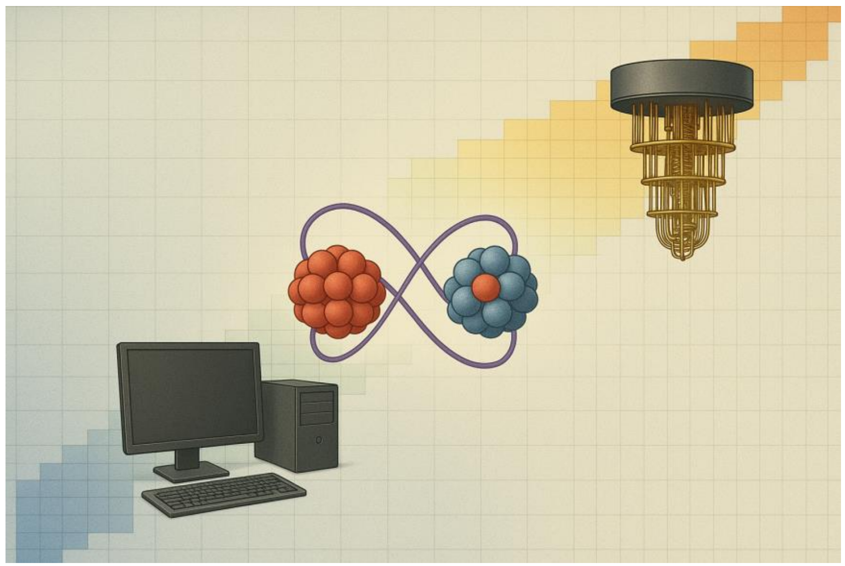
Using quantum computers for nuclear structure studies

Denis Lacroix

IJCLab Irène Joliot-Curie
Laboratoire de Physique des 2 Infinis



université PARIS-SACLAY

cnrs

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, EPJA 59 (2023)
Symmetry and QC – D. Lacroix, A. Ruiz Guzman and P. Siwach, Symmetry breaking/symmetry preserving circuits and symmetry restoration on quantum computers, EPJA 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)

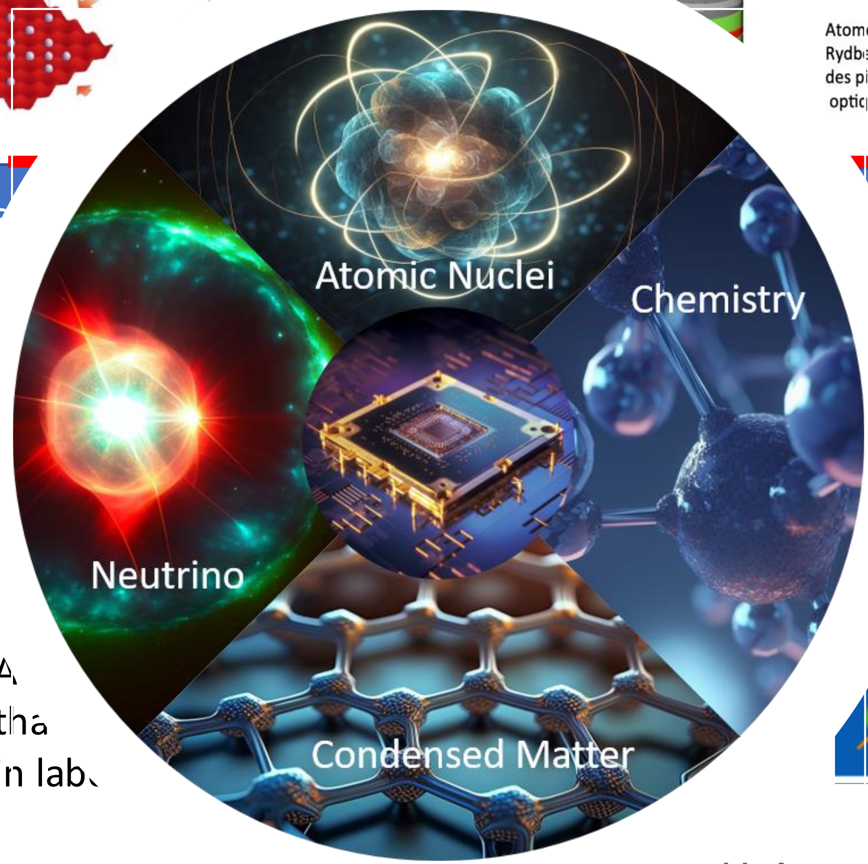
What means quantum devices today?

There are many types of quantum computers: ***analog versus digital quantum computers***

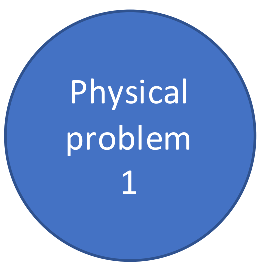
Quantum machines are often themselves many-body systems

Analog quantum s

quantum simulator

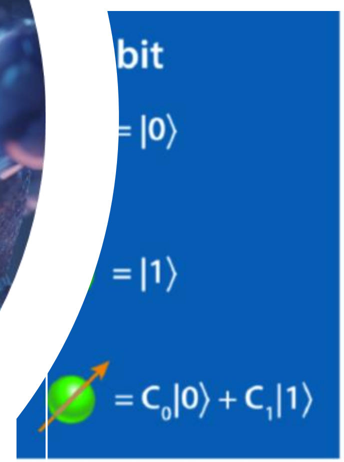


Analog System



Complex problem that cannot or hardly be simulated on classical computers

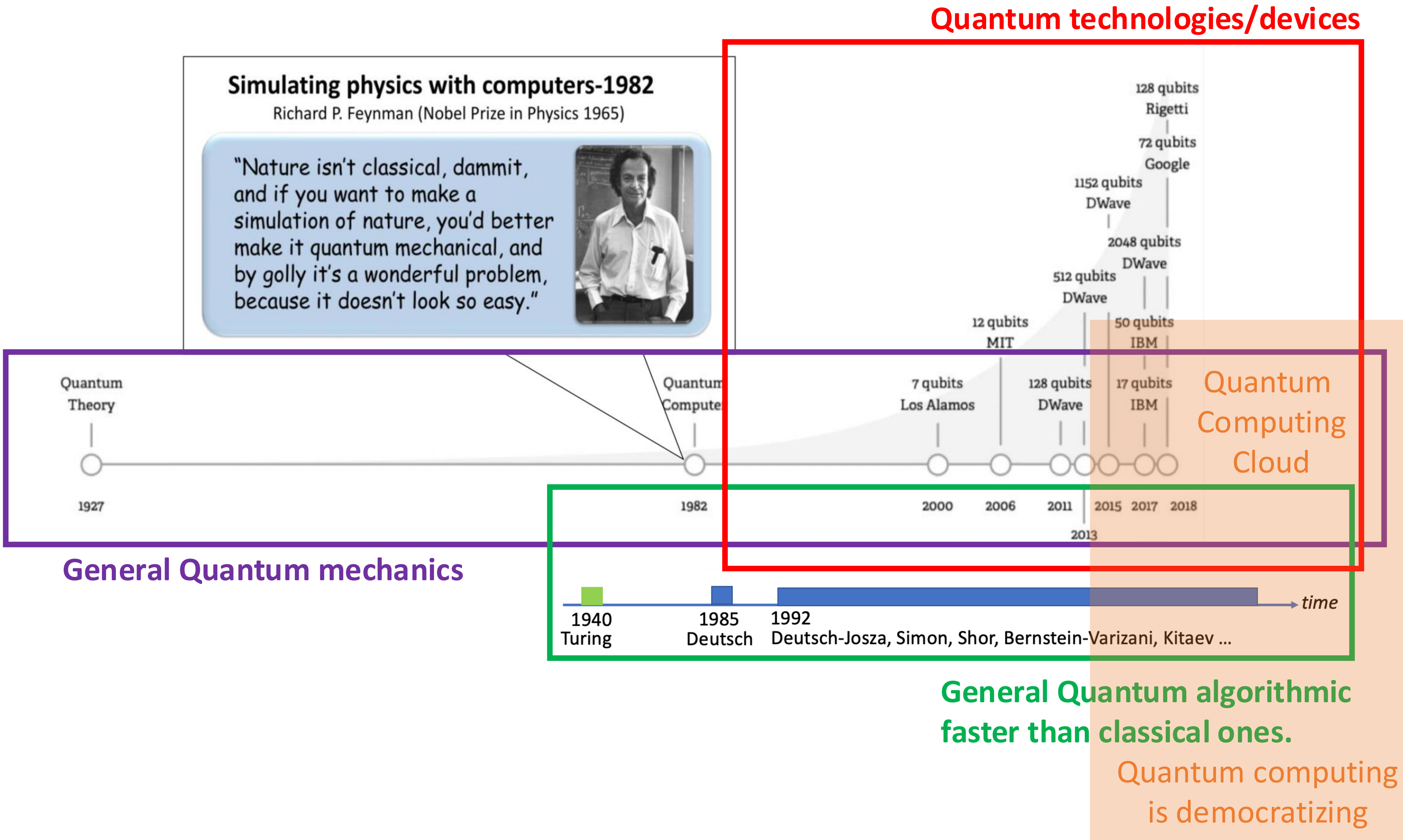
A
tha
in lab



Non-universal

Universal Quantum simulation

Why quantum computing is becoming mature now ?



What can be done on a *perfect* digital quantum computer?

