UNIVERSITAT DE BARCELONA

Nuclear shell-model Hamiltonians in a quantum computer

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Motivation

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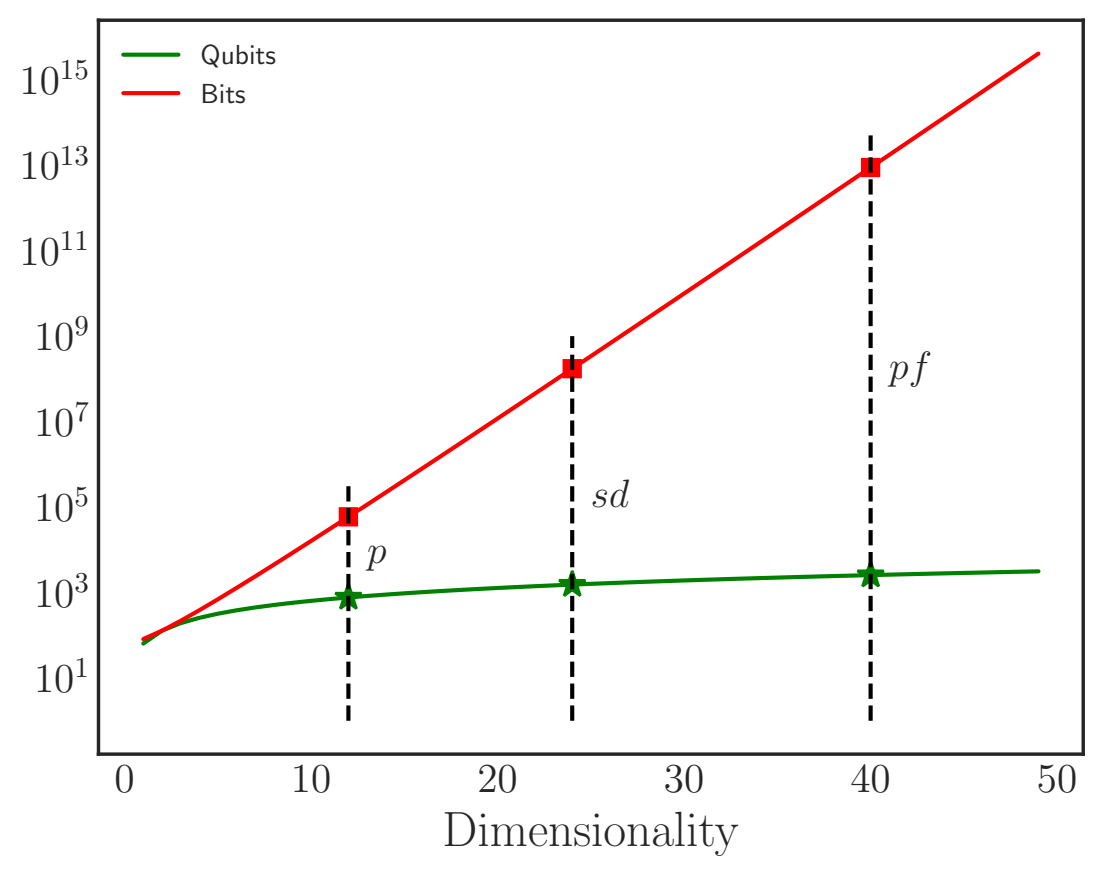
- Quantum algorithms may facilitate the solution to physical problems that scale exponentially in a classical computer. The shell-model is a textbook example.



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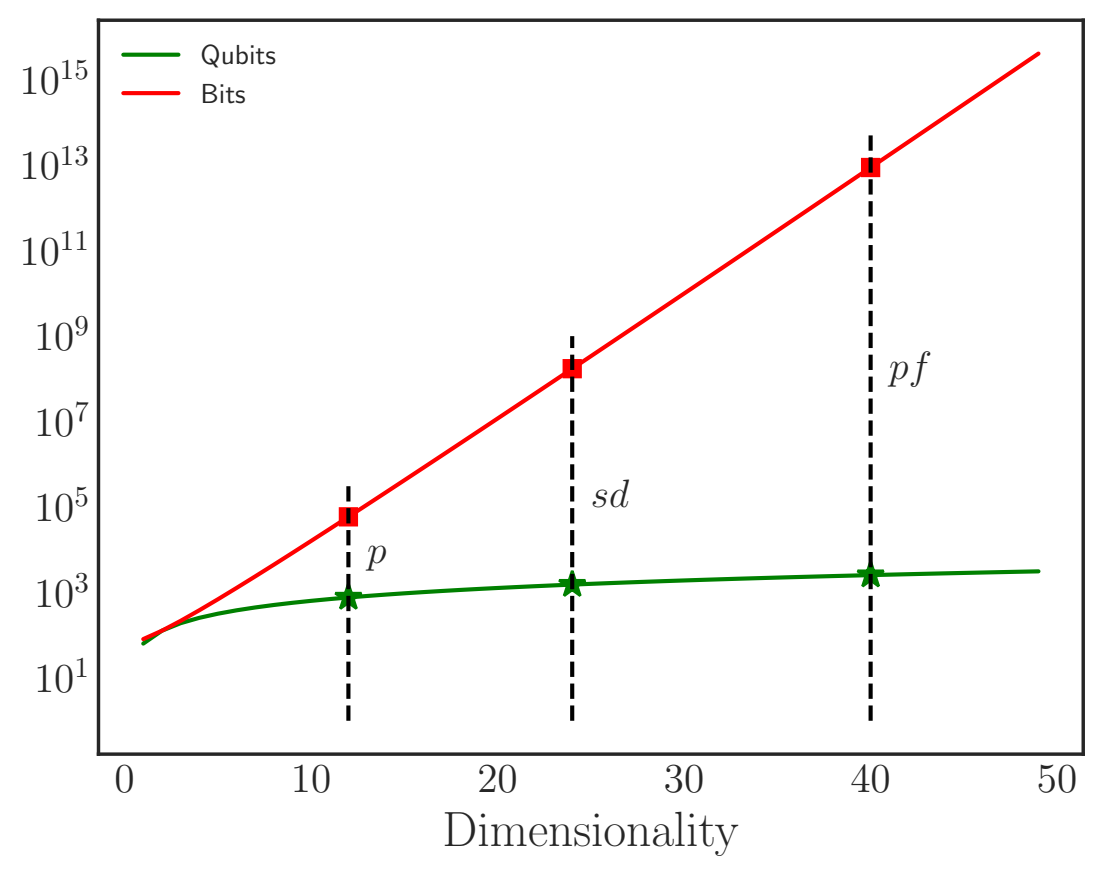

