Simulation of lattice Hamiltonians with qubits

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ATOMTRONICS, Benasque, May 21st 2024

Outline

1. Introduction: quantum simulation with qubits
2. Adiabatic algorithm for graphene

Pérez-Obiol et al, Phys. Rev. A 106, 052408 (2022)

Tang et al arXiv:2405.09225 (2024)

3. Variational algorithm for the nuclear shell model

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

Pérez-Obiol et al, Eur. Phys. J. A 59, 240 (2023)

4. Summary

Motivation: quantum many-body problem

Find ground states / dynamics of lattice Hamiltonians

$$\mathscr{H} = \sum_{ij} t_{ij}\, a_i^\dagger a_j + \sum_{ij} t_{ijkl}\, a_i^\dagger a_j^\dagger a_k a_l$$

(molecules, crystals, nuclei, optical lattices, etc.)

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Hilbert space scales factorially

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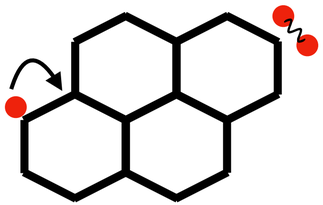
➡ Use quantum bits instead of bits: e.g. one qubit per orbital

➡ Use universal set of quantum gates: e.g. rotations + CNOT

$$\mathscr{H} = \sum_{ij} t_{ij}\, a_i^\dagger a_j + \sum_{ij} t_{ijkl}\, a_i^\dagger a_j^\dagger a_k a_l$$

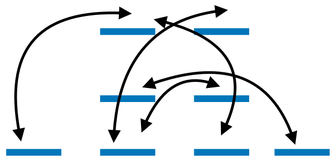
Fermi-Hubbard type (1D, 2D, square/hexagonal, 2nd neighbors, electric field, tilting)

$a_{i\uparrow}^\dagger a_{i+1\uparrow}$ $\quad$ $a_{i\uparrow}^\dagger a_{i\uparrow}\, a_{i\downarrow}^\dagger a_{i\downarrow}$



All to all couplings
(molecular hamiltonian, nuclear shell model)

$a_i^\dagger a_j^\dagger a_k a_l$



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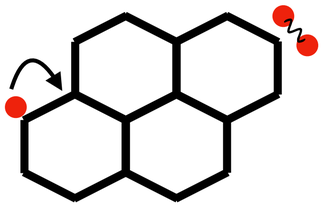

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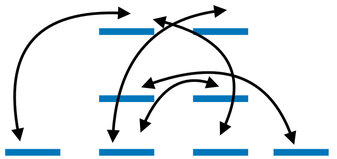

$$a_i^\dagger a_j^\dagger a_k a_l$$

Algorithms

Adiabatic evolution

$$|\psi(T)\rangle = \hat{T} e^{-i\int_0^T H(t)dt}\,|\psi(0)\rangle$$

$$H(t) = H_i(T-t) + \frac{t}{T} H_f$$

➡ Choose H_i

➡ Avoid degeneracy

Variational

$$|\psi(\vec{\theta})\rangle = \prod_{k=1}^{n} e^{i\theta_k A_k}\,|\psi_0\rangle$$

$$E = \min_{\theta_k} \frac{\langle \Psi(\theta_k)|H|\Psi(\theta_k)\rangle}{\langle \Psi(\theta_k)|\Psi(\theta_k)\rangle}$$

➡ Choose ansatz

➡ Minimize energy

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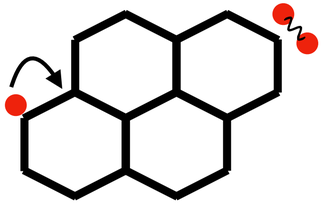

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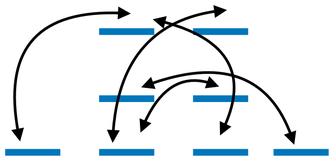

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➡ graphene ground states

Phys. Rev. A 106, 052408 (2022)

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➡ nuclear ground states

Sci Rep 13, 12291 (2023) *Eur. Phys. J. A* 59, 240 (2023)

Simulation of (artificial) graphene

1. Map fermions to qubits with Jordan-Wigner: $a_j = \left(\prod_{k=0}^{j-1} \sigma_k^{(z)} \right) \frac{1}{2} (\sigma_j^{(x)} - i\sigma_j^{(y)})$

Fermions operators

$\{a_i, a_j^\dagger\} = \delta_{ij}$

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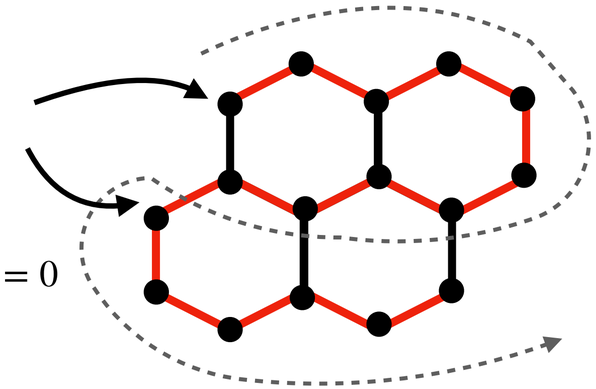