We can essentially solve the Schroedinger equation

Practical solution on a classical computer

$$i\hbar\frac{d}{dt}|\Psi\rangle = H|\Psi\rangle \xrightarrow[\{|j\rangle\}_{j=0,\cdots}]{\text{In a basis}}$$

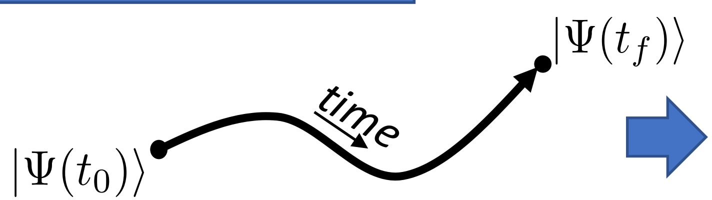
$$F_j(t) = \langle j|\Psi(t)\rangle$$

$$i\hbar\dot{F}_j(t) = \sum_i \langle j|H|i\rangle F_i(t)$$

$$i\hbar\dot{\mathbf{F}}(t) = \mathbf{H}\times\mathbf{F}(t)$$

Schroedinger Eq. is a Linear algebra problems

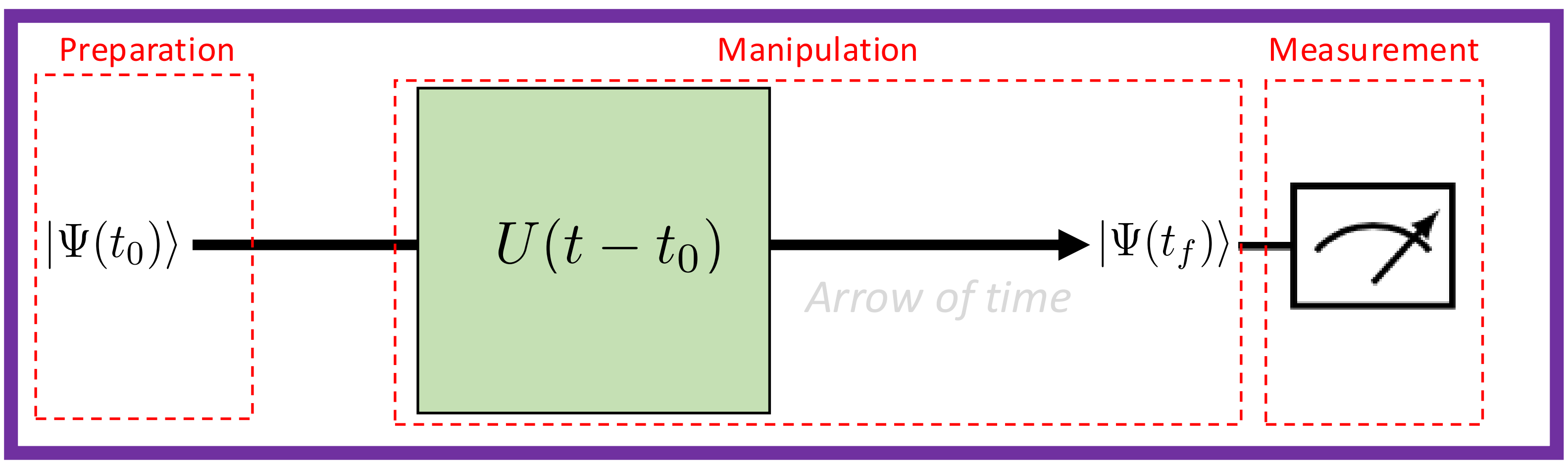
Formal solution



$$|\Psi(t)\rangle = e^{\frac{1}{i\hbar}(t-t_0)H}|\Psi(t_0)\rangle$$

$$= U(t-t_0)|\Psi(t_0)\rangle$$

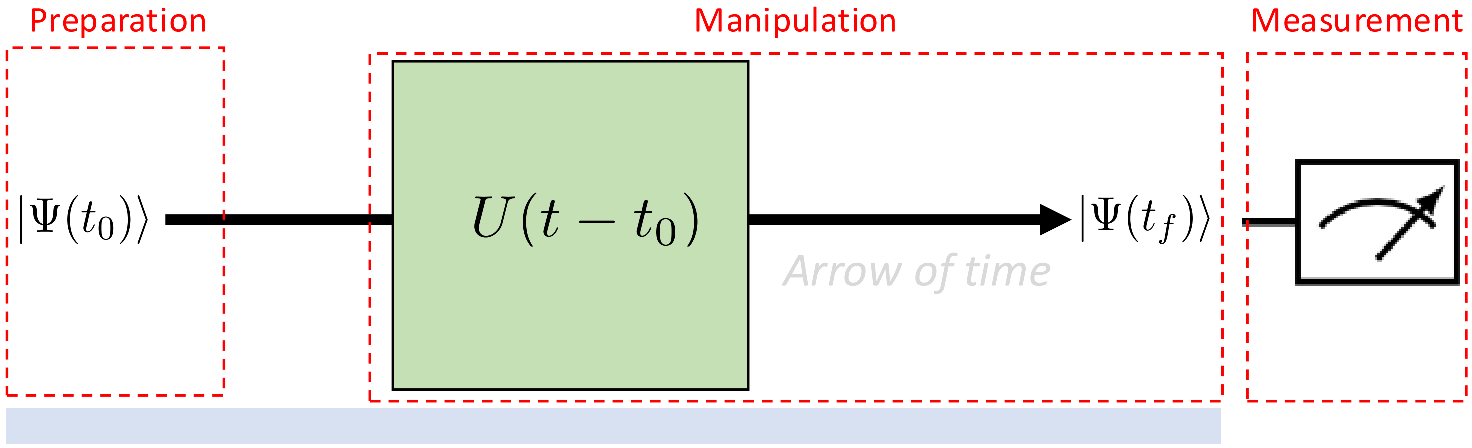
Having information on the w.f. means measuring it.

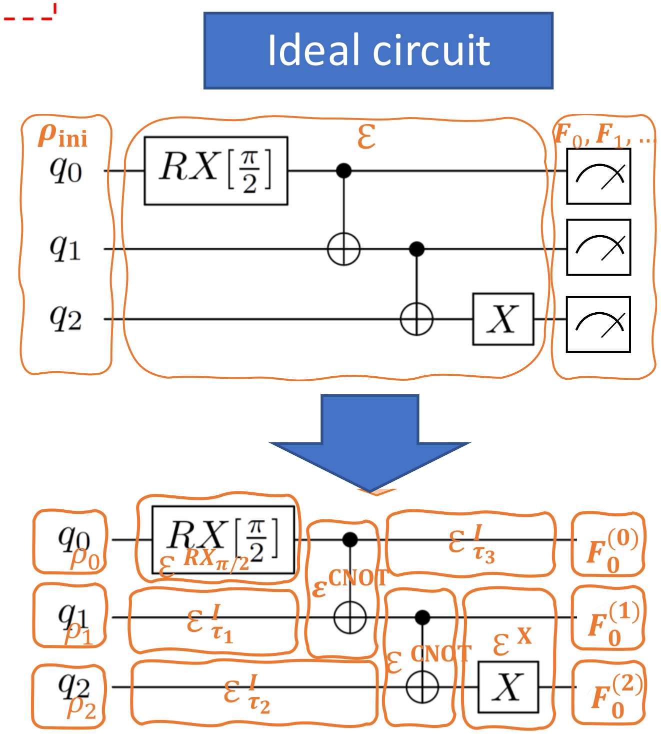


Quantum Circuit

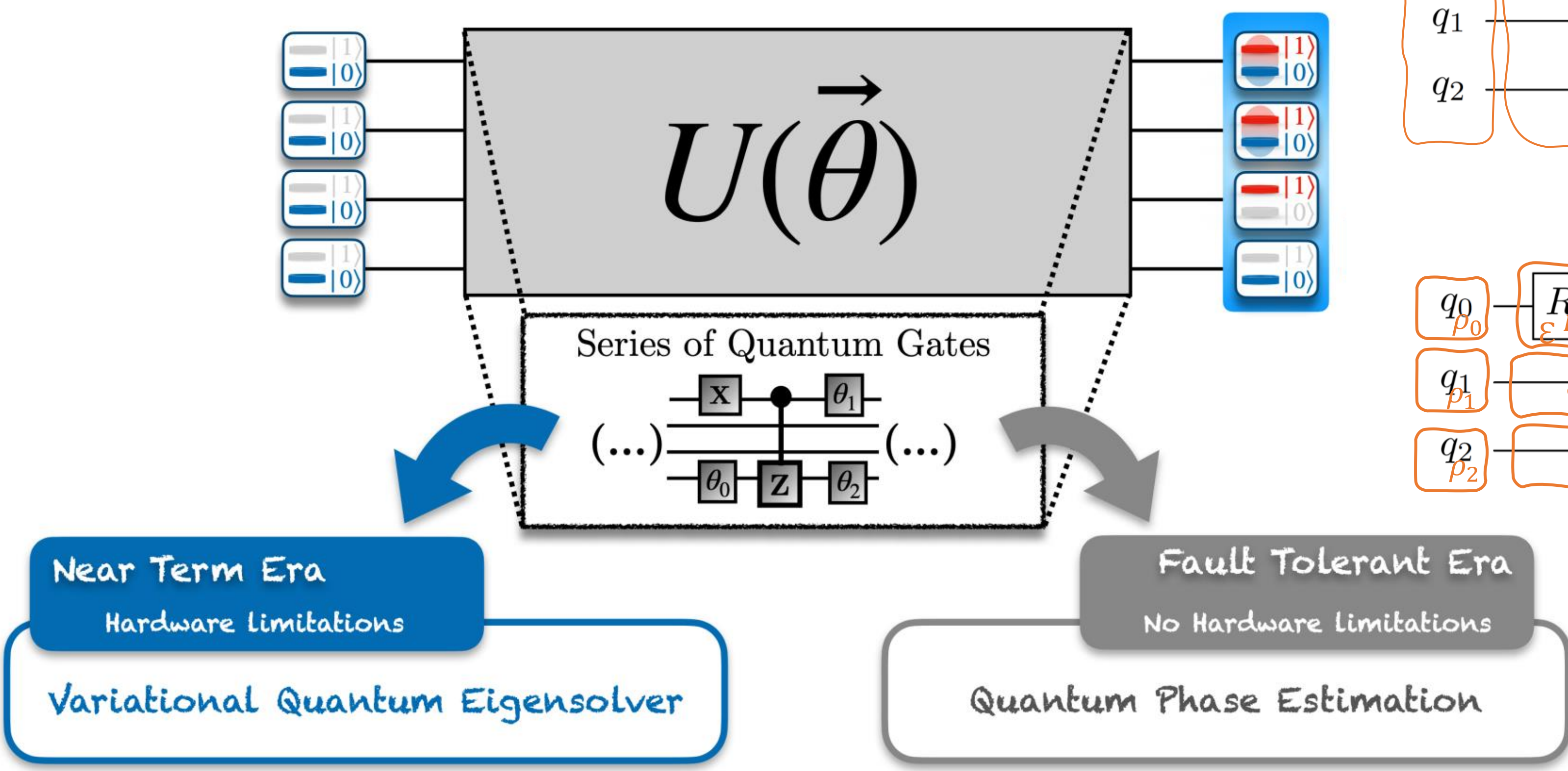
↓

Digital Quantum Circuit





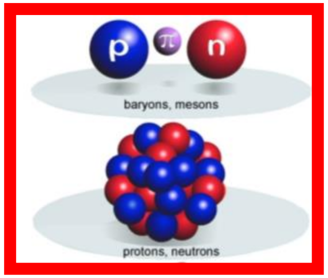
State preparation and manipulation are replaced by elementary quantum gates on one and two qubits

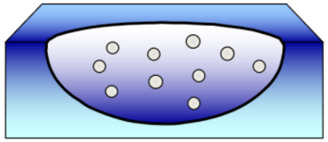


(credit: Y. Saad)

