High-precision nuclear structure simulations on NISQ quantum devices

Author: Arnau Morón Rodriguez

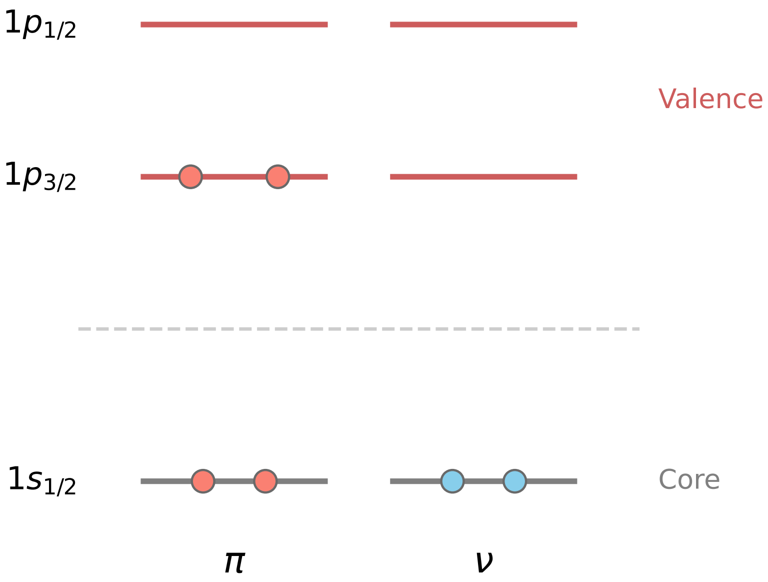
Supervisors: Javier Menéndez, Arnau Rios

Collaborators: Emanuele Costa, Kerman Gallego, Joan Ainaud

Outline

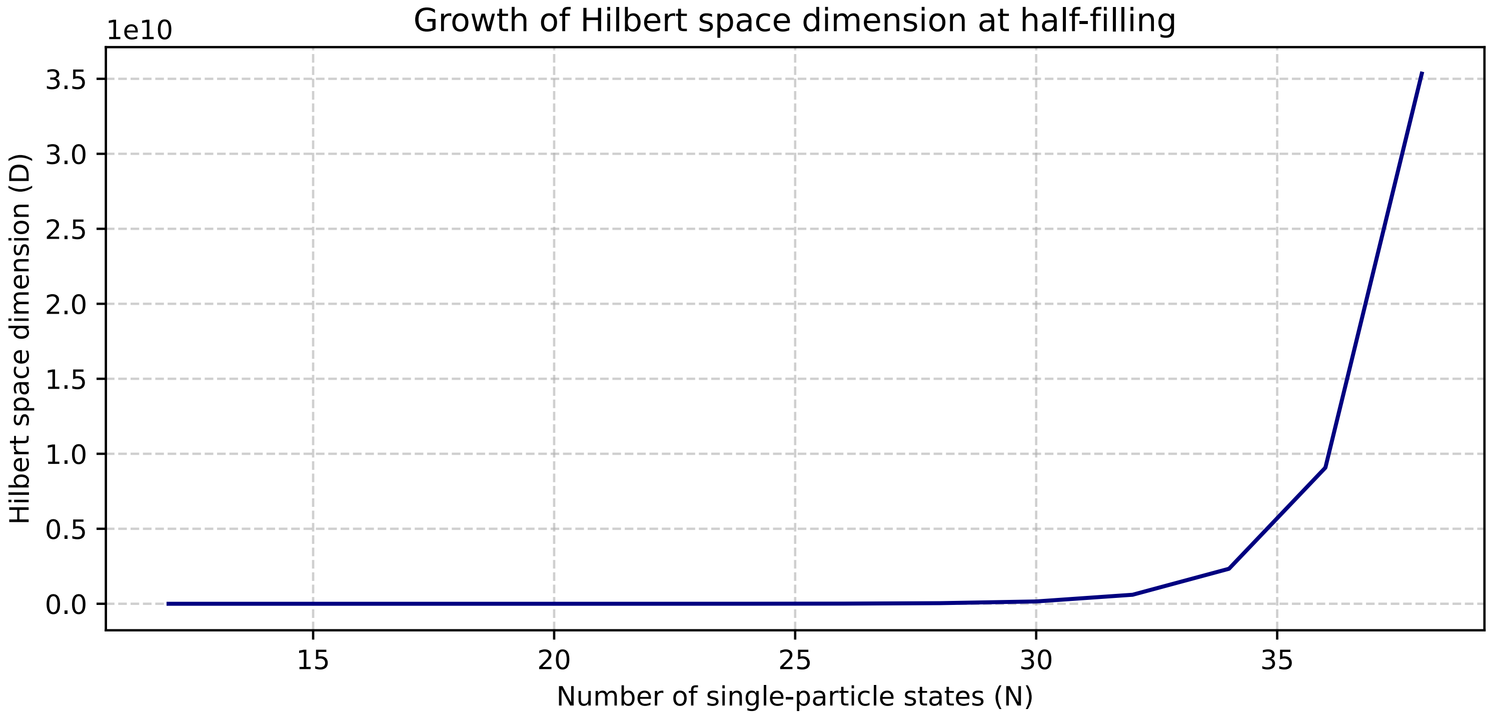
- Nuclear Shell Model
- Quantum Computing
- ADAPT-VQE
- Real Hardware executions

The Nuclear Shell Model



$$\hat{H} = \sum_i \epsilon_i \hat{a}_i^\dagger \hat{a}_i + \frac{1}{4} \sum_{ijkl} \bar{V}_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k$$

The Combinatorial Challenge in Nuclear Physics

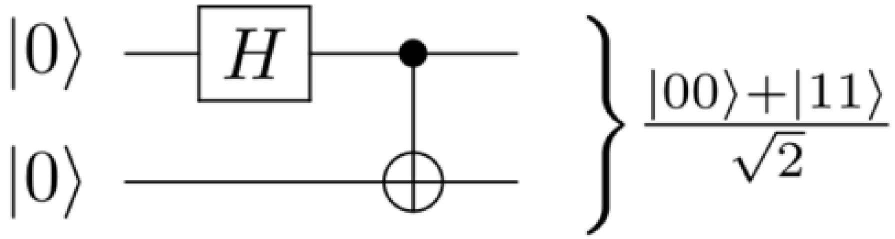


Quantum Computing

- Superposition

$$|0\rangle = \binom{1}{0} \qquad |1\rangle = \binom{0}{1} \quad \Rightarrow \quad |\Psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

- Entanglement



Why Quantum Computing?

