Using Machine Learning for Noise Resilient Optimization of Variational Quantum Eigensolvers

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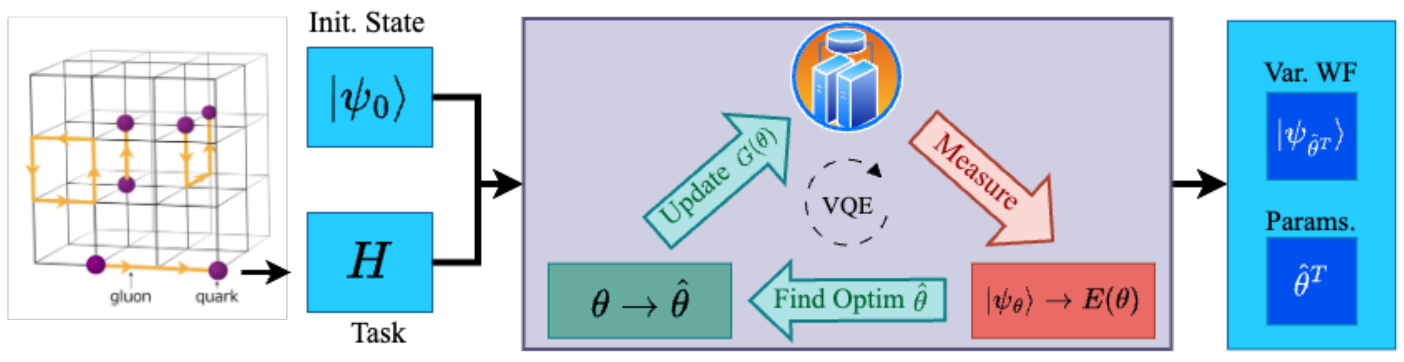
Motivation — VQEs on NISQ Devices

Noisy Intermediate Scale Quantum **(NISQ)** devices may be harnessed to **outperform classical hardware** for specific optimization tasks.

Especially, hybrid quantum-classical algorithms like Variational Quantum Eigensolvers **(VQEs)** can compute **ground state energies** of quantum Hamiltonians, or complex **minimization tasks** in general.



Background — VQEs and NFT Baseline

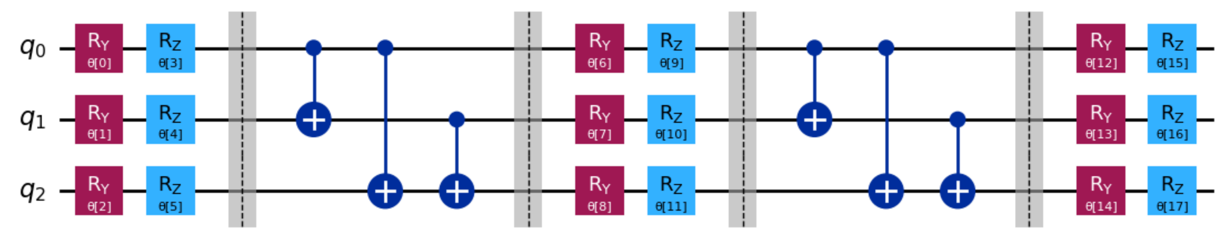
Goal:

- Find ground state and excited states of Hamiltonian H.

Quantum Device:

- Measure variational quantum circuit: get objective function $f^*(\boldsymbol{\theta}) = \langle\psi(\boldsymbol{\theta})|H|\psi(\boldsymbol{\theta})\rangle$

$|\psi(\boldsymbol{\theta})\rangle =$



Classical Computer:

- Optimize parameters $\boldsymbol{\theta}$, given $f^*(\boldsymbol{\theta})$ – improvement by new **EMICoRe** method [1]
- Baseline method (NFT [2]) uses VQE's functional form for sequential optimization:

$$f^*(\boldsymbol{\theta}) = \boldsymbol{b}^{\mathrm{T}} \cdot \mathbf{vec}\left(\bigotimes_{d=1}^{D}\begin{pmatrix}\cos(\theta_d)\\ \sin(\theta_d)\\ 1\end{pmatrix}\right), \quad \forall \boldsymbol{\theta} \in [0, 2\pi)^D$$

- Sequential optimization of one parameter θ_d each → $f^*(\theta_d)$ becomes cosine
- Find subspace optimum: fit two equidistant measurements + previous optimum

