Finding Excitation Spectra Using a Quantum Computer

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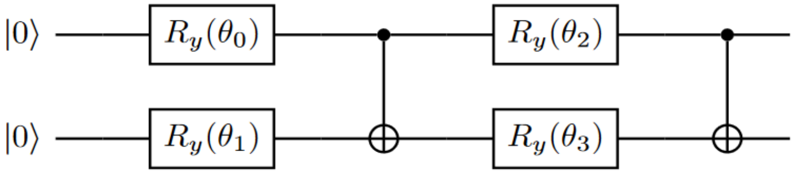
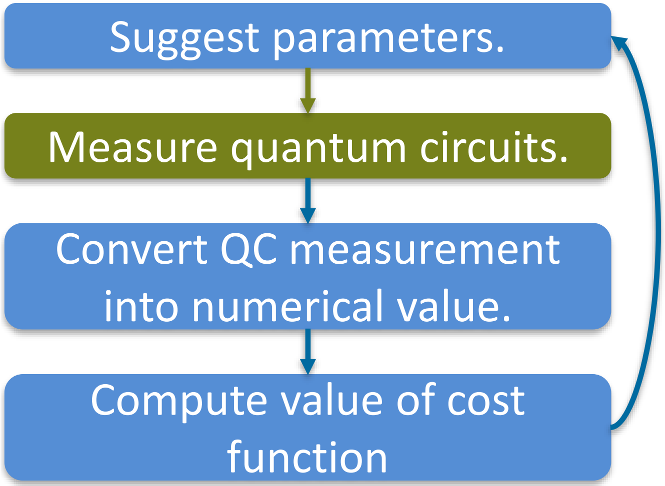
Variational Algorithms

- Noisy, Intermediate Scale Quantum (NISQ) era.
- Error prone, low coherence times.
- Variational algorithms help by reducing computational load on the QC.
- Hybrid Algorithms – utilise both quantum and classical computers
- Use short variational quantum circuits.
- Iterates until exit conditions are met.





Lipkin-Meshkov-Glick Model

- Simple shell model with two levels.
- Interactions that scatter a pair of particles from one level to the other.

$$H = \frac{1}{2}\epsilon \sum_{p\sigma} \sigma a^{\dagger}_{p\sigma} a_{p\sigma} + \frac{1}{2} V \sum_{pp'\sigma} a^{\dagger}_{p,\sigma} a^{\dagger}_{p',\sigma} a_{p',-\sigma} a_{p,-\sigma} + \frac{1}{2} W \sum_{pp'\sigma} a^{\dagger}_{p,\sigma} a^{\dagger}_{p',-\sigma} a_{p',\sigma} a_{p,-\sigma}$$

- The W term is commonly set to zero, and the Hamiltonian can be written in the quasi-spin basis.
- Block diagonal in quasi-spin basis.
- Hamiltonians label as H_N, where N is the number of particles.

H.J. Lipkin, N. Meshkov, and A.J. Glick. "Validity of many-body approximation methods for a solvable model: (I). Exact solutions and perturbation theory". In: Nuclear Physics 62.2 (1965), pp. 188–198. issn: 0029-5582.

Variational Quantum Eigensolver (VQE)

- Variational algorithm used to find ground state of an operator.
- For this work, the operators are the $N = 3$ and $N = 7$ LMG models.
- Operator expressed in terms of Pauli spin matrices.
- Cost function minimises the expectation energy of the operator.

$$H_{N=3A} = \begin{bmatrix} -1.5 & -0.866 \\ -0.866 & 0.5 \end{bmatrix}$$

$$H_{N=3A} = -0.5 - 1.0Z_0 - 0.8660254X_0$$

$$H_{N=7A} = \begin{bmatrix} -3.5 & -2.291 & 0 & 0 \\ -2.291 & -1.5 & -3.873 & 0 \\ 0 & -3.873 & 0.5 & -3.354 \\ 0 & 0 & -3.354 & 2.5 \end{bmatrix}$$

$$\begin{aligned} H_{N=7} = & -0.5 - 2.8225X_1 - 1.0Z_1 - 1.9365X_0X_1 \\ & - 1.9365Y_0Y_1 - 2.0Z_0 + 0.5315Z_0X_1. \end{aligned}$$

