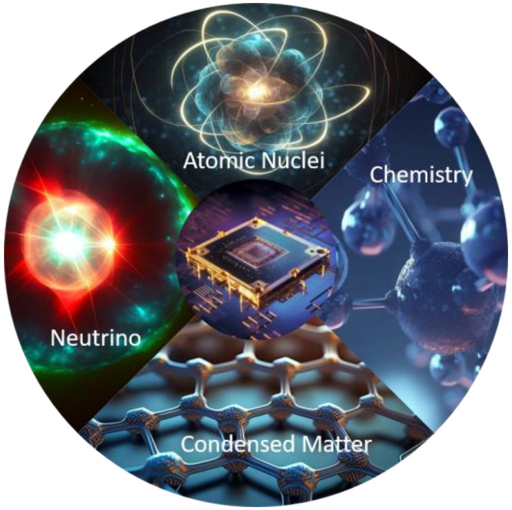
IJCLab Irène Joliot-Curie
Laboratoire de Physique des 2 Infinis

Some recent progress in the description of atomic nuclei using quantum computers

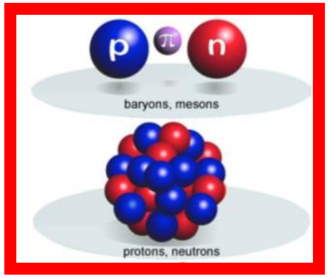
Denis Lacroix

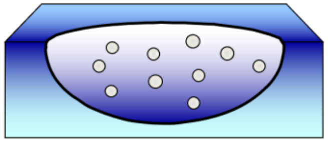


FRANCE HYBRID HPCQUANTUM INITIATIVE

Many-body physics and QC - T. Ayral, P. Besserve, D. Lacroix, and E.A. Ruiz Guzman ,
Quantum computing with and for many-body physics, Eur. Phys. J. A 59 (2023)
Symmetry and QC – D. Lacroix, A. Ruiz Guzman and P. Siwach,
Symmetry breaking/symmetry preserving circuits and symmetry restoration on quantum computers
Eur. Phys. J. A 59 (2023)
CERN Quantum Initiative – Di Meglio et al., Quantum Computing for High-Energy Physics: State of the Art and Challenges, PRX Quantum 5, 037001 (2024)

cnrs





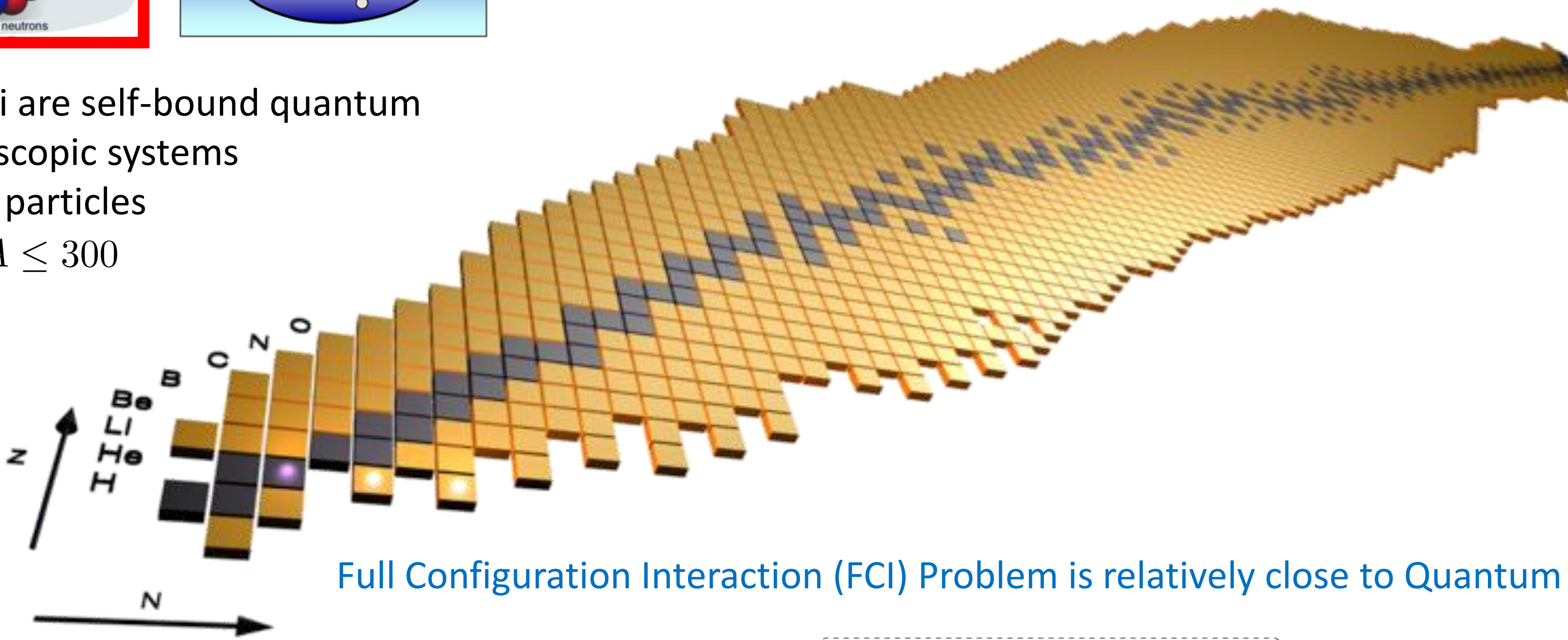
Quantum computing for atomic nuclei

Problematic and challenges

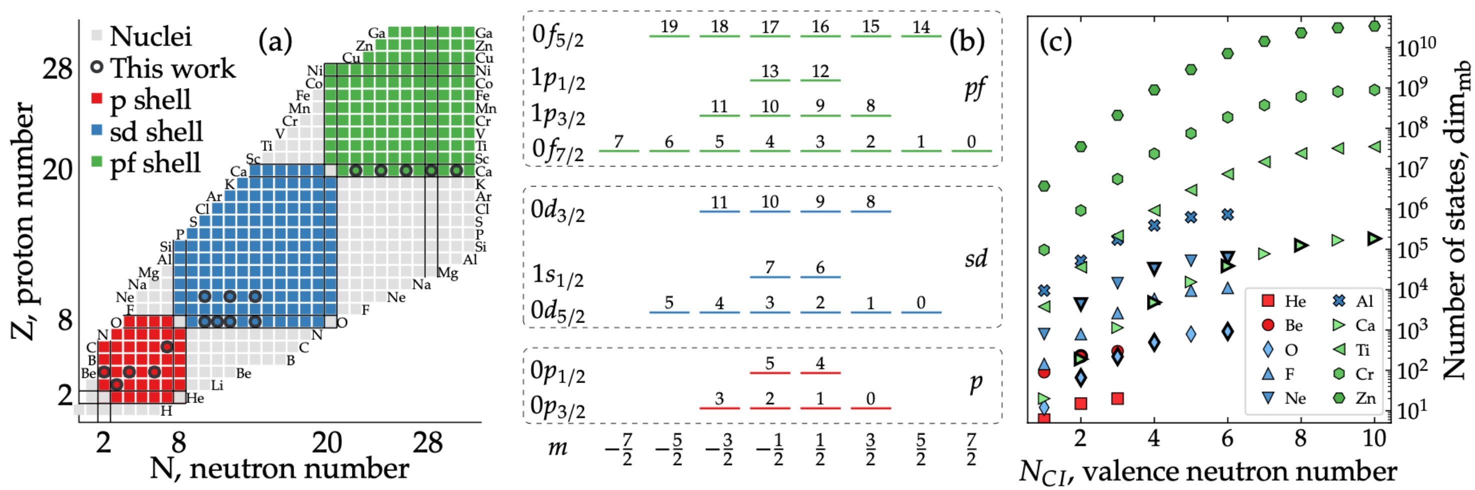
Nuclei are self-bound quantum mesoscopic systems

Nb of particles

$2 \leq A \leq 300$



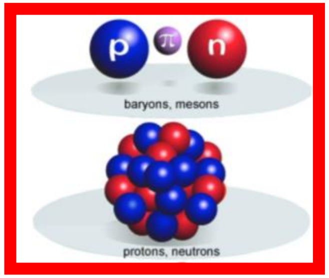
Full Configuration Interaction (FCI) Problem is relatively close to Quantum chemistry

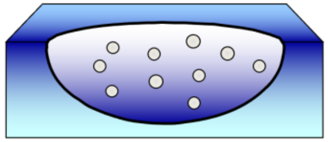


Perez-Obiol et al, Scientific Reports 13 (2023)

