@HadNucAtUB

Variational hybrid algorithms for nuclear shell model simulations

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Digital quantum computing

Instead of encoding information in classical bits, a digital quantum computer uses **qubits**, which can be held in a superposition of states $|0\rangle$ and $|1\rangle$.

Bit	**Qubit**
0 or 1	$\|\Psi\rangle = \alpha\|0\rangle + \beta\|1\rangle$

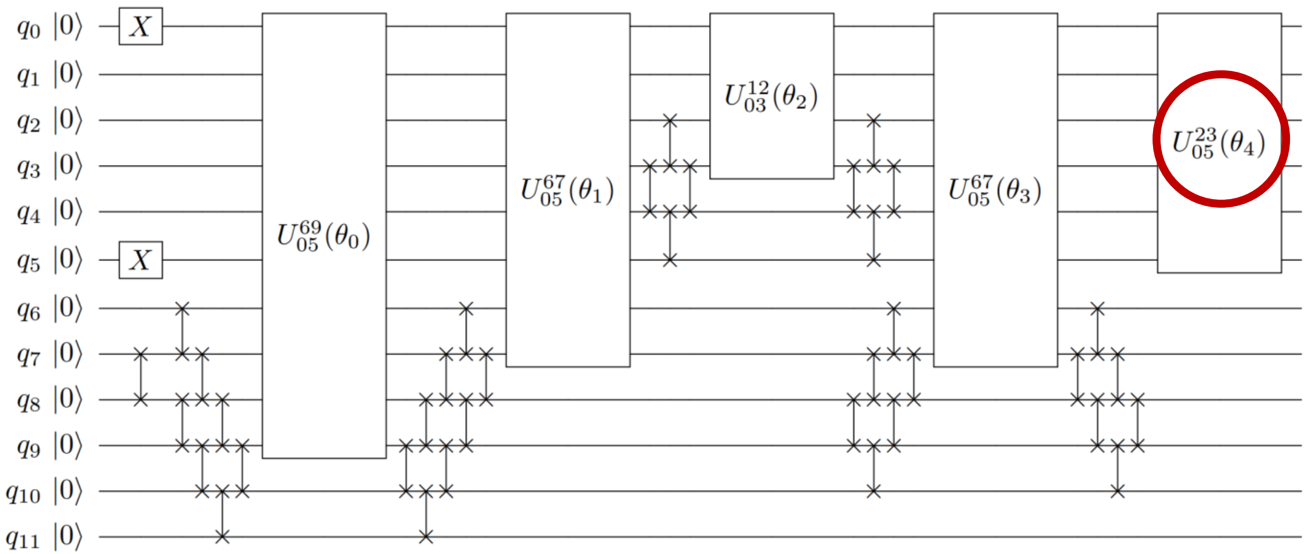
Moreover, a state of many qubits can be **entangled**.

$$|\Psi\rangle = \alpha|00\rangle + \beta|11\rangle$$

Michael A. Nielsen and Isaac L. Chuang. Quantum Computation and Quantum Infor-mation: 10th Anniversary Edition. Cambridge University Press, 2010.

Quantum circuits

To operate with qubits, quantum devices use **quantum gates** that represent **unitary transformations** on the qubits of a circuit.

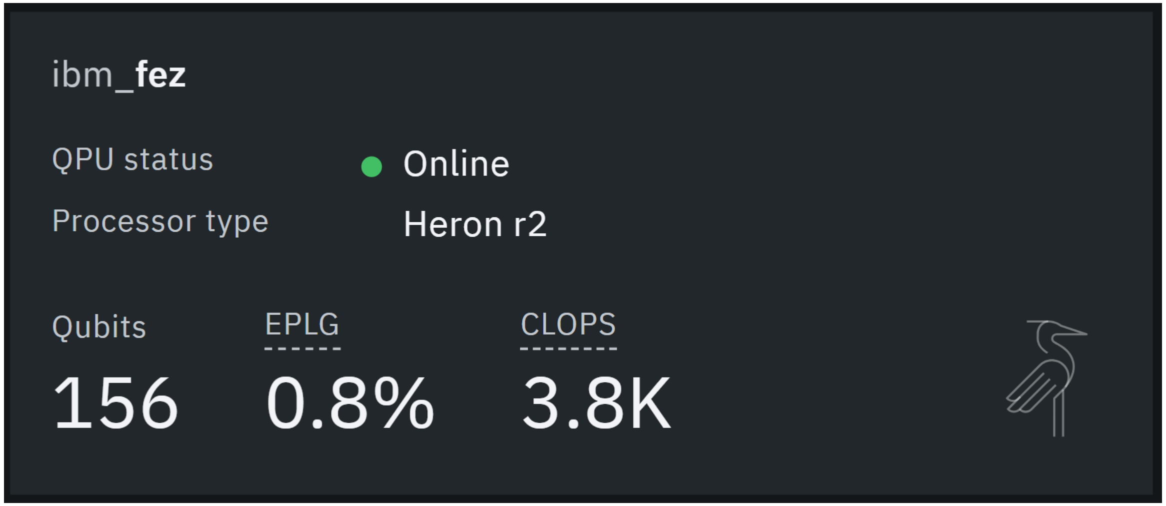


A circuit can be parametrized!