- Implementation in quantum devices comes with other challenges.

Specifics of the project

- Variational quantum eigensolvers (VQE) are a promising tool for the description of nuclear structure with quantum circuits.

[1] J Tilly, et al., The variational quantum eigensolver: a review of methods and best practices. Phys. Reports 986, 1–128 (2022)

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  - Iterative optimization and convergence
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  - Error mitigation
- Our algorithm of choice is the recent Adaptive Derivative-Assemled Problem-Tailored Variational Quantum Eigensolver (ADAPT-VQE). Adequate for the NISQ era.

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Simulation

Adaptive variational quantum eigensolver (ADAPT-VQE) [1]

Starting ingredients: a reference state $|\Psi_{\text{ref}}\rangle$ and a pool of operators $\hat{A}_m : a_i^+ a_j,\, a_i^+ a_j^+ a_l a_k \ldots$

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Algorithm:

$$|\Psi_0\rangle = |\Psi_{\text{ref}}\rangle$$

$$|\Psi_1\rangle = e^{i\theta_1 \hat{A}_1} |\Psi_0\rangle$$

$$|\Psi_2\rangle = e^{i\theta_2 \hat{A}_2} |\Psi_1\rangle = e^{i\theta_2 \hat{A}_2} e^{i\theta_1 \hat{A}_1} |\Psi_0\rangle$$

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$$|\Psi_n\rangle = e^{i\theta_n \hat{A}_n} \cdots e^{i\theta_1 \hat{A}_1} |\Psi_0\rangle$$

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Operators $\hat{A}_m$ selected according to the largest gradient

$$\left.\frac{\partial E^{(k)}}{\partial \theta_m}\right|_{\theta_m = 0} = i\langle \Psi_k | [H, \hat{A}_m] | \Psi_k \rangle$$

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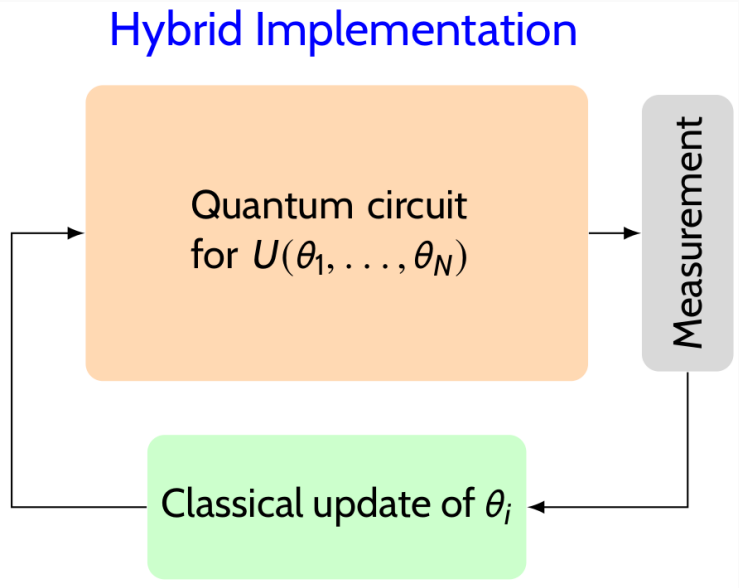

Courtesy of Jon Engel

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Parameters θ_m obtained minimizing the energy surface at every iteration.