Quantum computing for atomic nuclei

Problematic and challenges





Nuclei are self-bound quantum mesoscopic systems
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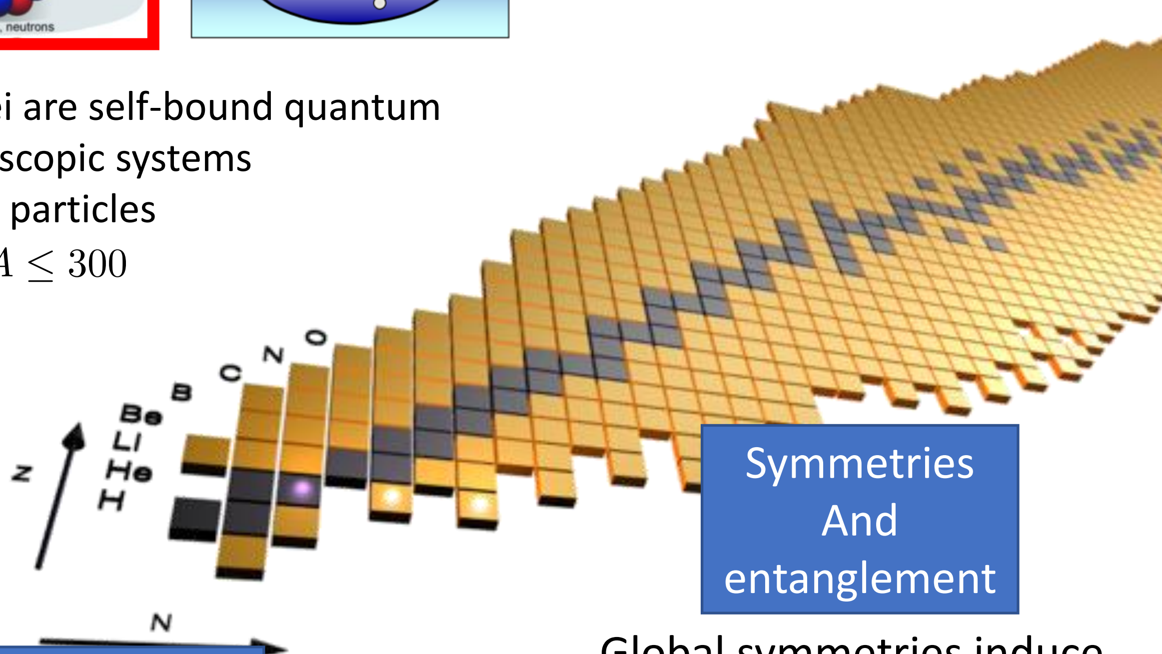
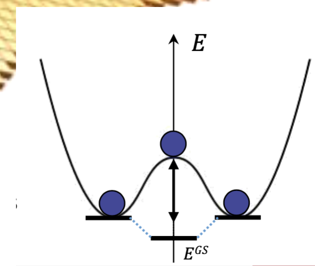
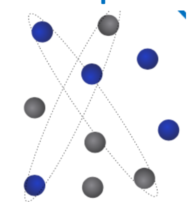




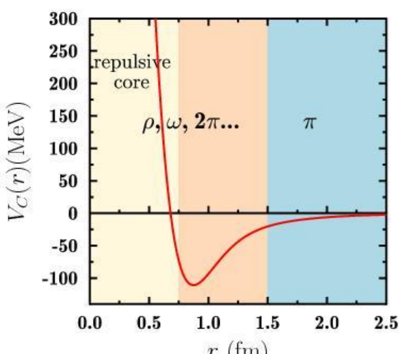
Spontaneous Broken symmetries (SB)

Small superfluid



(particle number SB)

Interaction

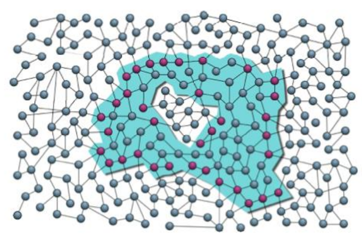


The problem is highly non-perturbative

Symmetries And entanglement

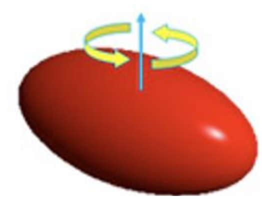
Global symmetries induce All-to-all entanglement

$S,\ T,\ J,\ \pi$



Nuclei are subject to entanglement volume law

Deformation can happen



(rotational invariance SB)

...

Developing variational approaches based on symmetry-breaking (SB)/symmetry restoration (SR)

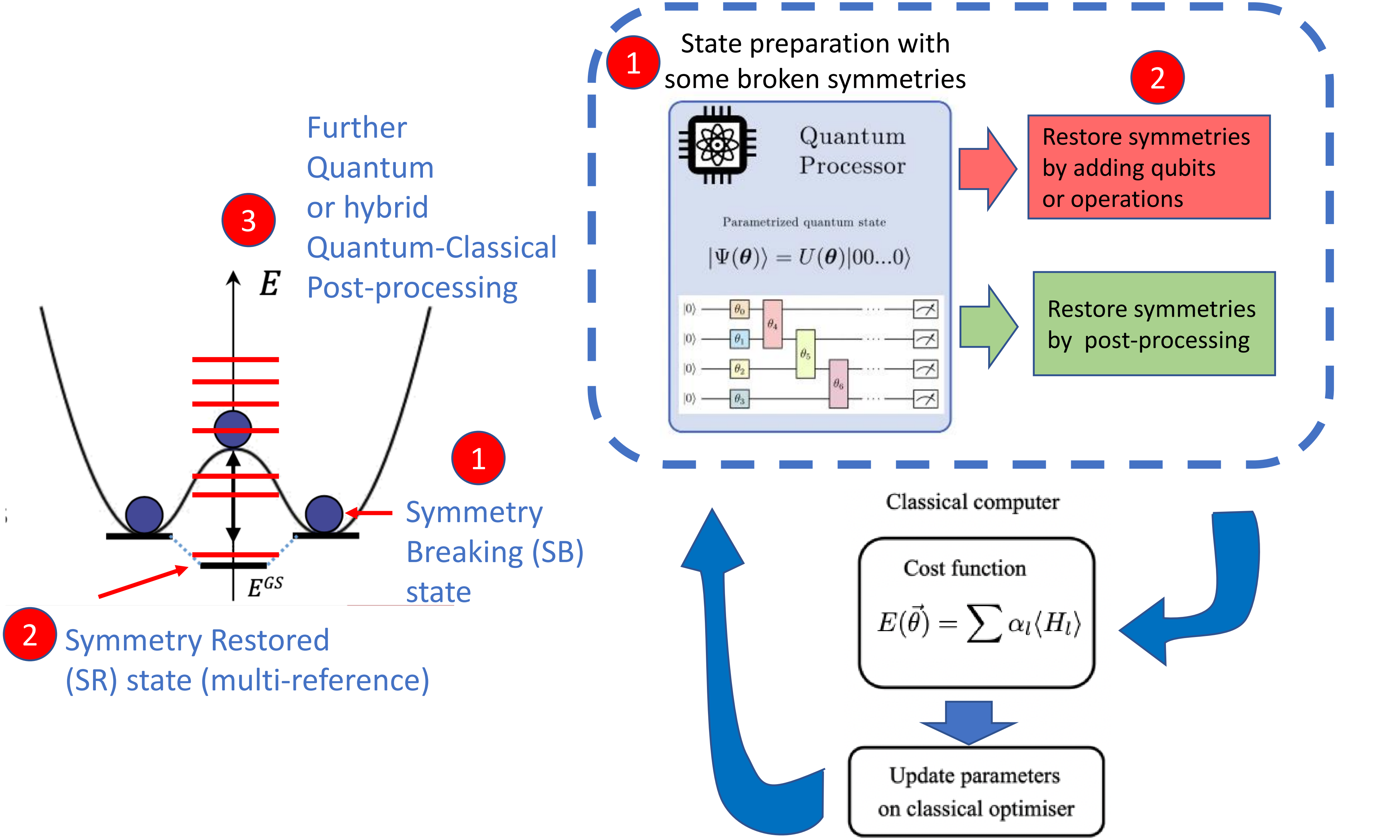


Illustration with small superconductors

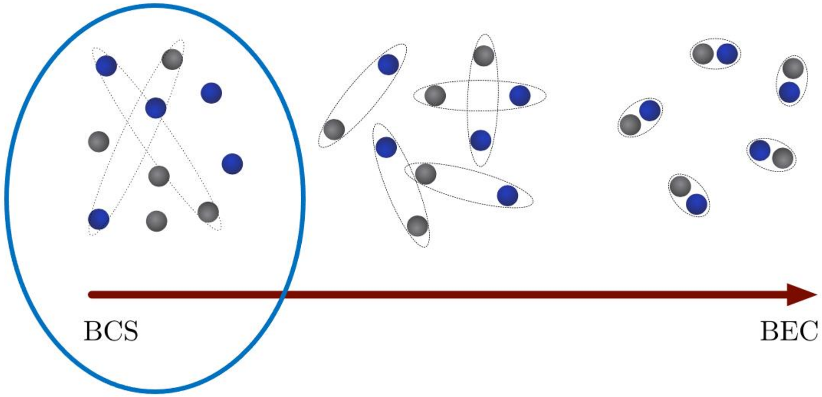
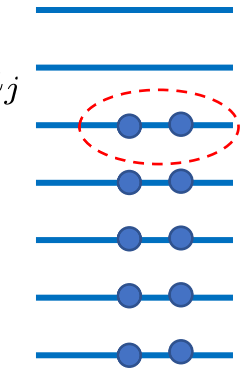
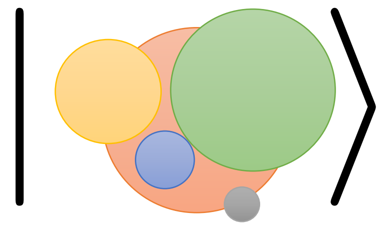


Illustration with the Richardson Hamiltonian

$$H_{\rm P} = \sum_{i>0} \varepsilon_i (a_i^\dagger a_i + a_{\bar{i}}^\dagger a_{\bar{i}}) - g \sum_{i,j>0} a_i^\dagger a_{\bar{i}}^\dagger a_{\bar{j}} a_j$$

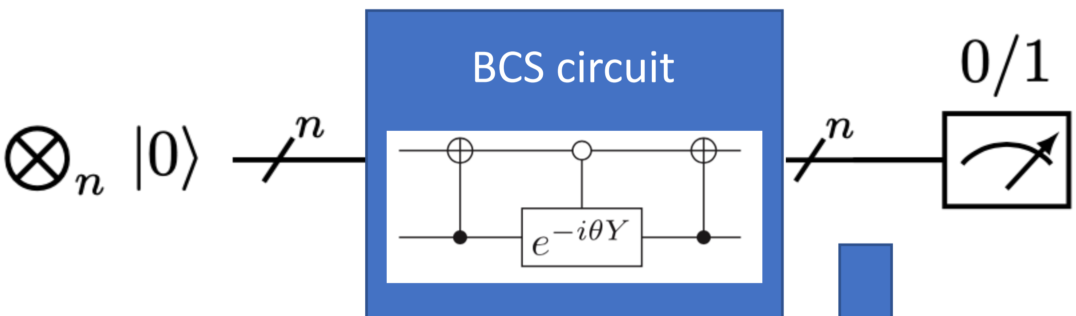


BCS state $|\Phi_0\rangle = \Pi_i (u_i + v_i a_i^\dagger a_{\bar{i}}^\dagger)|-\rangle$