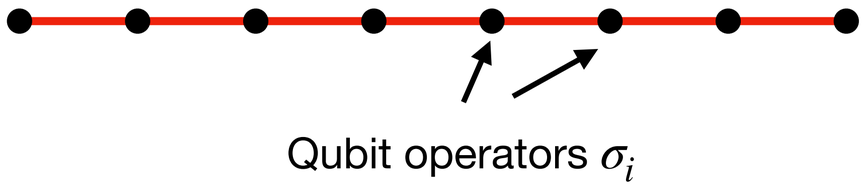

Qubit operators σ_i

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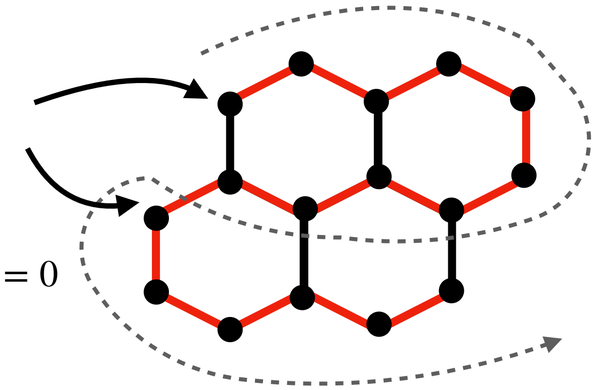

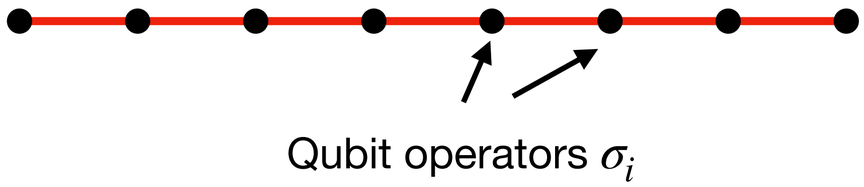

Qubit operators σ_i

2. Prepare ground state of U=0, depth scales as $\mathcal{O}(N_{hex})$

Z. Jiang et al., Phys. Rev. Applied 9, 044036 (2018)

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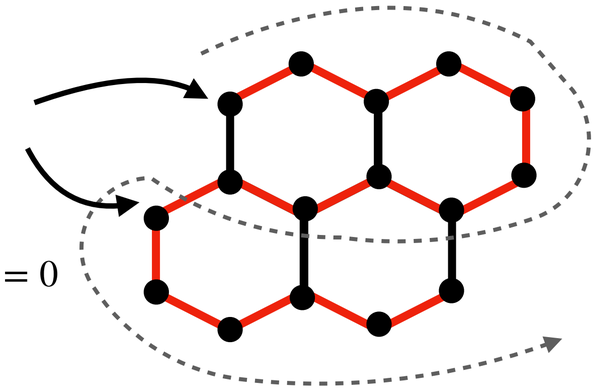

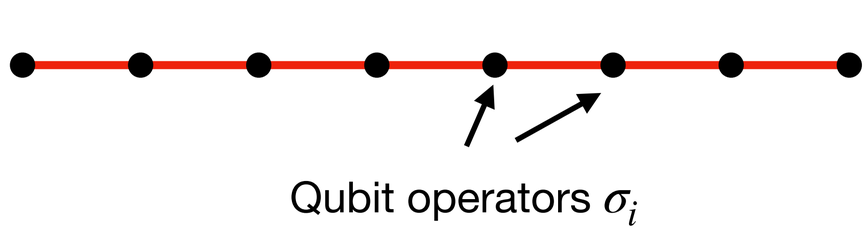

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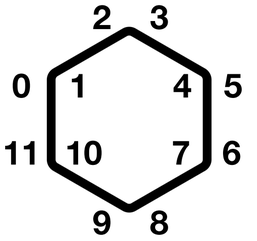
3. Adiabatic evolution (U=0 —> U=1)

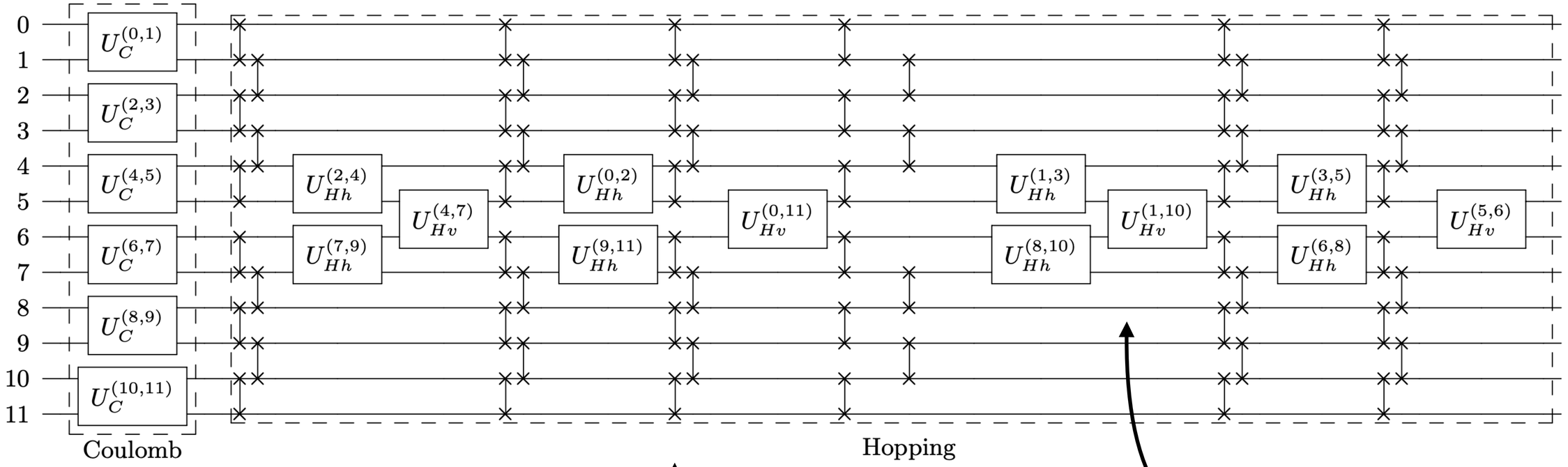
$$|\psi(T)\rangle = \hat{T}e^{-i\int_0^T \mathscr{H}(t)dt}|\psi(0)\rangle \approx \prod_{j=0}^{N} e^{-i\mathscr{H}(j\delta t)\delta t}|\psi(0)\rangle \approx \prod_{i,\sigma} e^{-iUs\delta_t a_{i,\uparrow}^\dagger a_{i,\downarrow}^\dagger a_{i,\uparrow} a_{i,\downarrow}} \times \prod_{\langle ij\rangle,\sigma\sigma'} e^{it\delta_t a_{i,\sigma}^\dagger a_{j,\sigma}} \times \prod_{\langle ij\rangle,\sigma} e^{-i\frac{2i\lambda_R}{3}\delta_t a_{i,\sigma}^\dagger a_{j,\sigma'}[(\vec{\sigma}\times\vec{d}_{ij})_z]_{\sigma,\sigma'}}|\psi(0)\rangle$$