Native Representation

Can represent many-body quantum states

Exponential to linear (polynomial)

$O(2^D)$ vs $O(D)$

Key Limitations Today

NISQ Devices

Noisy Intermediate-Scale Quantum processors have limited coherence time and gate errors.

Deep Circuits

Standard fermionic mappings require circuit depths that exceed current device capabilities

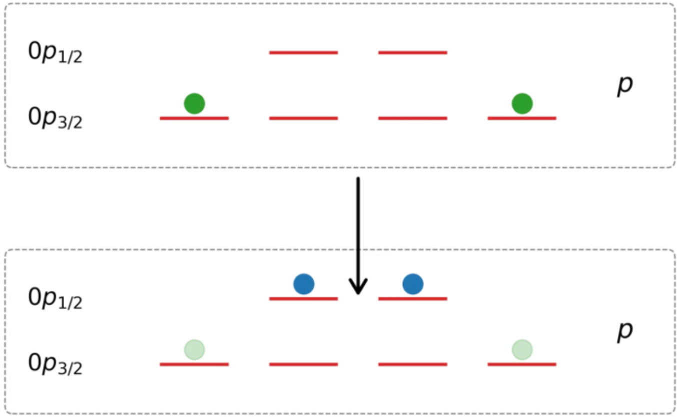
Noise Accumulation

Errors increase with each gate, degrading state fidelity and limiting accuracy

ADAPT-VQE

$$|\Psi\rangle = \prod_{i=1}^{N} e^{-i\,\theta \hat{A}_k} |\Phi_{ref}\rangle$$

$$\hat{A}_k = \hat{a}_i^\dagger \hat{a}_j - \hat{a}_j^\dagger \hat{a}_i \quad ; \quad \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l - \hat{a}_k^\dagger \hat{a}_l^\dagger \hat{a}_i \hat{a}_j$$

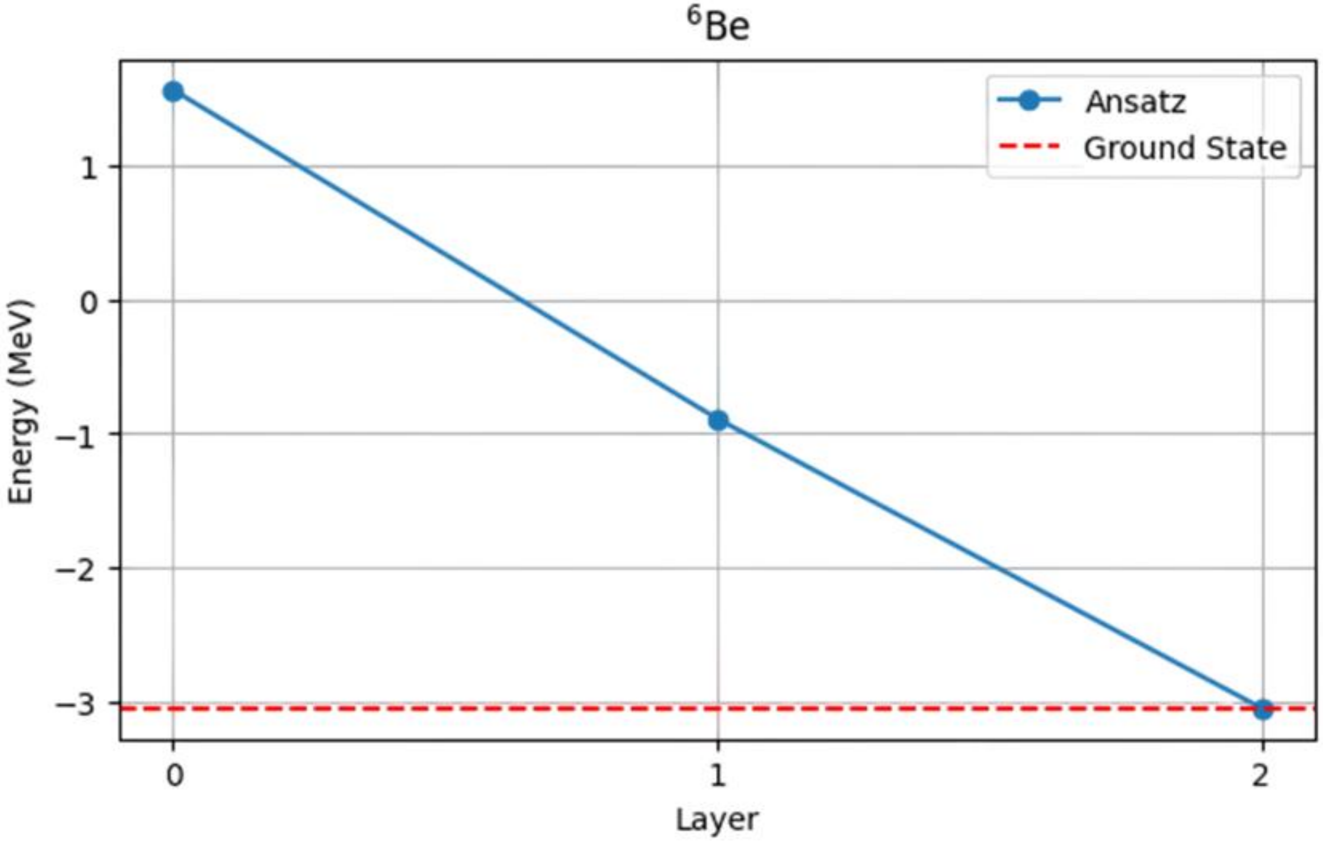


Optimized Efficiency

Minimizes circuit depth while maintaining high ground-state accuracy.

Adaptive Circuit Building

Selects (the most important) operators at each step to grow the quantum circuit (wave-function ansatz).