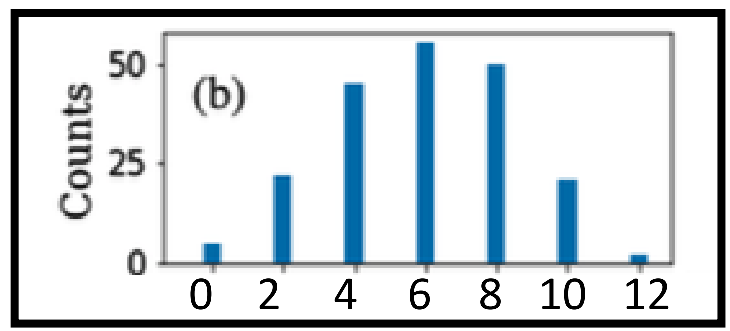
→ Mixes states with 0, 2, 4, … particles

BCS state in a circuit



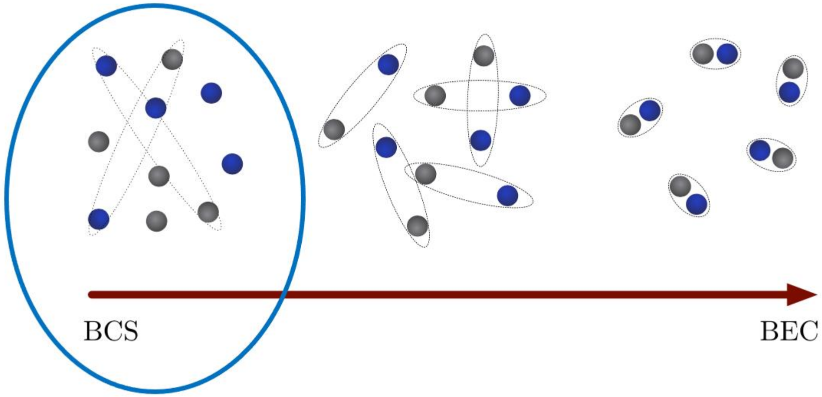
$$|\Psi_0\rangle = \bigotimes_i (\cos(\theta)|00\rangle + \sin(\theta)|11\rangle)_{i\bar{i}}$$

Example of mixing for 12 qubits (with IBM qiskit)



But ultimately symmetries should be restored!

Illustration with small superconductors



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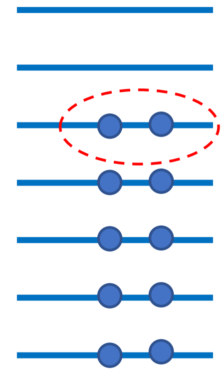
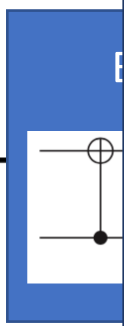


BCS state $|\Phi_0\rangle = \Pi$

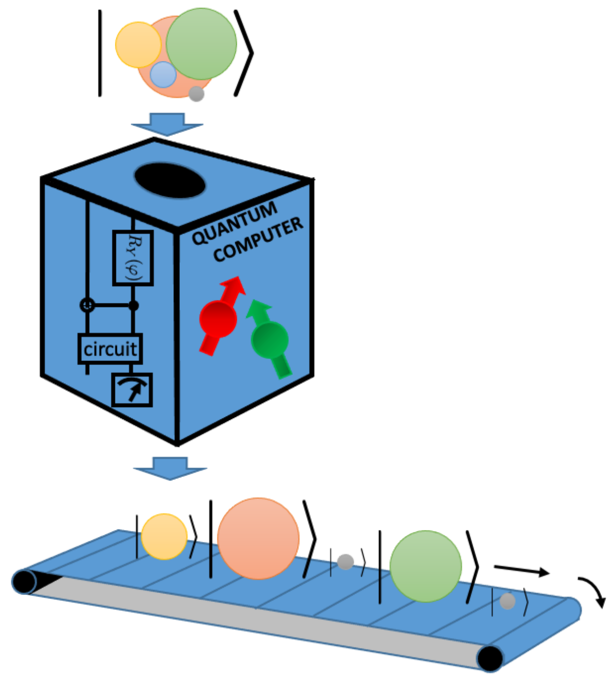
Mixes states with

BCS state in a circuit

$\bigotimes_n |0\rangle$ n

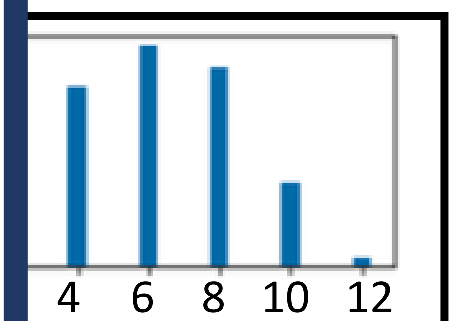


Symmetry restoration factory on QC



D. Lacroix, PRL 125, 230502 (2020)

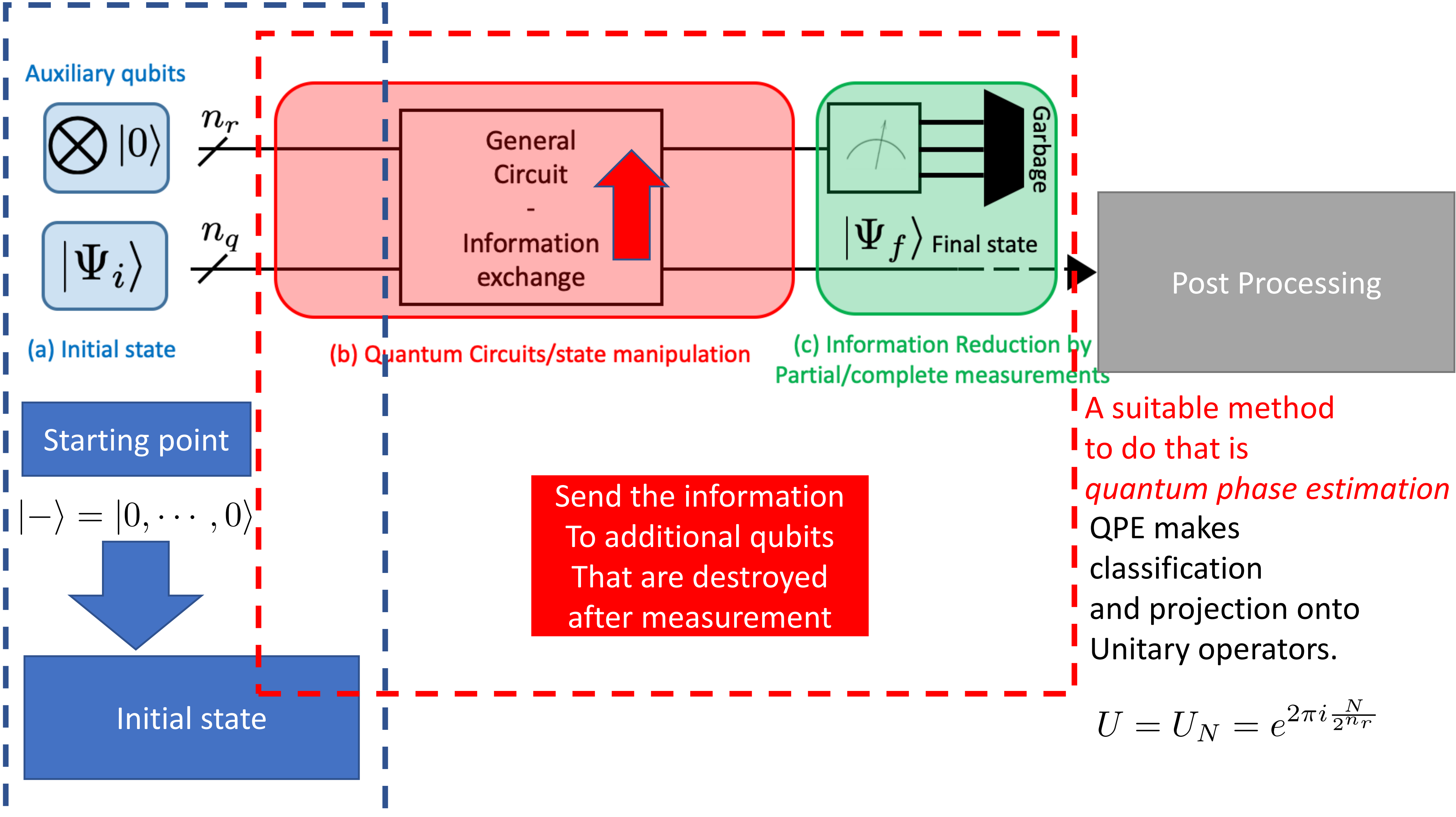
r 12 qubits (with IBM qiskit)



i

But ultimately symmetries should be restored!

Non-destructive counting on a quantum computer



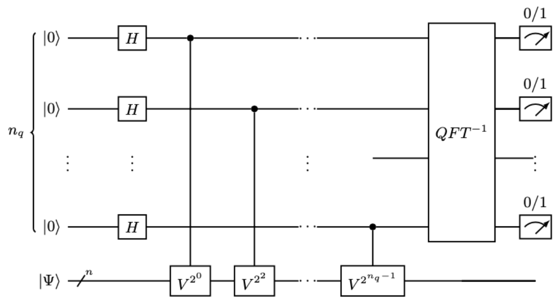
A suitable method to do that is *quantum phase estimation*

QPE makes classification and projection onto Unitary operators.

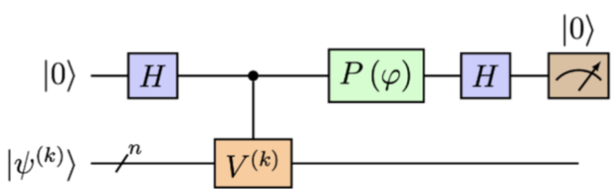
$$U = U_N = e^{2\pi i \frac{N}{2^{n_r}}}$$

D. Lacroix, *"Symmetry-Assisted Preparation of Entangled Many-Body States on a Quantum Computer"*, PRL 125, 230502 (2020).