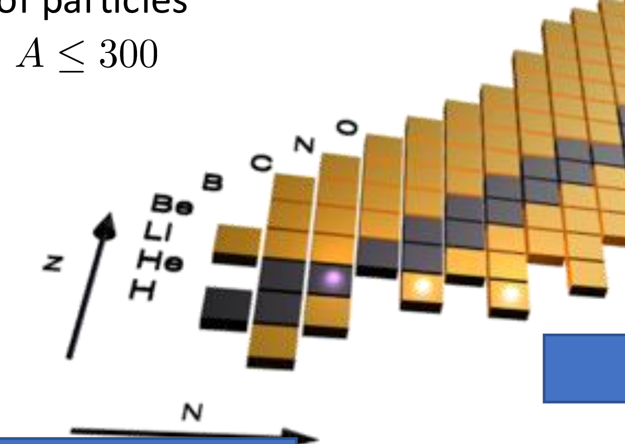
Quantum computing for the description of static and dynamical properties of atomic nuclei

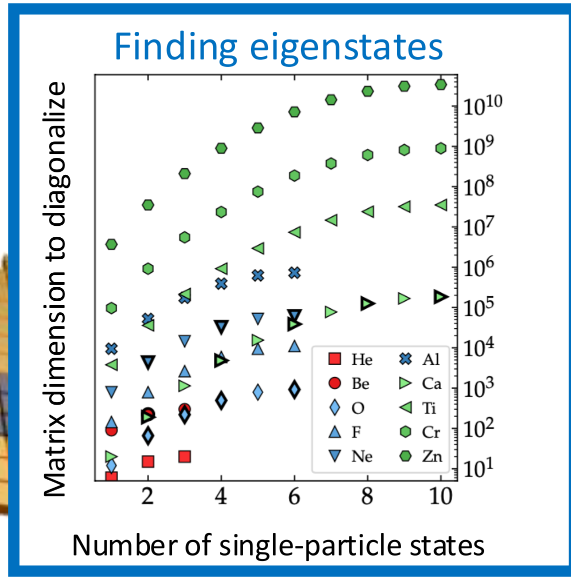
Problematic and challenges

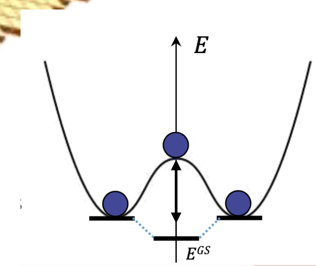




Nuclei are self-bound quantum mesoscopic systems
Nb of particles
$2 \leq A \leq 300$

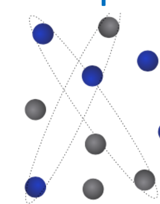






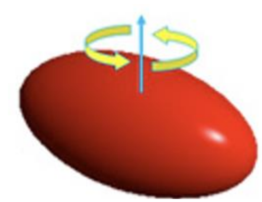
Spontaneous Broken symmetries (SB)

Small superfluid



(particle number SB)

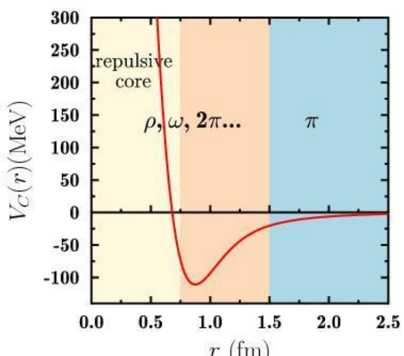
Deformation can happen



(rotational invariance SB)

...

Interaction

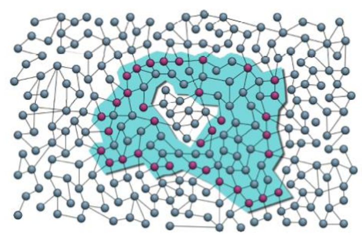


The problem is highly non-perturbative

Symmetries /Entanglement

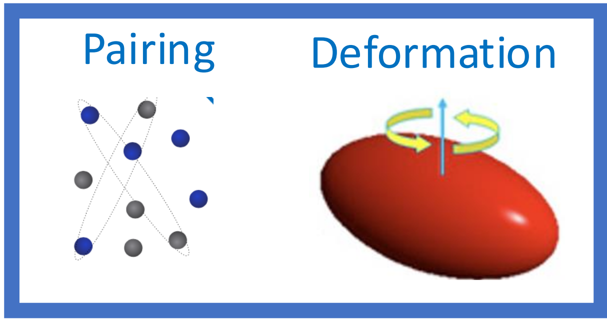
Global symmetries induce
All-to-all entanglement

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



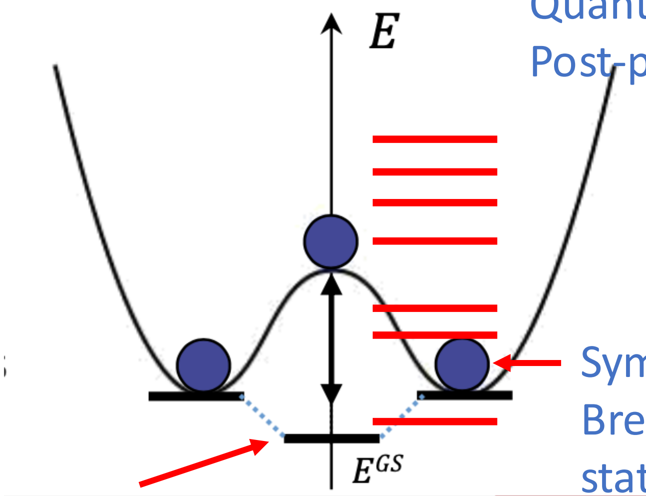
Nuclei are subject to entanglement volume law
(bad candidate for Tensor Network)

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



D. Lacroix, A. Ruiz Guzman and P. Siwach,
Symmetry breaking/symmetry preserving circuits
and symmetry restoration on quantum computers
EPJA 59 (2023)

3 Further Quantum or hybrid Quantum-Classical Post-processing



1 Symmetry Breaking (SB) state

2 Symmetry Restored (SR) state (multi-reference)

Variational optimization

1 Preparation of SB states on QC

2 Symmetry restoration on QC

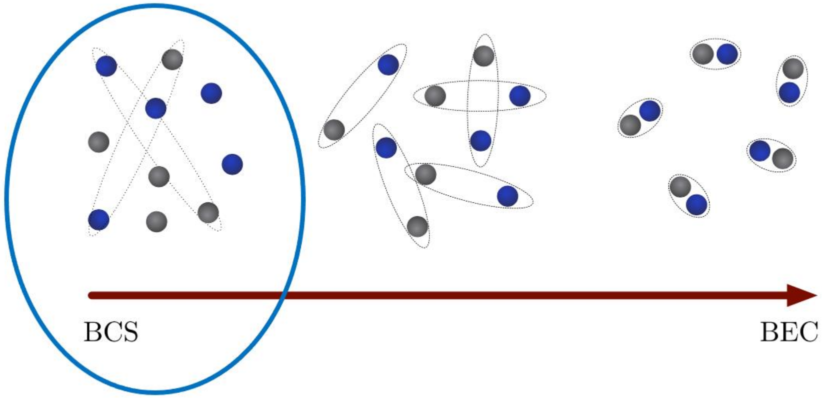
3 Post-processing for Improved ground state or excited States (QPE, Quantum Krylov, ...)

Which symmetries ?

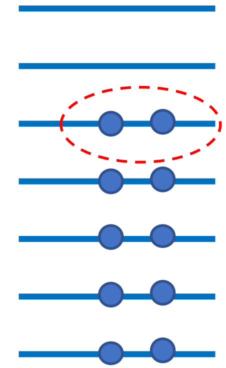
Many-Body

Particle Number
Parity
Total Spin

Illustration with the pairing Hamiltonian

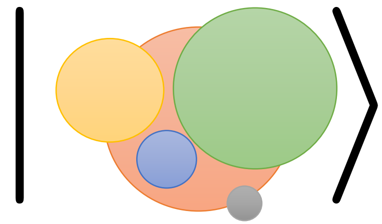


$$H_{\mathrm{P}} = \sum_{i>0} \varepsilon_i (a_i^\dagger a_i + a_{\bar{i}}^\dagger a_{\bar{i}}) - g \sum_{i,j>0} a_i^\dagger a_{\bar{i}}^\dagger a_{\bar{j}} a_j$$



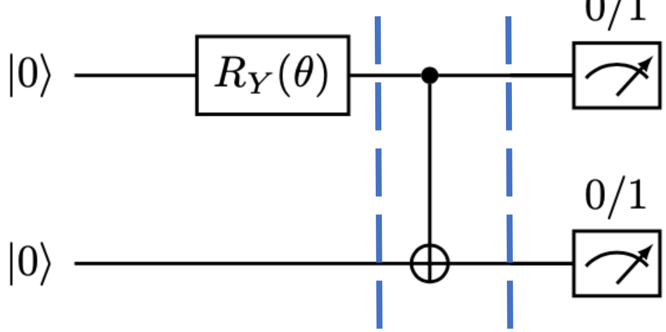
Example $|\Phi_0\rangle = \Pi_i (u_i + v_i a_i^\dagger a_{\bar{i}}^\dagger)|-\rangle$