^{6}Be
Ansatz
Ground State
Energy (MeV)
1
0
−1
−2
−3
0
1
2
Layer

Standard Approach: Jordan-Wigner

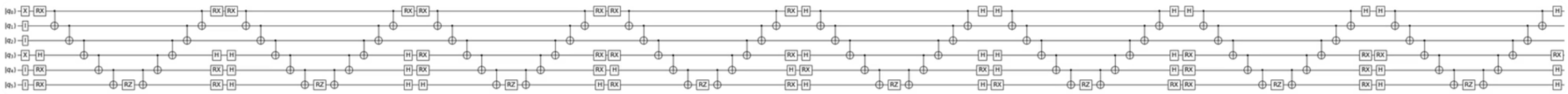
Jordan-Wigner Transformation

Maps fermionic operators to qubit (spin) operators

$$\hat{A}_k = a_i^\dagger a_j^\dagger a_k a_l - a_k^\dagger a_l^\dagger a_i a_j$$

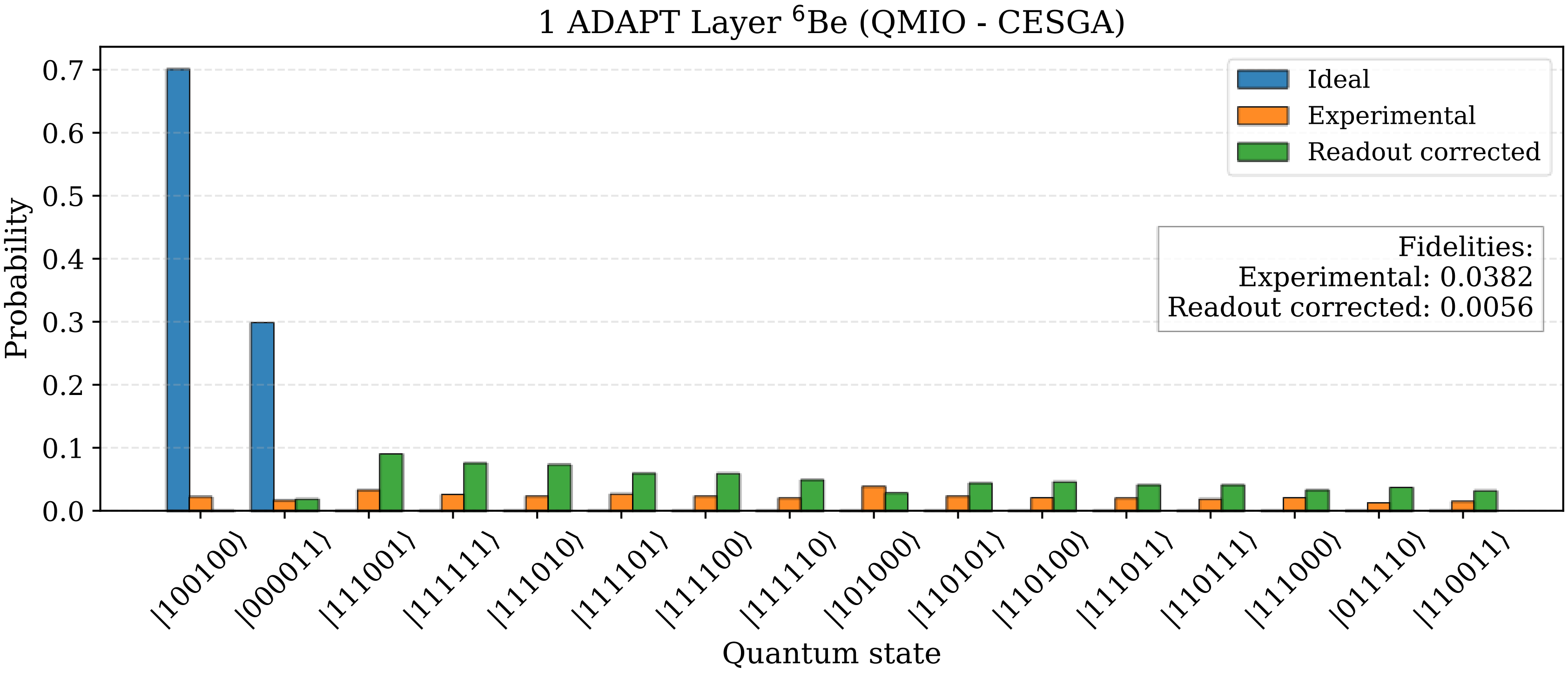
$$\hat{a}_i^\dagger = \left(\prod_{p=0}^{i-1} \hat{Z}_p\right) \frac{1}{2}\left(\hat{X}_i - i\hat{Y}_i\right)$$

$$\hat{a}_i = \left(\prod_{p=0}^{i-1} \hat{Z}_p\right) \frac{1}{2}\left(\hat{X}_i + i\hat{Y}_i\right)$$



Circuit depth

Non-local interactions


1 ADAPT Layer ^{6}Be (QMIO - CESGA)
Ideal
Experimental
Readout corrected
Fidelities:
Experimental: 0.0382
Readout corrected: 0.0056
Probability
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
|100100⟩
|000011⟩
|111001⟩
|111111⟩
|111010⟩
|111101⟩
|111100⟩
|111110⟩
|101000⟩
|110101⟩
|110100⟩
|111011⟩
|110111⟩
|111000⟩
|011110⟩
|110011⟩
Quantum state

Hard-Core Bosons

$$\hat{H}_{HCB} = \mathbb{Q}\hat{H}\mathbb{Q} \qquad \mathbb{Q} \equiv \text{Projector over the Seniority 0 states}$$