The quantum device **measures the qubits and forces them collapse** into states $|0\rangle$ and $|1\rangle$.

NISQ Era

The current quantum devices consist of $\sim \mathbf{10^2/10^3}$ **qubits.** However, the **error per gate is** $\sim \mathbf{1\%}$**.**



An actual quantum device available online

We are living the **Noise Intermediate-Scale Quantum (NISQ) Era.**

We can **split computations** between quantum and classical devices.

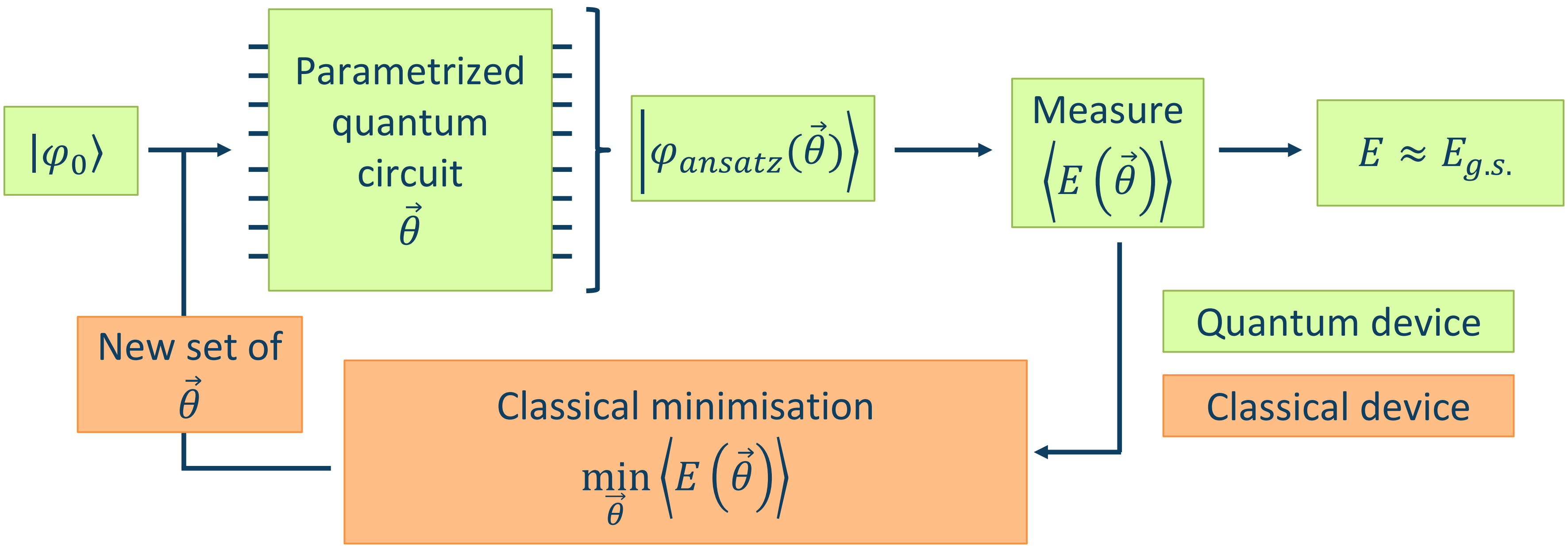
John Preskill. Quantum computing in the NISQ era and beyond. Quantum, 2:79, August 2018

Variational Quantum Eigensolvers

VQEs are hybrid algorithms based on the **variational principle:**

$$\frac{\langle \varphi | \hat{H} | \varphi \rangle}{\langle \varphi | \varphi \rangle} \geq E_{g.s.}$$

Parametrized ***ansatz*** $\left| \varphi(\vec{\theta}) \right\rangle$ $\longrightarrow$ $\min_{\vec{\theta}} \frac{\left\langle \varphi(\vec{\theta}) \middle| \hat{H} \middle| \varphi(\vec{\theta}) \right\rangle}{\left\langle \varphi(\vec{\theta}) \middle| \varphi(\vec{\theta}) \right\rangle} \approx E_{g.s.}$



