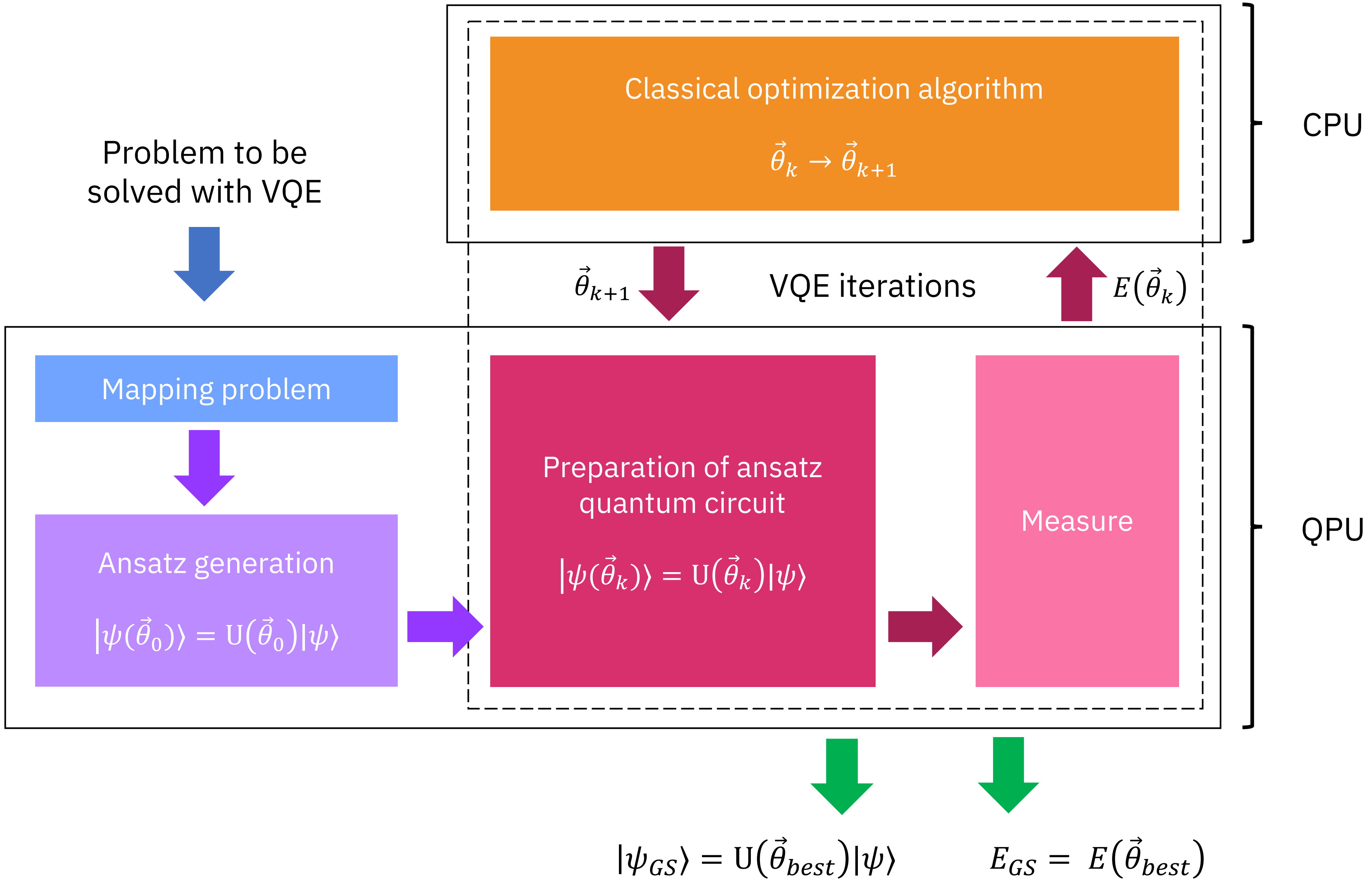
Variational Quantum Eigensolver introduction

