Surrogate Optimization of Quantum Circuits

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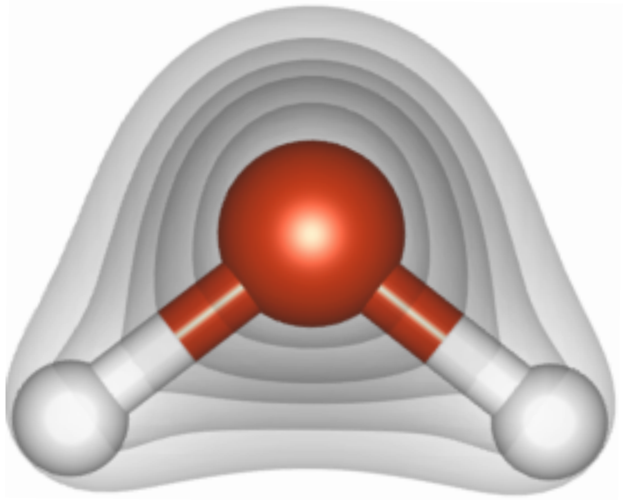
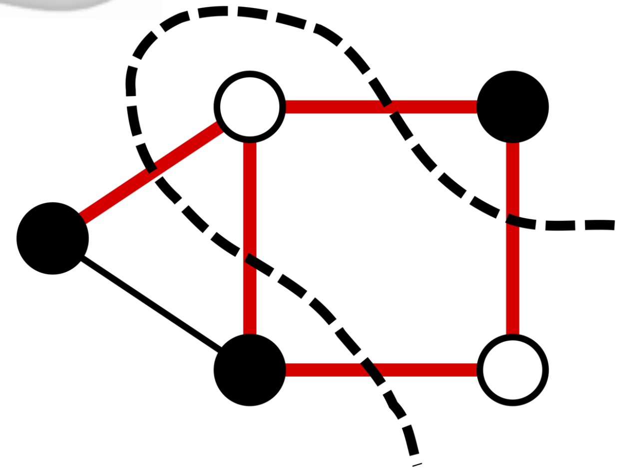
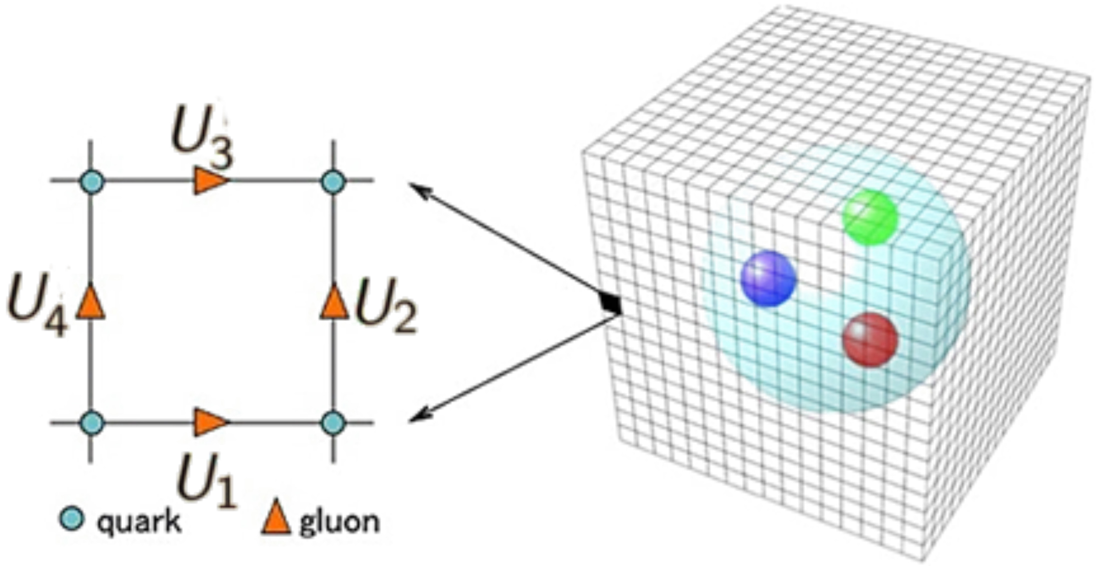
VQEs are proposed target for NISQ state preparation