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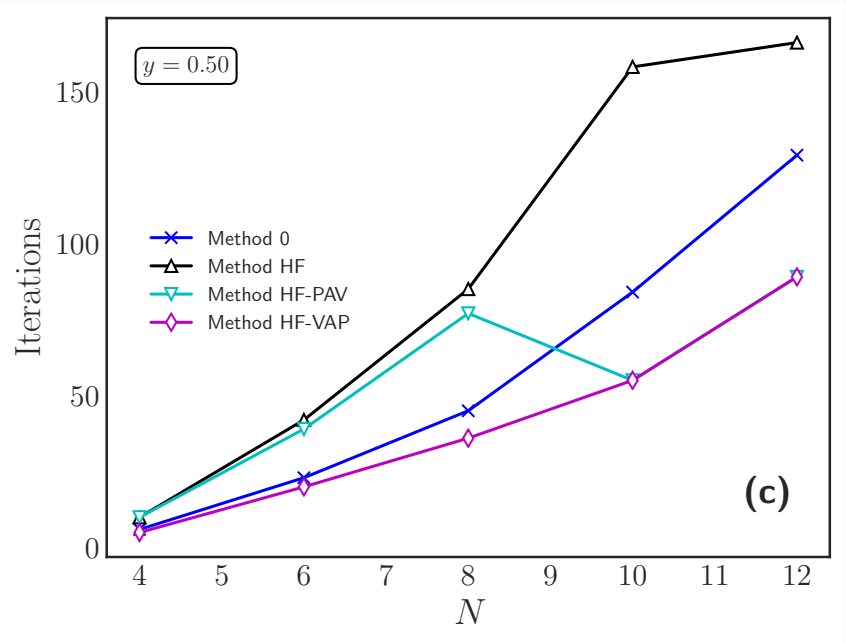
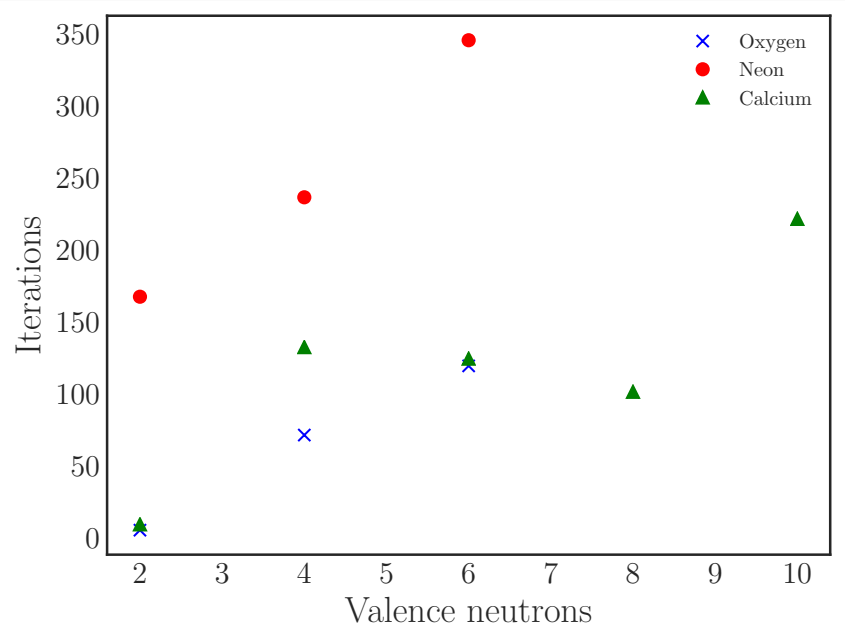
Good scaling!

Previous work with ADAPT-VQE in the Lipkin and shell-model[2]:

Lipkin model of N particles with interaction strength y



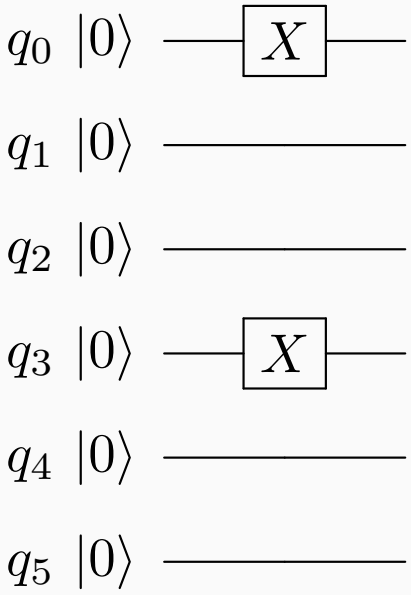
USDB, KB3G phenomenological interactions



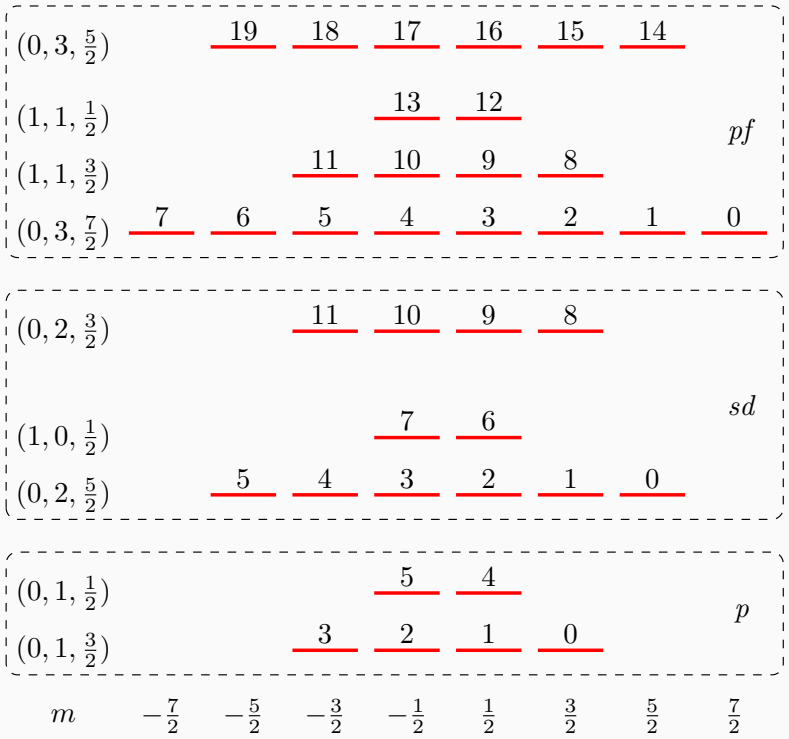
[2]A. M. Romero, J. Engel, Ho Lun Tang, and Sophia E. Economou. Phys. Rev. C 105, 064317