adiabatic errors

adiabatic+circuit errors

circuit for $e^{-i\mathscr{H}(s)\delta t}$ for 1 hexagon





$$e^{-iUh_C} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{-iU} \end{pmatrix}$$

$$h_C = a_0^\dagger a_1^\dagger a_0 a_1$$

$$\text{FSWAP} = 1 + a_0^\dagger a_1 + a_1^\dagger a_0 - a_0^\dagger a_0 - a_1^\dagger a_1$$

$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$e^{-ith_H} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(t) & -i\sin(t) & 0 \\ 0 & -i\sin(t) & \cos(t) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

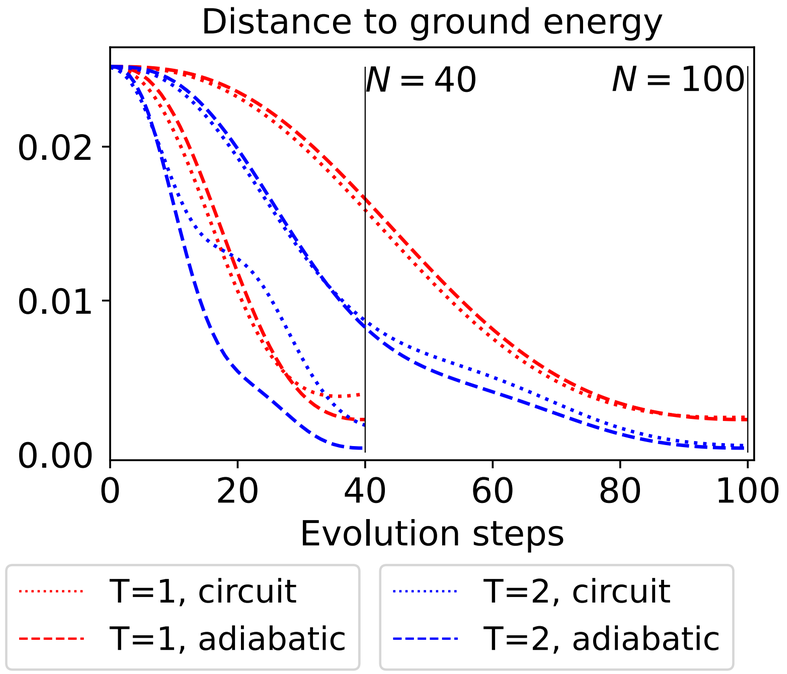
$$h_H = a_0^\dagger a_1 + a_1^\dagger a_0$$

Search for the optimal Trotterizations and periods with circuit simulations

Phys. Rev. A 106, 052408 (2022)

Cirq (Google) **+ openfermion** (prepares initial states)
Qibo, Quantum Science and Technology 7, 015018 (2021). (fast simulator)

example of 1x1 lattice (but simulations up to 4 hexagons)



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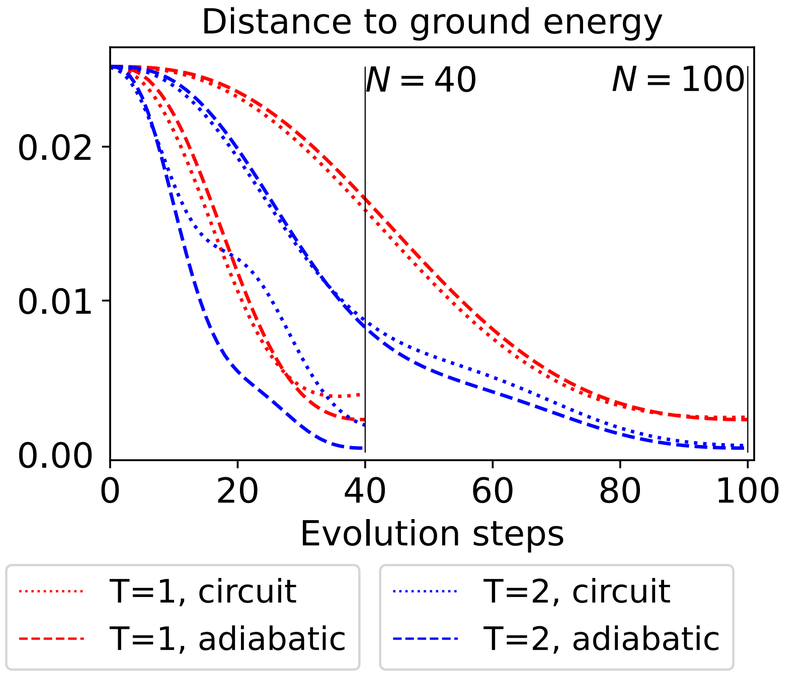