Background — GP Regression and VQE Kernel

- Gaussian Process Regression use **Multivariate Gaussian** distribution
  - **Goal:** infer mean and variance of function values $f(\Theta')$ from N measured noisy points $\{\Theta, f^*(\Theta) + \epsilon\}$, with $\Theta = \{\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_N\}$.

$$p\left(\boldsymbol{f}' \mid \Theta, \boldsymbol{y}\right) = \mathcal{N}_M\left(\boldsymbol{f}'; \boldsymbol{\mu}'_\Theta, \boldsymbol{S}'_\Theta\right), \quad \text{with}$$

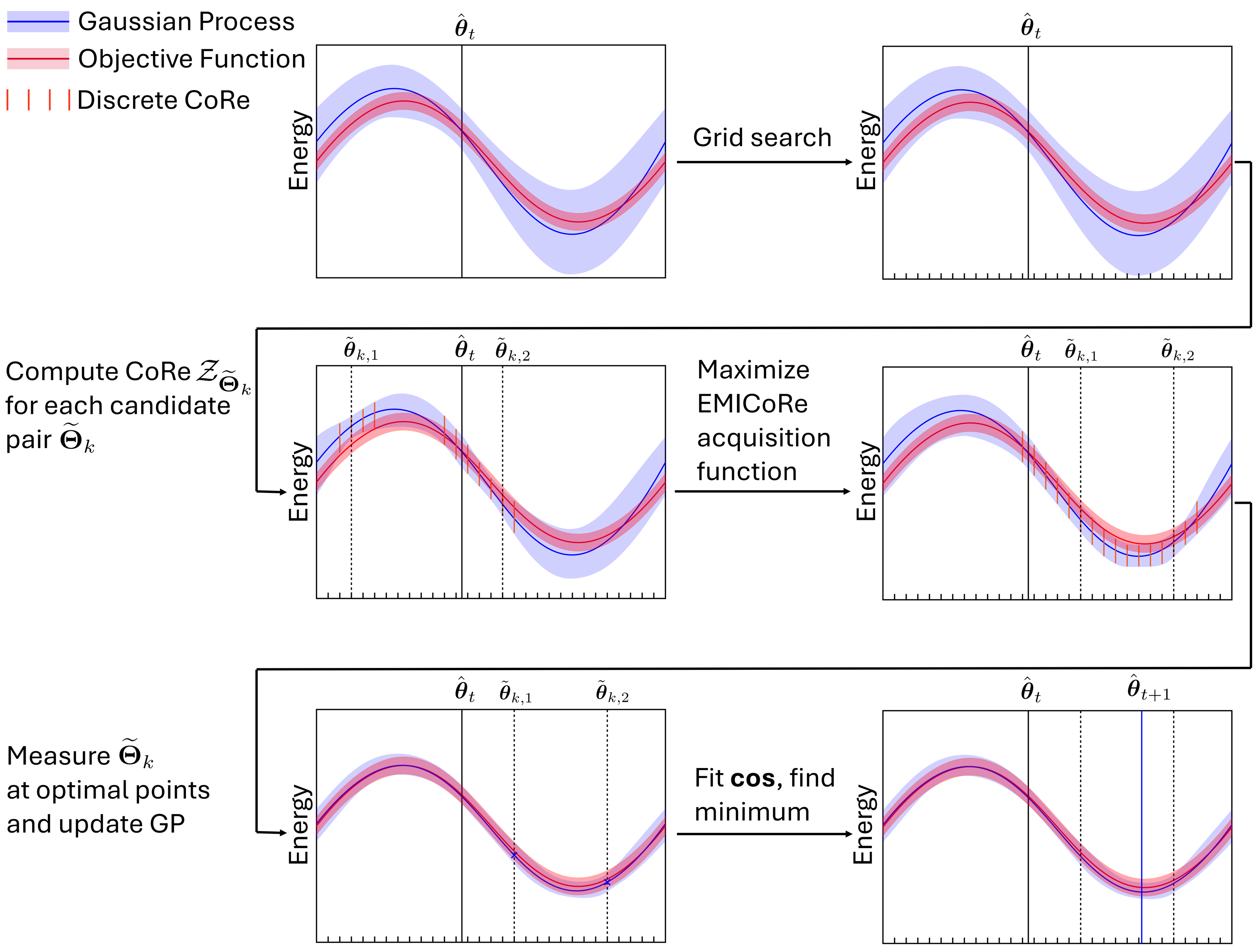
$$\boldsymbol{\mu}'_\Theta = \boldsymbol{K}'^{\top}\left(\boldsymbol{K} + \sigma^2 \boldsymbol{I}_N\right)^{-1}\boldsymbol{y}, \quad \boldsymbol{S}'_\Theta = \boldsymbol{K}'' - \boldsymbol{K}'^{\top}\left(\boldsymbol{K} + \sigma^2\boldsymbol{I}_N\right)^{-1}\boldsymbol{K}' \text{ and}$$

$$\boldsymbol{K} = k(\Theta, \Theta), \quad \boldsymbol{K}' = k\left(\Theta, \Theta'\right), \text{ and } \boldsymbol{K}'' = k\left(\Theta', \Theta'\right)$$