- **Ansatz**: a parameterized circuit used as Ansatz for the wave function
- **Optimizer**: a classical optimizer. Can either be a Qiskit optimizer or a callable that takes an array as input and returns a Qiskit or SciPy optimization result
- **Initial points**: an optional initial point (i.e. initial parameter values) for the optimizer. If *None* then VQE will look to the ansatz for a preferred point, and if *Not* will simply compute a random one
- **Callback**: a callback that can access the intermediate data during the optimization
- **Quantum instance**: the backend



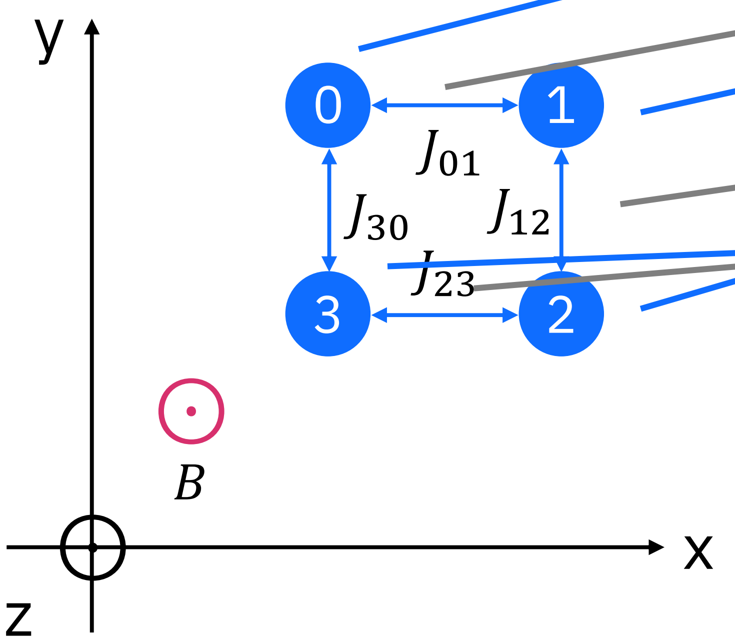
https://qiskit.org/documentation/stubs/qiskit.algorithms.VQE.html

Simulating Static and Dynamic Properties of Magnetic Molecules with Prototype Quantum Computers – L. Crippa et al., Magnetochemistry 7, 117 (2021)