➡ Mixes states with 0, 2, 4, ... particles



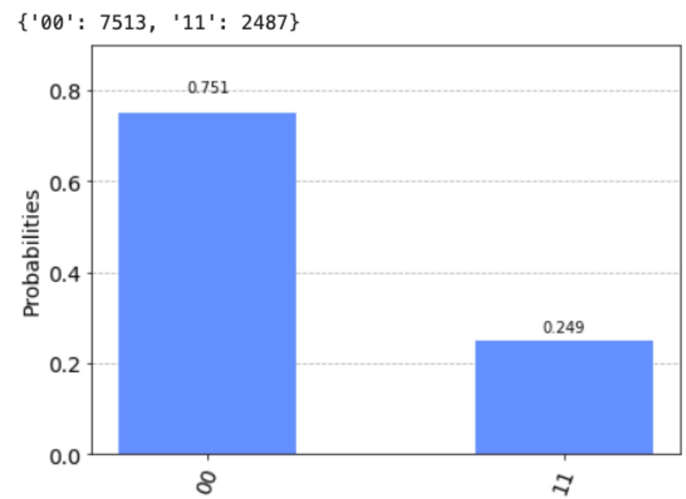
BCS states are generalized Bell states

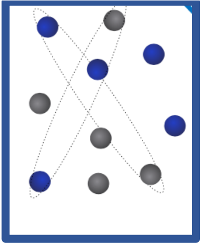
$$(\alpha|0\rangle + \beta|1\rangle) \otimes |0\rangle$$



$$(\alpha|00\rangle + \beta|11\rangle)$$

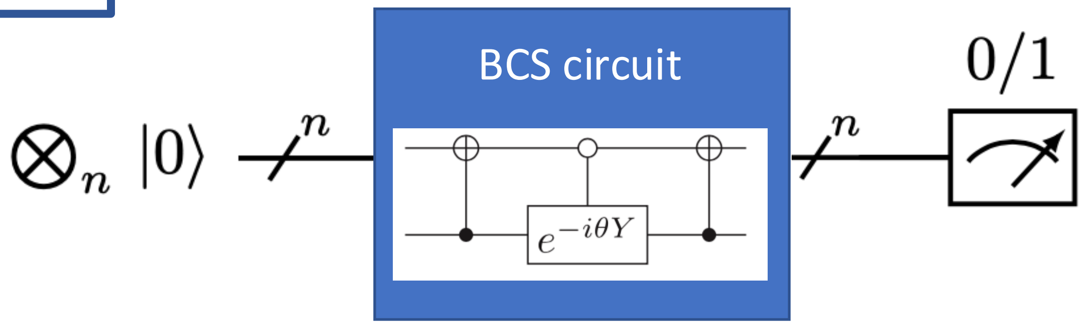
Here I created a Bell state



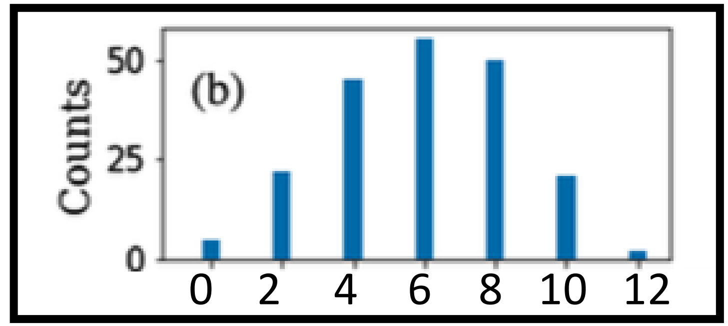


Quantum computing for atomic nuclei

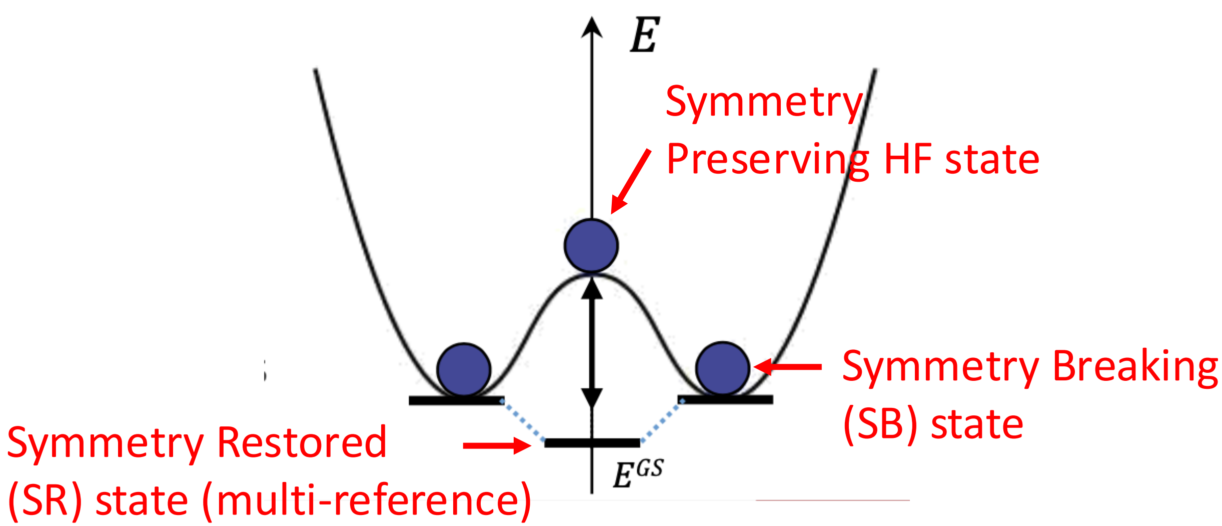
Illustration for small superfluids

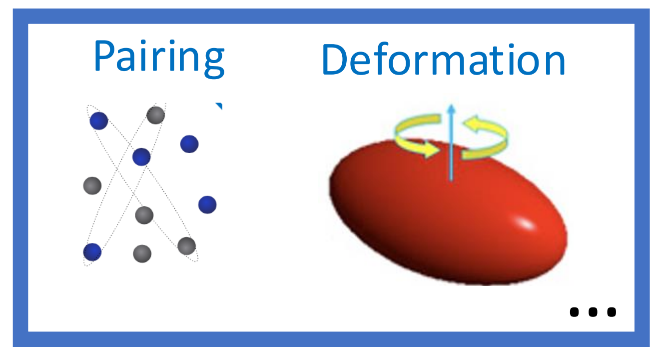


Example of mixing for 12 qubits



Restoring symmetries on a quantum computer?





D. Lacroix, A. Ruiz Guzman and P. Siwach, Symmetry breaking/symmetry preserving circuits and symmetry restoration on quantum computers EPJA 59 (2023)

A brief overview of the symmetry restoration problem and its solution

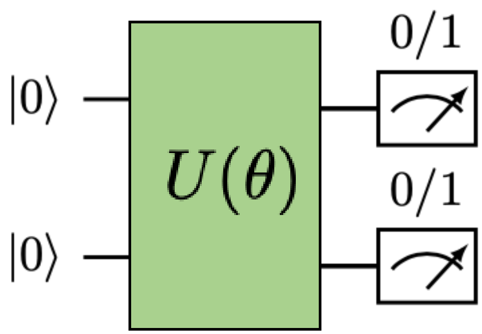
The particle number case

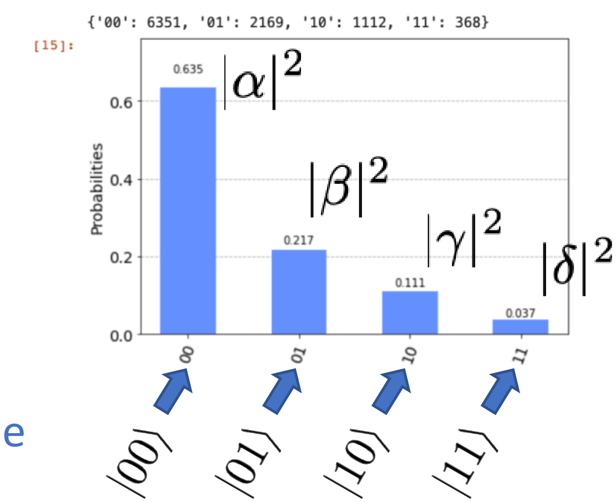
$$|\Psi\rangle = \sum_N c_N |N\rangle \Rightarrow |N\rangle \Rightarrow$$

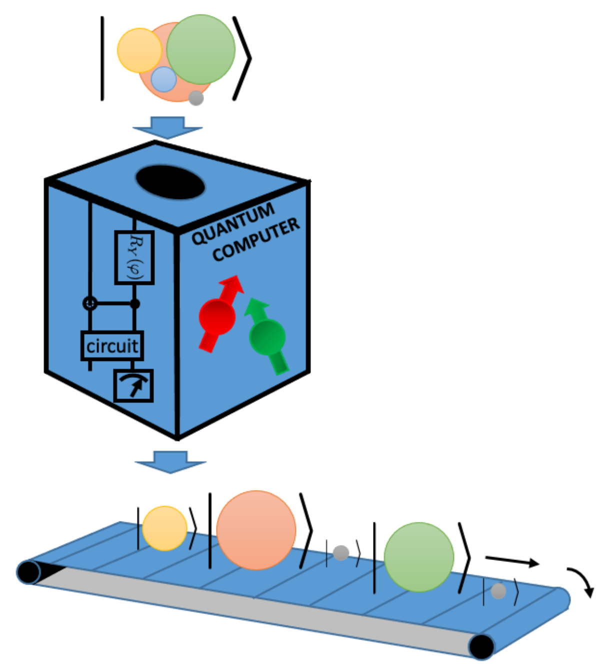
Use it for evolution,
Energy minimization, …

For 2 qubits

$$|\Psi\rangle = \underbrace{\alpha|00\rangle}_{|N=0\rangle} + \underbrace{\beta|01\rangle + \gamma|10\rangle}_{\propto |N=1\rangle} + \underbrace{\delta|11\rangle}_{|N=2\rangle}$$





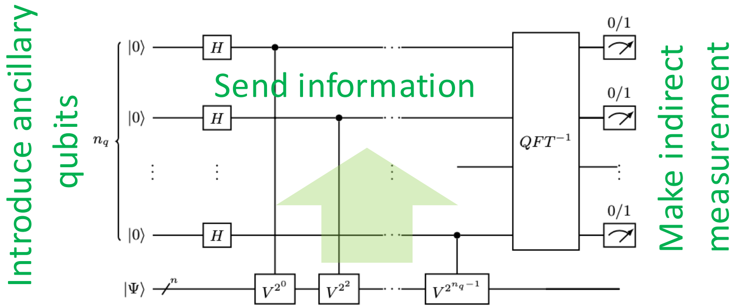


Difficulty – wave-function collapse

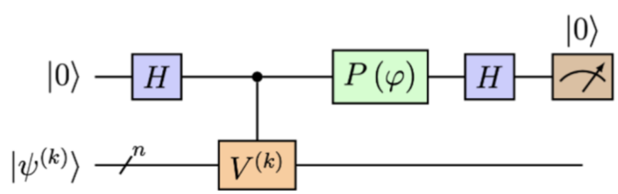
D. Lacroix, *"Symmetry-Assisted Preparation of Entangled Many-Body States on a Quantum Computer"*, PRL 125 (2020).