- Kernel function of the VQE can be infered from its functional form [1]:

$$k^{\mathrm{VQE}}\left(\boldsymbol{\theta}, \boldsymbol{\theta}'\right) = \sigma_0^2 \prod_{d=1}^{D}\left(\frac{\gamma^2 + \cos\left(\theta_d - \theta'_d\right)}{1 + \gamma^2}\right)$$

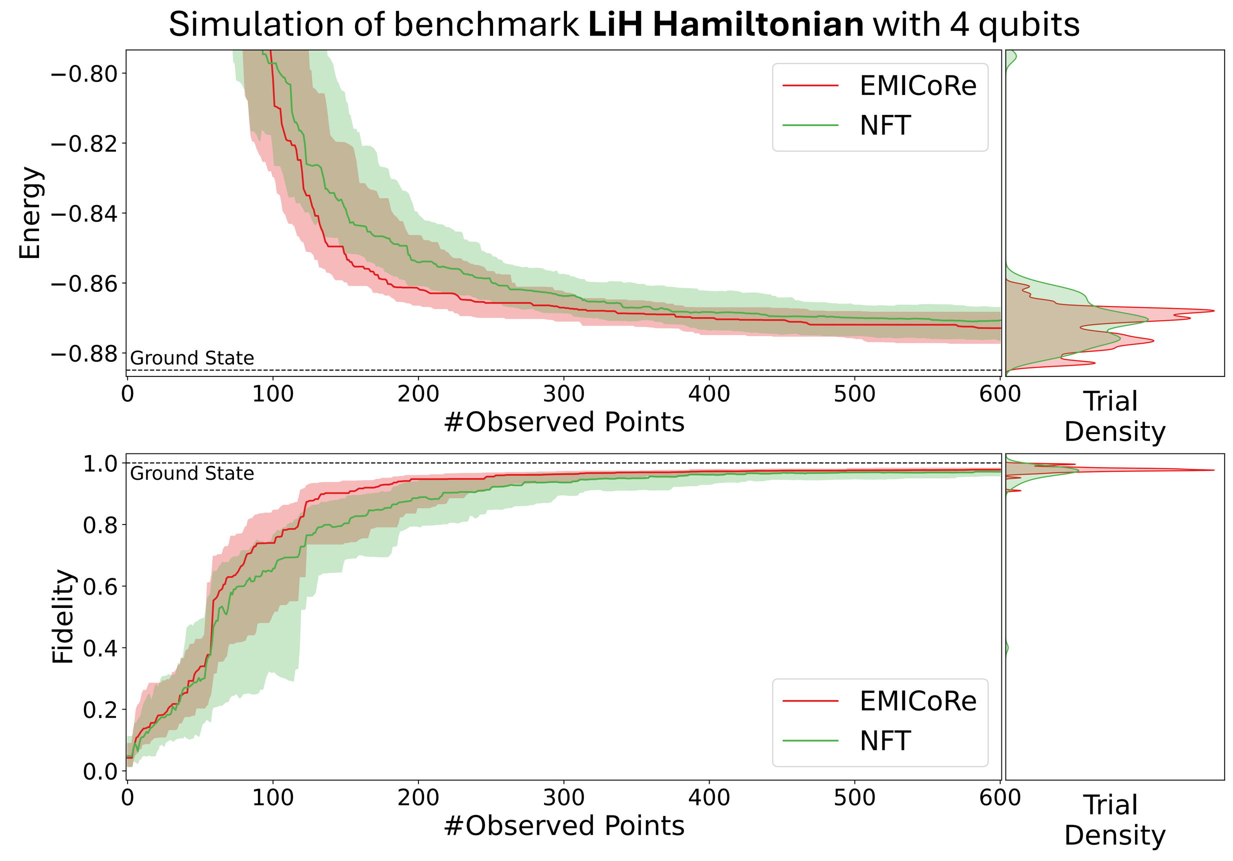
Method — EMICoRe's Algorithmic Procedure