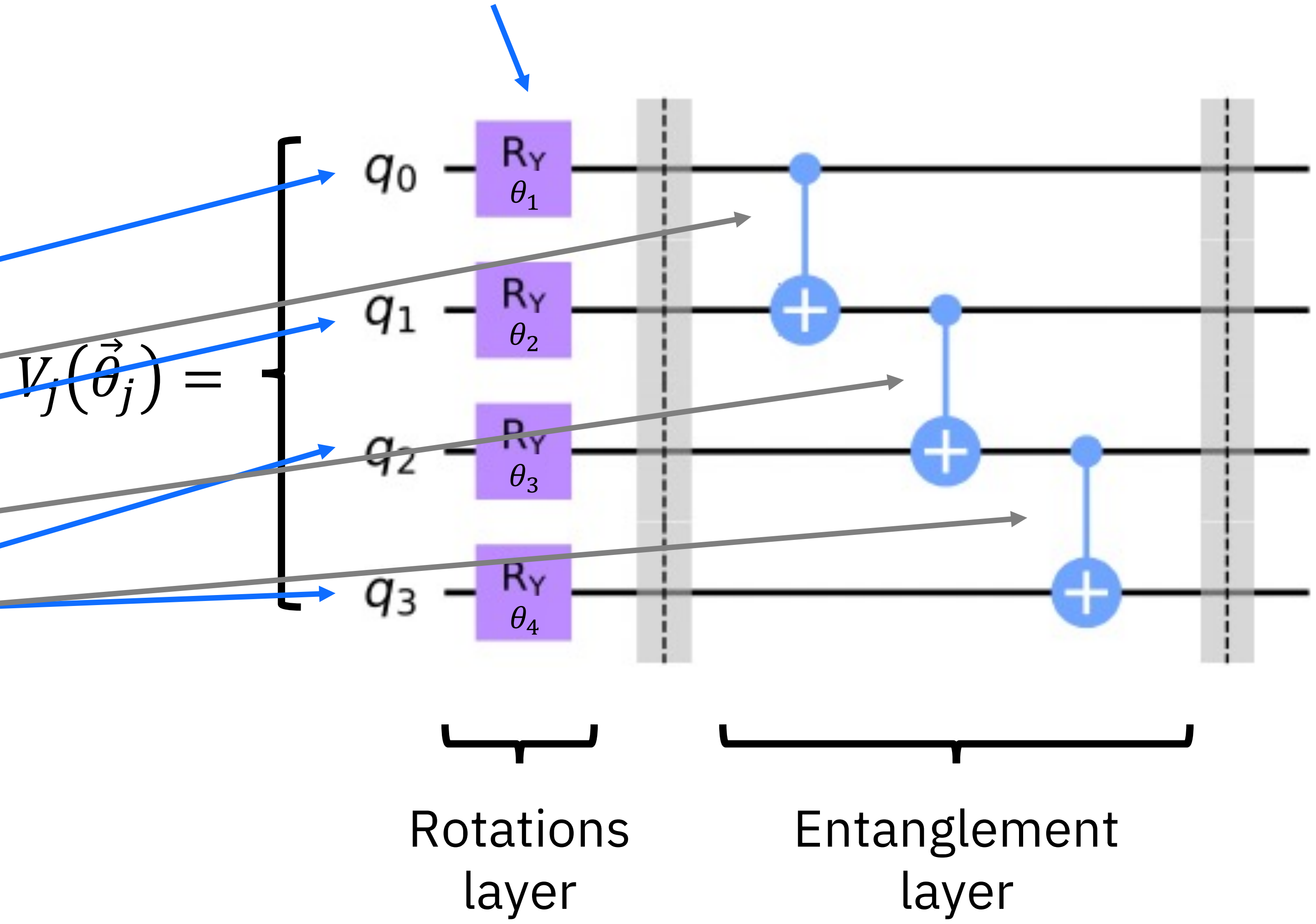
VQE setup: ansatz determination

Operator: finite-size spin ½ Heisenberg chains

$$\mathcal{H} = 2J \sum_{i=1}^{4} \vec{s}_i \cdot \vec{s}_{i+1} + B \sum_{i=1}^{4} s_i^z$$



$\theta_1, \theta_2, \ldots$ **Initial points**: initial parameters



Ansatz: parametrized circuit

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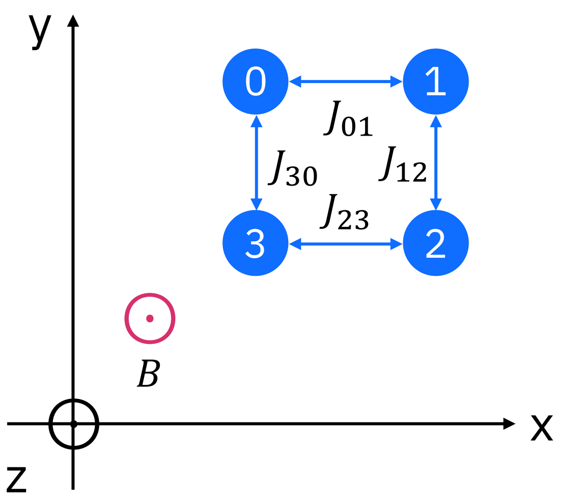


