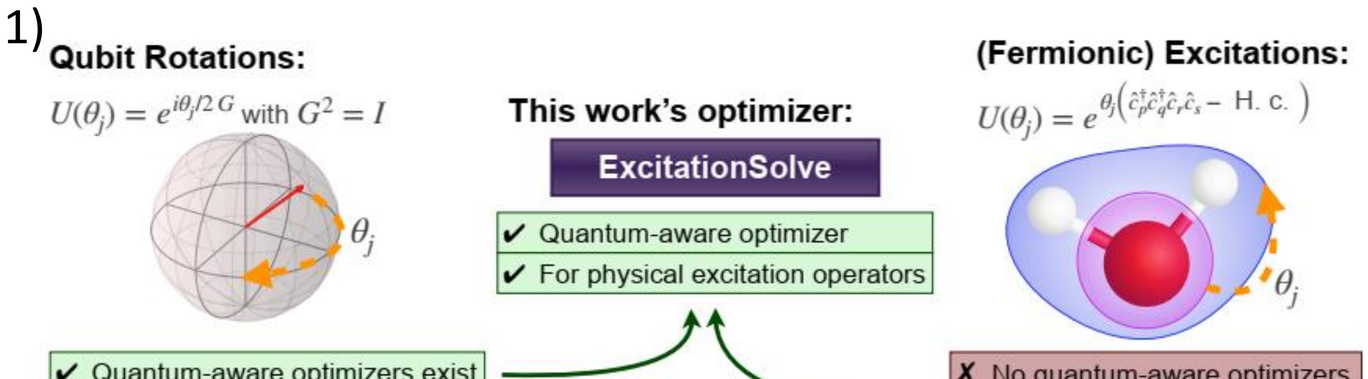
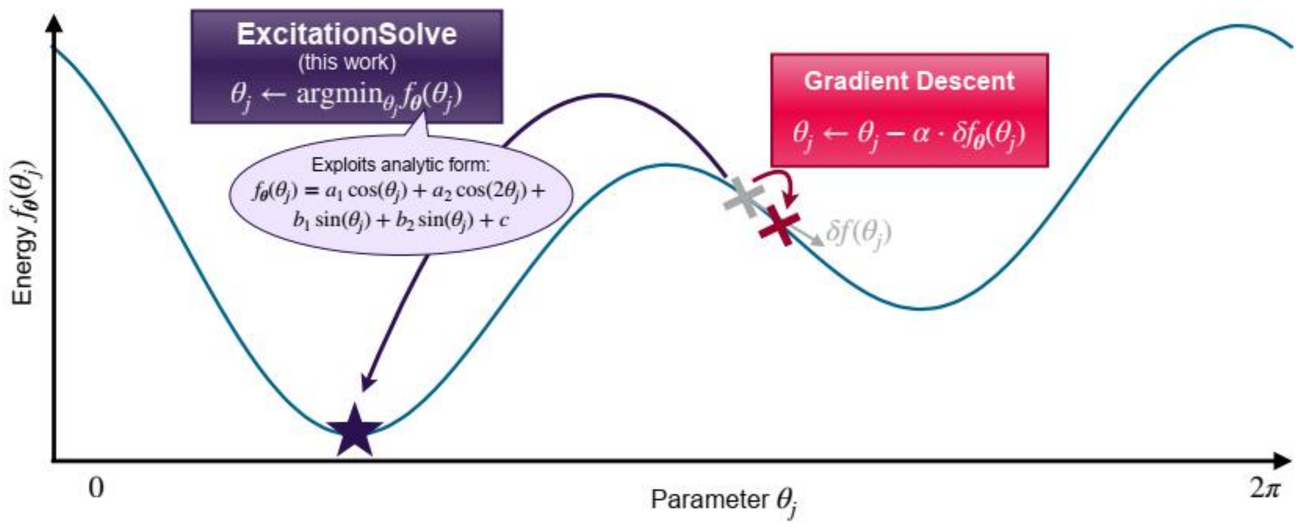
ExcitationSolve – A fast gradient-free optimizer for excitations in fixed and adaptive VQEs

Max Haas [1], Jonas Jäger,[1] Thierry N. Kaldenbach [1], Erik Schultheis [1], Thomas Hammerschmidt [2], Daniel Barragan-Yani [1]
[1] Institute of Materials Research, DLR Köln-Porz
[2] Ruhr University Bochum, ICAMS, Bochum