M. Cerezo et al., Variational quantum algorithms. Nature Reviews Physics, 3(9):625–644, August 2021

We can build a parametrized *ansatz* $|\varphi(\theta)\rangle$ **using a reference state and layering unitary operators**.

$$|\varphi(\theta)\rangle = e^{\theta\hat{T}}|\varphi_0\rangle$$

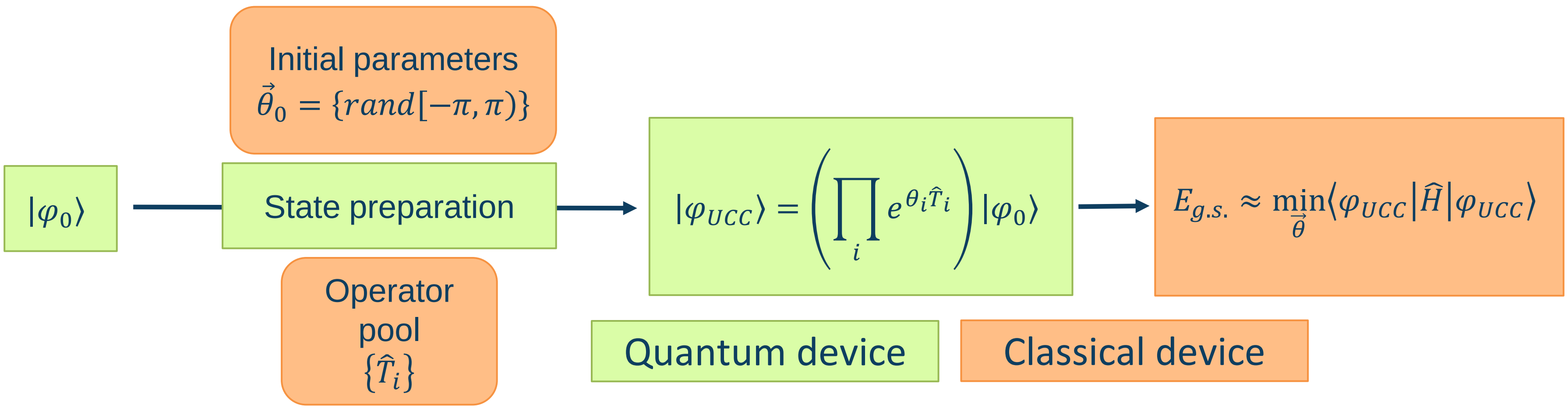
- Each layer has **a parameter and an operator**.
- Each many-body system has a **different operator pool**.

- We use **many-body basis Slater determinants** for the reference state.

The layers must be unitary →
$$\hat{T}_{ij}^{kl} = \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k - \hat{a}_k^\dagger \hat{a}_l^\dagger \hat{a}_j \hat{a}_i$$

UCC method

In the UCC method, the *ansatz* is **layered with all the operators in the pool**.