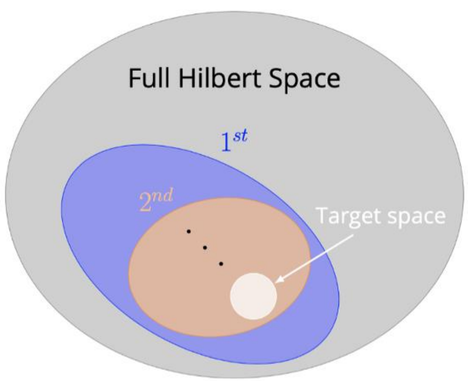
Standard Quantum Phase estimation



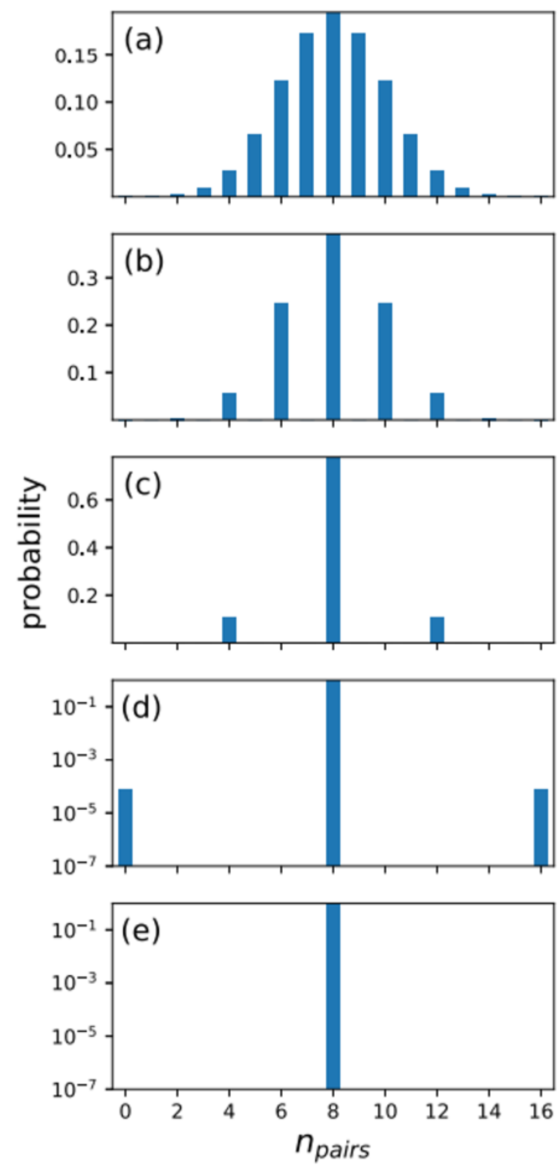
Iterative Quantum Phase estimation



$$\hat{V}^{(k)} = e^{i\phi_k \hat{N}} \qquad \phi_k = \frac{\pi}{2^k}$$

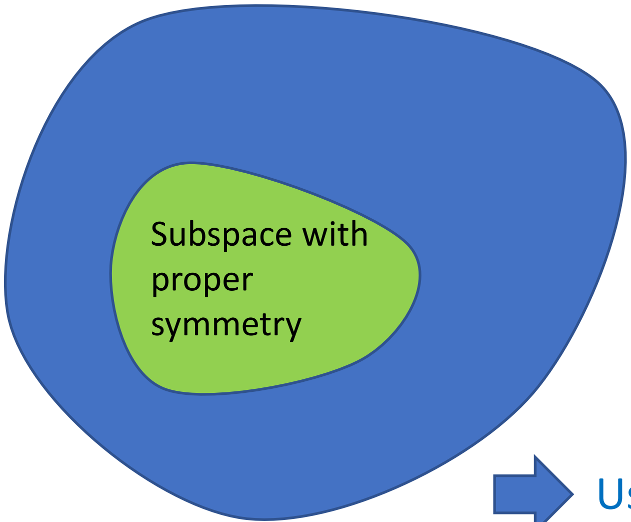


16 qubits, N = 8



Exploration of different methods for the symmetry restoration

Complete Hilbert space



Systematic Exploration of Phase-Estimation based methods for symmetry restoration (Kitaev method, Rodeo algorithms)

Eur. Phys. J. A (2023) 59:3
https://doi.org/10.1140/epja/s10050-022-00911-7
THE EUROPEAN PHYSICAL JOURNAL A
Regular Article - Theoretical Physics

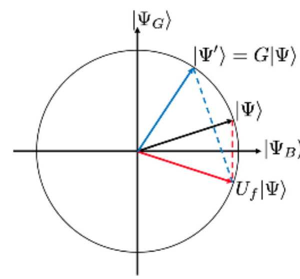
Symmetry breaking/symmetry preserving circuits and symmetry restoration on quantum computers

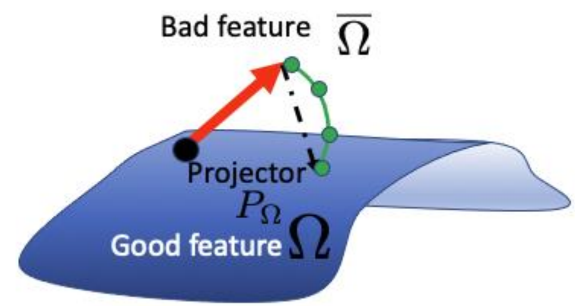
A quantum many-body perspective

Denis Lacroix[1,a], **Edgar Andres Ruiz Guzman**[1,b], **Pooja Siwach**[2,c]

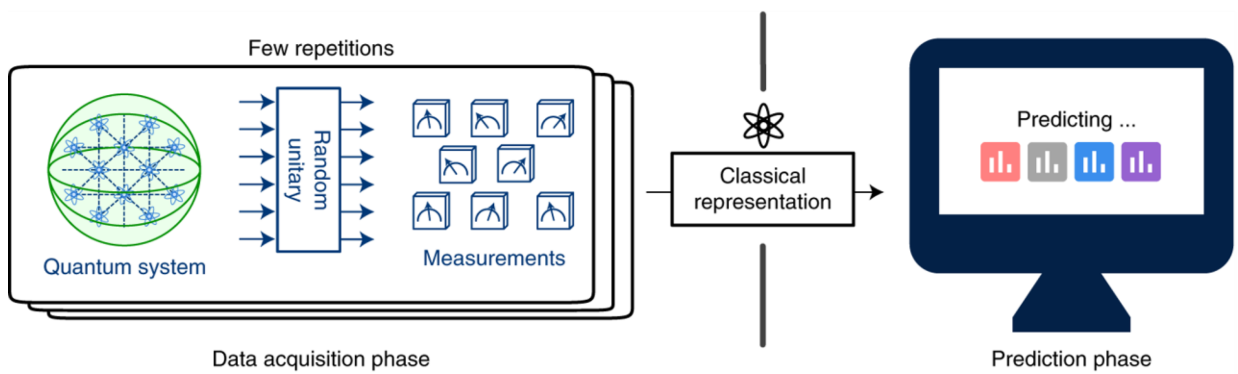
Use Oracle's and Grover-based methods for projection onto a subspace

Grover and Oracle





Use quantum tomography techniques (Classical Shadow method)



Restoring broken symmetries using quantum search "oracles"

Edgar Andres Ruiz Guzman and Denis Lacroix

Phys. Rev. C **107**, 034310 (2023) - Published 16 March 2023

H.-Y. Huang, R. Kueng and J. Preskill; Nat. Phys. 16, 1050 (2020)

E.A. Ruiz Guzman and DL, Eur. J. Phys. A 60 (2024)

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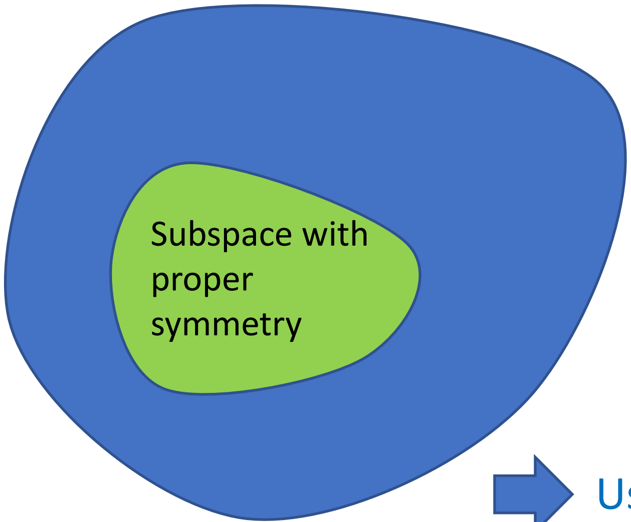

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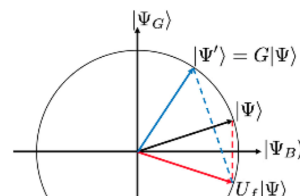

