Toward simulating the shell model in a quantum computer

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Institute of Cosmos Sciences

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“Cutting edge developments in nuclear structure physics”

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Agencia Estatal de Investigación
ICCUB

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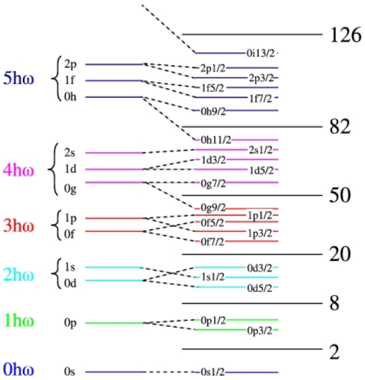
A. Pérez-Obiol

A. M. Romero

Nuclear shell model



Nuclear shell model configuration space only keep essential degrees of freedom

- High-energy orbitals: always empty
- Valence space: where many-body problem is solved
- Inert core: always filled

$$H\,|\Psi\rangle = E\,|\Psi\rangle \;\rightarrow H_{eff}\,|\Psi\rangle_{eff} = E\,|\Psi\rangle_{eff}$$

$$|\Psi\rangle_{eff} = \sum_{\alpha} c_\alpha\,|\phi_\alpha\rangle\,, \quad |\phi_\alpha\rangle = a^+_{i1}a^+_{i2}...a^+_{iA}\,|0\rangle$$

Shell model diagonalization:

$\sim 10^{12}$ Slater dets. Caurier et al. RMP77 (2005)

$\gtrsim 10^{30}$ Slater dets. with MCSM or variational

Otsuka, Shimizu, Tsunoda: PScr. 92 063001 (2017)
Dao, Nowacki: PRC 105, 054314 (2022)
Bally, Rodríguez: EPJA 60 62 (2024) **D. Frycz talk Thursday**

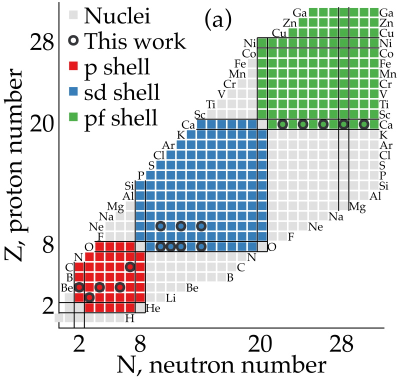
H_{eff} includes effects of

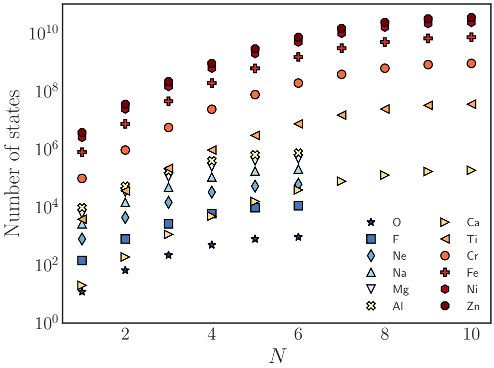
- inert core
- high-energy orbitals

Shell-model scaling

Even for medium-mass nuclei
shell-model calculations become demanding toward the mid-shell

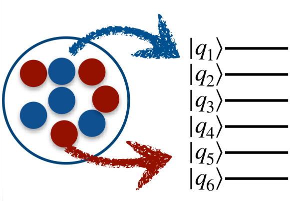
with number of Slater determinants (many-body basis states) reaching $\sim 10^{10}$ for relatively simple nuclei

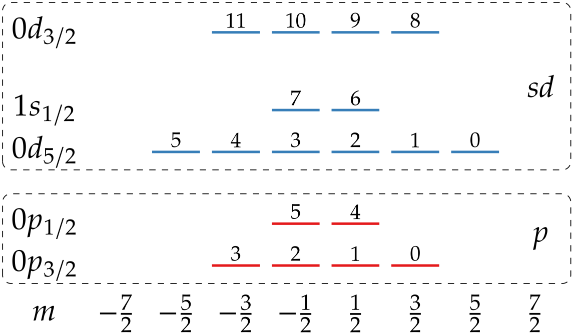




Quantum Computing

Since atomic nuclei are quantum systems
more naturally encoded into quantum computer in terms of qubits
than in classical computer in terms of bits





Jordan-Wigner mapping:

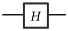
$|0\rangle \equiv$ empty orbital
$|1\rangle \equiv$ occupied orbital

Need as many qubits as single-particle orbitals in valence space
Only as many occupied qubits as protons and neutrons in the nucleus

Circuits, gates and measurements

Simulate the nuclear ground state
by acting with quantum gates on the system's qubits

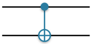
Logic gates



$$|0\rangle \mapsto \frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

$$|1\rangle \mapsto \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

2 qubit gates

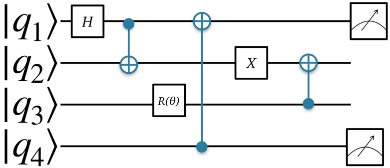


$$|00\rangle \mapsto |00\rangle$$
$$|01\rangle \mapsto |01\rangle$$
$$|10\rangle \mapsto |11\rangle$$
$$|11\rangle \mapsto |10\rangle$$

Finite set of universal gates sufficient
to build a general quantum circuit

Kitaev, Russ.Math.Surv.52 1191 (1997)
Nielsen, Chuang
Quantum Computation and Quantum Information

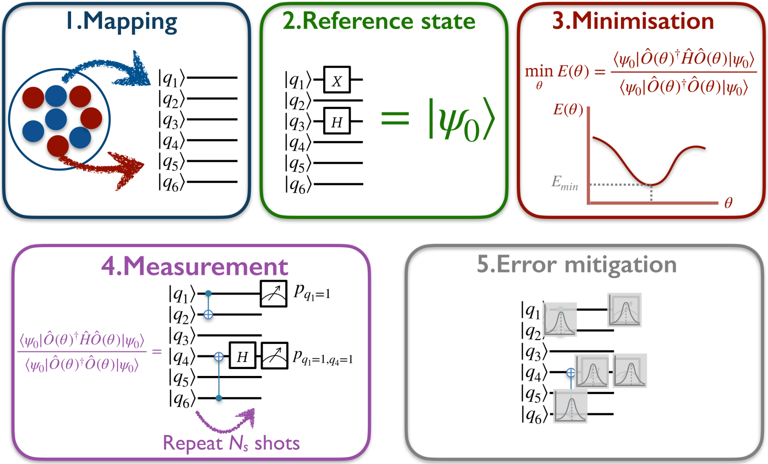
building a quantum circuit
which is measured to obtain the system's properties



Measurement
needs to be repeated N_s shots
in order to obtain energies with errors

Variational Quantum Eigensolvers (VQEs)

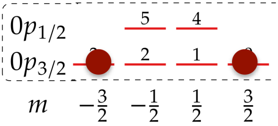
Simulate the nucleus variationally with minimization algorithm: VQE

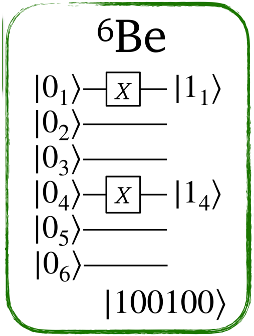


Reduce quantum computational burden, minimization performed classically: hybrid approach

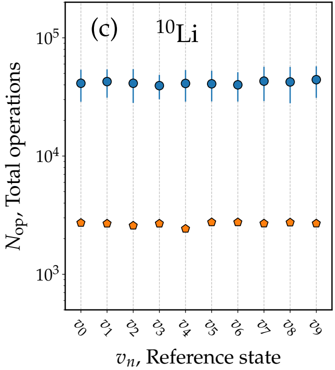
Reference state

Take reference state easily encoded in circuit: Slater determinant
in particular, we take Slater determinant with lowest energy





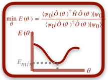
Similar results for other reference states:



Several previous works use Unitary Coupled Cluster method

Dumitrescu et al. PRL120 210501('18), Stetcu et al. PRC105 064308('22)
Kiss et al PRC106 034325('22), Sarma et al PRC108 064305('23)...