Quantum implementation

Implementation in quantum devices: fermionic mapping



$$X|0\rangle = |1\rangle$$



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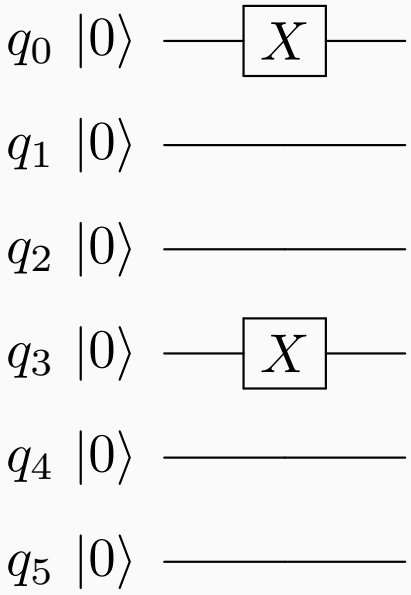

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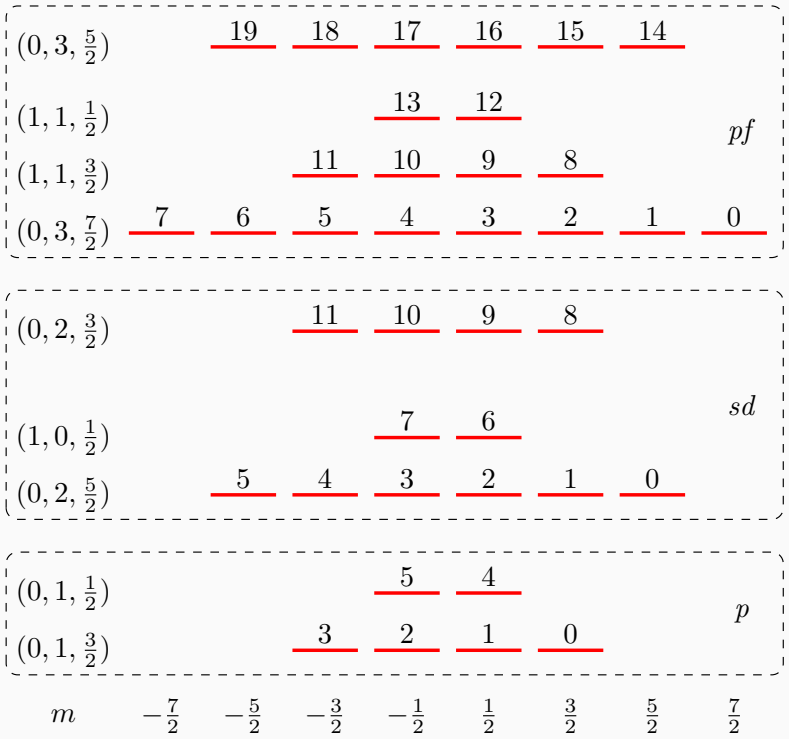

Jordan-Wigner mapping is used for convenience:

$$a_i^\dagger = \left(\prod_{k=0}^{i-1} Z_k\right)\sigma_i^-, \quad a_i = \left(\prod_{k=0}^{i-1} Z_k\right)\sigma_i^+,$$

but leads to unnecessarily large matrices and number of qubits

Choice of ansatz

We simply chose the lowest-energy Slater determinant. Straightforward to implement

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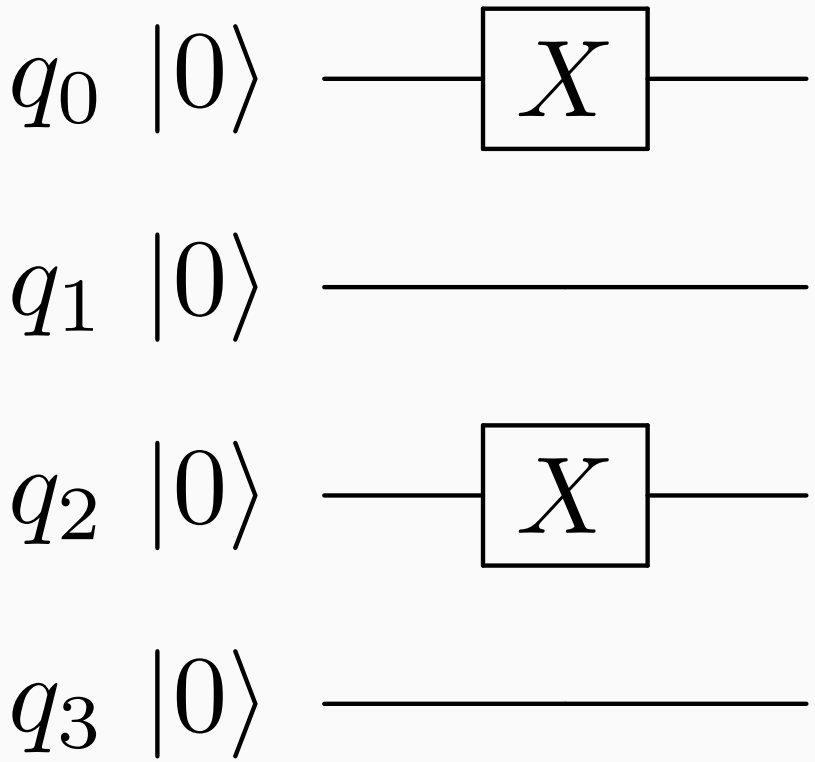
Example: Two particles in a four-state space

$$|\psi\rangle = |02\rangle$$



Variational part: pool operators

Implementation of ADAPT pool operators is straightforward. We chose all the possible two-body excitations

$$T_{rs}^{pq} = i(a_p^\dagger a_q^\dagger a_r a_s - a_r^\dagger a_s^\dagger a_p a_q)$$