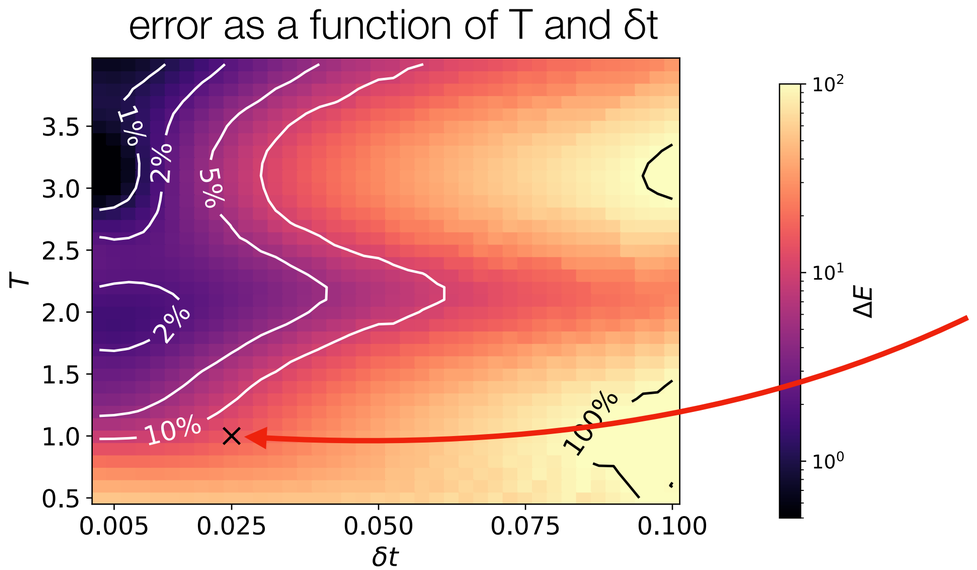

$$\Delta E = \left| \frac{\langle \psi_{FH} | \mathcal{H}_{FH} | \psi_{FH} \rangle - \langle \psi(t) | \mathcal{H}_{FH} | \psi(t) \rangle}{\langle \psi_{FH} | \mathcal{H}_{FH} | \psi_{FH} \rangle - \langle \psi_{TB} | \mathcal{H}_{FH} | \psi_{TB} \rangle} \right|$$

Using counter diabatic driving

arXiv:2405.09225

Jialiang Tang, Ruoqian Xu, Yongcheng Ding, Xusheng Xu, Yue Ban, Manhong Yung, Axel Pérez-Obiol, Gloria Platero, Xi Chen

$$H(t) = H_{kin} + \lambda(t)\, H_{int} + \lambda'(t)\, A(t) \qquad A(t) = i\,\alpha\,[H_{kin}, H_{int}] \qquad \lambda(t) = \sin\left(\frac{\pi\, t}{2T}\right)$$

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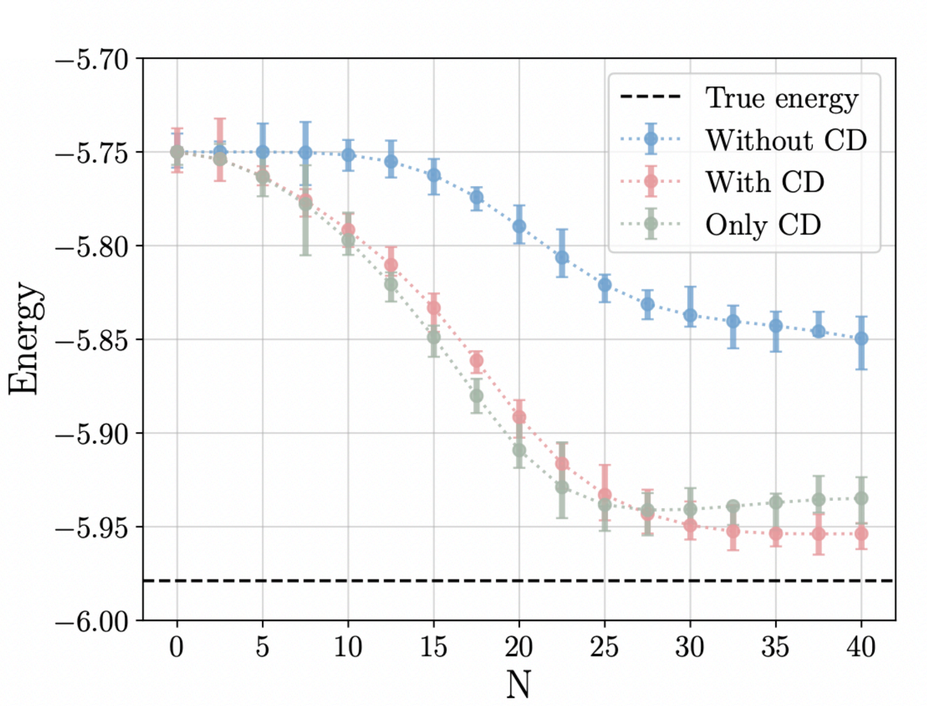
in terms of number of steps