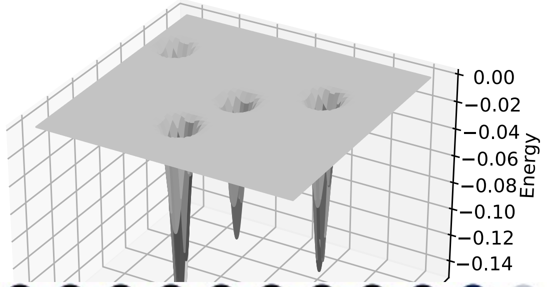




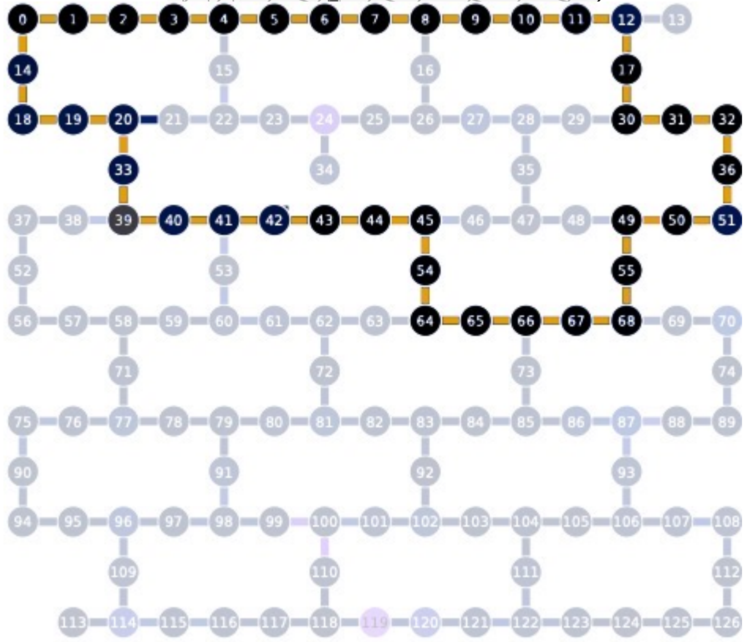
Max Cut: Author Miym: Used under [CC-BY-SA-3.0](CC-BY-SA-3.0)
https://en.wikipedia.org/wiki/Maximum_cut#/media/File:Max-cut.svg