Nuclear Pairing

Nucleon pairing entanglement in the qubit definition

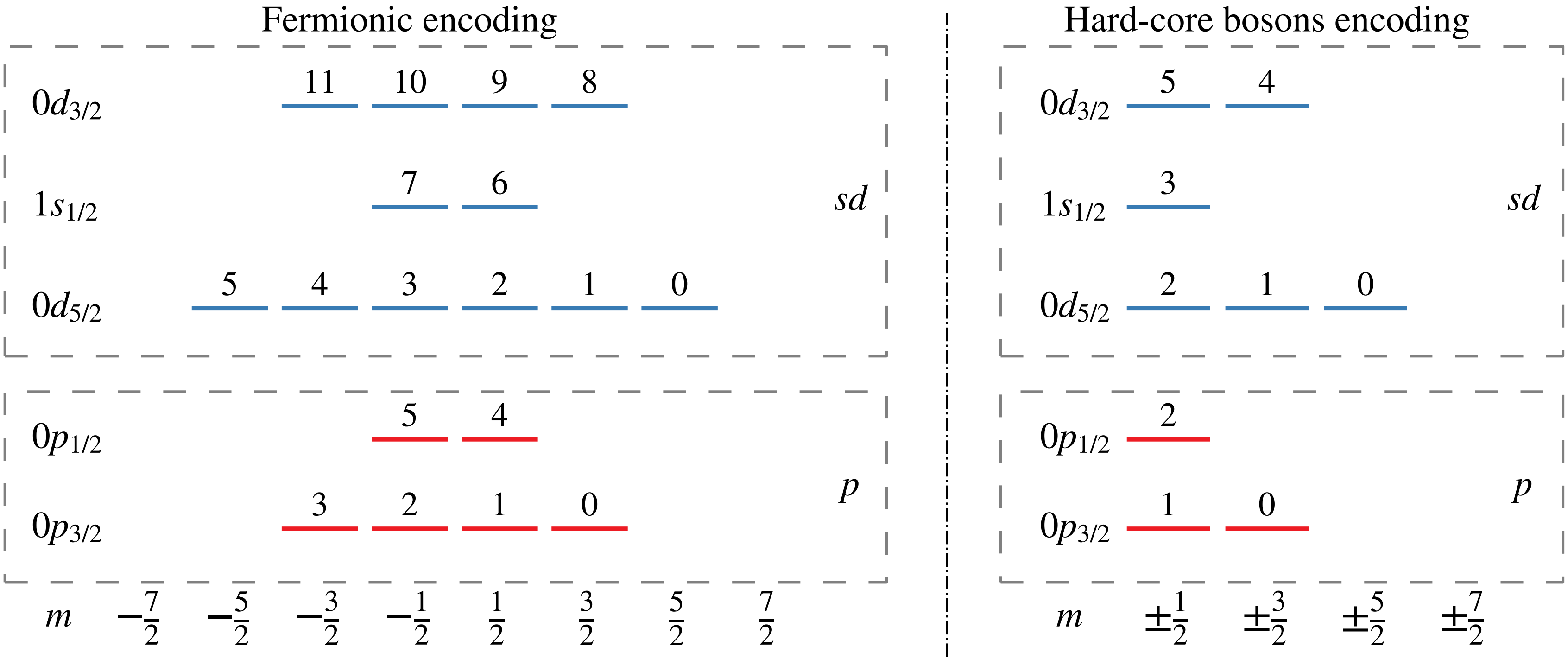
Hard-Core Boson Mapping

E. Costa et al. — quasiparticle pairing encoding for quantum annealing

Reduced Circuit

Qubits reduced by half

Depth reduced by **orders of magnitude** vs. Jordan-Wigner

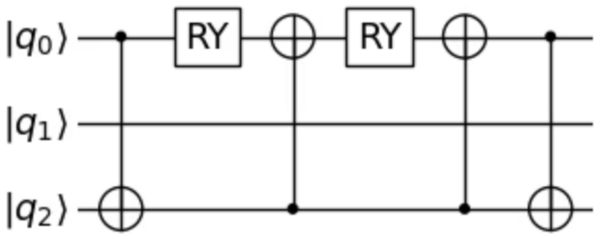

Fermionic encoding
Hard-core bosons encoding
$0d_{3/2}$ 11 10 9 8
$1s_{1/2}$ 7 6
$0d_{5/2}$ 5 4 3 2 1 0
sd
$0p_{1/2}$ 5 4
$0p_{3/2}$ 3 2 1 0
p
m $-\frac{7}{2}$ $-\frac{5}{2}$ $-\frac{3}{2}$ $-\frac{1}{2}$ $\frac{1}{2}$ $\frac{3}{2}$ $\frac{5}{2}$ $\frac{7}{2}$
$0d_{3/2}$ 5 4
$1s_{1/2}$ 3
$0d_{5/2}$ 2 1 0
sd
$0p_{1/2}$ 2
$0p_{3/2}$ 1 0
p
m $\pm\frac{1}{2}$ $\pm\frac{3}{2}$ $\pm\frac{5}{2}$ $\pm\frac{7}{2}$

Hard-Core Bosons Transformation

$$a_i^\dagger a_j^\dagger a_k a_l - a_k^\dagger a_l^\dagger a_i a_j \rightarrow Q_A^\dagger Q_B - Q_B^\dagger Q_A$$

$$Q_A^\dagger = a_a^\dagger a_{\tilde{a}}^\dagger = \frac{1}{2}\left(\hat{X}_A - i\hat{Y}_A\right)$$

$$Q_A = a_a a_{\tilde{a}} = \frac{1}{2}\left(\hat{X}_A + i\hat{Y}_A\right)$$



Circuit depth

Local interactions

Noise Mitigation Techniques

Readout Mitigation

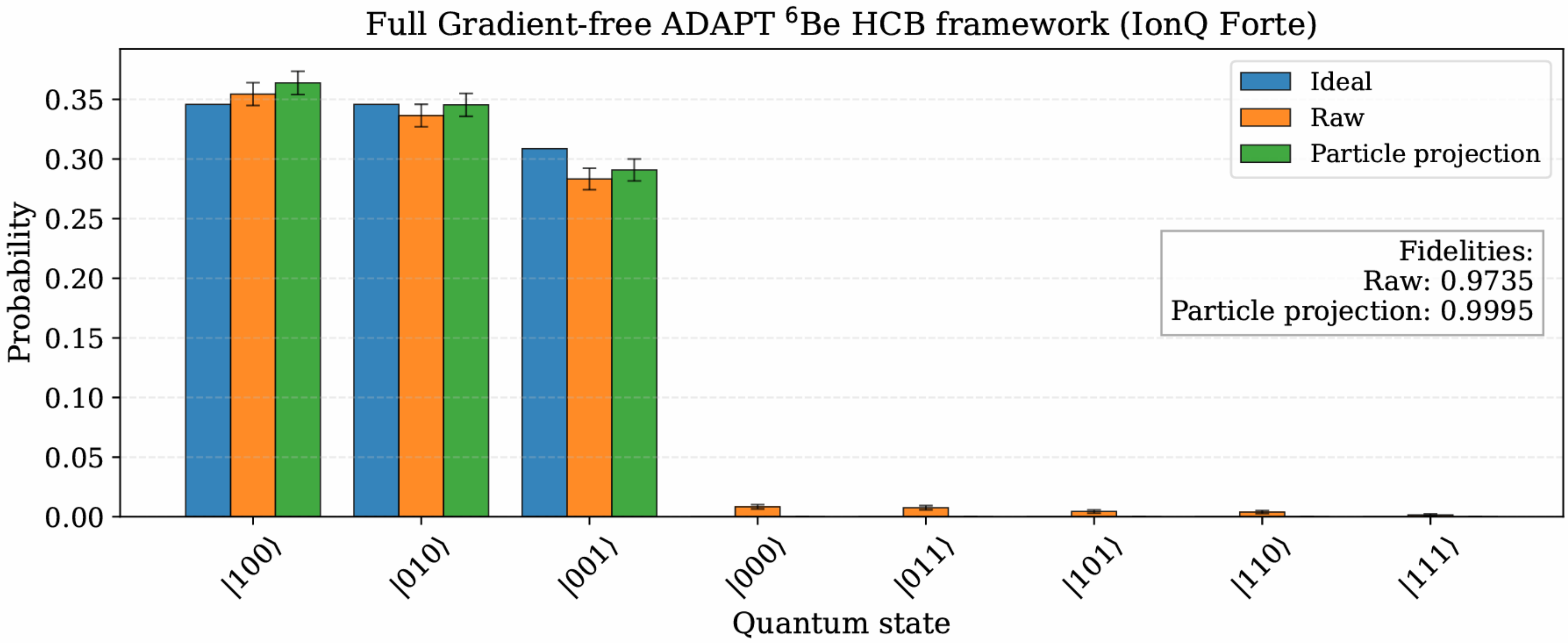
Mitigate errors that occur during measurements.