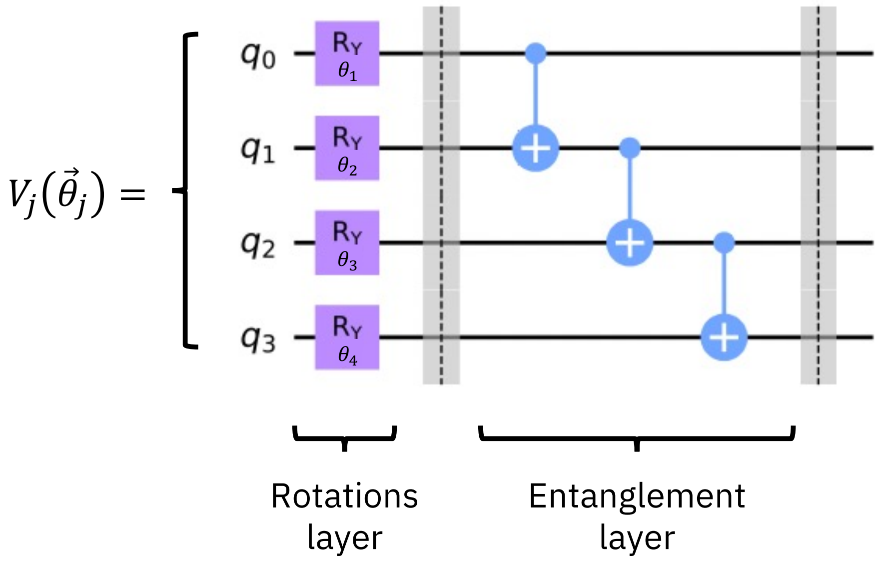
Heuristic Ansatz – HA

Pros:

- Easily fitted with hardware configuration
- Can in principle reproduce very well the target waveform

Cons:

- The number of layers needed could easily increase



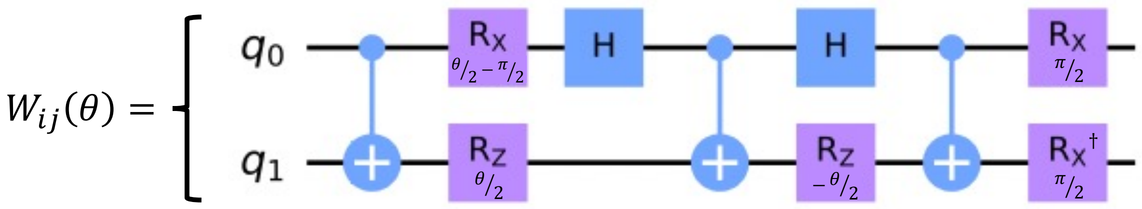
Physically Motivated Ansatz – PMA [3] [4]

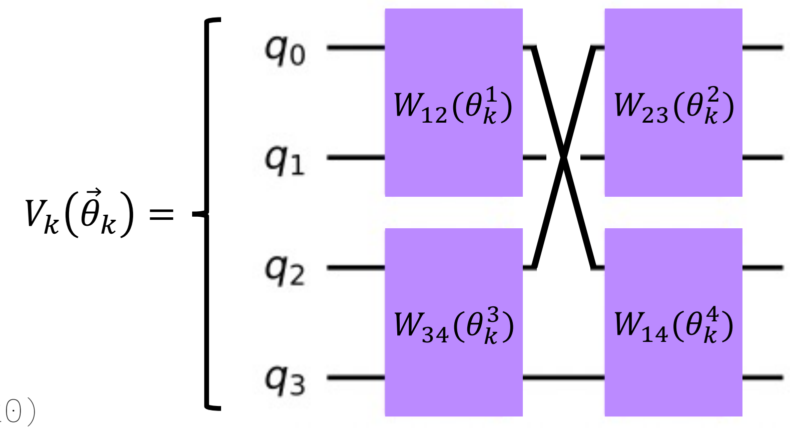
Pros:

- Preservation of S and m quantum numbers
- More scalable, and should take less iterations to converge

Cons:

- Not so easy to apply on hardware





Ansatz initialisation required:

- Low B: S = 0, m = 0
- Intermediate B: S = 1, m = −1

[3] Bryan T. Gard et al., npj Quantum Information 6, 10 (2020)
[4] Kazuhiro Seki et al., Phys. Rev. A 101, 052340 (2020)