Results — Quantum Chemistry Hamiltonian

$$H = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2}\sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s \qquad \text{Adapted from [3]}$$

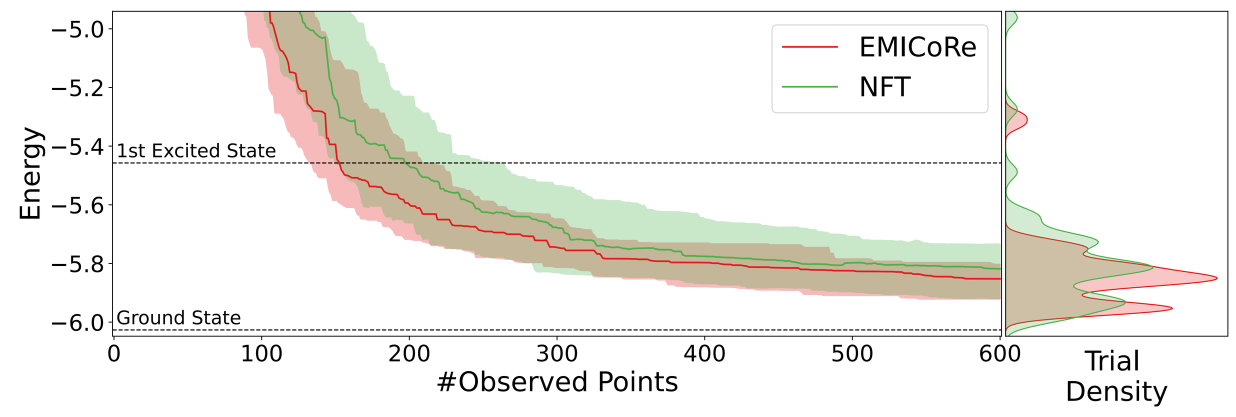
Simulation of benchmark **LiH Hamiltonian** with 4 qubits



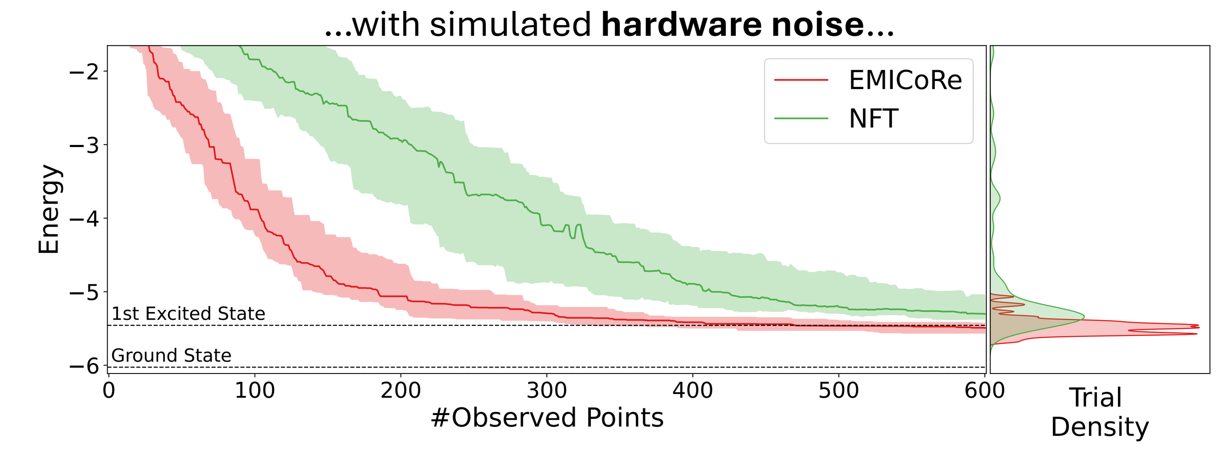
Results — Simulated Hardware Noise

$$H_{\text{Ising}} = \sum_{j=1}^{Q-1}\sigma_j^X\sigma_{j+1}^X + \sum_{j=1}^{Q}\sigma_j^Z$$