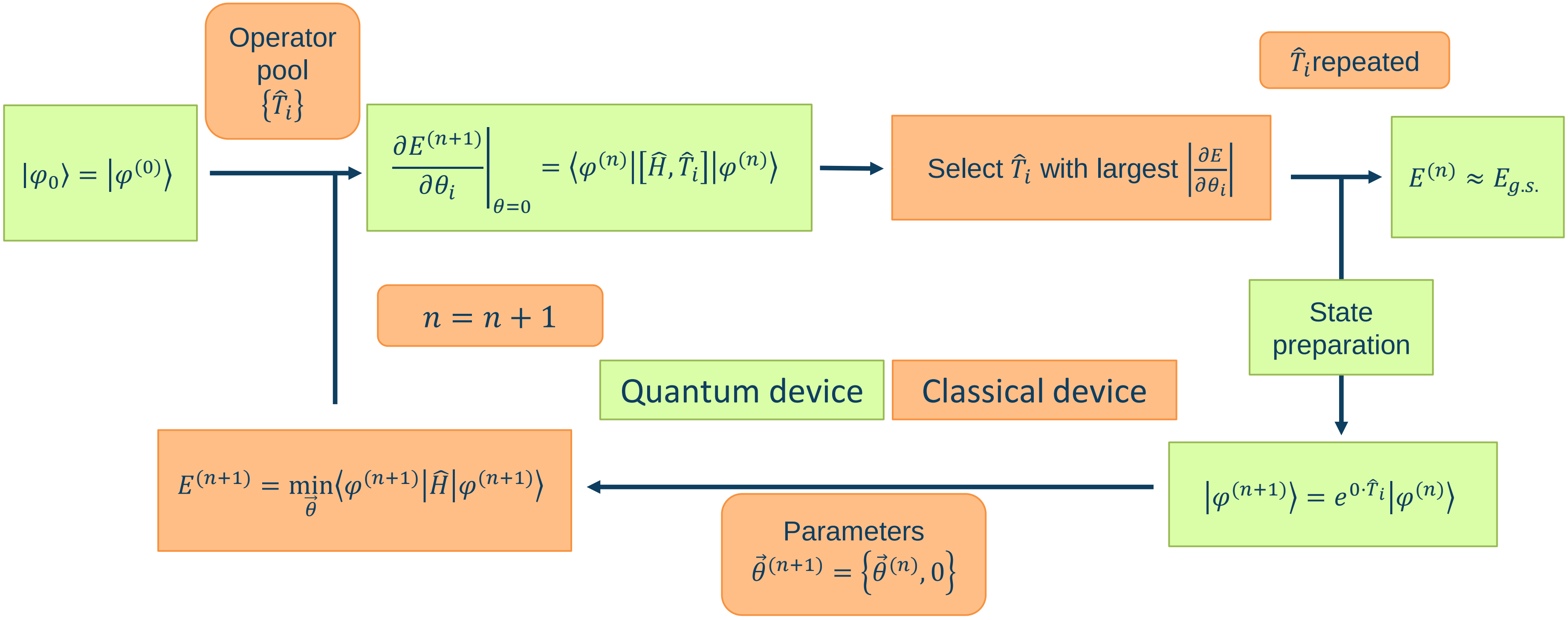


Number of operators in the pool = Number of *ansatz* layers

M. Cerezo et al., Variational quantum algorithms. Nature Reviews Physics, 3(9):625–644, August 2021

Instead of layering the entire operator pool, the ADAPT method **adds layers to the *ansatz* iteratively**.

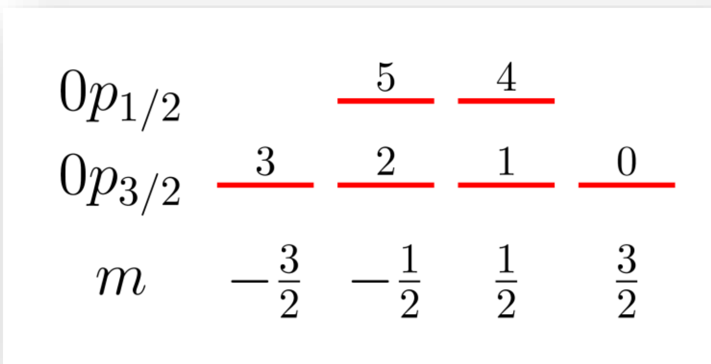
Each step, the ADAPT method selects the **operator with the largest energy gradient**.



H. R. Grimsley, S. E. Economou, E. Barnes, and N. J. Mayhall, An adaptive variational algorithm for exact molecular simulations on a quantum computer, Nat. Commun. 10, 3007 (2019).

Nuclear many-body problem

We want to compute the **ground state of energy of light nuclei** in the *p* shell.



The **valence space** consists of the single particle states in the p shell.

Nuclear shell model Hamiltonian

$$\hat{H}_{eff} = \sum_{ij} \varepsilon_i \hat{a}_i^\dagger \hat{a}_i + \frac{1}{4} \sum_{ijkl} \tilde{v}_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k$$