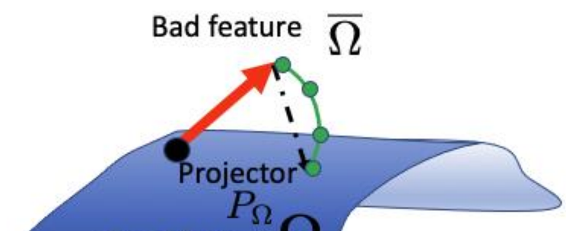

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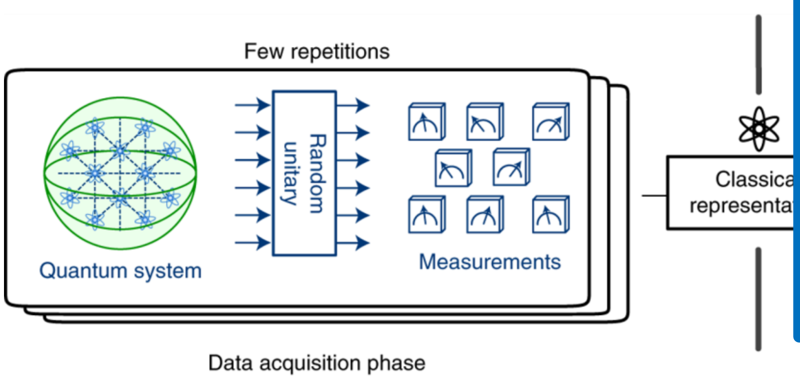
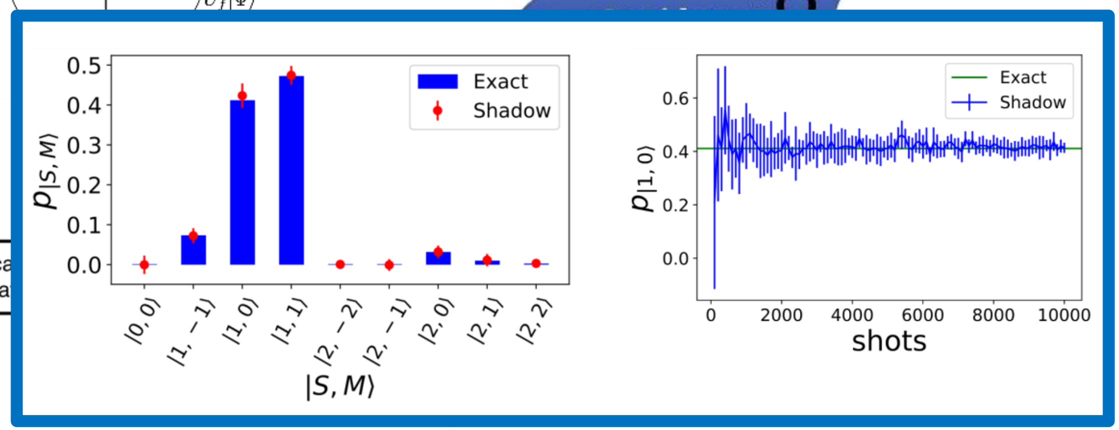




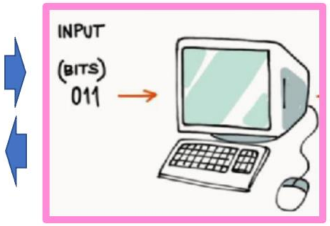
H.-Y. Huang, R. Kueng and J. Preskill; Nat. Phys. 16, 1050 (2020)

E.A. Ruiz Guzman and DL, Eur. J. Phys. A 60 (2024)

Coming back to our superconducting problem

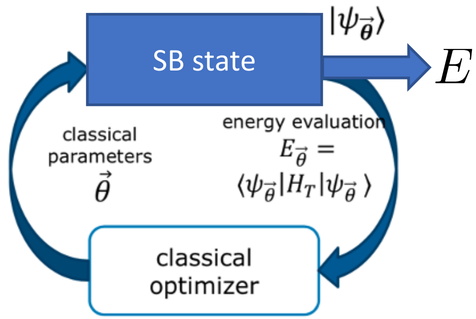
Combining projection with variational method

Classical optimization

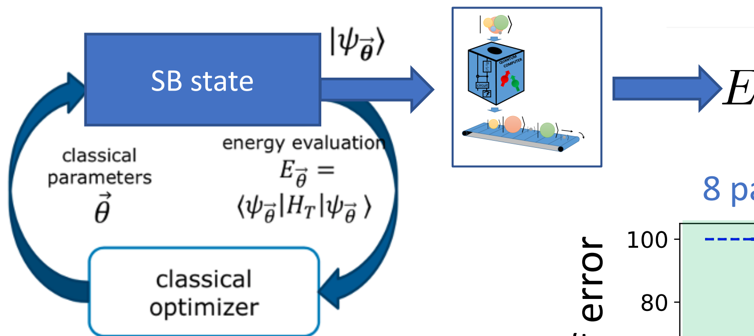


Quantum-Classical optimizers

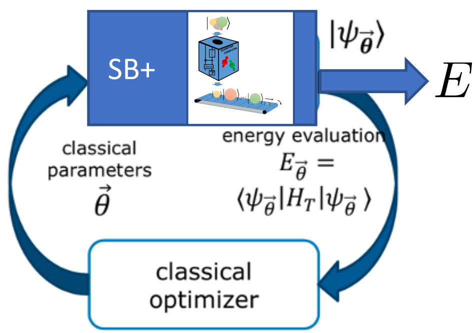
- Standard BCS theory

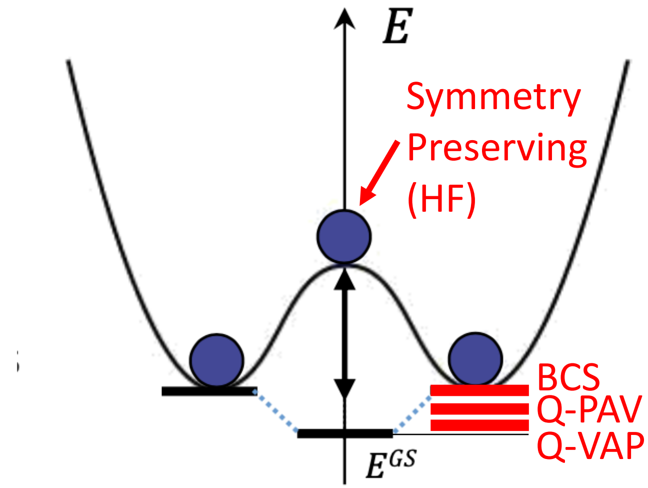


- Project after optimization
  Q-PAV: Quantum Projection After Variation

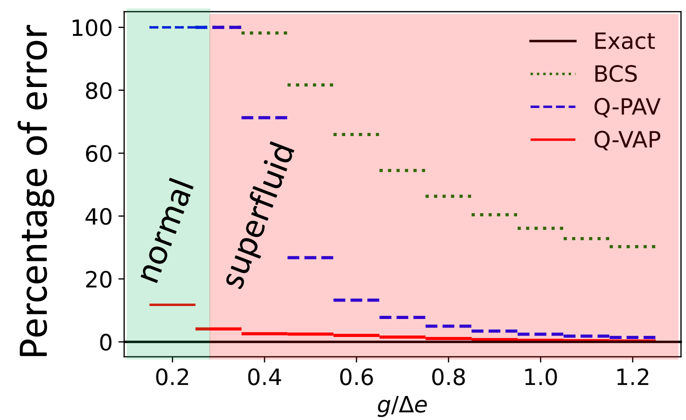


- The optimization is made on the Symmetry restored state.
  Q-VAP: Quantum Variation After Projection





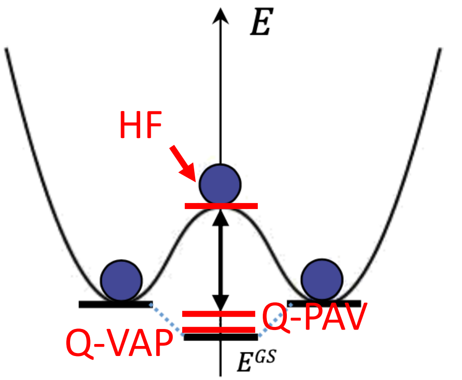
8 particles on 8 equidistant levels



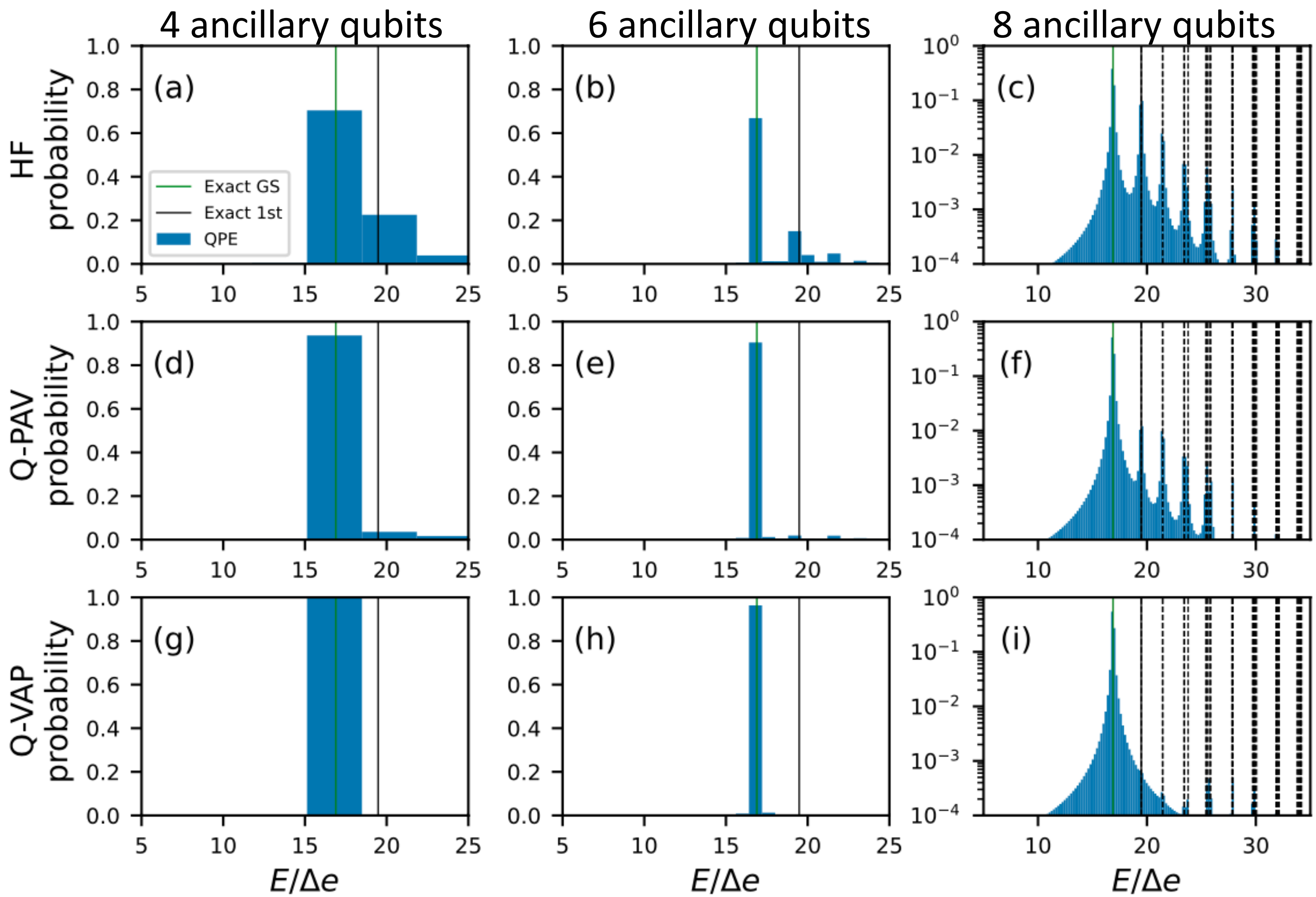
Ruiz Guzman and Lacroix, PRC 105 (2022)