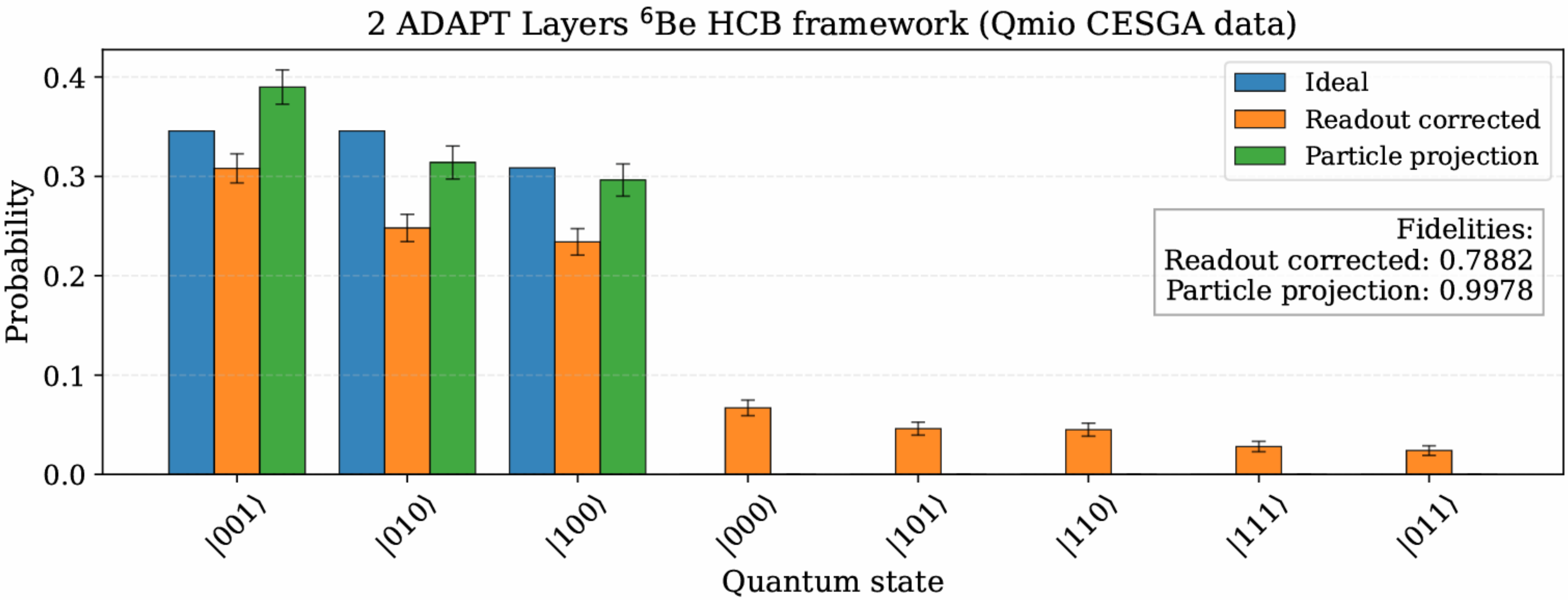
Post-selection

Discard experimental runs where qubits break the symmetries of the operators.

Symmetry Projection

Reconstruct the Wave function from a post-selected experimental run.


Full Gradient-free ADAPT ^{6}Be HCB framework (IonQ Forte)
Ideal
Raw
Particle projection
Fidelities:
Raw: 0.9735
Particle projection: 0.9995
Probability
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
|100⟩
|010⟩
|001⟩
|000⟩
|011⟩
|101⟩
|110⟩
|111⟩
Quantum state


2 ADAPT Layers ^{6}Be HCB framework (Qmio CESGA data)
Probability
0.0
0.1
0.2
0.3
0.4
Ideal
Readout corrected
Particle projection
Fidelities:
Readout corrected: 0.7882
Particle projection: 0.9978
|001⟩
|010⟩
|100⟩
|000⟩
|101⟩
|110⟩
|111⟩
|011⟩
Quantum state

Ground-State Energy Accuracy on $^{6}\mathrm{Be}$

0.2%

Trapped Ion

IonQ — ground-state energy error after mitigation

0.4%

Superconducting

Qmio-CESGA — ground-state energy error after mitigation

Summary

Optimized encoding

Hard-Core Boson approach to halve qubit requirements and circuit depth

Error Mitigation Strategies

Readout, post-selection, and symmetry projection to reconstruct wave functions

Real Hardware Validation

Highly accurate ground-state energies on noisy hardware

Outlook

Non-semi-magic nuclei

Extend beyond current limitations to more complex nuclear systems (proton-neutron correlations).

Scalability of the algorithm

Assess how the method scales to larger systems and more qubits.

Optimize the parameters

Improve parameter optimization techniques for better convergence.