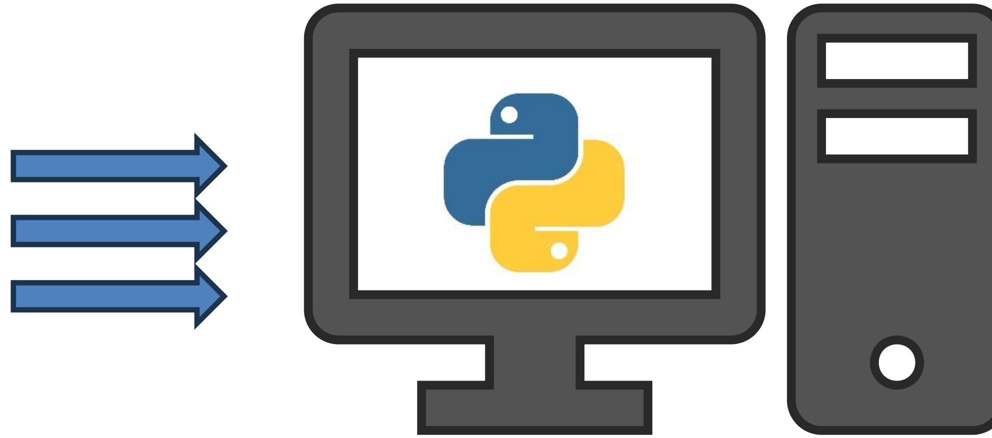
Schrödinger equation

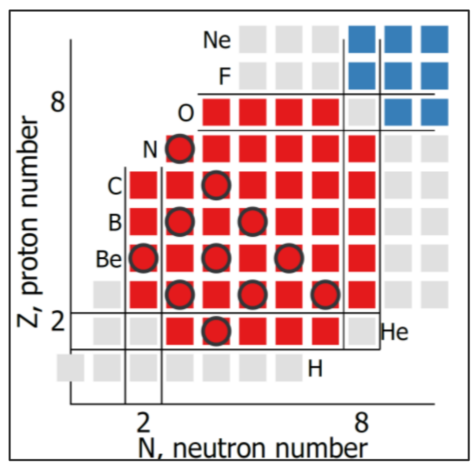
$$\hat{H}_{eff} |\Psi\rangle = E |\Psi\rangle$$

Classical simulation

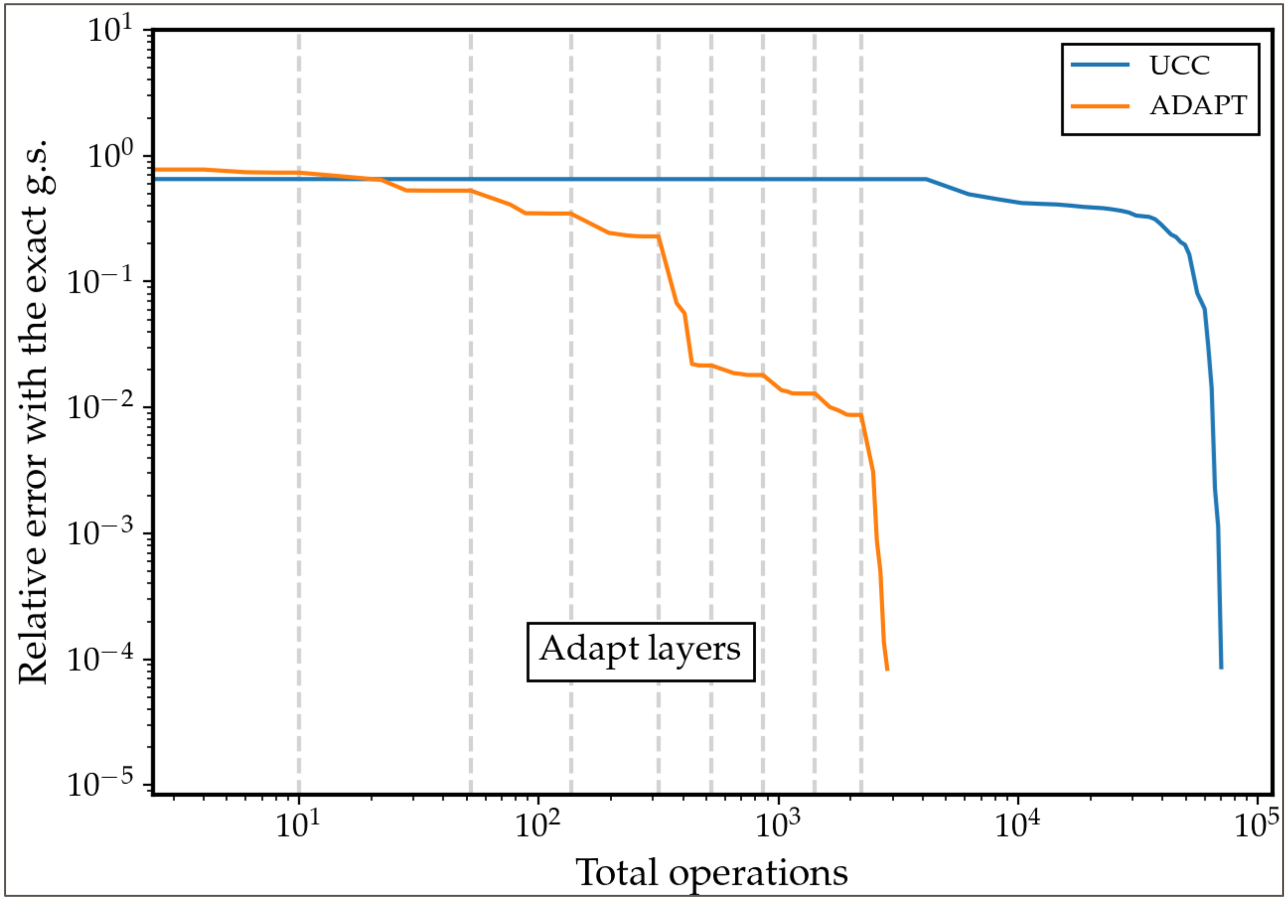
Quantum computer

Classical computer





Our results are **compared with exact g.s. energies,** computed by diagonalising the Hamiltonian