1)



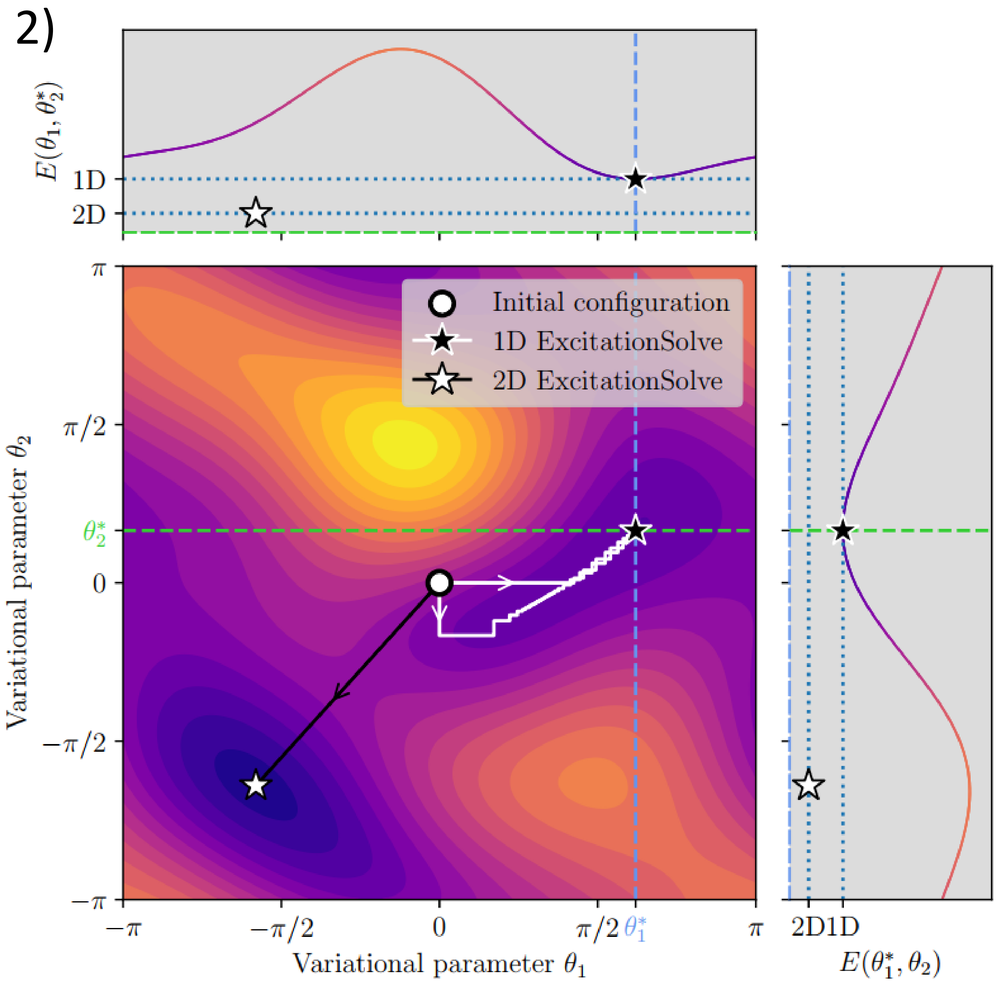
Optimization step of (fermionic) excitation operator: *(same quantum resources)*



Introduction

ExcitationSolve is a fast globally-informed gradient-free optimizer for physically-motivated ansätze constructed of excitation operators, a common choice in variational quantum eigensolvers. This new optimizer determines the global optimum along each variational parameter using the same quantum resources that gradient-based optimizers require for one update step (Fig. 1).