THANKS

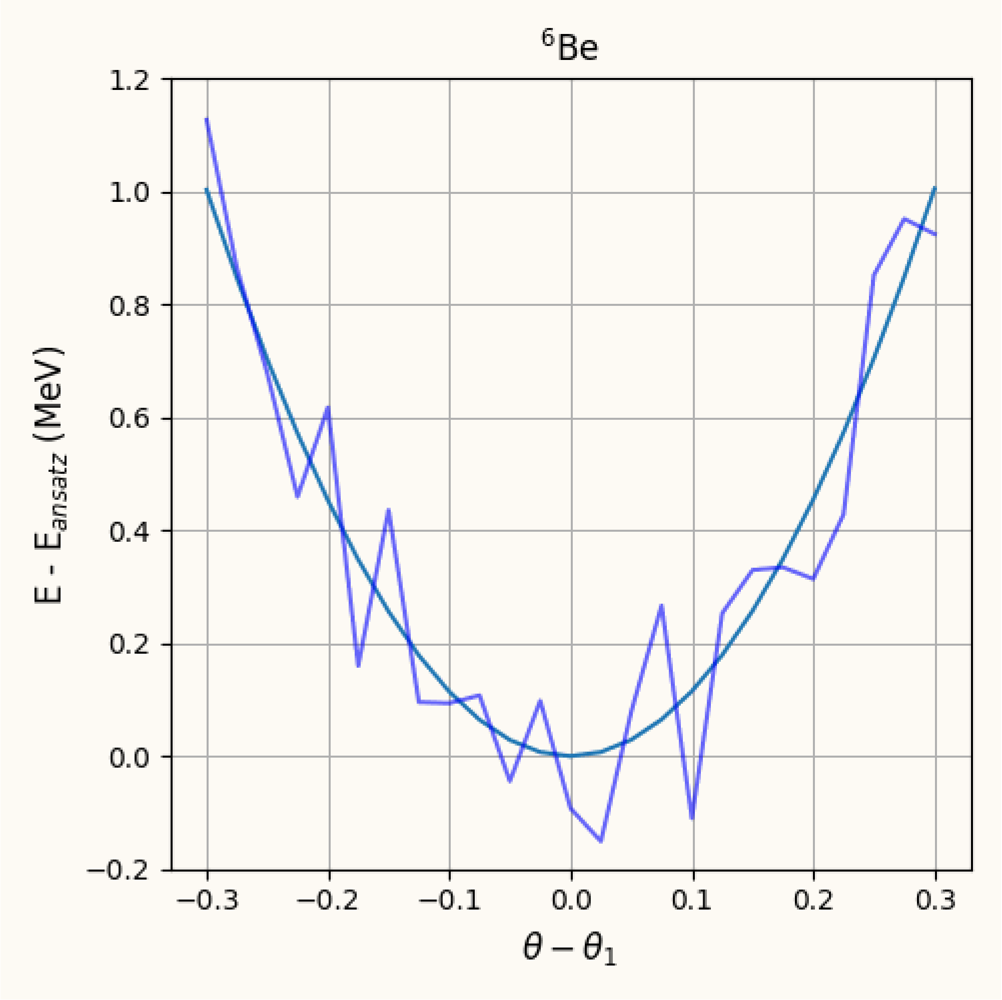
Simulation of Atomic Nuclei in Noisy Digital Quantum Hardware

Operator selection & Parameter optimization

$$E(\theta) = \langle\psi|e^{i\theta\hat{A}}\hat{H}e^{-i\theta\hat{A}}|\psi\rangle$$

- Gradient evaluation

$$\left.\frac{\partial E}{\partial \theta_k}\right|_{\theta_k=0} = i\,\langle\Psi_{k-1}|\left[\hat{H}, \hat{A}_k\right]|\Psi_{k-1}\rangle$$

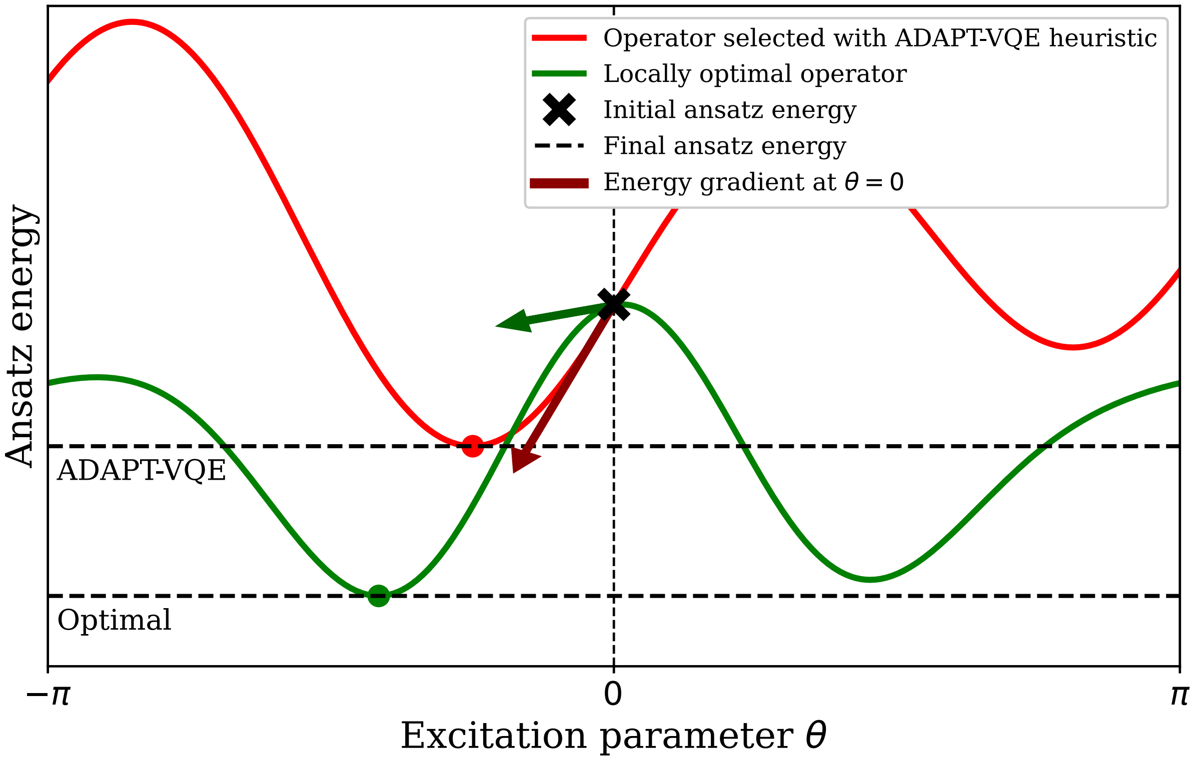


^{6}Be
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
−0.3
−0.2
−0.1
0.0
0.1
0.2
0.3
E - E$_{ansatz}$ (MeV)
$\theta - \theta_1$