Here we use ADAPT: iteratively build ground state

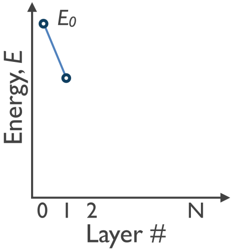


Layer 1

Operator pool

$\hat{A}_m : i(a_p^\dagger a_q^\dagger a_r a_s - a_r^\dagger a_s^\dagger a_p a_q)$

M operators (respecting symmetry)



1. Ansatz

$$|\psi_1(\theta_1)\rangle = e^{i\theta_1 \hat{A}_k} |\psi_0\rangle$$

2. Compute gradients

for k=1,M:

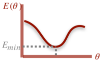
$$\left.\frac{\partial E}{\partial \theta_k}\right|_{\theta_k=0} = i\langle\psi(\theta)|[\hat{H}_{\text{eff}}, \hat{A}_k]|\psi(\theta)\rangle\Big|_{\theta_k=0}$$

3. Keep the operator with largest gradient

$$|\psi_1(\theta_1)\rangle = e^{i\theta_1 \hat{A}_{k_1}} |\psi_0\rangle$$

4. Minimise the energy (classically)

$$\min_{\theta_1} E(\theta_1) = \langle\psi_0|e^{-i\theta_1 \hat{A}_{k_1}} \hat{H} e^{i\theta_1 \hat{A}_{k_1}} |\psi_0\rangle$$



Grimsley, Economou, Barnes & Mayhall, Nat Comms **10** 3007 (2019)

ADAPT VQE

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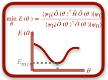

Layer 2

Operator pool

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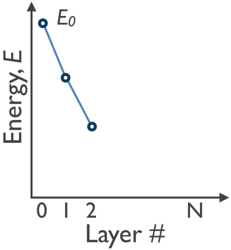


1. Ansatz

$$|\psi_2(\theta_1,\theta_2)\rangle = e^{i\theta_2 \hat{A}_k} e^{i\theta_1 \hat{A}_{k_1}} |\psi_0\rangle$$

2. Compute gradients

```
for k=1,M:
```

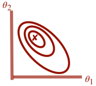
$$\left.\frac{\partial E}{\partial \theta_k}\right|_{\theta_k=0} = i\langle\psi(\theta)|[\hat{H}_{\text{eff}}, \hat{A}_k]|\psi(\theta)\rangle\Big|_{\theta_k=0}$$

3. Keep the operator with largest gradient

$$|\psi_2(\theta_1,\theta_2)\rangle = e^{i\theta_2 \hat{A}_{k_2}} e^{i\theta_1 \hat{A}_{k_1}} |\psi_0\rangle$$

4. Minimise the energy (classically)

$$\min_{\theta_1,\theta_2} E(\theta_1,\theta_2) = \langle\psi_0| e^{-i\theta_1 \hat{A}_{k_1}} e^{-i\theta_2 \hat{A}_{k_2}} \hat{H} e^{\theta_2 \hat{A}_{k_2}} e^{\theta_2 \hat{A}_{k_2}} |\psi_0\rangle$$



Grimsley, Economou, Barnes & Mayhall, Nat Comms **10** 3007 (2019)

ADAPT VQE

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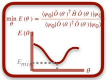

Layer N

Operator pool

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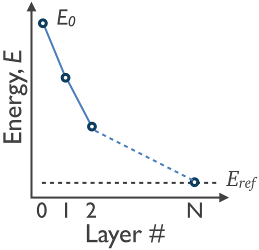
M operators (respecting symmetry)



1. Ansatz

$$|\psi_N(\vec{\theta})\rangle = \Pi_{l=1}^{N} e^{i\theta_l \hat{A}_l} |\psi_0\rangle$$

2. Compute gradients

```
for k=1,M:
```

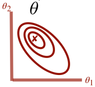
$$\left.\frac{\partial E}{\partial \theta_k}\right|_{\theta_k=0} = i\langle\psi(\theta)|[\hat{H}_{\rm eff}, \hat{A}_k]|\psi(\theta)\rangle\Big|_{\theta_k=0}$$

3. Keep the operator with largest gradient

$$|\psi_N(\vec{\theta})\rangle = e^{i\theta_M \hat{A}_{k_N}} |\psi_{N-1}(\vec{\theta})\rangle$$