Systematic of Symmetry filtering methods

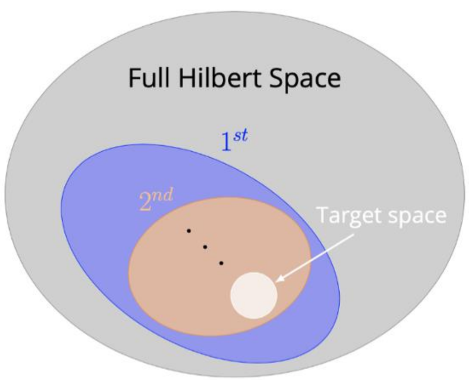
Standard Quantum Phase estimation



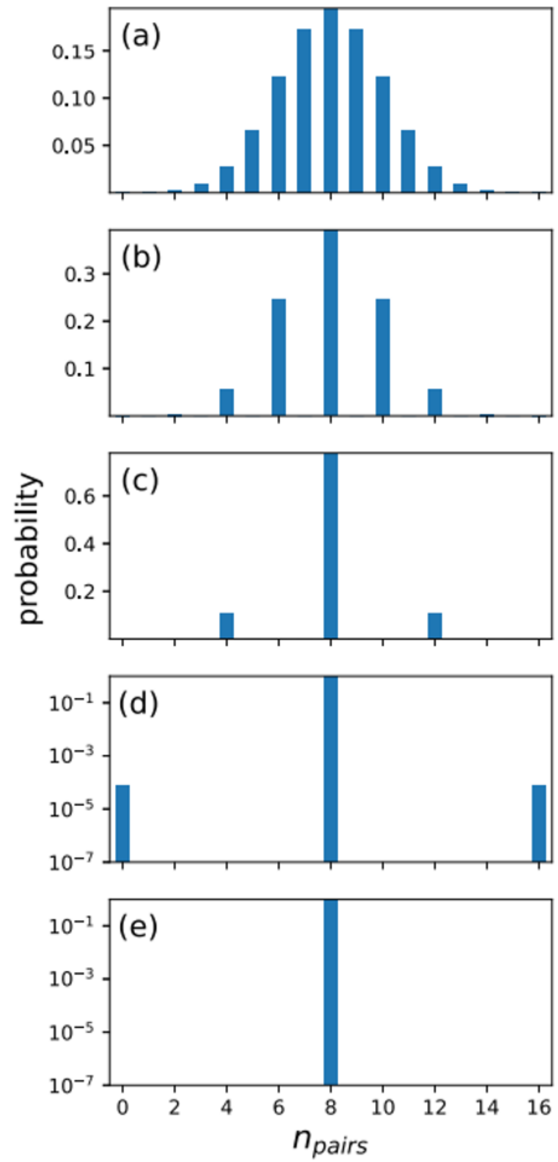
Iterative Quantum Phase estimation



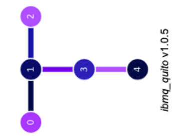
$$\hat{V}^{(k)} = e^{i\phi_k \hat{N}} \qquad \phi_k = \frac{\pi}{2^k}$$



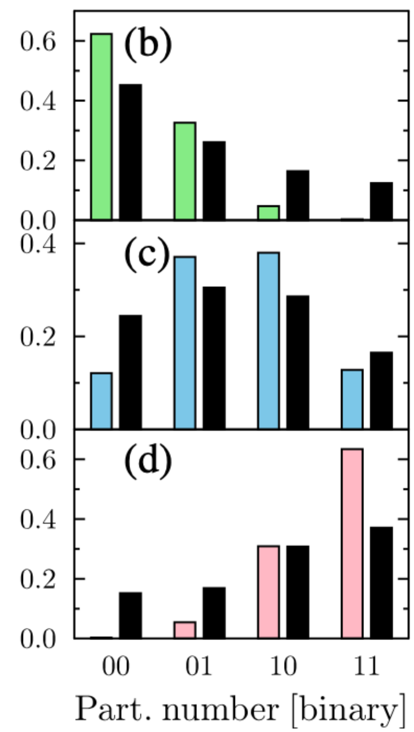
16 qubits, N = 8



Test on real devices



IBM Q5 (5 qubits)

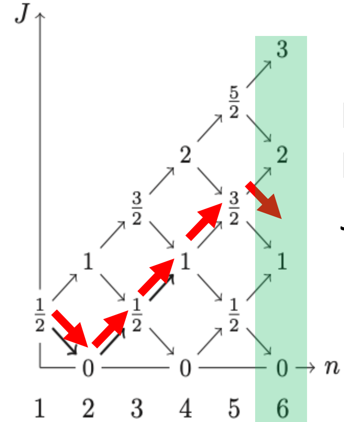


D. Lacroix, Phys. Rev. Lett. 125 (2020).

Summary of achieved work on symmetry restoration

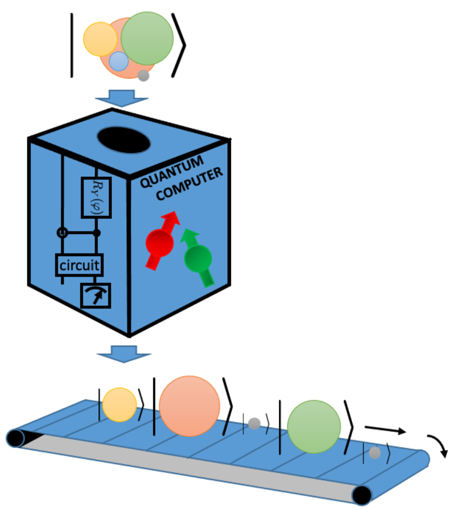
1. Preparation of SB states on QC
2. Symmetry restoration on QC
3. Post-processing for Improved ground state or excited States (QPE, Quantum Krylov, …)

Total spin symmetry

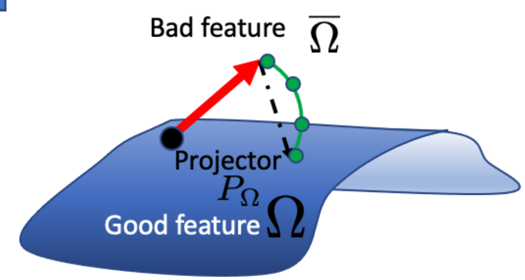


P. Siwach and DL, Phys. Rev. A 104, (2021)
Ruiz Guzman, DL, Eur. J. Phys. A 60 (2024)
J. Zhang, PhD thesis Paris-Saclay Univ. (2025)

2 Restoring symmetries



Various methods being developed



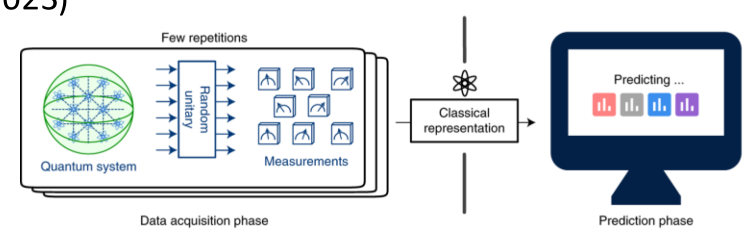
-With phase-estimation

D. Lacroix, PRL 125, 230502 (2020).

-Using quantum Oracles

Ruiz Guzman, Lacroix, PRC 107 (2023)

-Using classical post-processing (shadows)

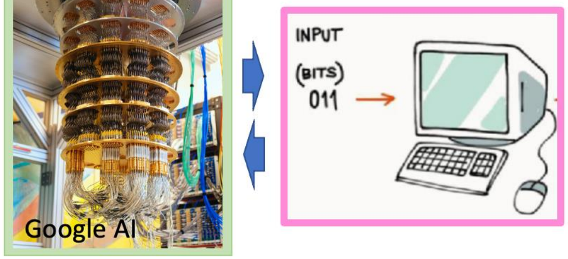


Ruiz Guzman, Lacroix, Eur. J. Phys. A 60 (2024)

Coming back to our superconducting problem

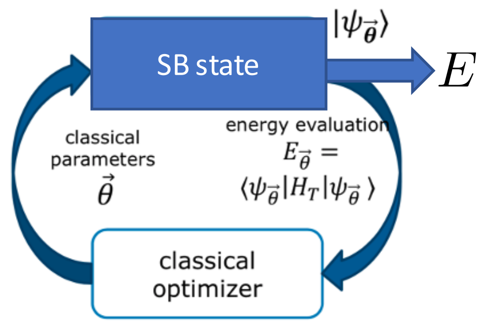
Combining projection with variational method

Classical optimization

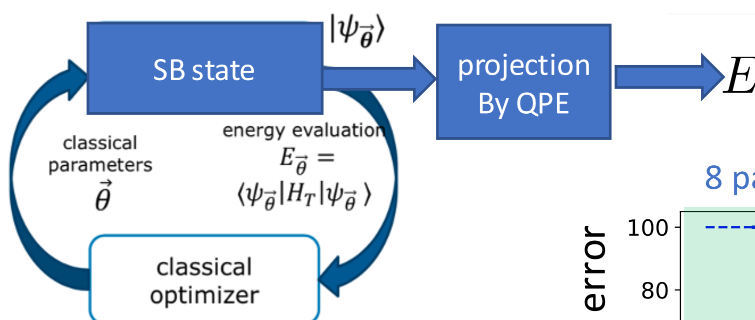


Quantum-Classical optimizers

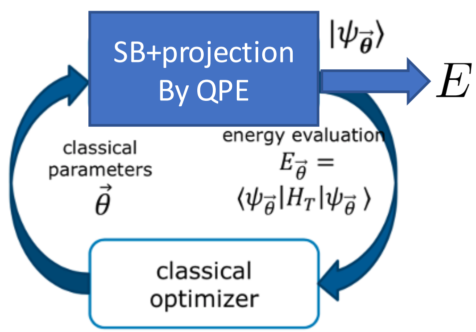
- Standard BCS theory

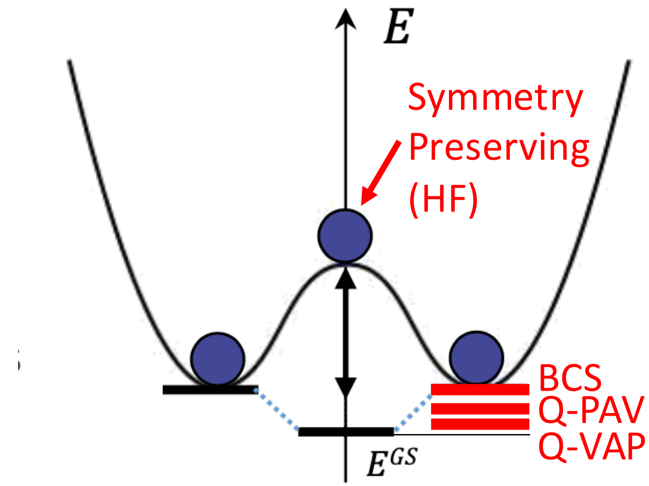


- Project after optimization
  Q-PAV: Quantum Projection After Variation

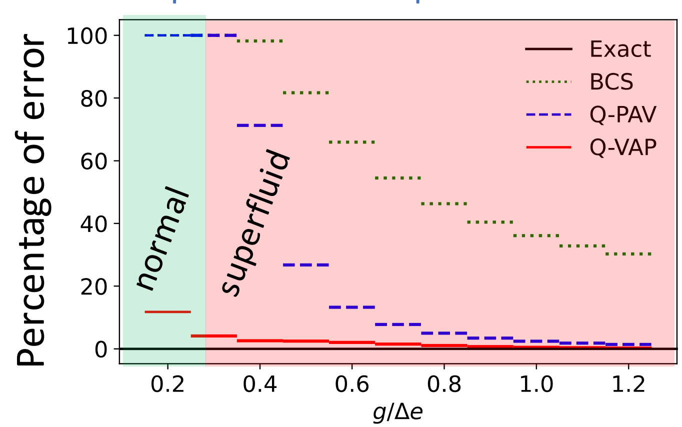


- The optimization is made on the Symmetry restored state.
  Q-VAP: Quantum Variation After Projection