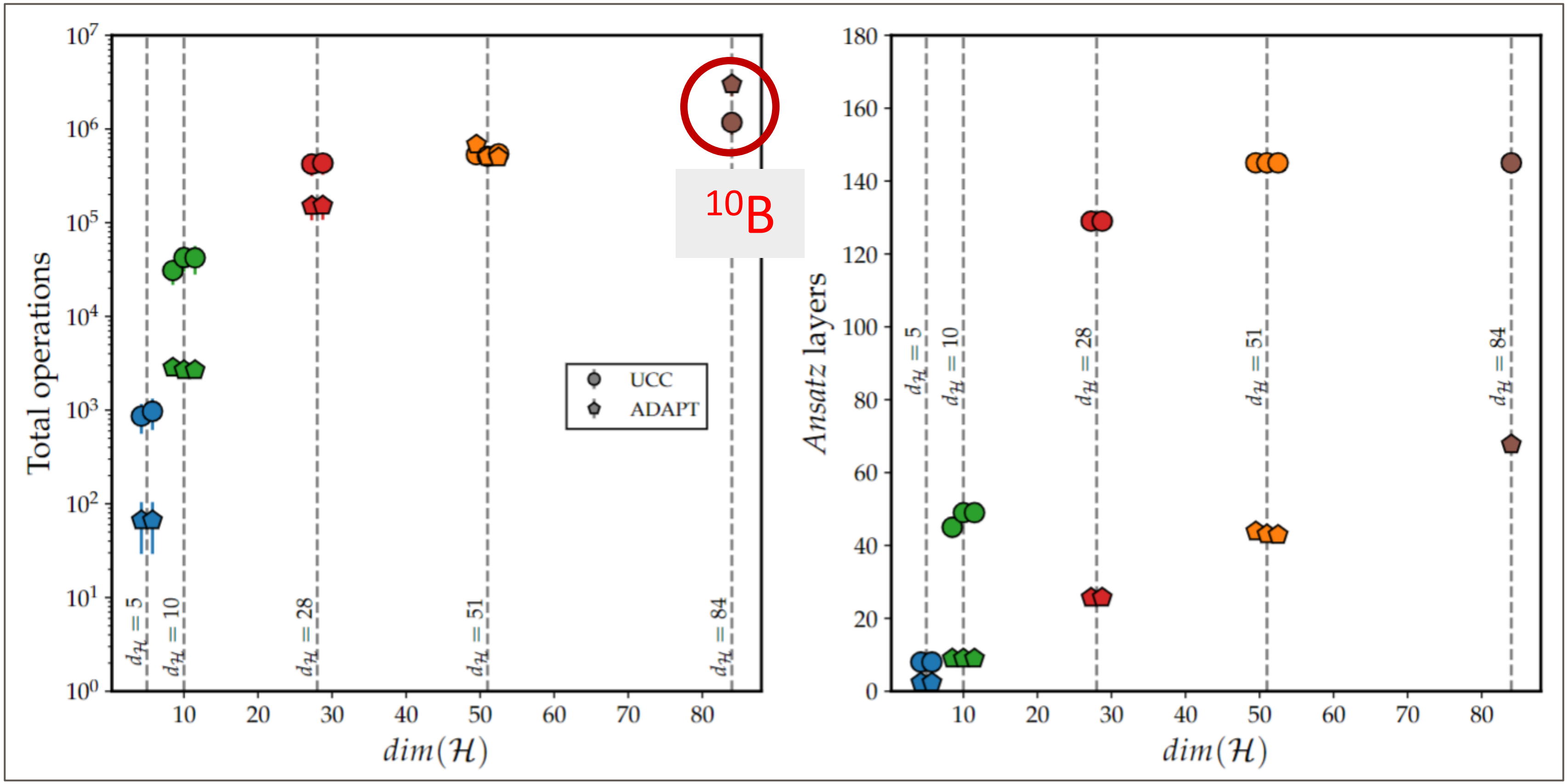


We consider the methods to be successful if they converge to the g.s. with a **relative error** $< \mathbf{10^{-4}}$

We quantify the efficiency of the methods using the number of **total operations**.

