact Quadratic Truncation of the Baker-Campbell-Hausdorff Expansion
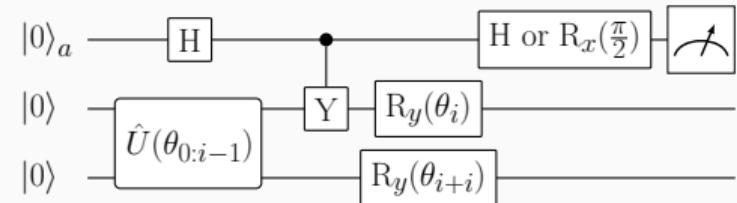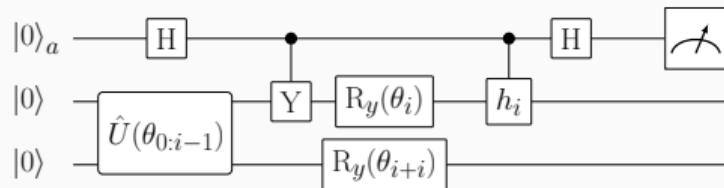
Robert A. Lang, Ilya G. Ryabinkin, and Artur F. Izmaylov*

$$e^{i\hat{O}}\hat{H}e^{-i\hat{O}} = \hat{H} + a[\hat{H}, \hat{O}] + b[[\hat{H}, \hat{O}], \hat{O}]$$

Kumar *et al.*, J. Chem. Theory Comput. 2022, 18, 9, 5312; McArdle and Tew, arXiv:2006.11181, 2020; Lang *et al.*, J. Chem. Theory Comput. 2021, 17, 1, 66;

QITE with non-Hermitian $\bar{H}$

Gradient in the Hermitian case: $\qquad C_i = \dfrac{\partial \langle \Phi |}{\theta_i} \hat{H} |\Phi\rangle$

In the TC case: split non-Hermitian Hamiltonian in Hermitian and anti-Hermitian part:

$$\hat{H}_{TC}^+ = \hat{H}_{TC} + \hat{H}_{TC}^\dagger, \qquad \hat{H}_{TC}^- = \hat{H}_{TC} - \hat{H}_{TC}^\dagger$$

$$C_i = \frac{1}{2} \left(\langle \partial_{\theta_i} \Phi | \hat{H}_{TC} | \Phi \rangle + \langle \Phi | \hat{H}_{TC}^\dagger | \partial_{\theta_i} \Phi \rangle \right) = \frac{C_i^+ + C_i^-}{4}$$

$$C_i^+ = 2 \langle \partial_{\theta_i} \Phi | \hat{H}_{TC}^+ | \Phi \rangle, \qquad C_i^- = 2 \langle \partial_{\theta_i} \Phi | \hat{H}_{TC}^- | \Phi \rangle$$

McArdle and Tew, arXiv:2006.11181, 2020; Sokolov, **WD**, Luo, Alavi, Tavernelli, arXiv:2201.03049 (2022); Schuld *et al.*, Phys. Rev. A 99, 032331 (2019)