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$$e^{i\theta T_{pq}^{rs}} = e^{i\theta P_{pq}^{rs} X_p Y_q Y_r Y_s} e^{i\theta P_{pq}^{rs} Y_p X_q Y_r Y_s} e^{-i\theta P_{pq}^{rs} Y_p Y_q X_r Y_s} e^{-i\theta P_{pq}^{rs} Y_p Y_q Y_r X_s}$$
$$\times e^{-i\theta P_{pq}^{rs} Y_p X_q X_r X_s} e^{-i\theta P_{pq}^{rs} X_p Y_q X_r X_s} e^{i\theta P_{pq}^{rs} X_p X_q Y_r X_s} e^{i\theta P_{pq}^{rs} X_p X_q X_r Y_s}$$

$$P_{pq}^{rs} = \prod_{m=p+1, m\notin[r,s]}^{r-1} Z_m \prod_{n=r+1, n\notin[p,q]}^{s-1} Z_n$$

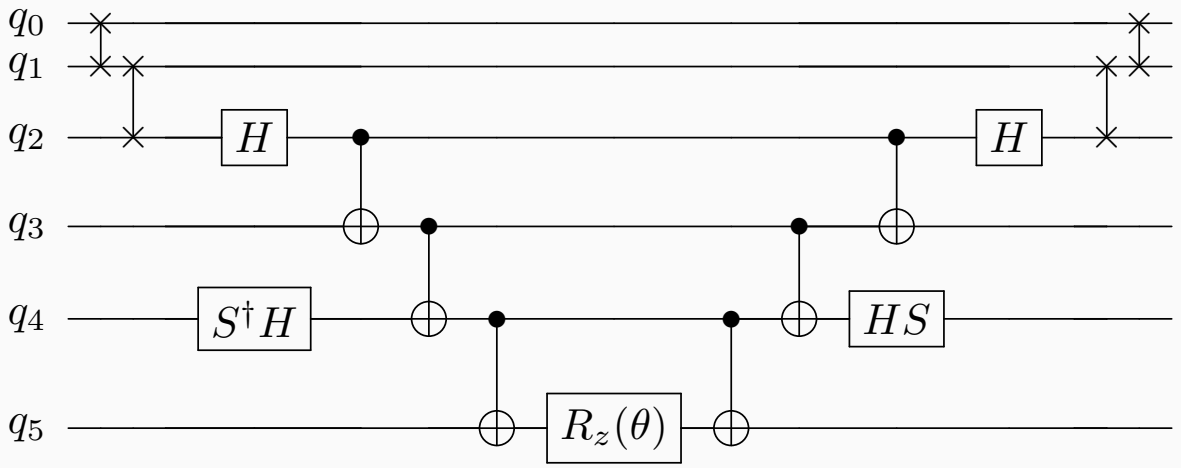

Figure 2: Quantum circuit to implement $e^{-i\theta X_0 Z_1 Y_4 Z_5}$

Measurement of the energy

$$H = \sum_i \varepsilon_i a_i^\dagger a_i + \frac{1}{4} \sum_{ijkl} \bar{v}_{ijkl} a_i^\dagger a_j^\dagger a_l a_k$$

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We disentangle them in terms of the form

$$\begin{aligned}
n_i &= a_i^\dagger a_i = \frac{1}{2}(1 - Z_i) \\
h_{ijij} &= -2 a_i^\dagger a_i a_j^\dagger a_j = -\frac{1}{2}(1 - Z_i)(1 - Z_j), \\
h_{ijki} &= a_i^\dagger a_i (a_j^\dagger a_k + a_k^\dagger a_j) \\
&= \frac{1}{2}(1 - Z_i) \left(\prod_{n=j+1}^{k-1} Z_n \right) \left(|01\rangle\langle 10| + |10\rangle\langle 01| \right)_{jk}, \\
h_{ijkl} &= P_{ij}^{kl} \left(|0011\rangle\langle 1100| + |1100\rangle\langle 0011| \right)_{ijkl},
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But this is not the problem!