VQEs have some issues

- Barren plateaus

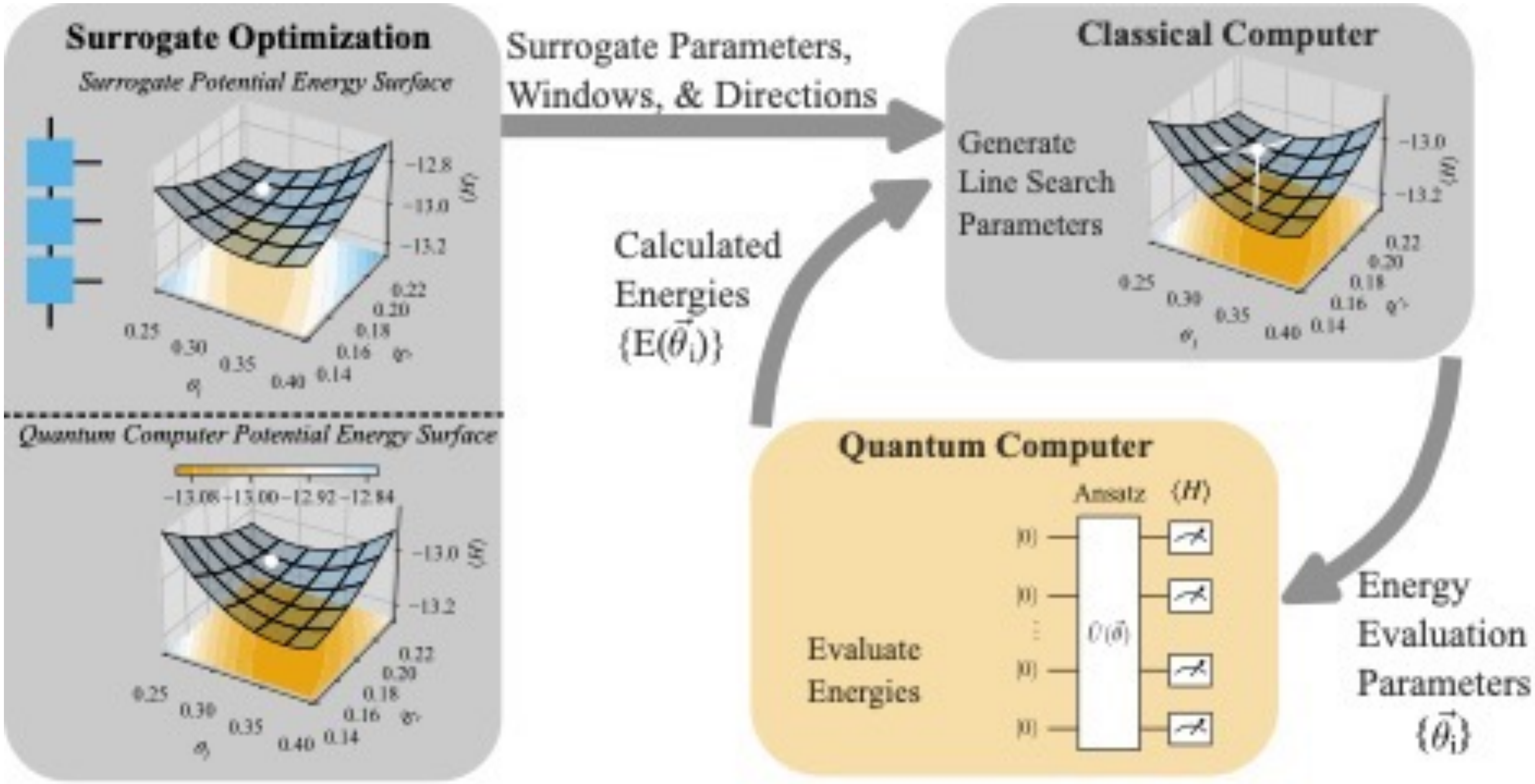


- Hardware constraints