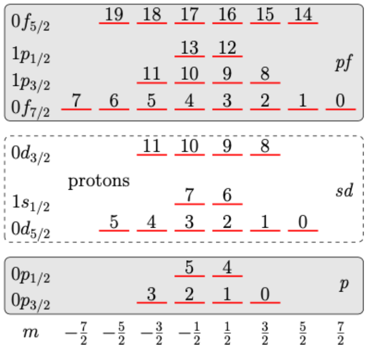
8 particles on 8 equidistant levels

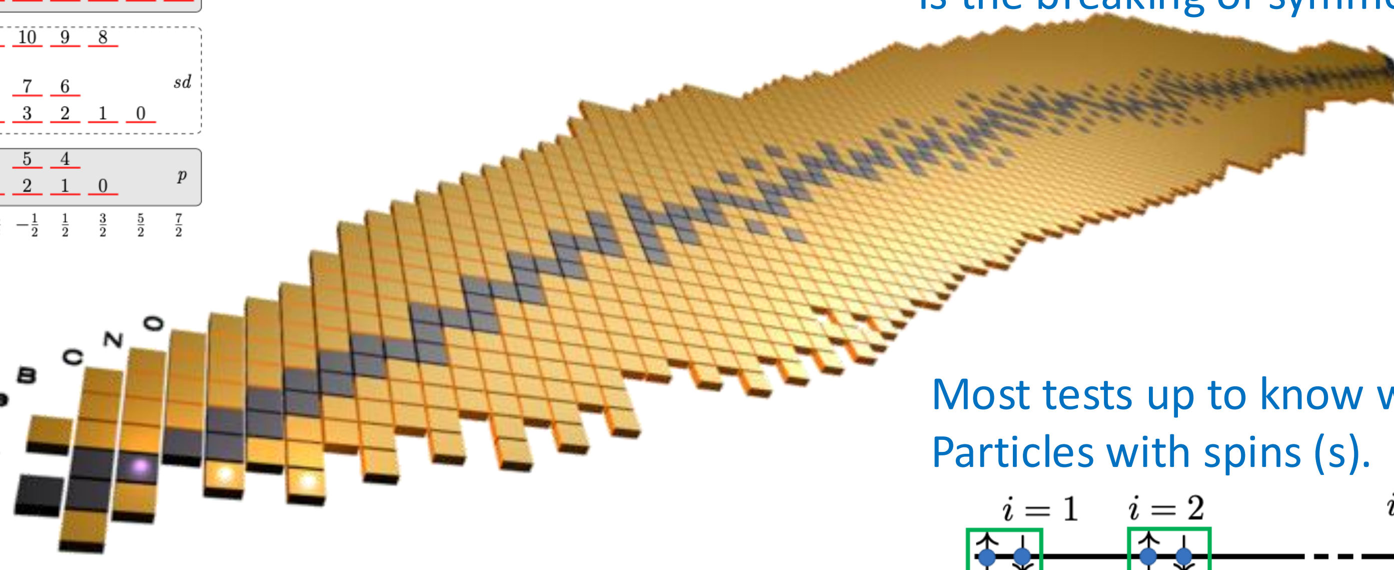


Ruiz Guzman and Lacroix, PRC 105 (2022)

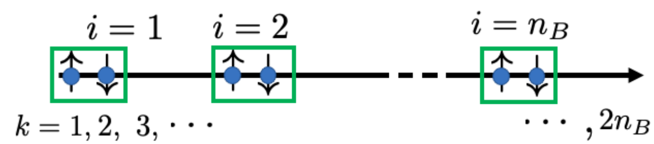
Getting closer to realistic problems

Is the breaking of symmetries always a good idea?

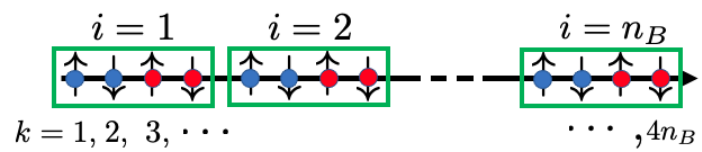




Most tests up to know were made on
Particles with spins (s).



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 Paris-Saclay Univ. (2025).

Going beyond traditional nuclear physics methods: Use of adaptative methods

Iterative construction of the ansatz

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

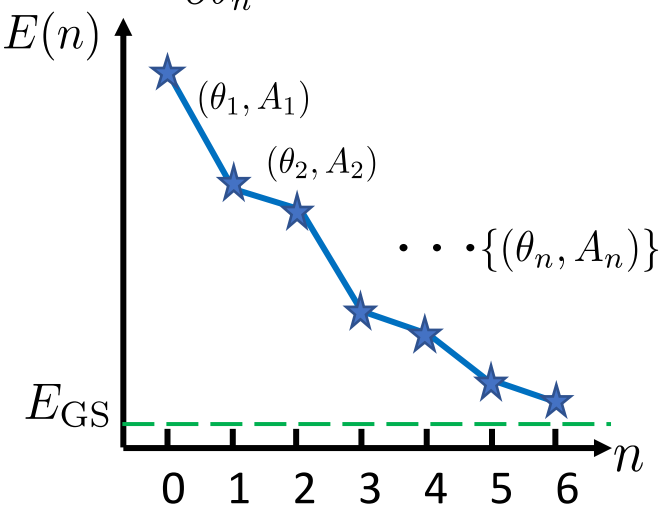
- Start from a state $|\Psi_0\rangle = |n=0\rangle$

- Built iteratively the ansatz such as:

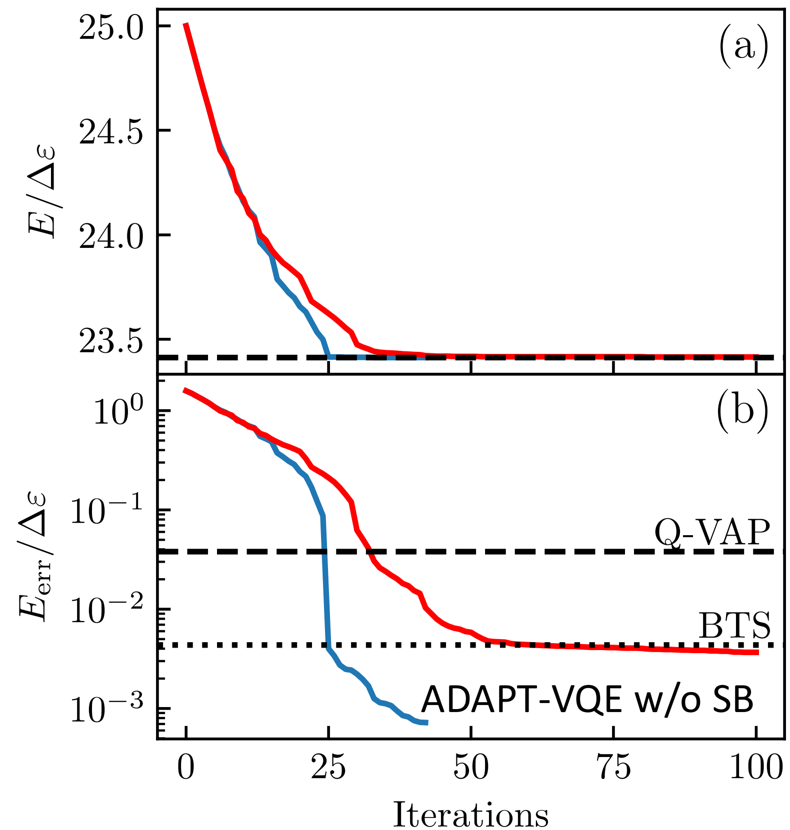
$$|n\rangle = e^{i\theta_n A_n}|n-1\rangle = \prod_{k=1}^{n} e^{i\theta_k A_k}|0\rangle$$

Such that $\quad A_n \in \{O_1, \cdots, O_\Omega\}$

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

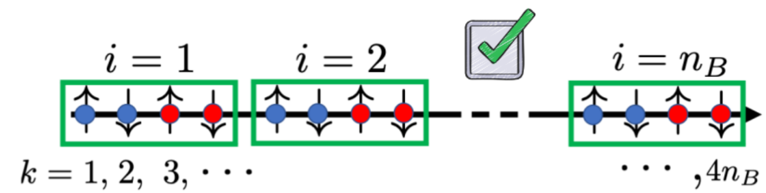


ADAPT-VQE applied to the Superfluid problems: only spins



J. Zhang, D. Lacroix, and Y. Beaujeault-Taudière, PRC (2025)

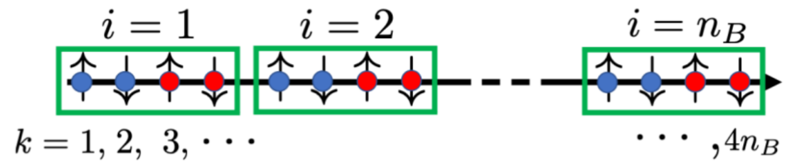
Extension to spin and isospin



Is breaking symmetries always a good idea?