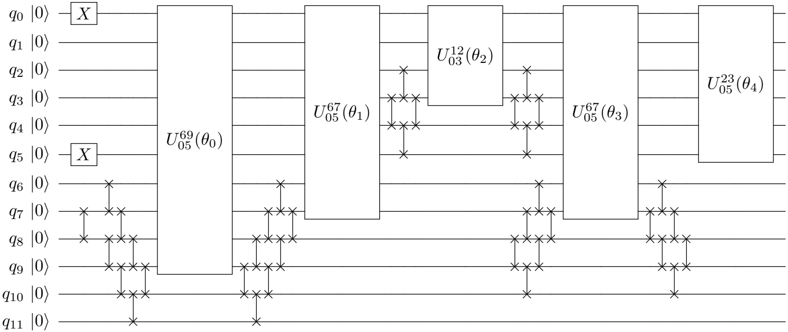
4. Minimise the energy (classically)

$$\min_{\vec{\theta}} E(\vec{\theta})$$

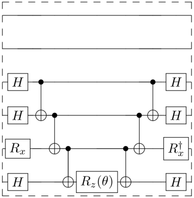


Grimsley, Economou, Barnes & Mayhall, Nat Comms **10** 3007 (2019)

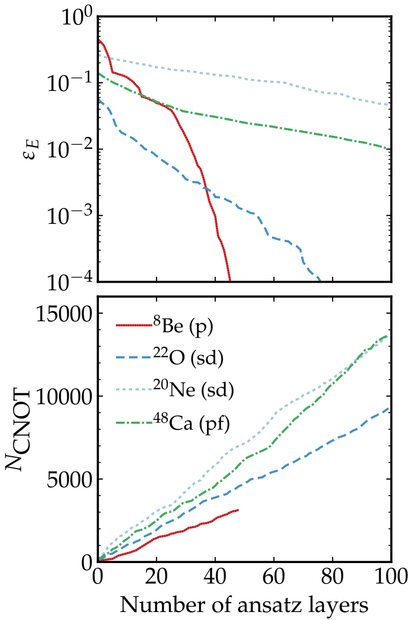
As a result, quantum circuit to simulate the nuclear ground state: eg ^{18}O



where the 5 unitary operators needed to obtain the nuclear ground state are combination of qubit gates:



Simulating nuclei with ADAPT (classically!)



Perform classical simulations
of the quantum systems to simulate
p-, *sd*- and *pf*-shell nuclei

Relative energy error ε_E
rapidly decresing for *p*-shell nuclei
and semimagic *sd*-shell systems

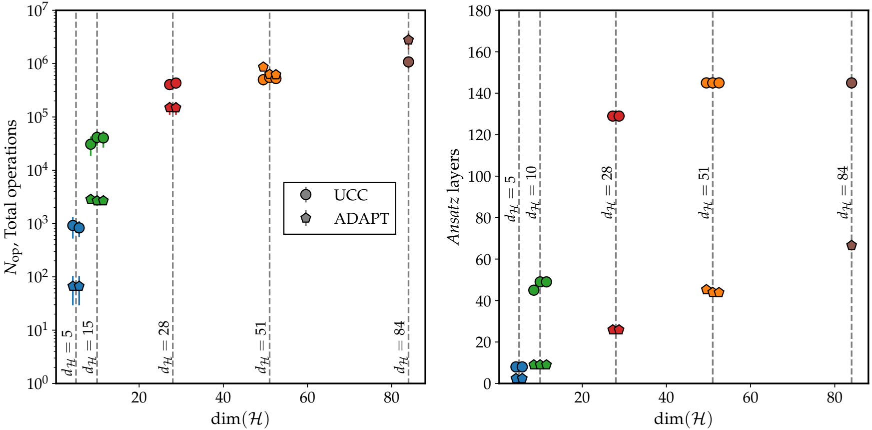
Energy convergence much slower
in open *sd*-shell and *pf* shell
requires more layers
and deeper (more CNOT gates) circuits

Pérez-Obiol et al. Sci. Rep. 13 12291 (2023)

Quantum resources: UCC vs ADAPT

Compare the quantum resources required by two VQEs:
Unitary Coupled Cluster (UCC) vs ADAPT

In simpler systems, ADAPT is more efficient
but toward the midshell UCC requires fewer quantum operations

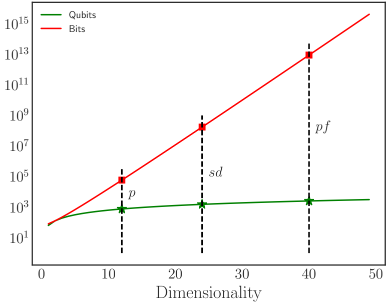


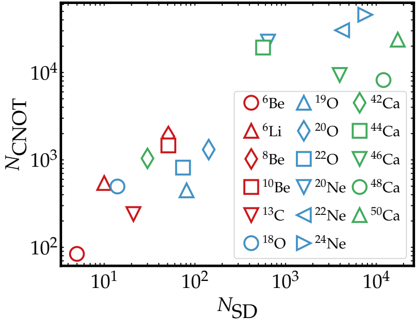
Carrasco et al. to be submitted

ADAPT simulations: scaling

Number of qubits needed to encode nuclei grows polynomially: relatively small number of qubits