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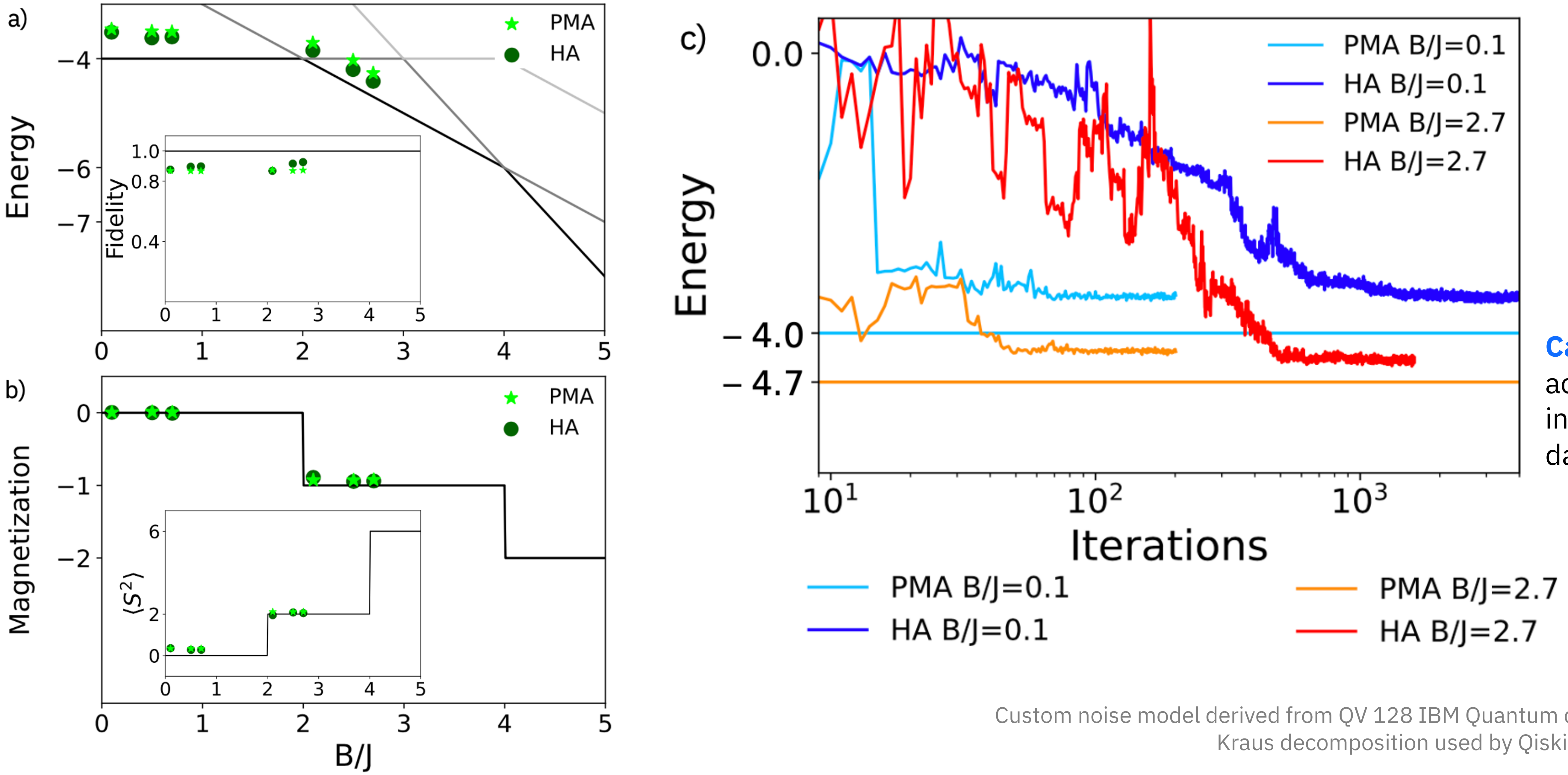
Four spin ½ Heisenberg closed ring

$$\mathcal{H} = 2J\sum_{i=1}^{4}\vec{s}_i\cdot\vec{s}_{i+1} + B\sum_{i=1}^{4}s_i^z$$

Noisy simulated VQE results



Callback: access intermediate data

Custom noise model derived from QV 128 IBM Quantum chip (early 2021)
Kraus decomposition used by Qiskit to model errors