Usefulness of the symmetry breaking strategy-symmetry restoration

To obtain expressive ansätze

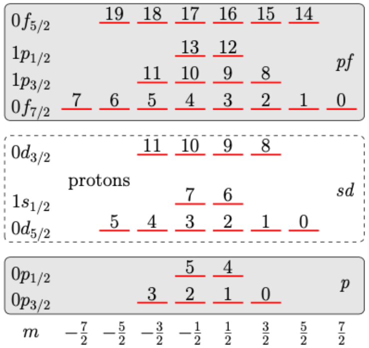


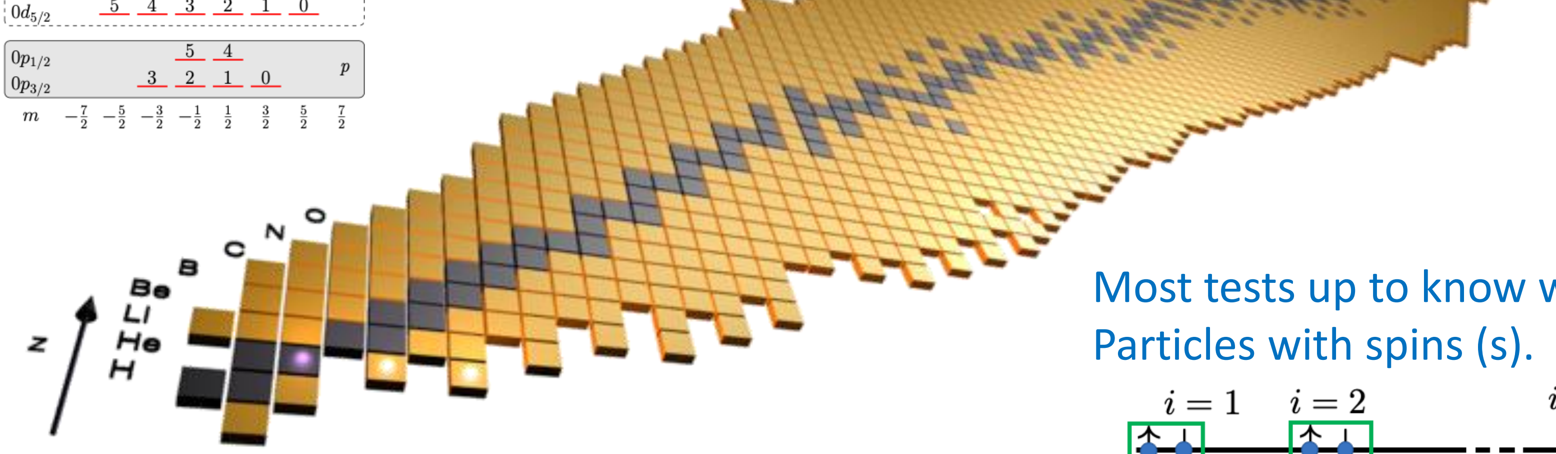
Quantum Phase estimate on energy after convergence



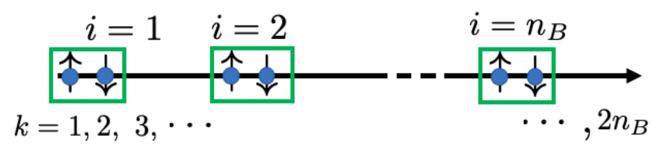
Getting closer to realistic problems

Is the breaking of symmetries always a good idea?

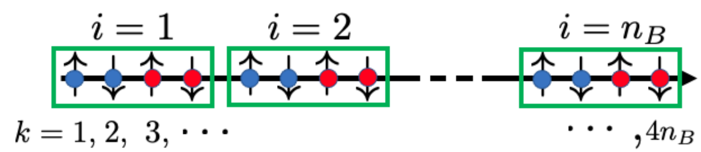




Most tests up to know were made on Particles with spins (s).



But nuclei have both spin (s) and isospin (t) (neutron/proton)



➡ This increases the number of qubits

$$S_z, \; S^2, \; \pi$$

➡ This increases the number of symmetries that could be broken

$$S_z, \; S^2, \; T_z, \; T^2, \; \pi$$

Symmetry-breaking states become extremely hard to control
Symmetry restoration becomes very demanding

J. Zhang, PhD thesis (2025).

Iterative construction of the ansatz

Grimsley, et al, Nat. Commun. 10 (2019)

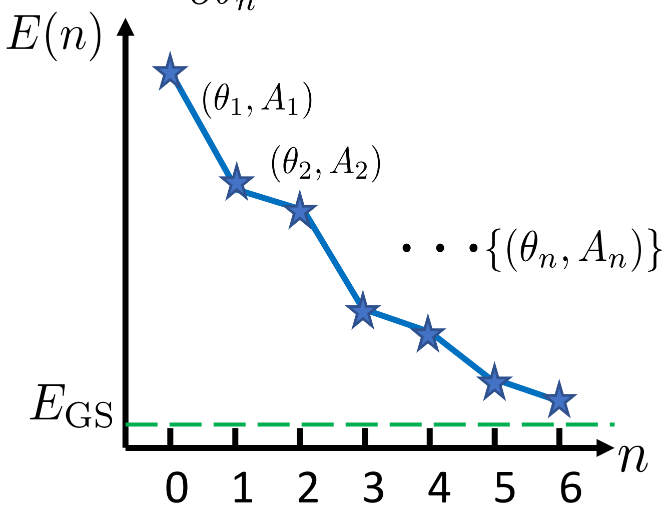
- Start from a state $|\Psi_0\rangle = |n=0\rangle$
- Built iteratively the ansatz such as:

$$|n\rangle = e^{i\theta_n A_n}|n-1\rangle = \prod_{k=1}^{n} e^{i\theta_k A_k}|0\rangle$$

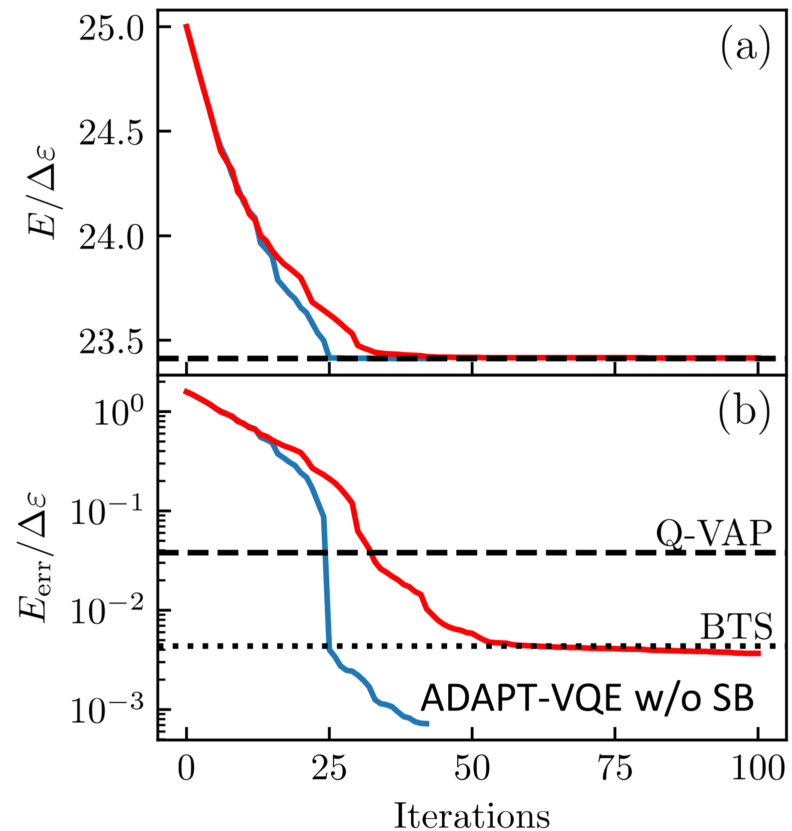
$$A_n \in \{O_1, \cdots, O_\Omega\}$$

Such that

$$\frac{\partial E(n)}{\partial \theta_n} = i\langle n|\,[H, A_n]\,|n\rangle \quad \text{is maximum}$$

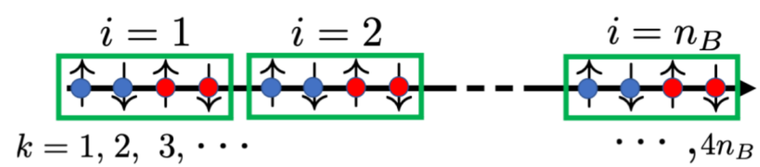


ADAPT-VQE applied to the Superfluid problems: only spins



Zhang, Lacroix,Beaujeault-Taudière, PRC 110, 064320 (2024)

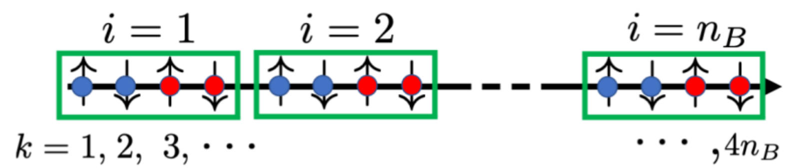
Extension to spin and isospin



Is breaking symmetries always a good idea?