2)



It can be used for both adaptive- and fixed ansätze

- ExcitationSolve both for operator selection and optimization (Fig. 3)
- Initialize new operators with optimal parameter
- Multi-parameter optimization can avoid and help escape local minima (Fig. 2)
- Combine with Energy Sorting [3] to build ansatz with a single iteration over operator pool

Publications:

Publication on ArXiv:

- Jäger, Kaldenbach, Haas, Schultheis *„Fast gradient-free optimization of excitations in VQEs"*
- Code on GitHub

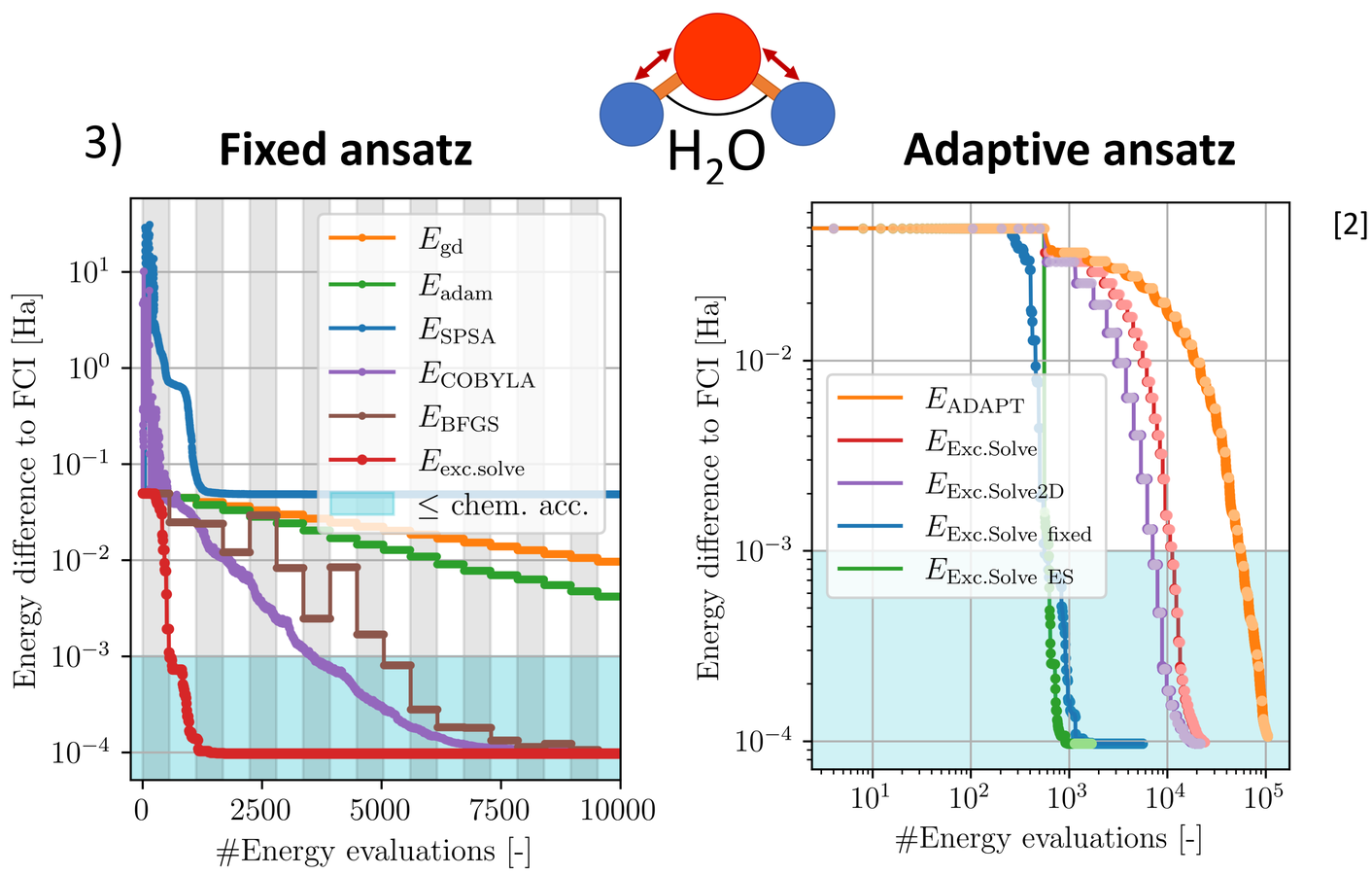
Paper

Code

Coming soon:

- Reviewed Journal publication
- Follow-up publication

3)



[2]

Sources

[1] Peruzzo et al., 2014, Nat. Comm.
[2] Grimsley at al., 2019, Nat. Comm.
[3] Fan et al., 2023, J. Phys. Chem. Lett.

Bundesministerium für Wirtschaft und Klimaschutz
DLR Quantencomputing Initiative
QuantiCoM
DLR