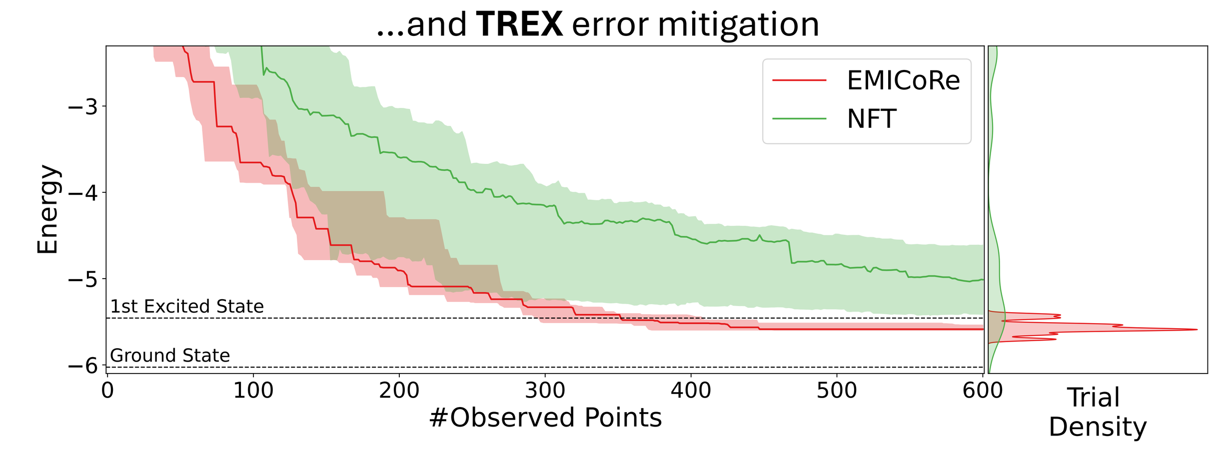
Simulation of benchmark **Ising Hamiltonian** with **5** qubits...



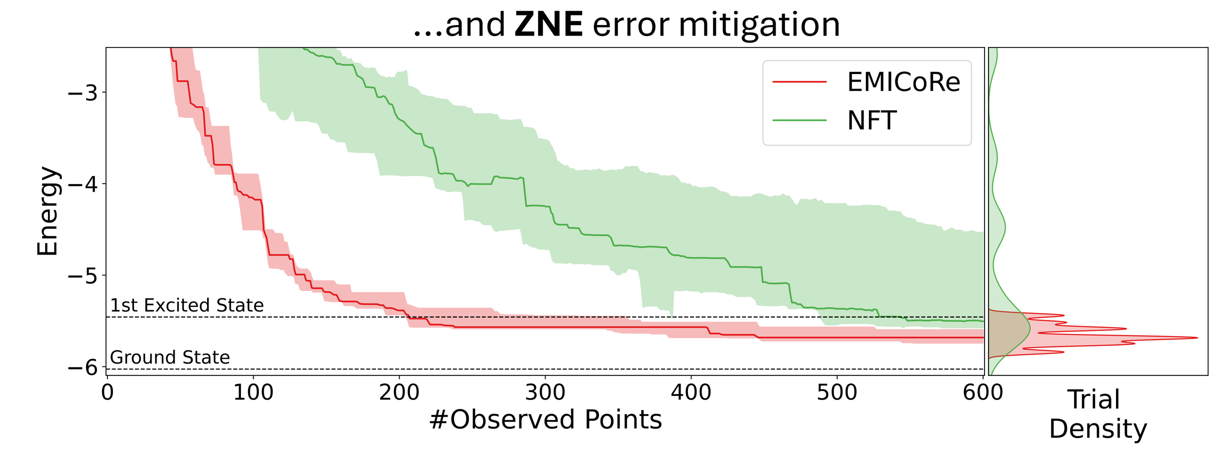
...with simulated **hardware noise**...



...and **TREX** error mitigation



...and **ZNE** error mitigation



Fake5QV1() backend from **qiskit.primitives** used for noisy simulations

Conclusion

1. VQE kernel with EMICoRe acquisition function: **powerful machine-learning-based method for optimising VQEs**
2. Outperformance of state-of-the-art baseline for benchmark **Ising model**, even stronger for more complex **quantum chemistry Hamiltonian**
3. Even **stronger outperformance** when applying **simulated hardware noise**
4. Future work on application to lattice field theories, e.g. **2+1D QED**

References

[1] Nicoli, Anders, Funcke, et al. "Physics-Informed Bayesian Optimization of Variational Quantum Circuits". Proceedings of 37th Conference on Neural Information Processing Systems (NeurIPS 2023)

[2] Nakanishi, et al. "Sequential minimal optimization for quantum-classical hybrid algorithms". *Phys. Rev. Research 2, 043158* (2020)

[3] Kandala, et al. "Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets". *Nature* 549, 242 (2017)