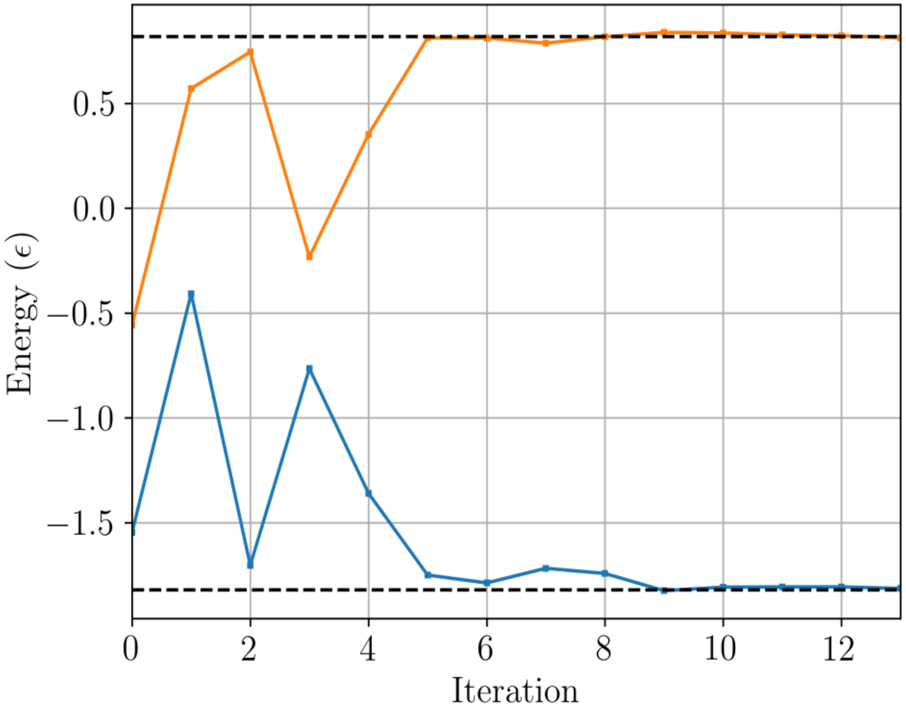
VQE: Finding Excited States

- Adjust cost function to minimise the variance of the Hamiltonian, instead of energy.

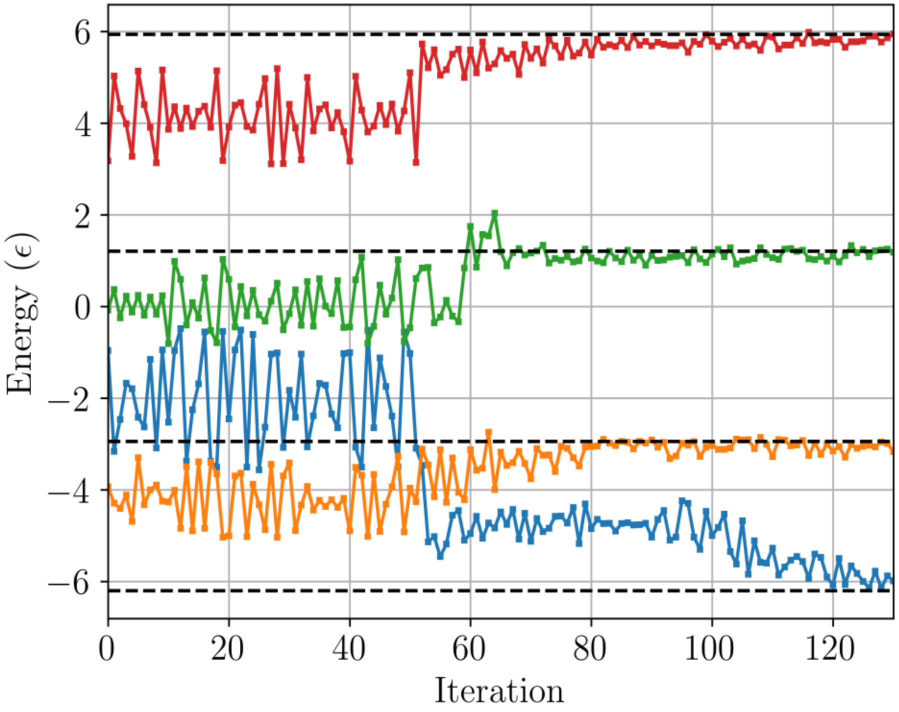
$$\sigma^2 = \langle H^2 \rangle - \langle H \rangle^2.$$

- Variance of Hamiltonian is zero at eigenstates.
- Introduces additional circuit measurements but no additional circuit complexity.
- Suitable for NISQ hardware.