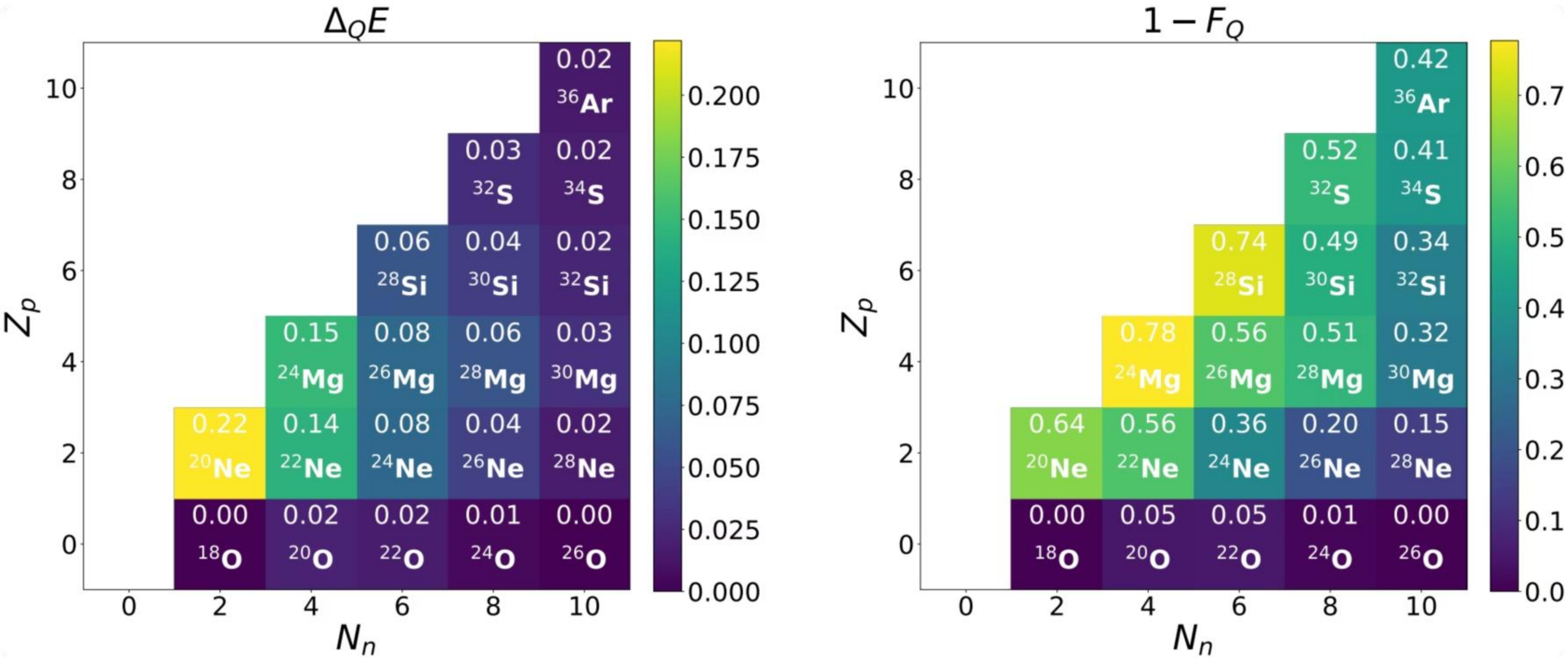
Operator selection & Parameter optimization

- Energy evaluation $E(\theta) = \langle\psi|e^{i\theta\hat{A}}\hat{H}e^{-i\theta\hat{A}}|\psi\rangle$ $\hat{A}^3 = \hat{A}$

$$E(\theta) = a_0 + c_1\cos(\theta) + s_1\sin(\theta) + c_2\cos(\theta) + s_2\sin(\theta)$$



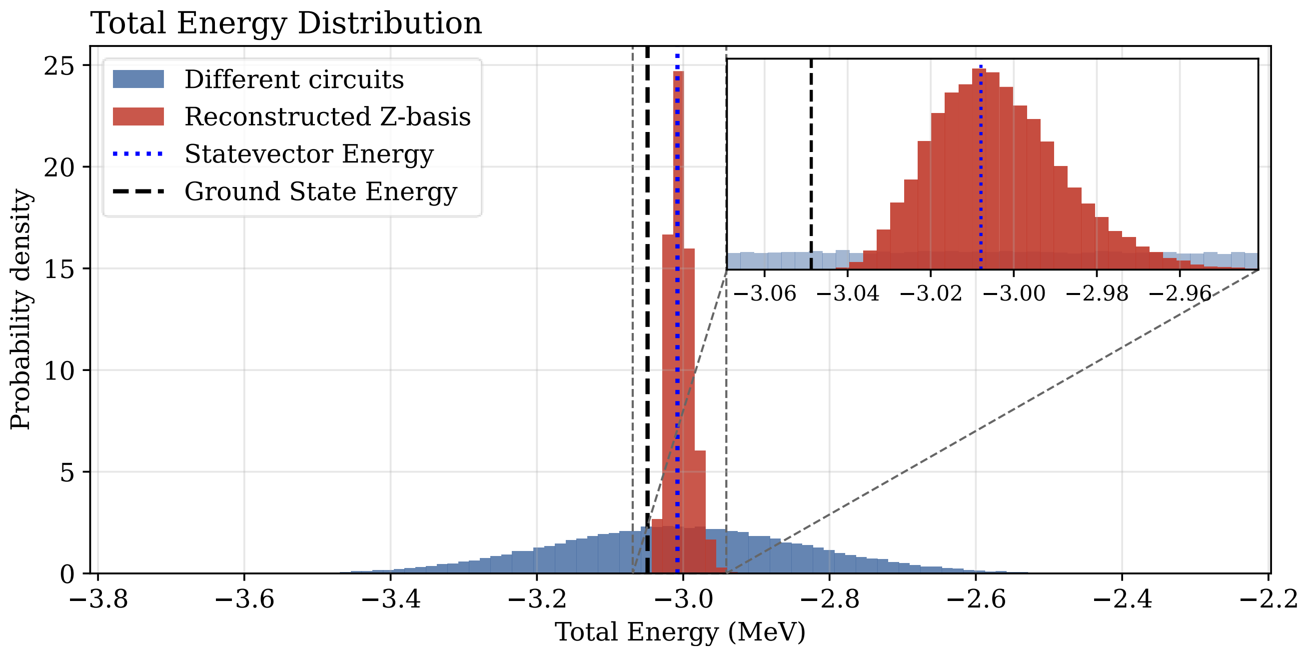
C. Feniou et al. Greedy gradient-free adaptive variational quantum algorithms on a noisy intermediate scale quantum computer