- Gradient Estimations

Surrogate Hessian Approach

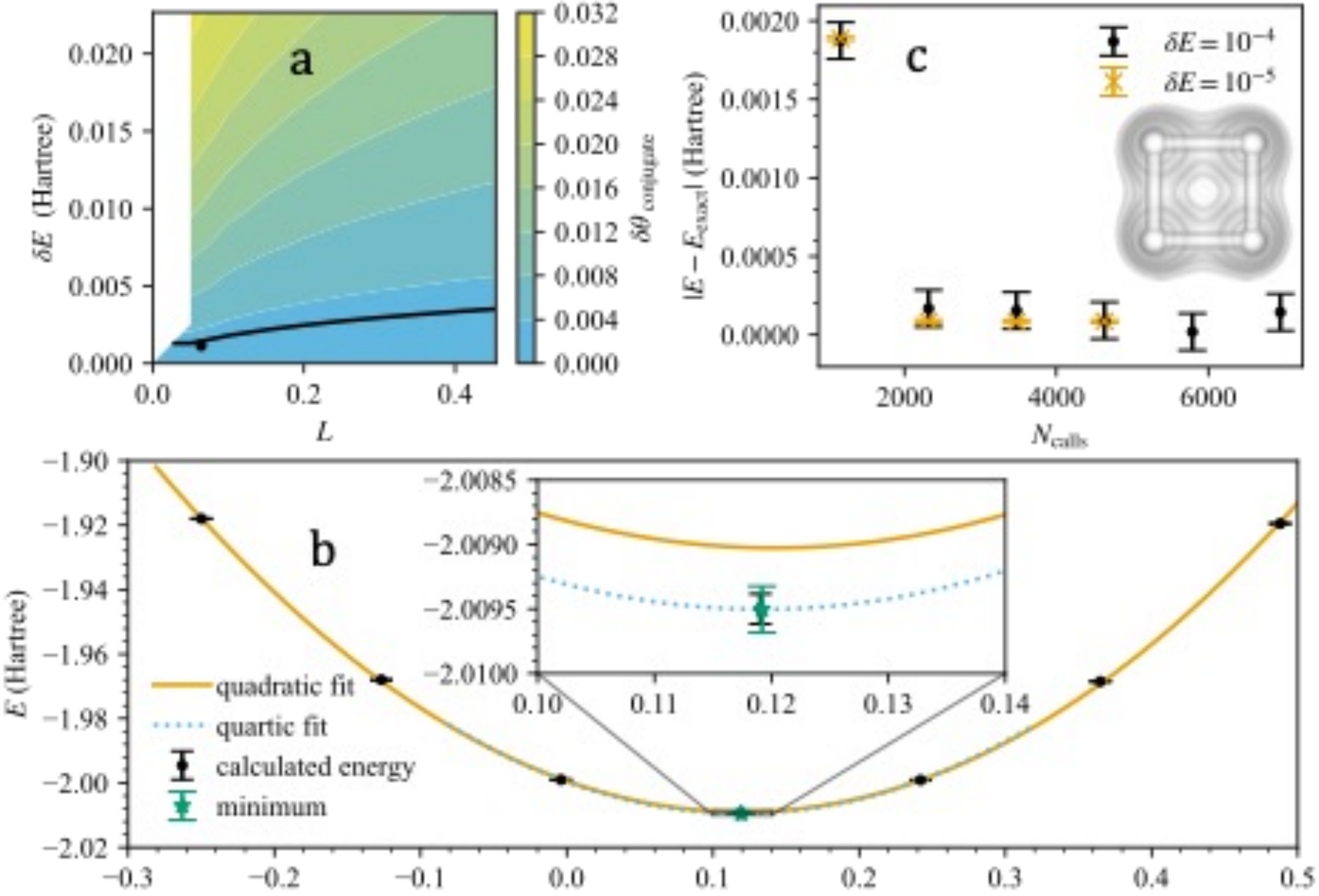


Optimization of chemical systems (H_4)