Extension to the proton-neutron pairing Hamiltonian problem

$$
\begin{aligned}
H \;=\; & \sum_{i=1}^{n_B} \left[\varepsilon_{i,n}(\nu_i^\dagger \nu_i + \nu_{\bar{i}}^\dagger \nu_{\bar{i}}) + \varepsilon_{i,p}(\pi_i^\dagger \pi_i + \pi_{\bar{i}}^\dagger \pi_{\bar{i}})\right] \\
& - \sum_{T_z=-1,0,1} g_V(T_z)\mathcal{P}_{T_z}^\dagger \mathcal{P}_{T_z} \\
& - \sum_{S_z=-1,0,1} g_S(S_z)\mathcal{D}_{S_z}^\dagger \mathcal{D}_{S_z}.
\end{aligned}
$$



Different Hamiltonian limits

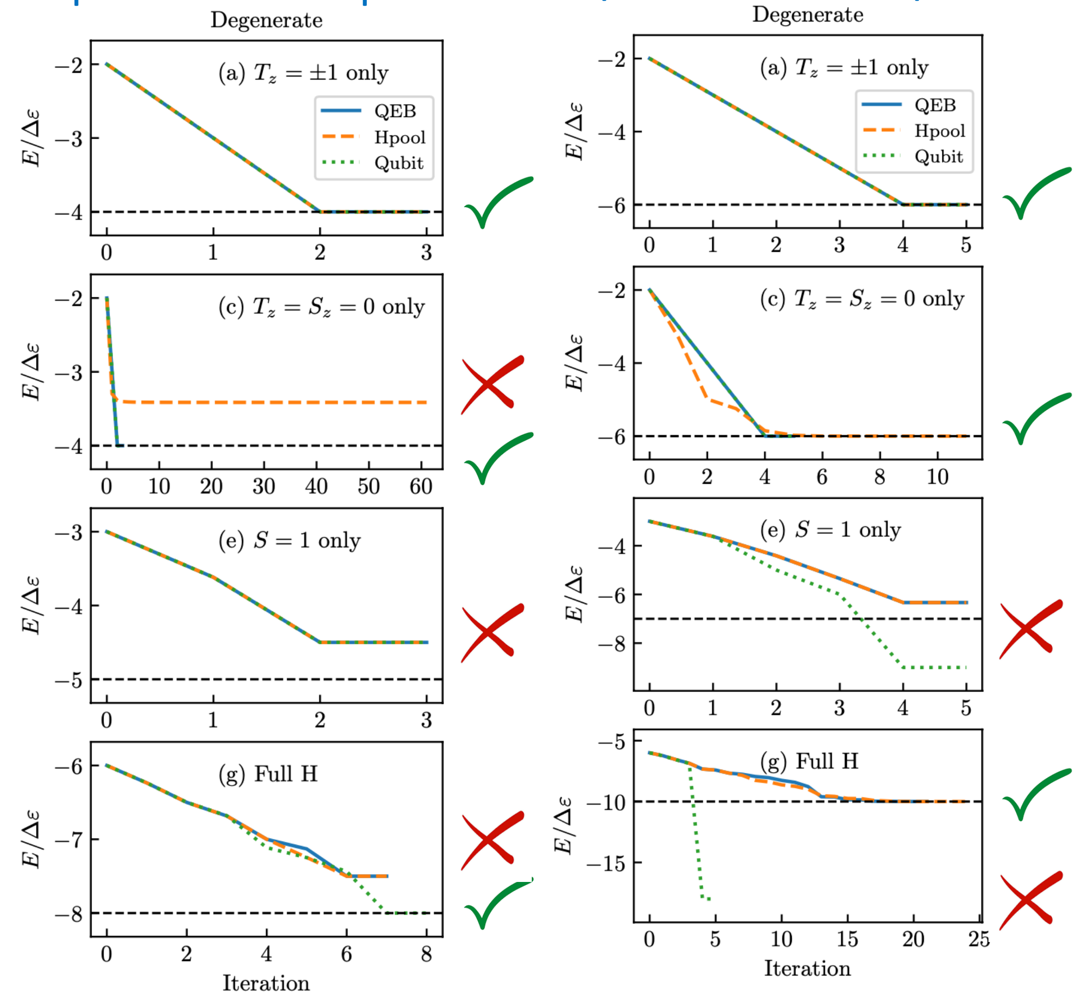
Case \ S_z/T_z	Isoscalar −1	Isoscalar 0	Isoscalar 1	Isovector −1	Isovector 0	Isovector 1
1				✓		✓
2		✓			✓	
3				✓	✓	✓
4	✓	✓	✓	✓	✓	✓

Different operator pool in ADAPT-VQE breaking or not symmetries

	Particle number	Seniority	Parity
H-pool	✓	✓	✓
QEB-pool	✓	×	✓
Qubit-pool	×	×	✓

4 particles on 8 qubits

4 particles on 12 qubits

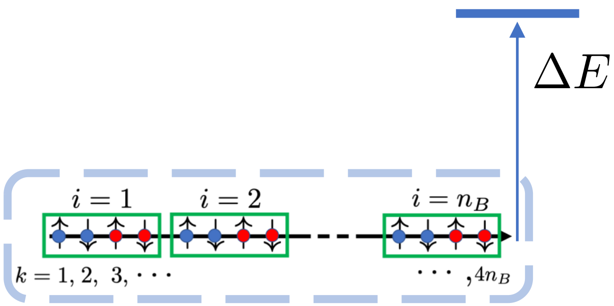


Zhang, Lacroix, Beaujeault-Taudière, PRC 110, 064320 (2024)

Specific methods to improving convergence

Going closer to nuclei: adding isospin

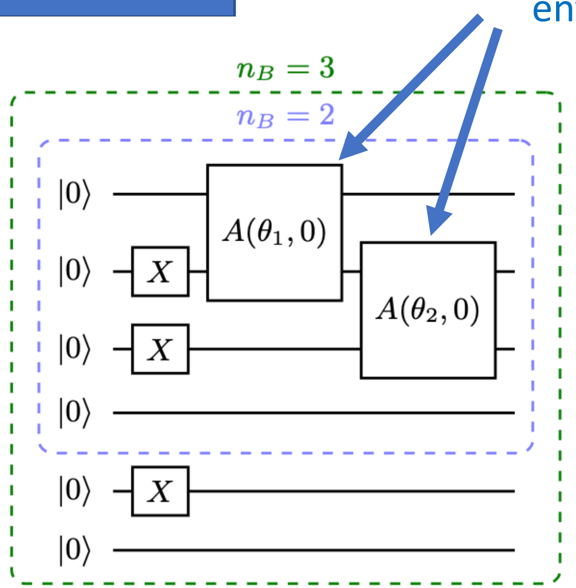
Embedding

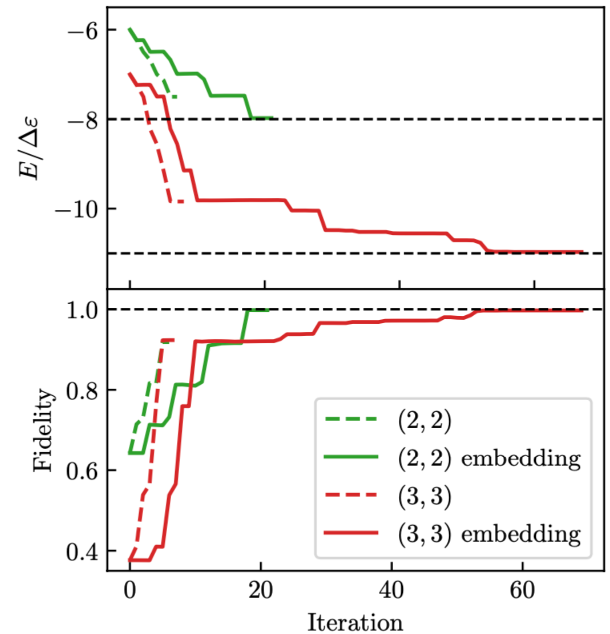


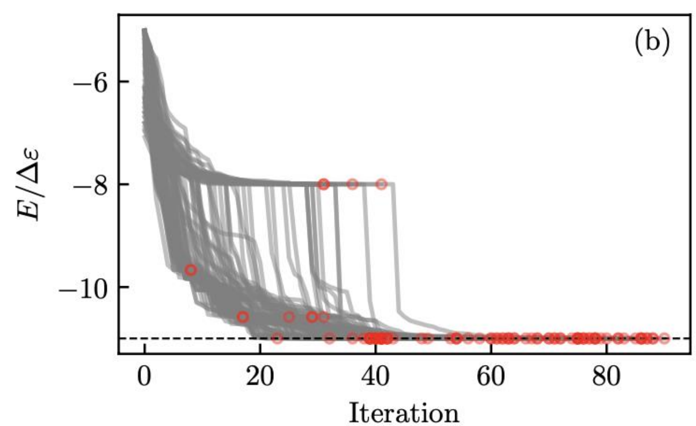
Fictitious
set of qubits

Initial condition Randomization

Initial random
entangler



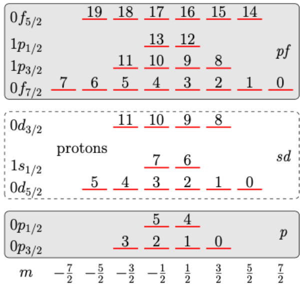




Zhang, Lacroix,Beaujeault-Taudière, PRC 110, 064320 (2024)