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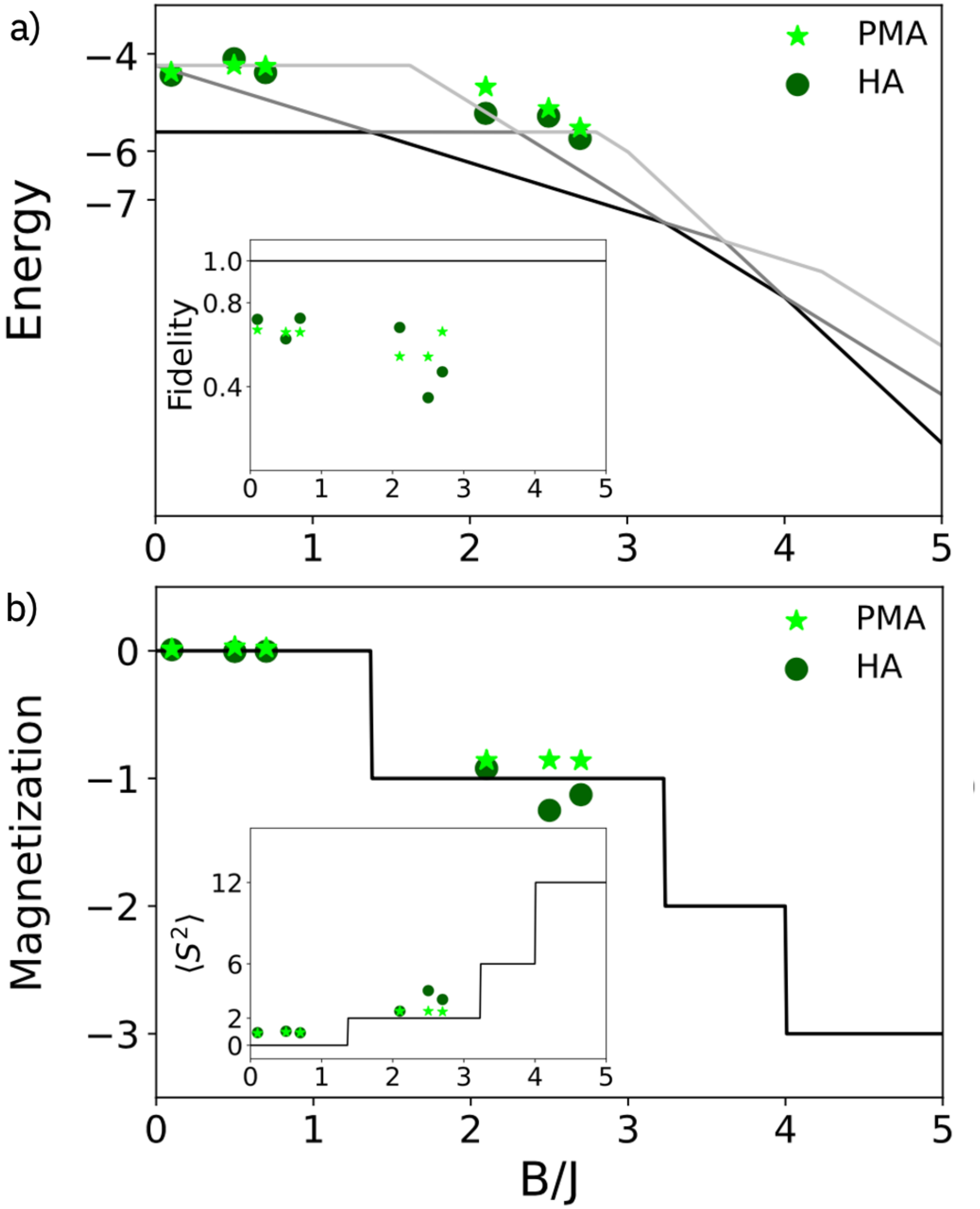
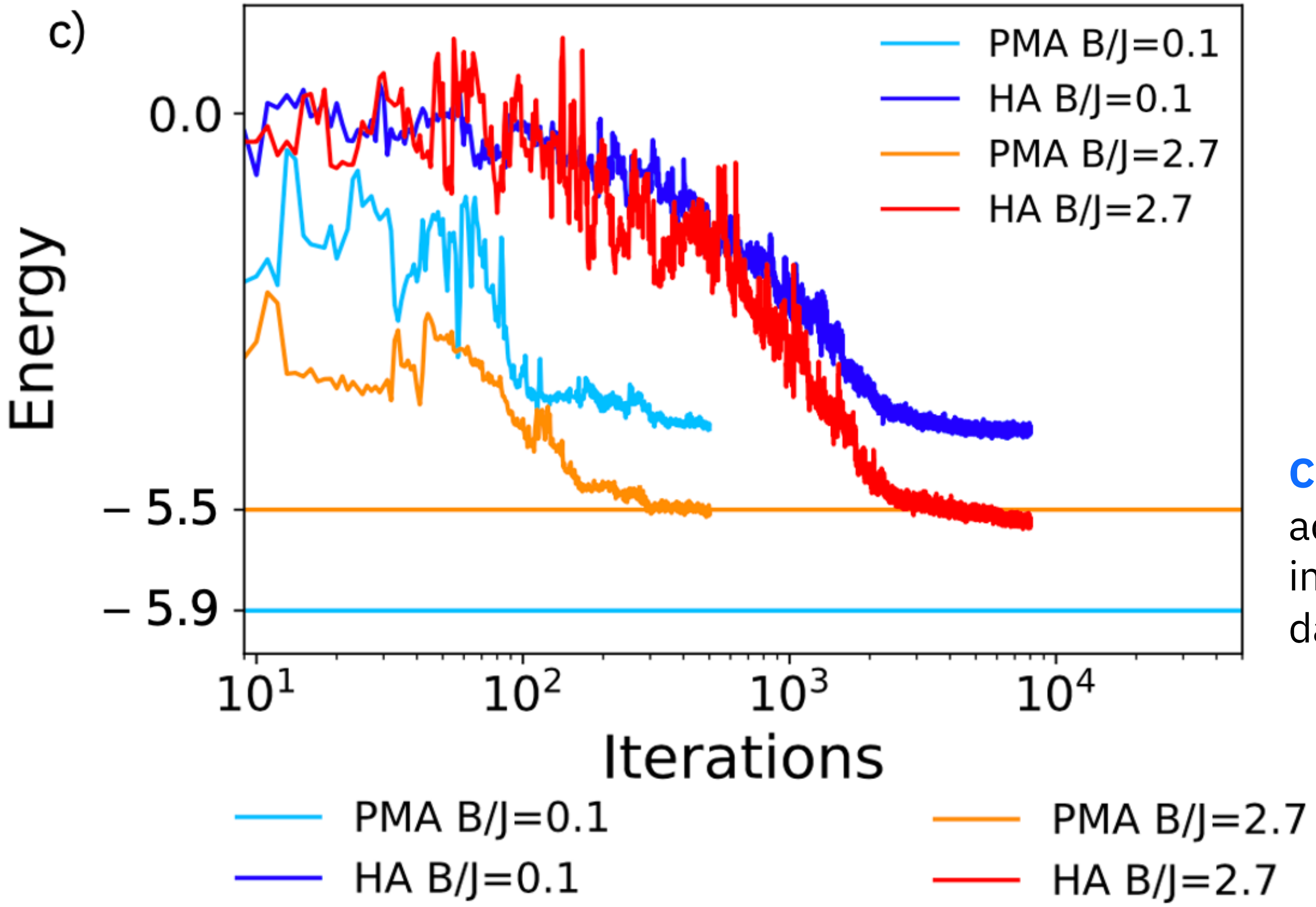
Six spin ½ Heisenberg closed ring

$$\mathcal{H} = 2J\sum_{i=1}^{6}\vec{s}_i\cdot\vec{s}_{i+1} + B\sum_{i=1}^{6}s_i^z$$

Noisy simulated VQE results





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