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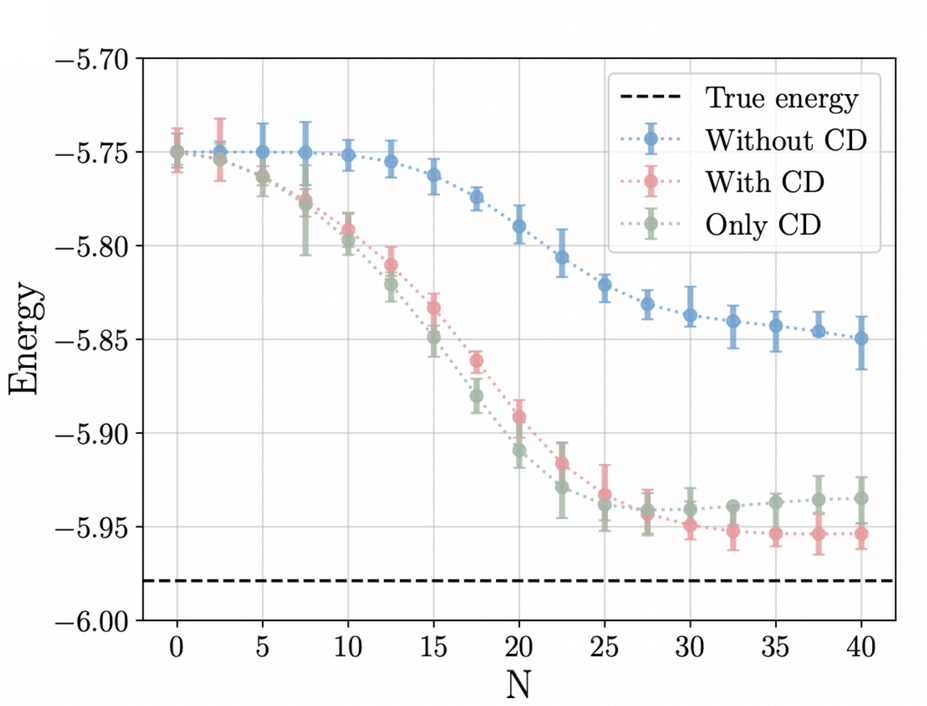
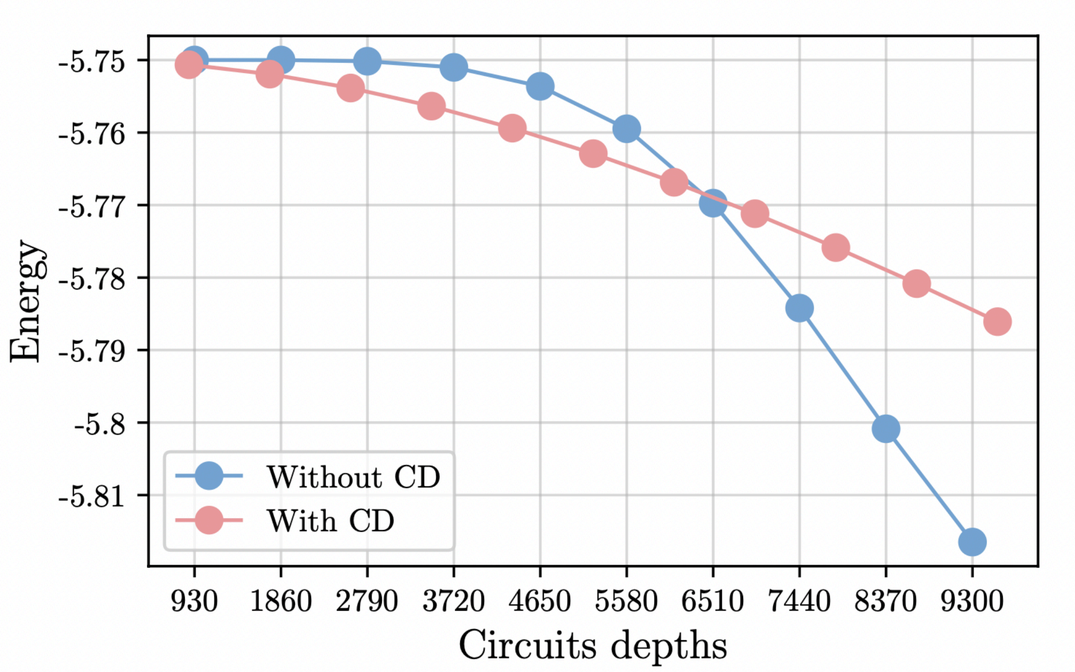


in terms of circuit depths:



Nuclear shell model

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

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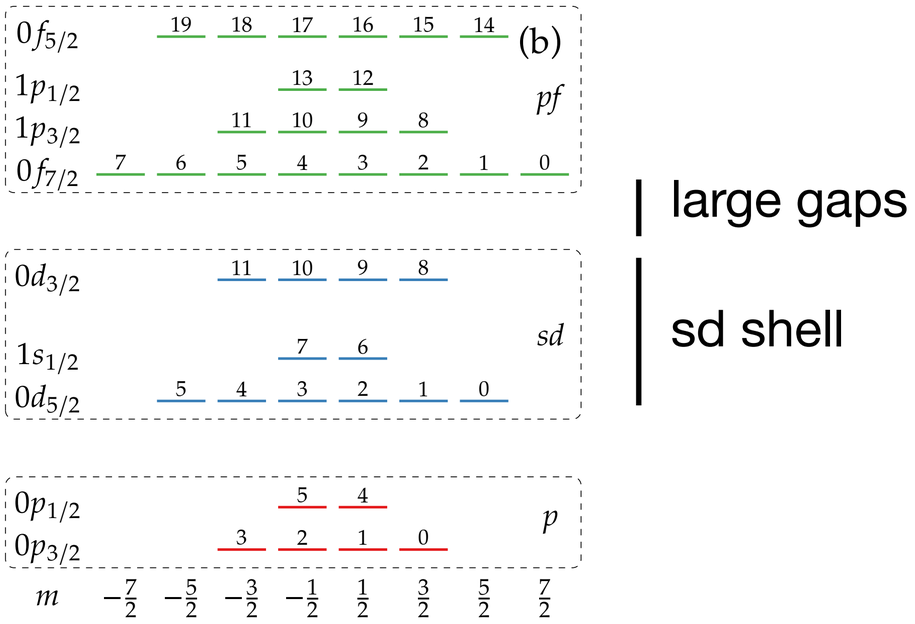
Magic numbers: numbers of neutrons that make nuclei specially bound/stable