Extension to the proton-neutron pairing Hamiltonian problem

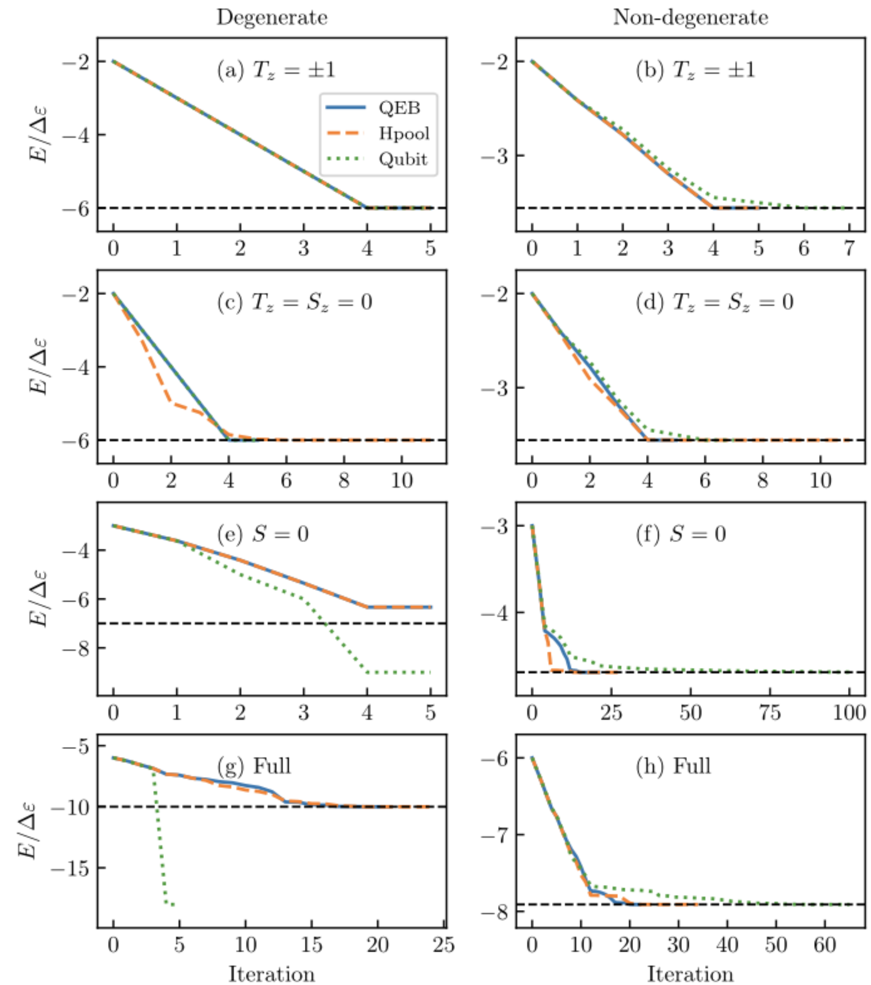
$$
\begin{aligned}
H \;=\; & \sum_{i=1}^{n_B}\Big[\varepsilon_{i,n}(\nu_i^\dagger \nu_i + \nu_{\bar{i}}^\dagger \nu_{\bar{i}}) + \varepsilon_{i,p}(\pi_i^\dagger \pi_i + \pi_{\bar{i}}^\dagger \pi_{\bar{i}})\Big] \\
& - \sum_{T_z=-1,0,1} g_V(T_z)\mathcal{P}_{T_z}^\dagger \mathcal{P}_{T_z} \\
& - \sum_{S_z=-1,0,1}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



Different Hamiltonian limit

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

4 particles on 12 qubits



Different operator pool in ADAPT-VQE breaking or not symmetries

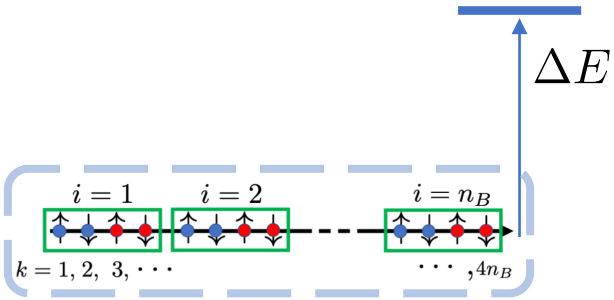
	Particle number	Seniority	Parity
H-pool	✓	✓	✓
QEB-pool	✓	×	✓
Qubit-pool	×	×	✓

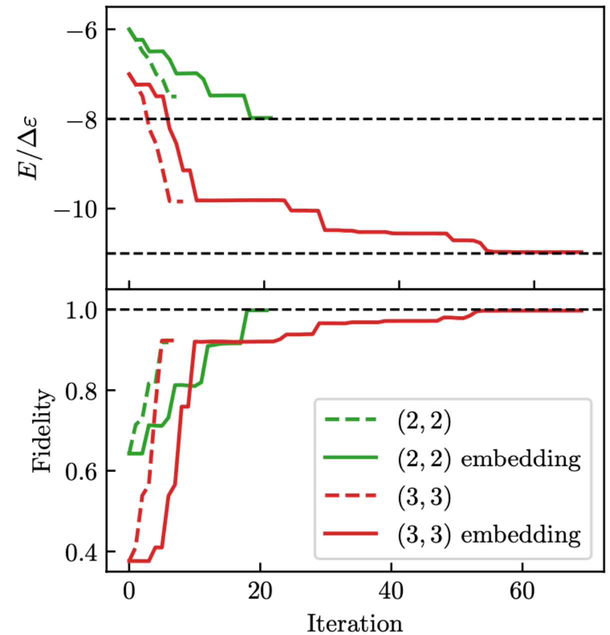
J. Zhang, D. Lacroix, and Y. Beaujeault-Taudière, PRC 110 (2024)

Going closer to nuclei: adding isospin

Embedding

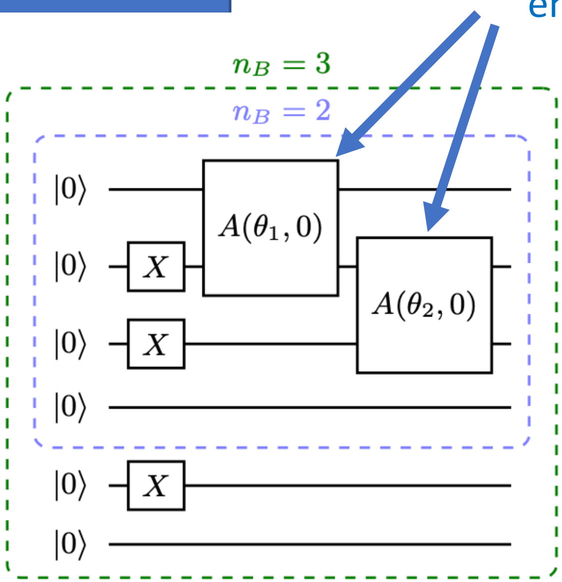
Fictitious
set of qubits

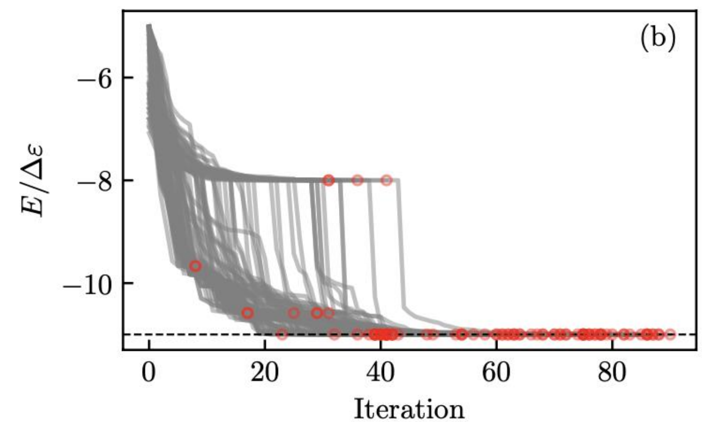




Initial condition Randomization

Initial random
entangler

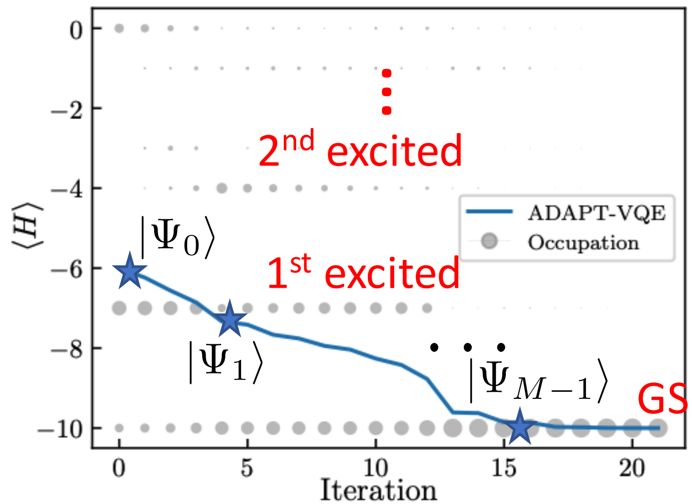




J. Zhang, D. Lacroix and Y. Beaujeault-Taudière, PRC 110 (2024)

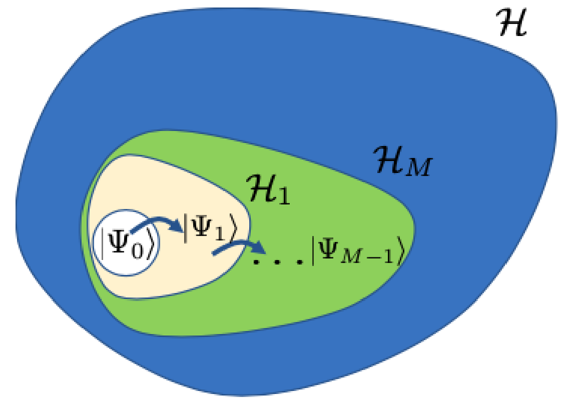
From ground state only to excited states

The states generated during the convergence contain information on excited states



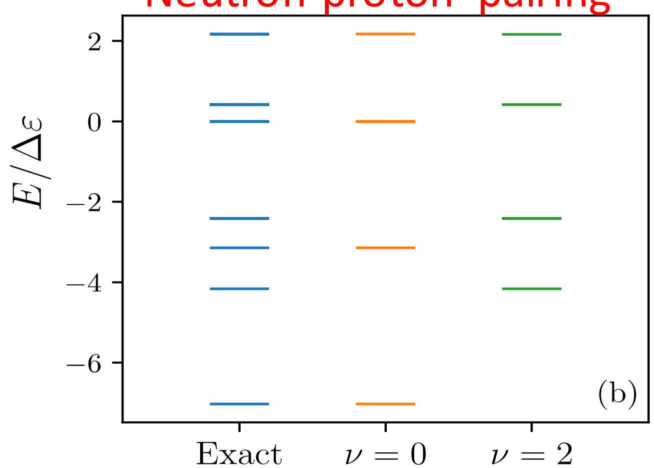
J. Zhang, D. Lacroix, Phys. Lett. B 869 (2025)

We used these states in a Quantum Subspace Diagonalization method (QSD)