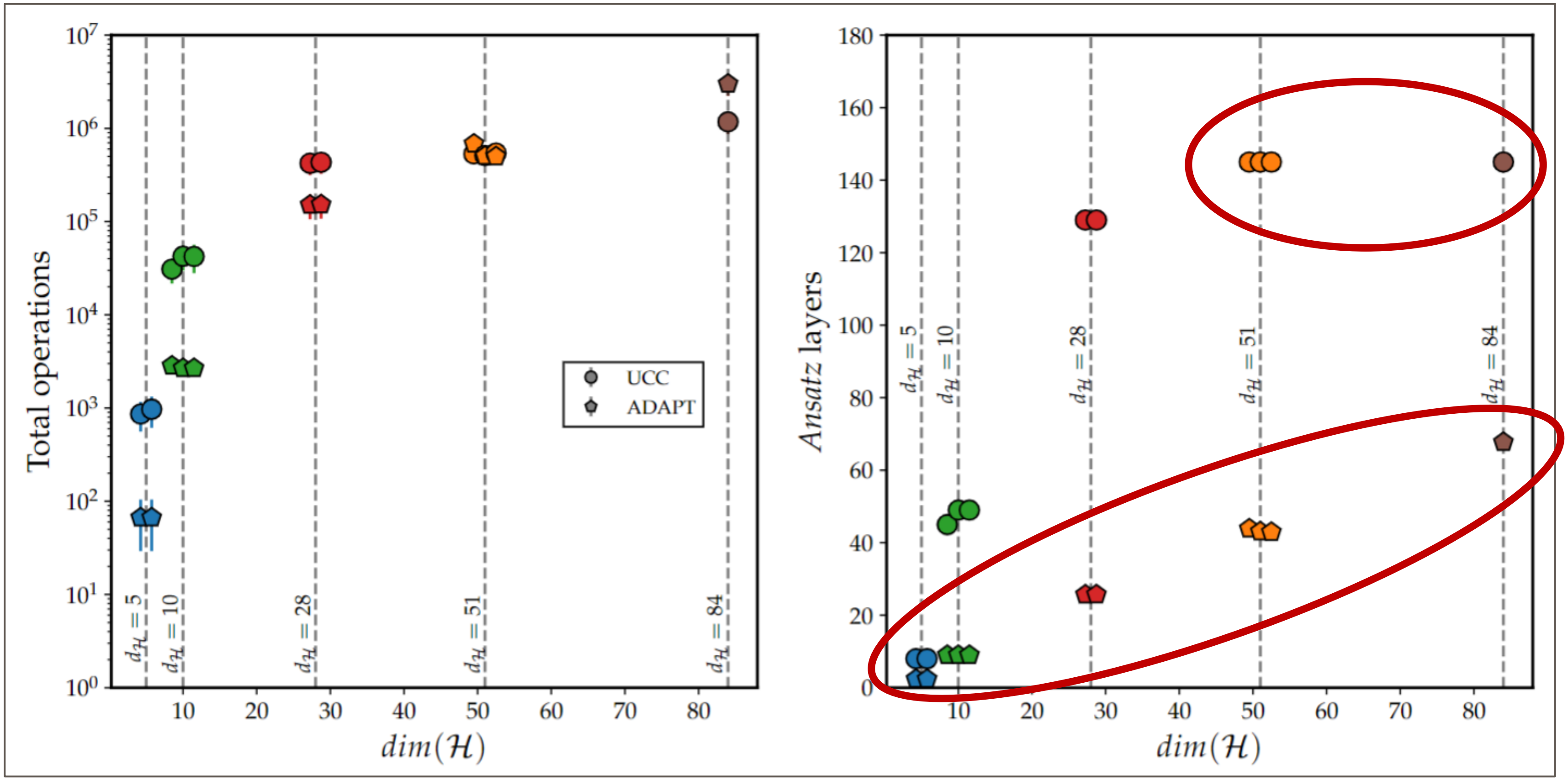
Using both UCC and ADAPT, we **are able to converge to the ground state of ^{6}Li with a relative error of 10^{-4}**. So far, **ADAPT needs less operations than UCC** to reach the g.s.

UCC vs ADAPT: *p*-shell nuclei



The ADAPT method needs less operations than the UCC method for nuclei with $\dim(\mathcal{H}) < 51$. For ^{10}B, the UCC **needs less operations to converge**.

UCC vs ADAPT: *p*-shell nuclei



The number of layers in the ADAPT *ansatz* **increases linearly** with the dimension of the Hilbert space.

The number of layers in the UCC *ansatz* **stops increasing** due to the limited size of the operator pool.

Conclusions & Outlook

We were able to compute the ground state of energy of *p*-shell nuclei with a precision of 10^{-4} using the UCC and the ADAPT methods.

The number of layers of the ADAPT *ansatz* grows linearly with $\dim(\mathcal{H})$ and the number of layers of the UCC *ansatz* is limited to the operators available in the valence space. This results in the ADAPT becoming less efficient than the UCC for $\dim(\mathcal{H}) > 51$.

Outlook:

- Simulate **nuclei in higher shells**. How a larger valence space affects the UCC and ADAPT performance?
- Perform UCC and ADAPT on a quantum device.