N=3

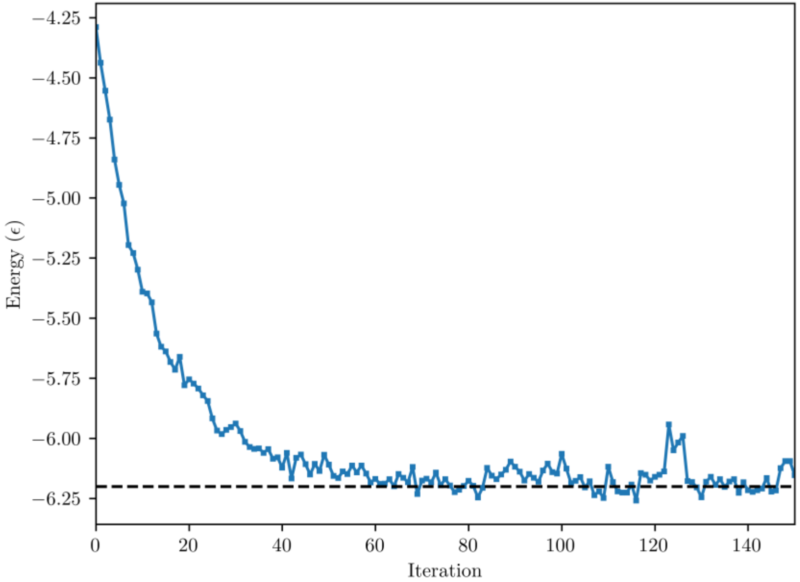

0.5
0.0
−0.5
−1.0
−1.5
Energy (ϵ)
0
2
4
6
8
10
12
Iteration

N=7


6
4
2
0
−2
−4
−6
Energy (ϵ)
0
20
40
60
80
100
120
Iteration

VarQITE

- Variational Quantum Imaginary Time Evolution.
- Original QITE is too expensive for NISQ hardware.
- Variational QITE encodes the time evolution into the quantum circuit parameters.
- Solves a series of liner equations $A\dot{\theta} = C$
- A and C are created using measurements from the quantum computer, $\dot{\theta}$ is the change in parameters of the variational circuit for the next iteration.
- Evolves over iterations to find the ground state of a given operator.



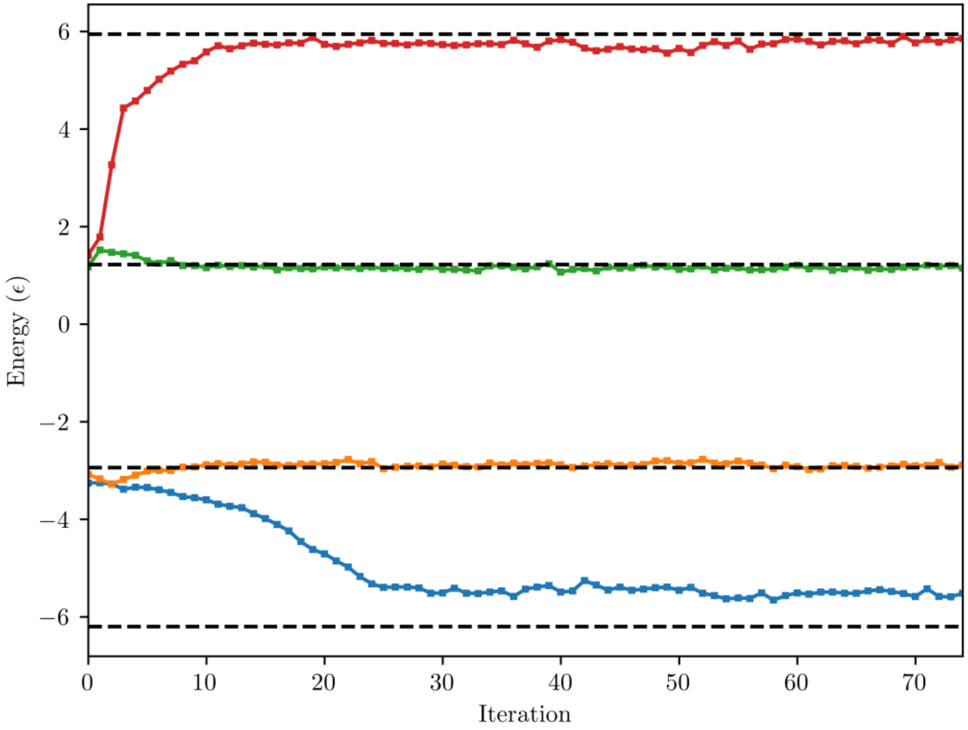
Xiao Yuan et al. “Theory of variational quantum simulation”. In: Quantum 3 (Dec. 2018), pp. 1–41

VarQITE: Finding Excited States

- Adjusting the creation of matrix C allows for excited states to be found.
- By default, C is a gradient matrix that represents the derivative of the operator w.r.t each parameter in the variational circuit.
- C can be altered to instead represent the derivative of the variance of the operator w.r.t each parameter in the variational circuit.
- This, like with the Variance VQE method, introduces additional circuit measurements over the original algorithm but does not increase circuit depth or qubit number.
- Suitable for NISQ hardware.

VarQITE Excited State Results

- Random initial parameters.
- IBM_Nairobi: 25000 shots.
- Good convergence to all but the ground state.
- For most states, convergence in small number of iterations.



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