1. Optimize the window size and parameter uncertainties for a given target energy

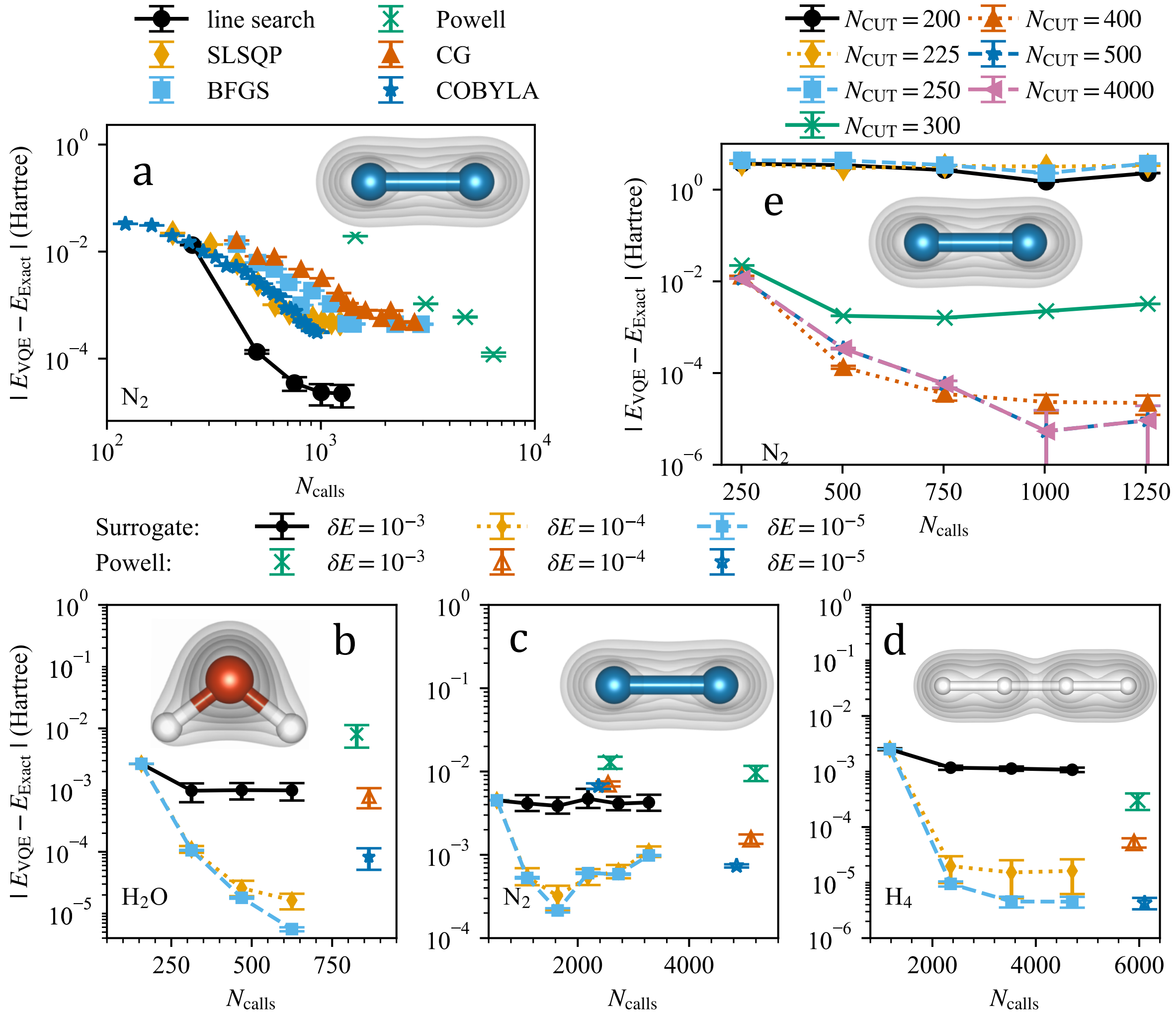
2. Perform line searches across the conjugate directions

3. Repeat until converged



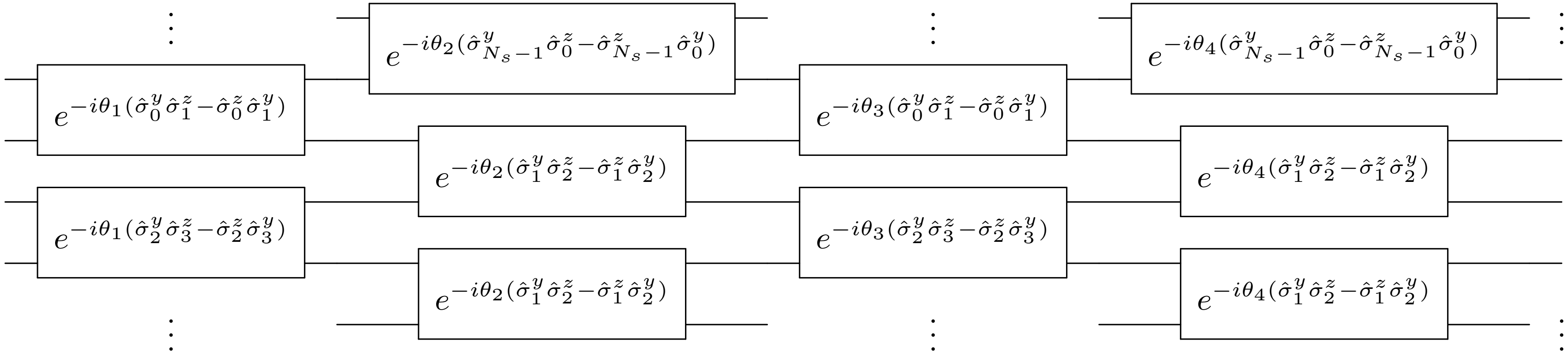
Optimization of chemical systems (H_2O, H_4, N_2)