Bharti Bhoy and Paul Stevenson. Shell-model study of ^{58}Ni using quantum computing algorithm, 2024

A. Pérez-Obiol, A. M. Romero, J. Menéndez, A. Rios, A. García-Sáez, and B. Juliá-Díaz. Nuclear shell-model simulation in digital quantum computers. Scientific Reports, 13(1), July 2023

Thank you!

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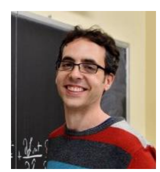
https://github.com/miquel-carrasco/Master-s-thesis-codes

A. Rios

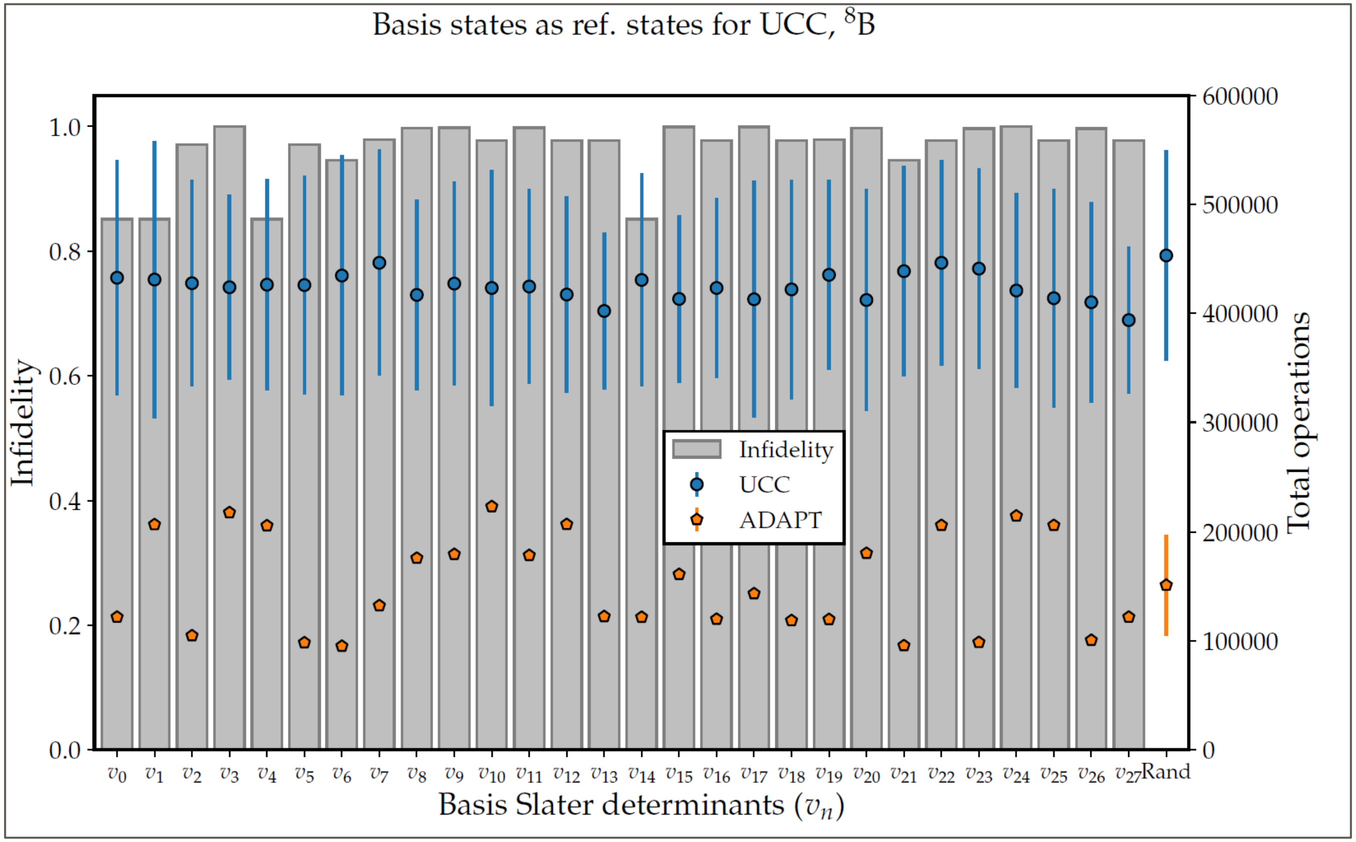
J. Menéndez



X. Roca

E. Costa

UCC vs ADAPT: ^{8}B



For the ^{8}B nucleus, the ADAPT method needs **3 times less operations** in order to converge to the g.s. than the UCC method.

The UCC error bars correspond to the *ansätze* with **randomised operator orderings and initial parameter values**

All states of the many-body basis perform very similar for the UCC.

For the ADAPT some states need half of the operations than others