Mean field: predicts these magic numbers and sets single-particle basis



large gaps

sd shell

Nuclear shell model

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

Hamiltonian coefficients adjusted phenomenologically
(e.g. nuclear ground energies)

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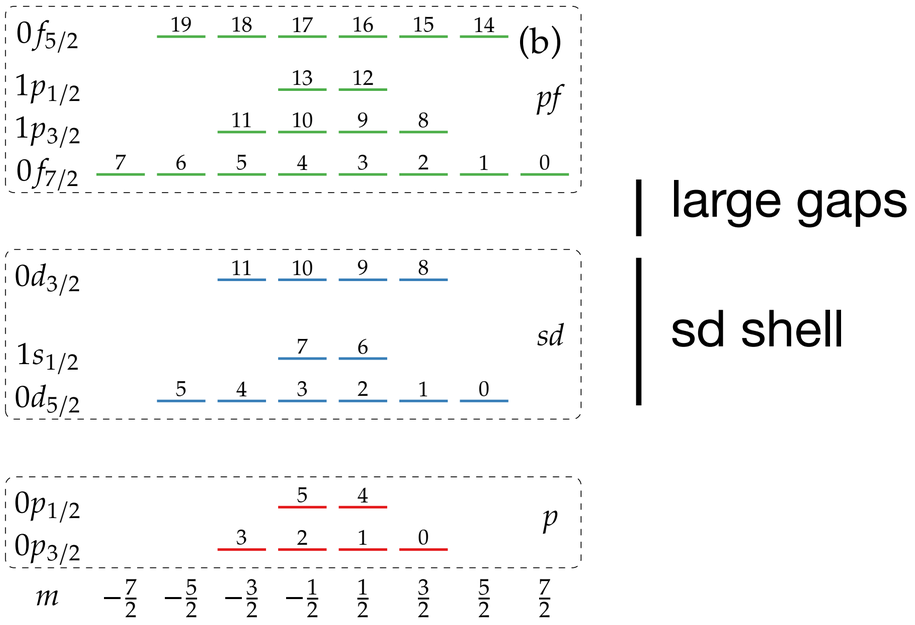

adapt-VQE for Nuclear shell model

1. As an initial we chose lowest energy basis state

$|\Psi_0\rangle = \prod_i a_i^\dagger |\text{vac}\rangle$, e.g. $|\psi_0\rangle = a_0^\dagger a_3^\dagger |0\rangle$

2. Pool of operators for the ansatz

$A_k = i(a_p^\dagger a_q^\dagger a_r a_s - a_r^\dagger a_s^\dagger a_p a_q)$

➡ Ansatz built adaptively: largest $\left.\frac{\partial E^{(n)}}{\partial \theta_k}\right|_{\theta_k=0}$

Grimsley et al., *Nat. comm.* **10**, 1–9 (2019)

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$$E = \min_{\theta_k} \langle \Psi(\theta_k) | H | \Psi(\theta_k) \rangle$$

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Sci Rep 13, 12291 (2023)

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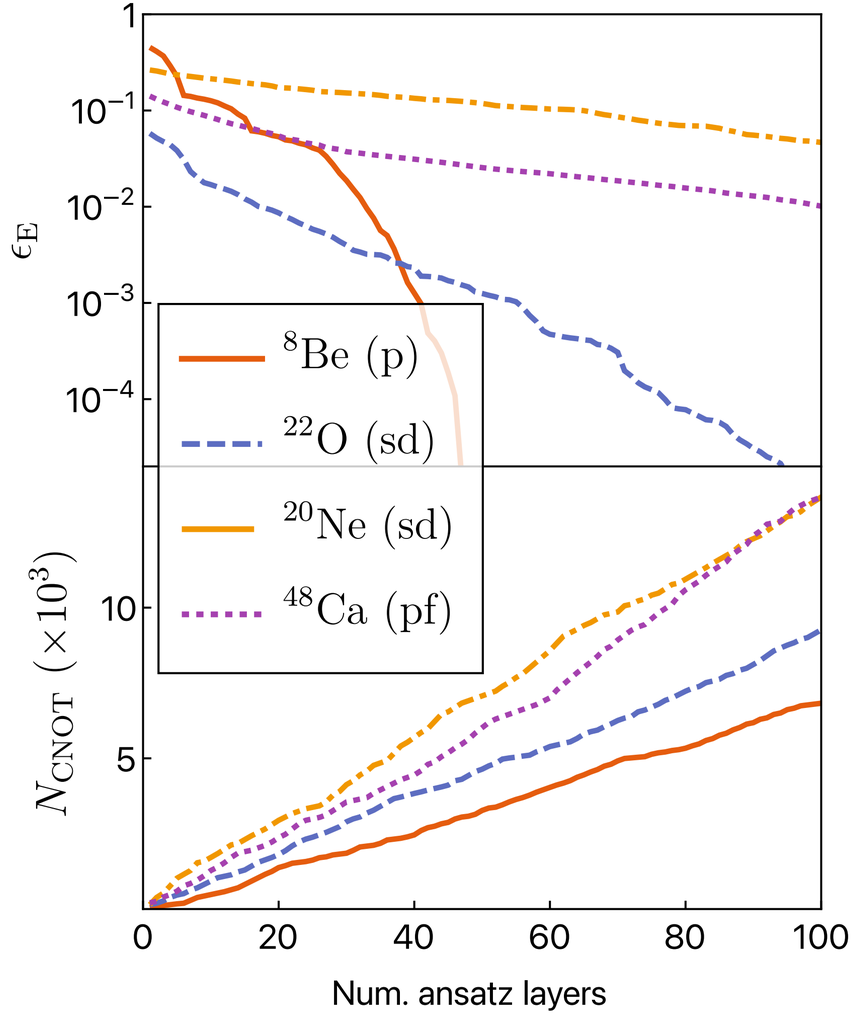
➡ Ansatz built adaptively: largest $\left.\frac{\partial E^{(n)}}{\partial \theta_k}\right|_{\theta_k=0}$