Measurement: minimum clique problem

Dimension of two-body excitation operators increases quartically with space dimensionality and can not be measured simultaneously. We need to find the minimum partition group of commuting operators

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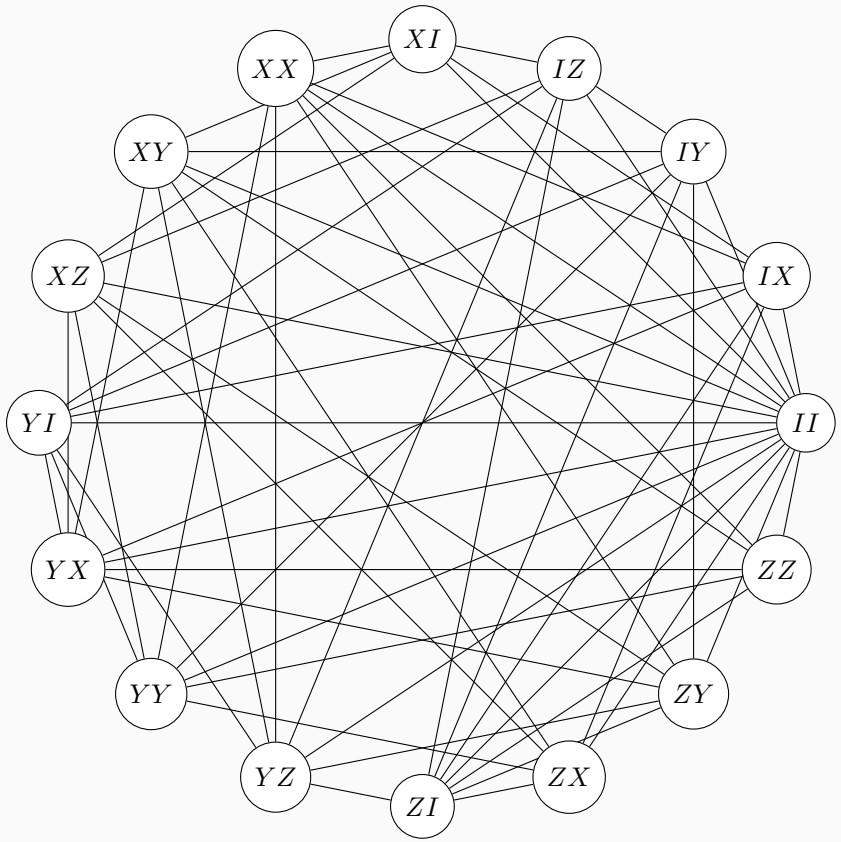

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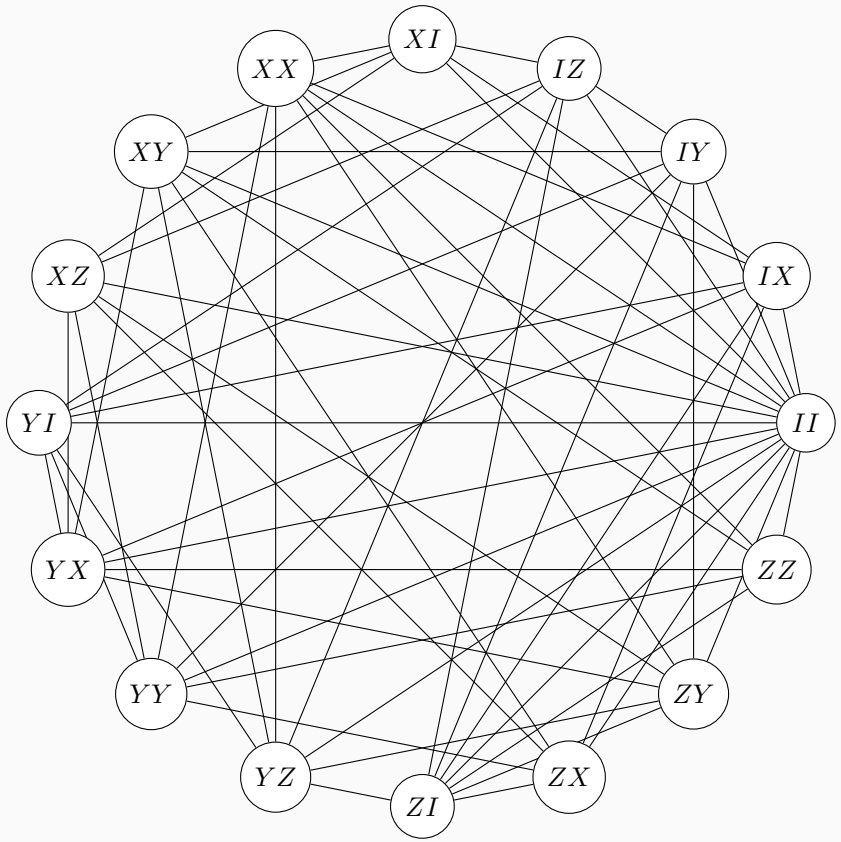
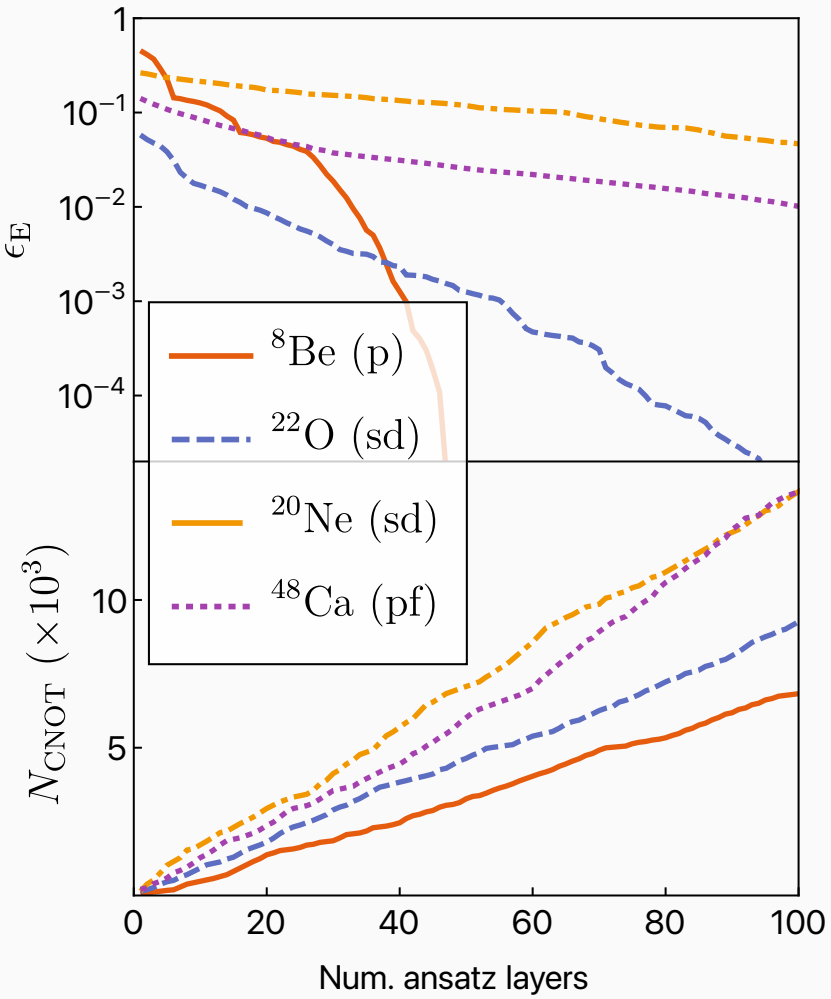