Complexity (depth) of the quantum circuits (measured by CNOT gates) scales similarly to number of Slater determinants (combinatorially)





Pérez-Obiol et al. Sci. Rep. 13 12291 (2023)

Try different approaches with better scaling: **E. Costa talk Thursday 15:35**

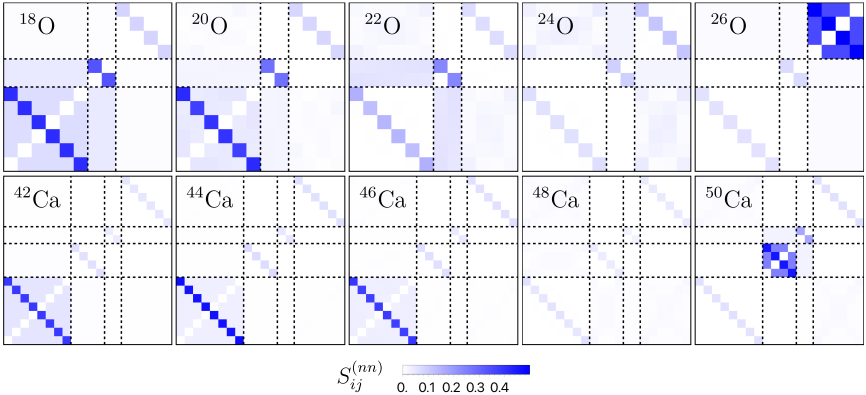
Entanglement in nuclei: mutual information

We can also use quantum information tools to analyze nuclear structure

Mutual information: measure of entanglement between orbitals

$$S_{ij} = S(i) + S(j) - S(ij)$$

Strong entanglement mainly between pairs

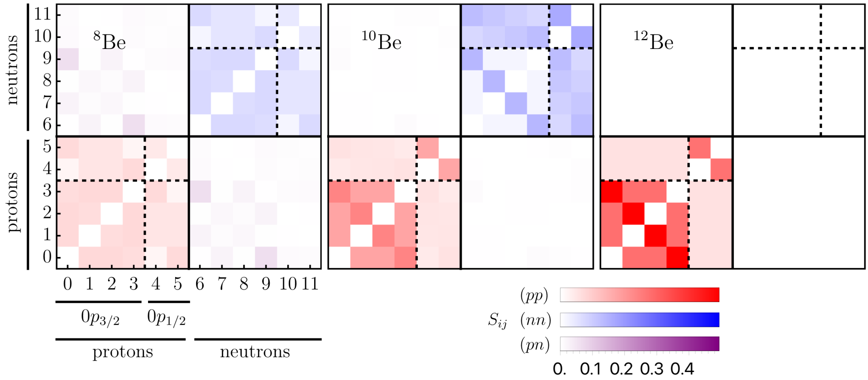


Pérez-Obiol et al. EPJA 59 240 (2023)

Nuclear entanglement: protons and neutrons

Weak entanglement between protons and neutrons
especially in neutron-rich nuclei

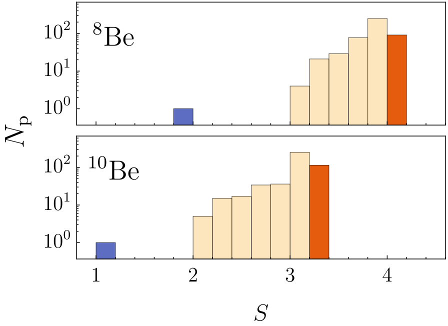
Gorton, Johnson, JPG 50 045110 (2023), PRC 110 034305 (2024)