Grimsley et al., *Nat. comm.* **10**, 1–9 (2019)

$$|\psi(\vec{\theta})\rangle = \prod_{k=1}^{n} e^{i\theta_k A_k} |\psi_0\rangle$$

$$E = \min_{\theta_k} \langle \Psi(\theta_k) | H | \Psi(\theta_k) \rangle$$

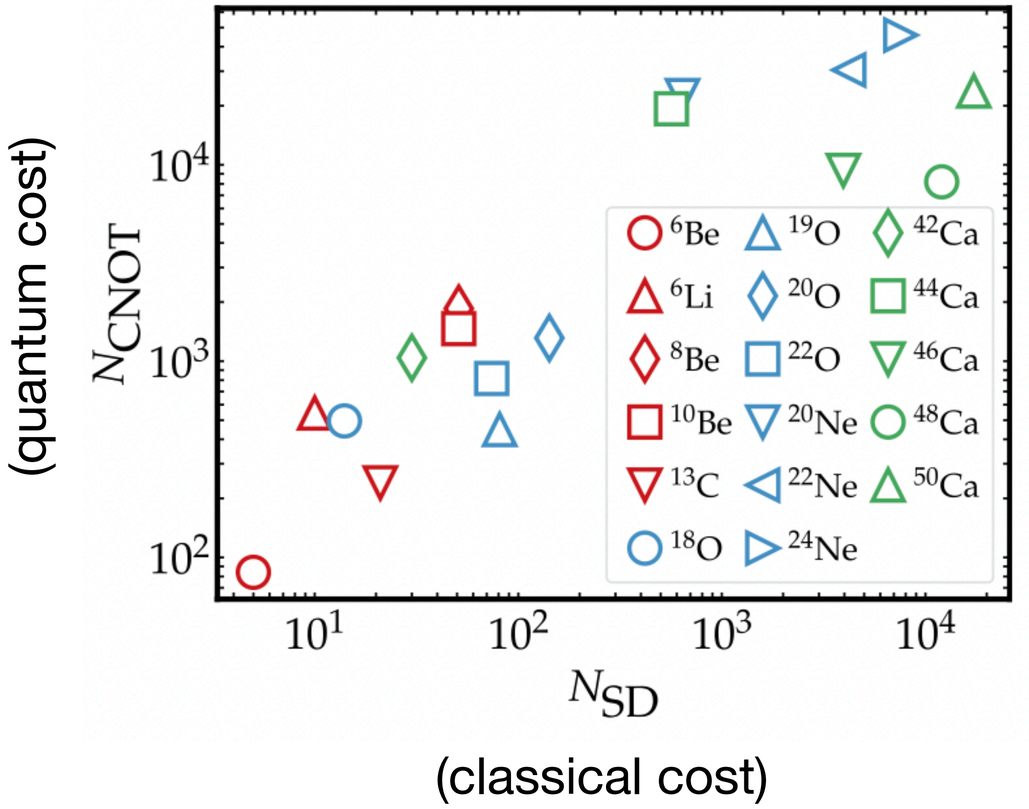


adapt-VQE for Nuclear shell model

num. parameters for each nuclei

shell	N_q	N_{SD}	nucleus	N_{layers}	ϵ_r bound
p	6	5	^{6}Be	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}
		74	^{19}O	32	10^{-6}
		81	^{20}O	70	10^{-6}
		142	^{22}O	119	10^{-6}
	24	640	^{20}Ne	167	2×10^{-2}
		4206	^{22}Ne	236	2×10^{-2}
		7562	^{24}Ne	345	2×10^{-2}
pf	20	30	^{42}Ca	9	10^{-8}
		565	^{44}Ca	132	10^{-2}
		3952	^{46}Ca	124	10^{-2}
		12022	^{48}Ca	101	10^{-2}
		17276	^{50}Ca	221	10^{-2}

scaling QC vs scaling ED



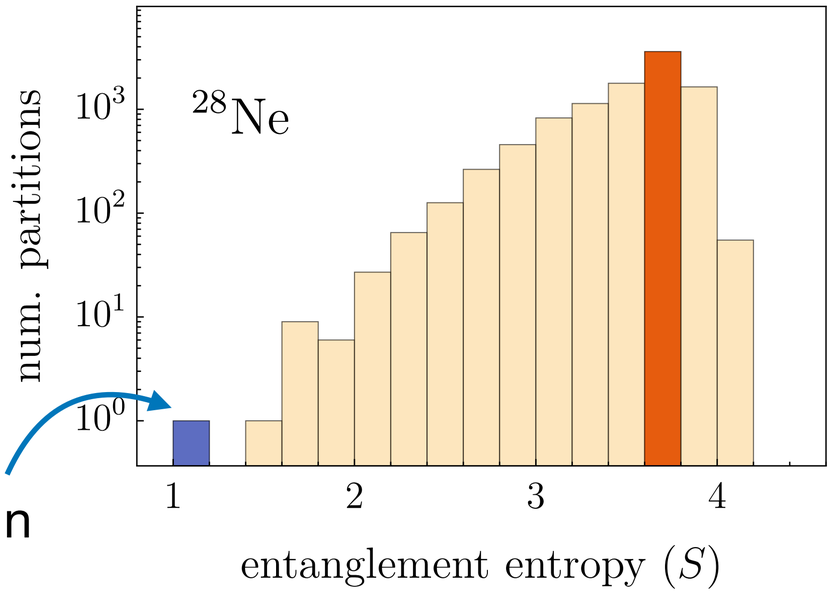
Nuclear entanglement & QC

Von Neumann entropy

$$S = -\sum_i \rho_i \log \rho_i$$

We find very low entanglement between proton and neutron orbitals, e.g.