NP-hard problem! We used a greedy algorithm for approximate solutions

Results

Quantum simulation of ADAPT-VQE

- Number of CNOTS grows linearly with the number of iterations!
- In lower dimensionality spaces, results converge quickly
- Different convergence behavior for different nuclei



A. Perez-Obiol, A. M. Romero et al, Nuclear shell-model simulation in a quantum device, TBP

Quantum simulation of ADAPT-VQE

shell	N_q	N_{SD}	nucleus	N_{iters}	ϵ_r bound
p	6	5	^{6}He	2	10^{-5}
	12	10	^{6}Li	9	10^{-7}
		51	^{8}Be	48	10^{-5}
		51	^{10}Be	48	10^{-5}
		42	^{13}C	17	10^{-5}
sd	12	14	^{18}O	5	10^{-6}
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Model circuit

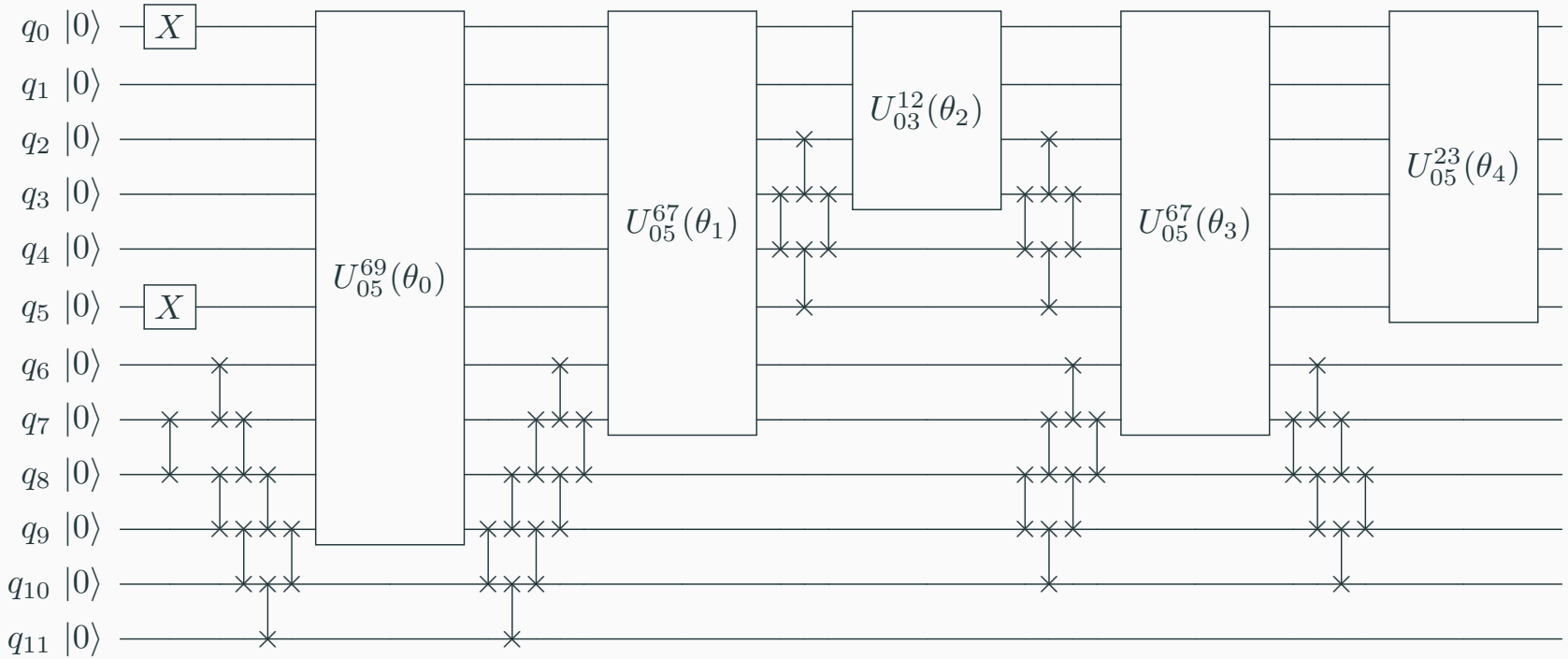

Figure 3: Quantum circuit to prepare the exact ground state for the *sd*-shell with two neutrons, ^{18}O. X gates prepare the reference state and FSWAPS are used to change basis so that exponentials of pool operators operate on adjacent qubits. Multiqubit gates in the boxes are defined as $U_{ij}^{kl}(\theta) \equiv e^{i\theta T_{ij}^{kl}}$ and $\theta_0 = -0.157263$, $\theta_1 = -0.437238$, $\theta_2 = 0.604663$, $\theta_3 = 0.214431$, $\theta_4 = -0.785469$.

Number of circuits for measurement

shell	N_q	N_h	N_hh	Total
p	6	2	10 (9)	13 (12)
	12	4	109 (44)	114 (49)
sd	12	8	203 (86)	212 (95)
	24	16	1389 (518)	1406 (535)
pf	20	20	1507 (570)	1528 (591)
	40	40	10572 (3459)	10613 (3500)

Table 1: Number of different circuits needed to measure the expectation value of the Hamiltonian. N_q indicates the number of qubits used, corresponding to the number of orbitals in the shell. N_h and N_hh are the number of single and double hopping terms in the Hamiltonian, defining the number of different circuits needed to measure these parts. The values in parenthesis correspond to the minimum number of groups containing $h_{ijkl}^{(hh)}$ terms found such that all operators in the group commute with each other and can be measured with the same circuit. In the last column, we list the total number of circuits corresponding to $N_\mathsf{h} + N_\mathsf{hh} + 1$, accounting also for the single circuit needed to measure $\langle h_i \rangle$.

Conclusions and ongoing work

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- Promising results were obtained using ADAPT-VQE applied with phenomenological shell-model interactions in the classical and quantum simulation of the algorithm.

[3] A. Perez-Obiol, A. M. Romero et al, Nuclear shell-model simulation in a quantum device, TBP

[4] Selection of six sites to host the first European quantum computers

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- We developed a baseline code with the quantum implementation of the nuclear shell-model to explore and study these upcoming challenges[3].

[3] A. Perez-Obiol, A. M. Romero et al, Nuclear shell-model simulation in a quantum device, TBP

[4] Selection of six sites to host the first European quantum computers