Spectral methods

Getting excited states

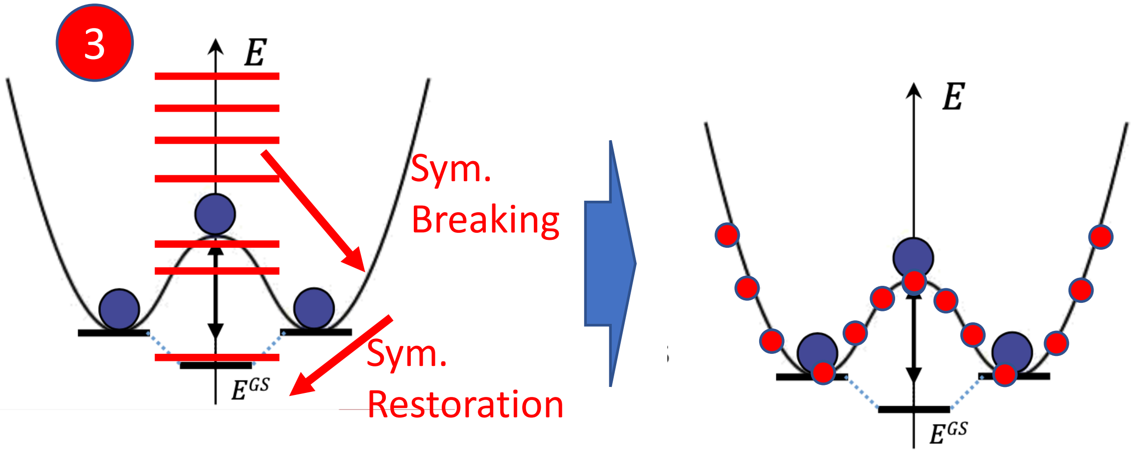


PHYSICAL REVIEW C **109**, 024327 (2024)

Solving the Lipkin model using quantum computers with two qubits only with a hybrid quantum-classical technique based on the generator coordinate method

Yann Beaujeault-Taudière
Université Paris-Saclay, CNRS/IN2P3, IJCLab, 91405 Orsay, France
and Laboratoire Leprince-Ringuet (LLR), École Polytechnique, CNRS/IN2P3, F-91128 Palaiseau, France

Denis Lacroix
Université Paris-Saclay, CNRS/IN2P3, IJCLab, 91405 Orsay, France

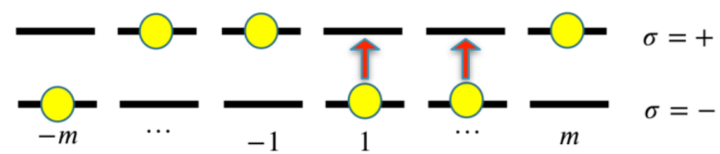


Quantum Generator Coordinate Method

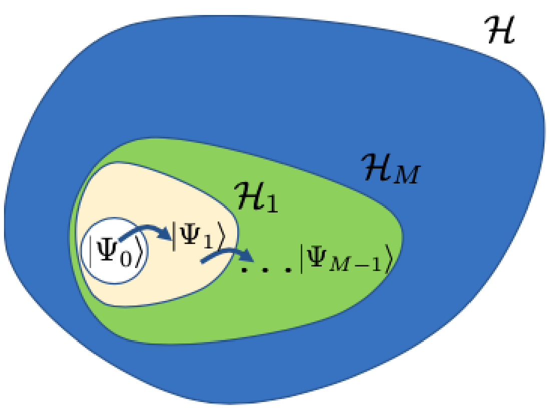
$$|\Psi\rangle = \int_{\mathbf{q}} f(\mathbf{q})|\Phi(\mathbf{q})\rangle d\mathbf{q}$$

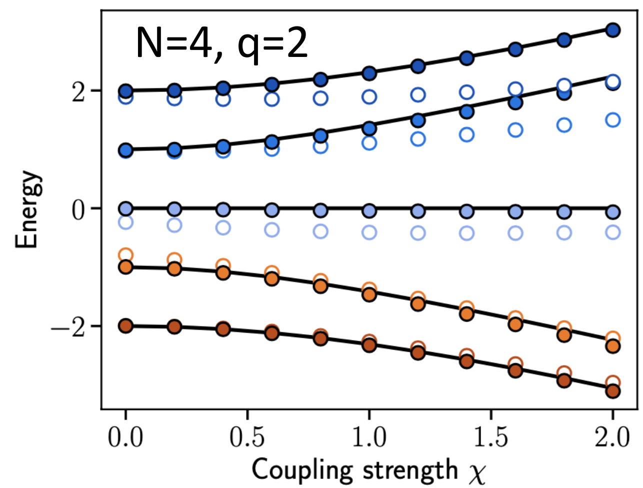
$$\int_{\mathbf{q}'} d\mathbf{q}' \left[\mathcal{H}(\mathbf{q},\mathbf{q}') - E\mathcal{N}(\mathbf{q},\mathbf{q}')\right] f(\mathbf{q}') = 0$$

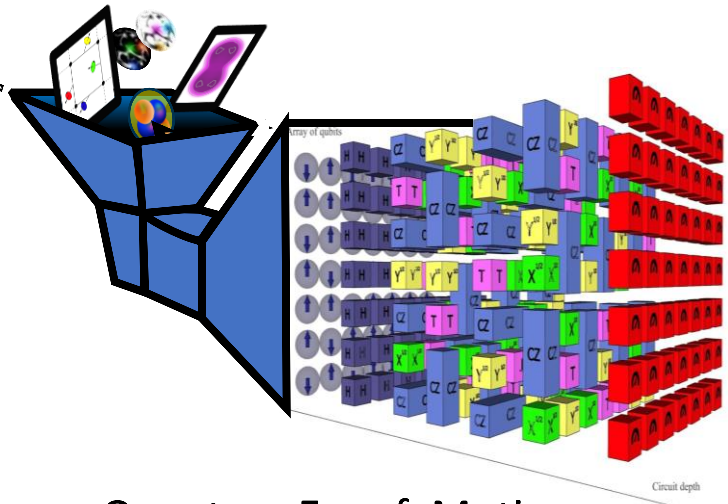
Application



Quantum Subspace expansion





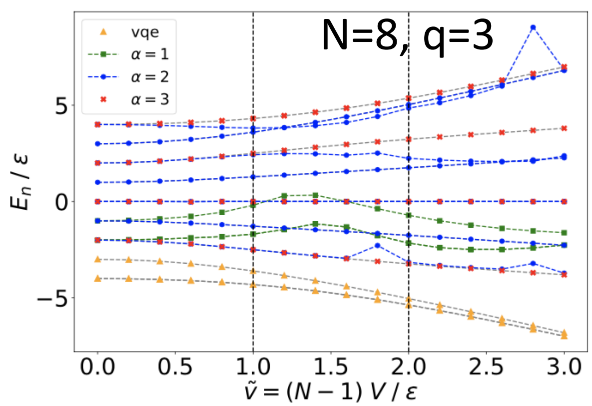


- We have explored many technique to enforce symmetries in many-body systems
- Our main focus was to have expressive variational ansätze for ground state preparation
- We are now developing algorithms also for excited states: ADAPT VQE, q-EOM, Green's function

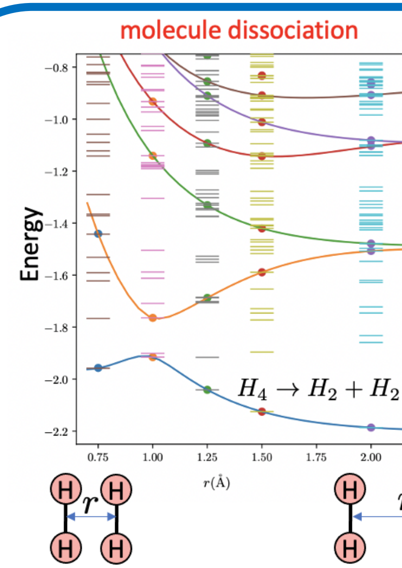
Quantum Eq. of Motion

ADAPT-VQE for excited states

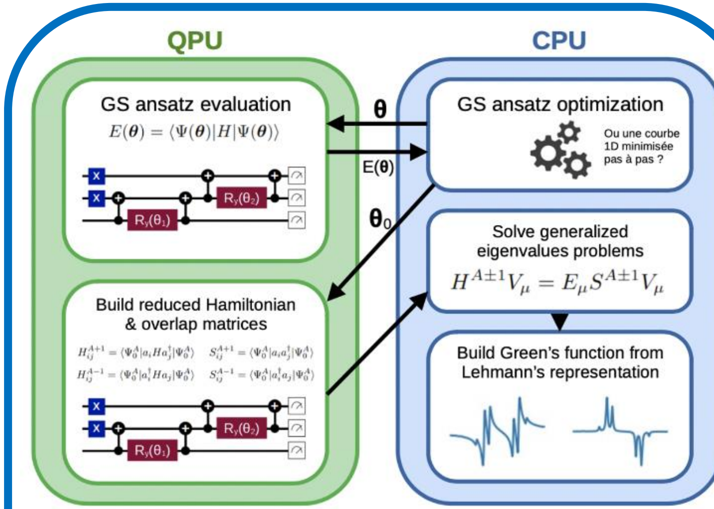
Green's function



Hlatshwayo et al, PRC 106 (2022), & PRC 109 (2024)



JZhang, et al, in preparation



Aychet-Claisse, et al, in preparation

Thanks to my Collaborators

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WESTERN MICHIGAN UNIVERSITY — Lawrence Livermore National Laboratory

E. A. Ruiz Guzman

J. Zhang

S. Aychet Claisse

Y. Beaujeault-Taudiere

M. O. Hlatshwayo

P. Siwach

EVIDEN an atos business — LPSC Grenoble Laboratoire de Physique Subatomique et de Cosmologie — WESTERN MICHIGAN UNIVERSITY — UNIVERSITÀ DI TRENTO

T. Ayral

P. Besserve

M. Mangin Brinet

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A. Roggero

Thank you!