Eur. Phys. J. A 59, 240 (2023)



p vs n

Nuclear entanglement & QC

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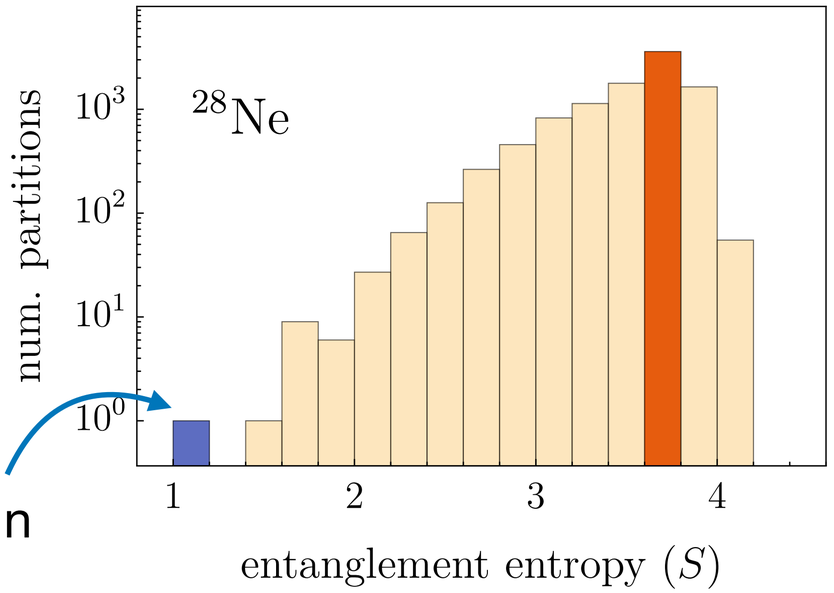
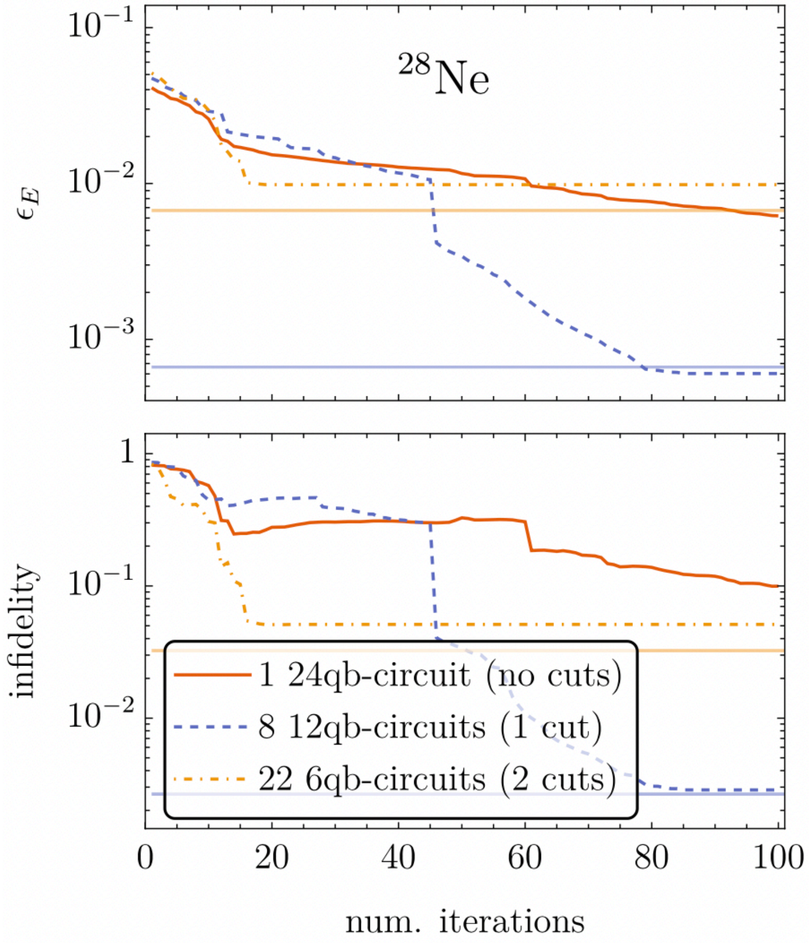


p vs n

$$|\psi\rangle = \sum_j c_j |\phi_j^{(p)}\rangle \otimes |\phi_j^{(n)}\rangle$$



Summary

1. Devised and simulated quantum **algorithms for nuclei and graphene**

—> Jordan Wigner mapping: one orbital per qubit

1. **Adiabatic evolution for graphene**

   Polynomial scaling of periods and time steps, efficient measurement

   Shortcuts to adiabaticity improve the efficiency but depending on time period

2. **Adaptive variational for nuclei**:

   Errors decrease exponentially fast with num. parameters

   No barren plateaus found

   Exponential speed up vs classical computers not clear when going to heavy nuclei