Conclusions

- Promising results were obtained using ADAPT-VQE applied with phenomenological shell-model interactions in the classical and quantum simulation of the algorithm.
- The quantum implementation of VQE carries challenges of its own that hopefully are easier to solve than the exponential scaling.
- We developed a baseline code with the quantum implementation of the nuclear shell-model to explore and study these upcoming challenges[3].
- Barcelona Supercomputing Center will host one of the first European quantum computers[4].

[3] A. Perez-Obiol, A. M. Romero et al, Nuclear shell-model simulation in a quantum device, TBP

[4] Selection of six sites to host the first European quantum computers

In collaboration with

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Virginia Tech: Sophia Economou and Ho Lun Tang

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University of Barcelona: Arnau Ríos, Javier Menéndez and Bruno Juliá

Barcelona Supercomputing Center: **Axel Pérez Obiol** and Artur García

Merci beaucoup!

Extra slides

Fermionic mapping: example and potential alternative

The general Hamiltonian:

$$H = \sum_i \varepsilon_i a_i^\dagger a_i + \frac{1}{4} \sum_{ijkl} \bar{v}_{ijkl} a_i^\dagger a_j^\dagger a_l a_k \,, \tag{1}$$

under a JW mapping, the corresponding matrix representation will have $2^{\mathrm{dim}} \times 2^{\mathrm{dim}}$ elements.

[5] RMN Pesce, PD Stevenson: H2ZIXY, arXiv:2111.00627

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Take the case of ^{6}Li in the M-scheme: ground-state is formed with 10 $M = 0$ states, but with JW the Hamiltonian matrix is $2^{12} \times 2^{12}$!

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Compact encoding of the Hamiltonian[5]:

$$H = 0.598IIII - 0.088IIIX + \ldots - 0.037ZZZX - 0.059ZZZZ. \tag{2}$$

Only 4 qubits are needed! But what do projections 0 and 1 represent?

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Why ADAPT and not Unitary Coupled Clusters approach?

$$|\Psi(\boldsymbol{\theta})\rangle = e^{\hat{T}(\boldsymbol{\theta})}|0\rangle \longrightarrow E_{\mathrm{UCC}} = \min_{\boldsymbol{\theta}} \frac{\langle\Psi(\boldsymbol{\theta})|H|\Psi(\boldsymbol{\theta})\rangle}{\langle\Psi(\boldsymbol{\theta})|\Psi(\boldsymbol{\theta})\rangle}, \tag{3}$$

[6] I. Stetcu et al. Phys. Rev. C 105, 064308
[7] O. Kiss et al, Phys. Rev. C 106, 034325

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$$e^{A+B} = \lim_{n\to\infty}\left(e^{A/n}e^{B/n}\right)^n, \tag{4}$$

  Good results are obtained with only one Trotter step[6]. Although symmetries can be broken in the wavefunction and be more crucial in strongly-correlated systems

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- ADAPT does not depend on the cluster operator order
- However, it is possible that ADAPT leads to deeper circuits[7]

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