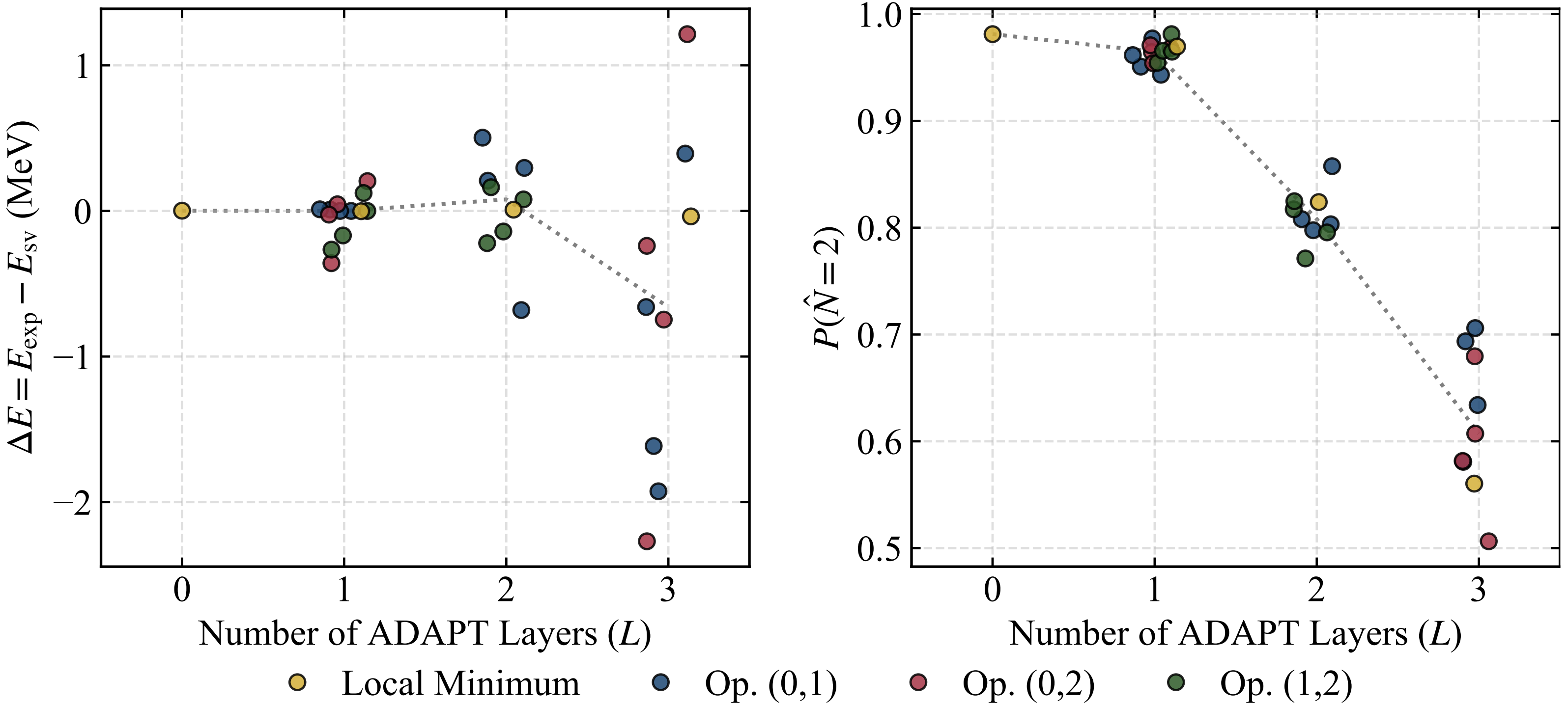
E. Costa et al. — quasiparticle pairing encoding for quantum annealing

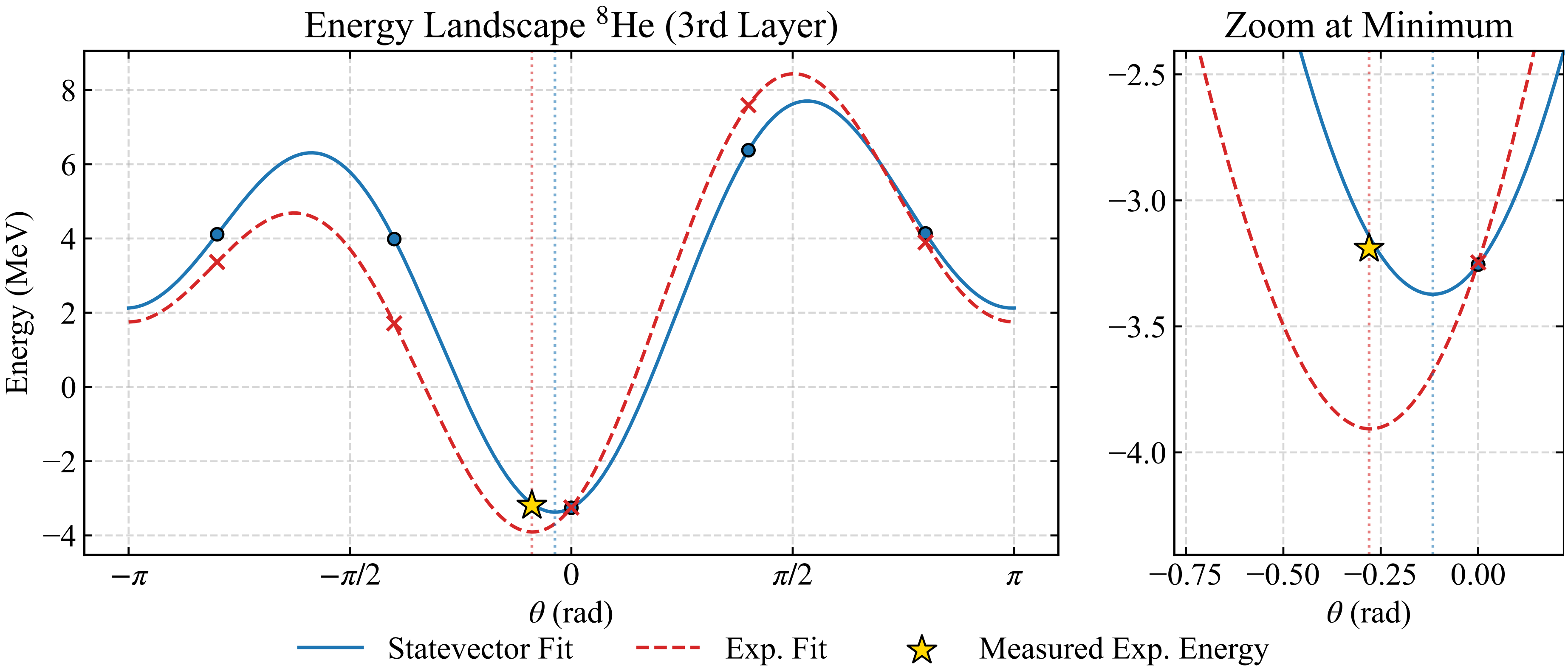
Other Advantages

- → Simpler Hamiltonian
- → Particle projected
- → Preciser energy measurements



Execution of ^{8}He on QMIO Quantum Computer (CESGA)




Energy Landscape ^{8}He (3rd Layer)
Zoom at Minimum
Energy (MeV)
8
6
4
2
0
−2
−4
−π
−π/2
0
π/2
π
θ (rad)
−2.5
−3.0
−3.5
−4.0
−0.75
−0.50
−0.25
0.00
θ (rad)
Statevector Fit
Exp. Fit
Measured Exp. Energy