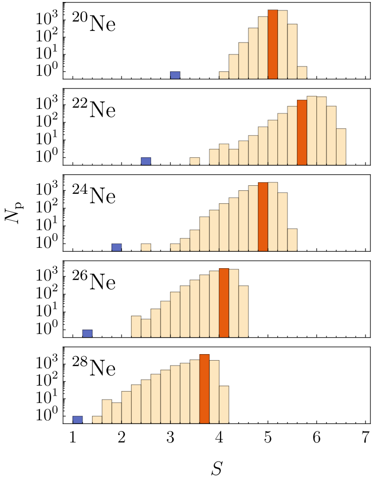
Pérez-Obiol et al. EPJA 59 240 (2023)

Nuclear entanglement: bipartitions

Indeed, among all possible bipartitions, the one with less mutual information between the two parts is the one of protons vs neutrons



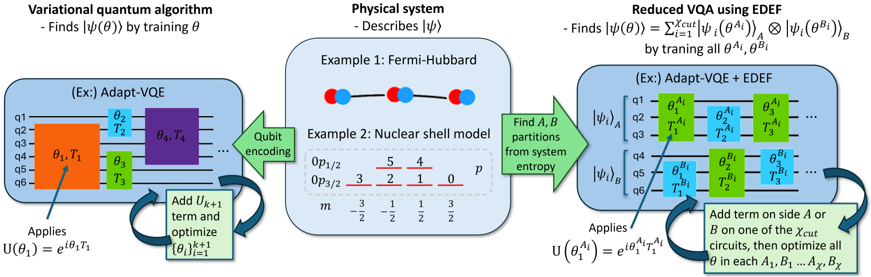
Pérez-Obiol et al. EPJA 59 240 (2023)



Application: entropy-driven entanglement forging

Use low-entanglement between different bipartitions of the nucleus to simplify the (quantum) simulation

Build different circuits for protons and neutrons and combine (forge) them together using symmetries (Schmidt decomposition)



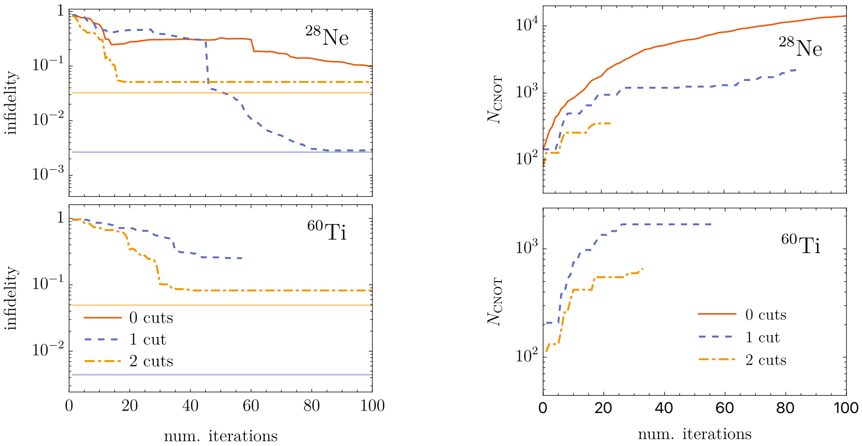
Pérez-Obiol et al. arXiv:2409.04510

Similar EDEF strategy can be used in condensed matter systems: eg Fermi-Hubbard in 1D

Entropy-driven entanglement forging (EDEF)

Separate simulation of protons and neutrons
allows for a more efficient simulation of neutron-rich nuclei

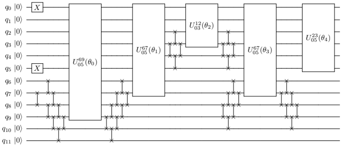
In some cases, calculation without EDEF even too demanding



Pérez-Obiol et al. arXiv:2409.04510

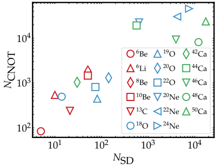
Summary

Classical simulations of building ground-states in digital quantum computer

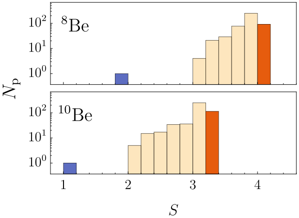


Converged ground-state energies of *p*-, *sd*- and selected *pf*-shell nuclei with relative high quantum resources

Scaling does not suggest quantum advantage with respect to classical simulations



Low proton-neutron entanglement exploit in EDEF: build quantum circuits separately



Outlook

Run first simulations in quantum computer (Barcelona Supercomputing Center, 15 qubits) mitigate noise, optimize quantum resources