1. Line search performs significantly better than traditional optimizers
2. Significantly better than noise resilient Powell
3. Accuracy of the surrogate is important for swift convergence

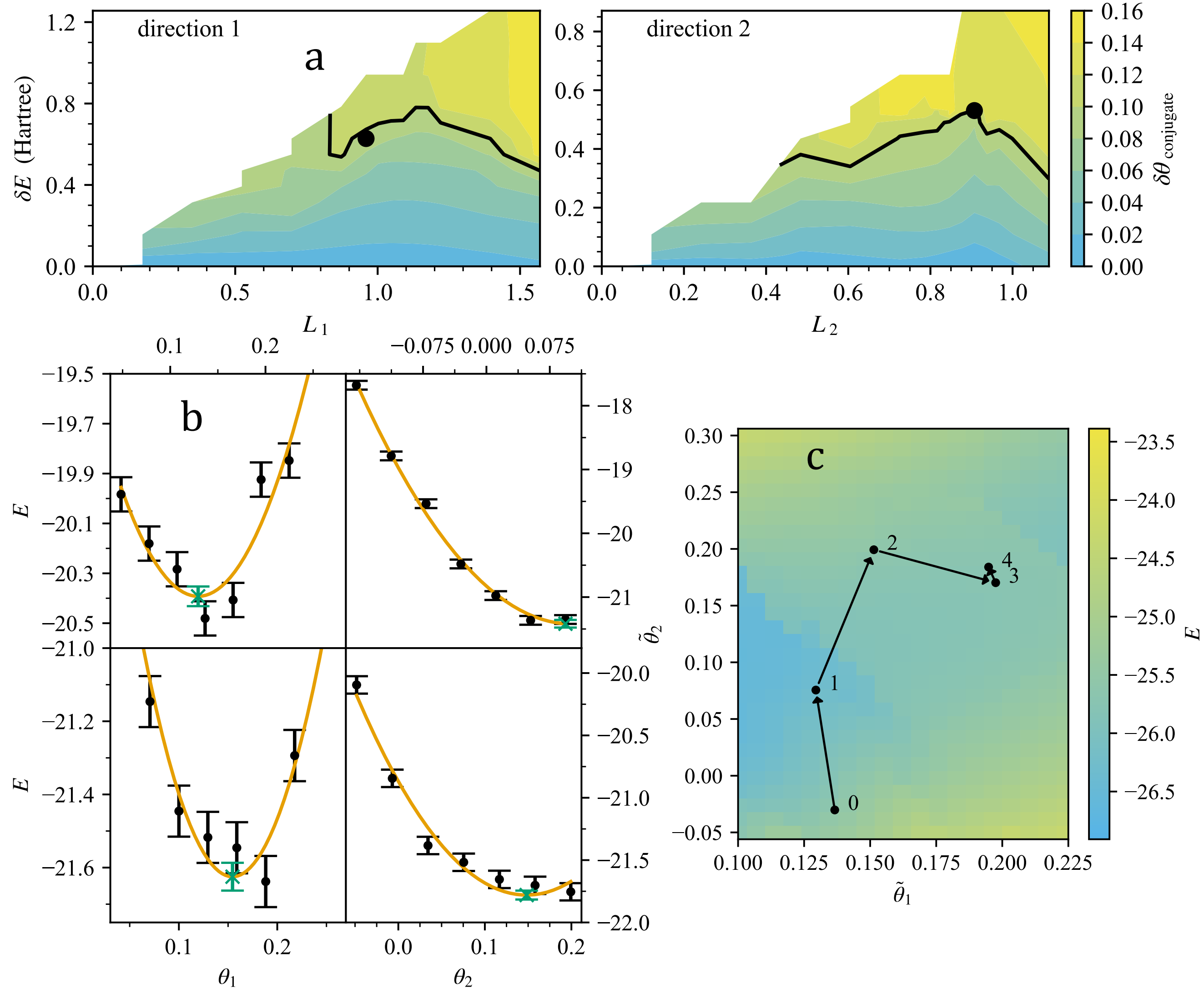


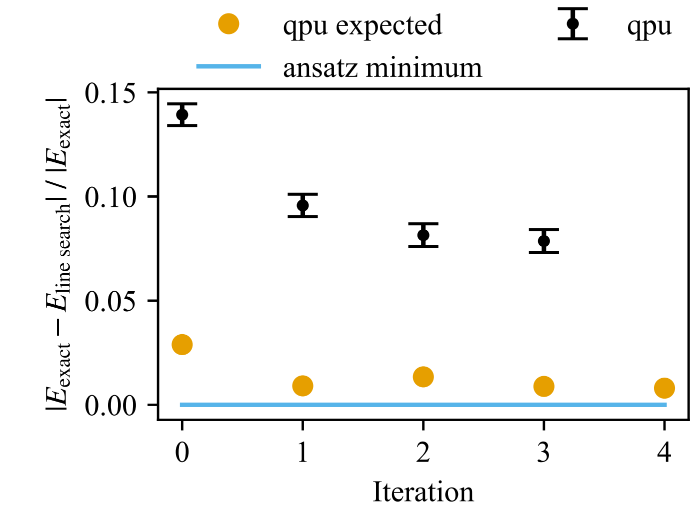
Optimization of transverse Ising model on QPU

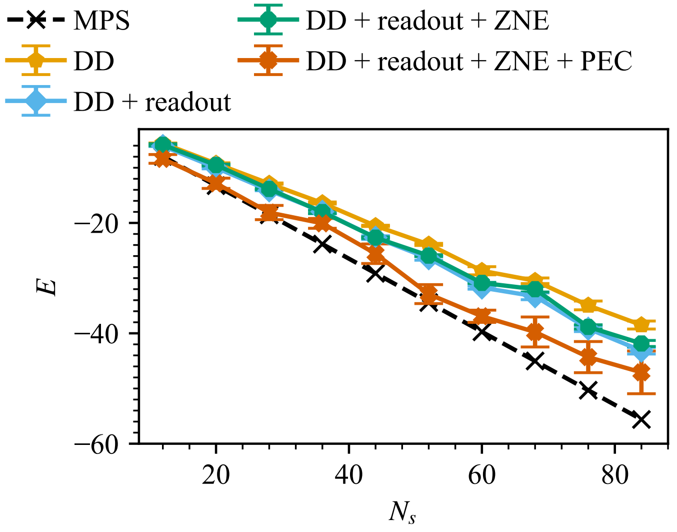
$$\hat{H} = J_1 \sum_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z + J_2 \sum_i \hat{\sigma}_i^z \hat{\sigma}_{i+2}^z + h_t \sum_i \hat{\sigma}_i^x$$



Optimization of transverse Ising model on QPU







Highlights

- Demonstrated an improvement over existing optimizers for electronic structure problems
- Proof-of-principle demonstration for the transverse Ising model using *40 qubits*
- Method is systematically improvable

Open Questions:

1. Scaling to sufficiently complex circuits
2. Can one semi-dynamically update the search directions?
3. Extensions to material systems?
4. Gauge theories?

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