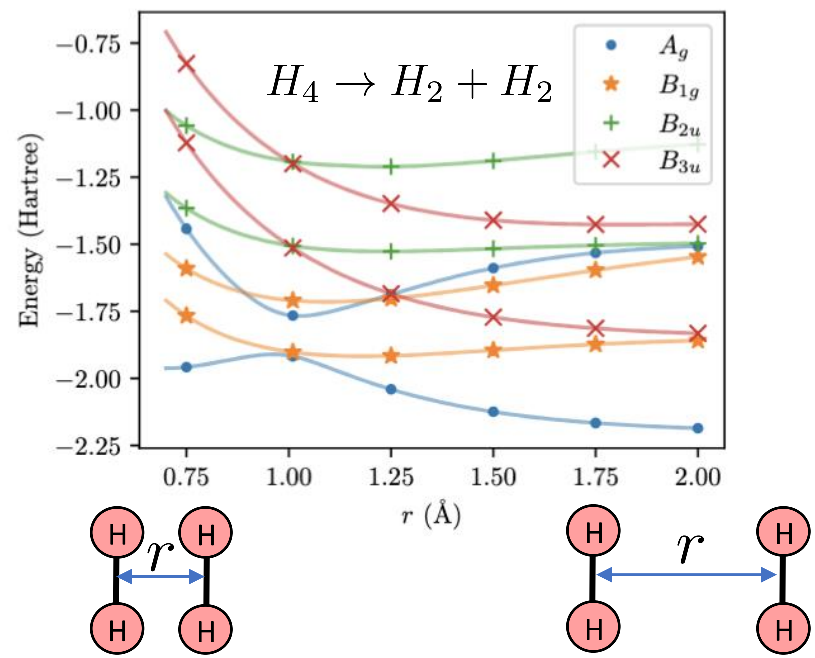


Applications

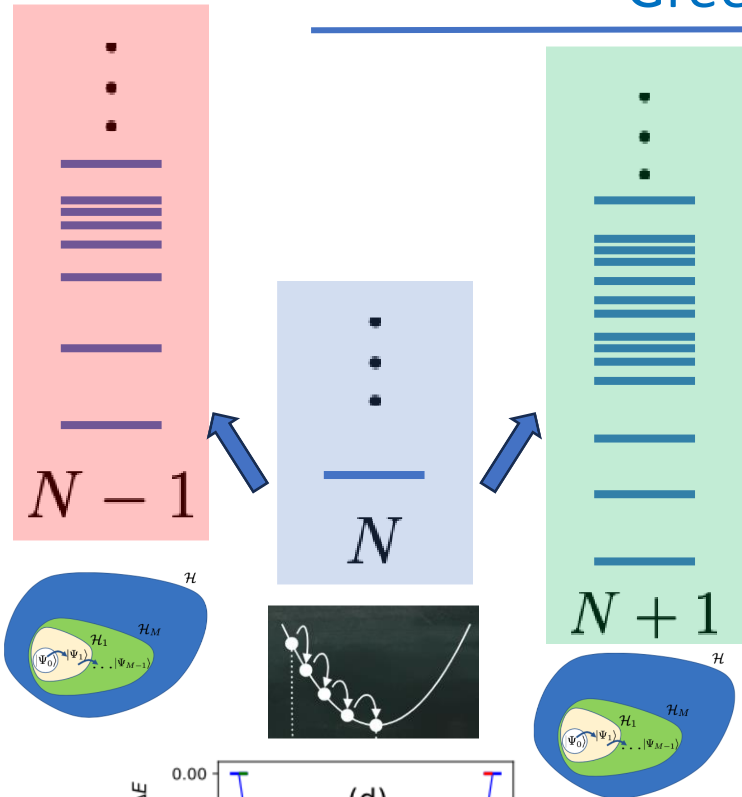
Neutron-proton pairing



molecule dissociation



Green's function estimated with a quantum computer

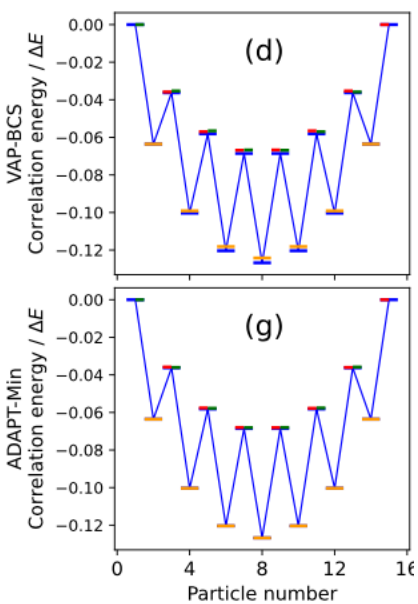


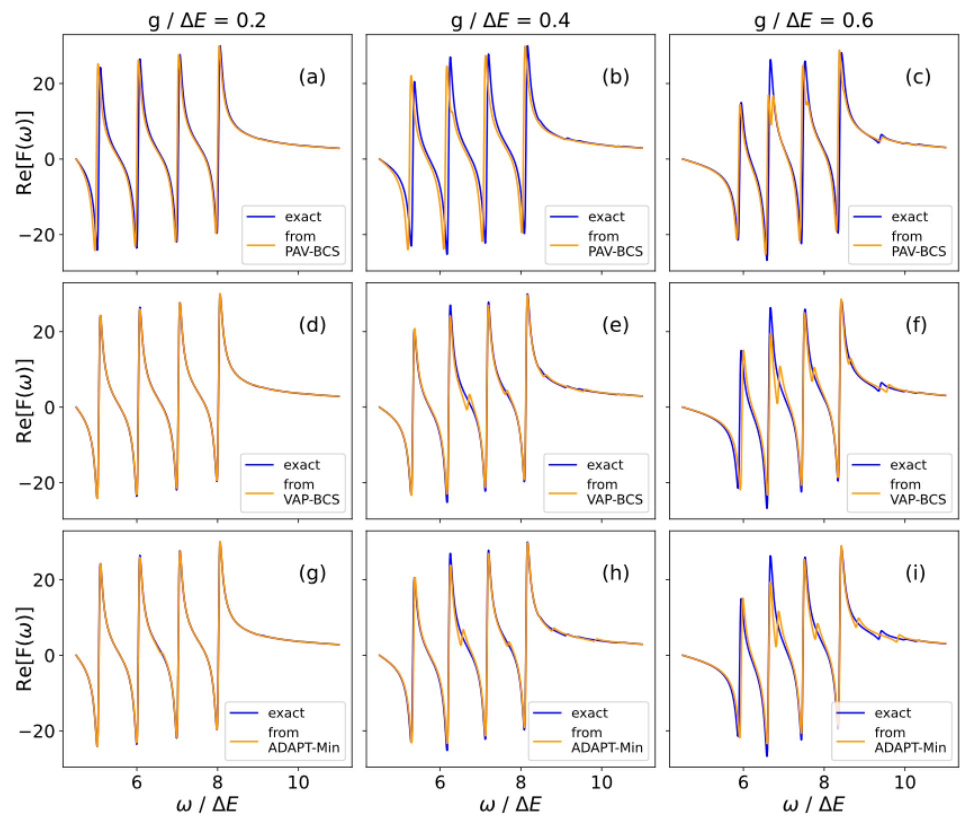
Green's function matrix elements $G_{ij}(t,t') = \langle \Psi_0 | \mathrm{T}[a_j^\dagger(t) a_i(t')] | \Psi_0 \rangle$

Lehman representation

$$G_{ij}(\omega) = \frac{\langle \Psi_0^N | a_i | \Psi_k^{N+1} \rangle \langle \Psi_k^{N+1} | a_j^\dagger | \Psi_0^N \rangle}{\omega - (E_k^{N+1} - E_0^N) + i\eta} + \sum_k \frac{\langle \Psi_0^N | a_j^\dagger | \Psi_k^{N-1} \rangle \langle \Psi_k^{N-1} | a_i | \Psi_0^N \rangle}{\omega - (E_0^N - E_k^{N-1}) - i\eta}.$$

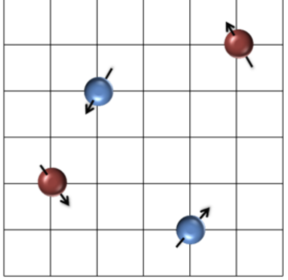
Illustration with the pairing Hamiltonian





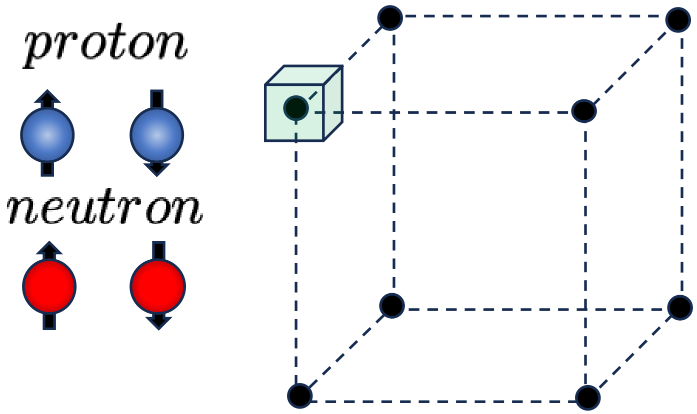
S. Aychet Claisse, D. Lacroix, V. Somà, Phys. Rev. C 113 (2026)

Ongoing work- Quantum simulation of nuclei on lattices



$L \times L \times L$ lattice
(here $L = 2$)

Number of single-particle states: $4L^3$

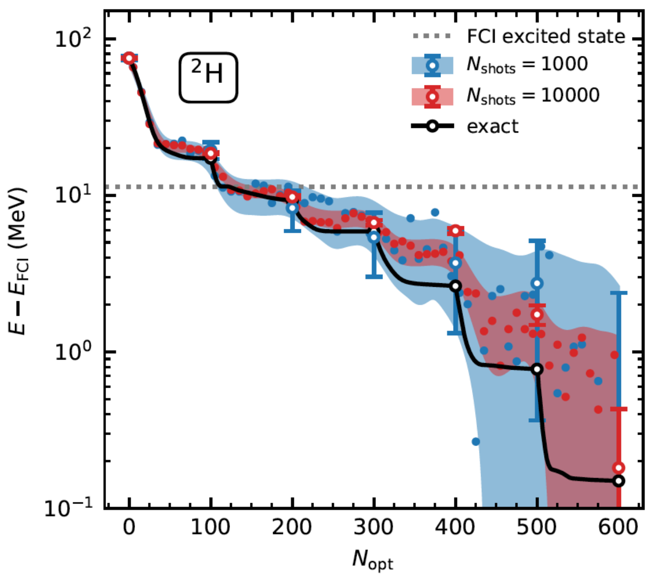


Pionless EFT Hamiltonian [Bedaque, van Kolck 2002]

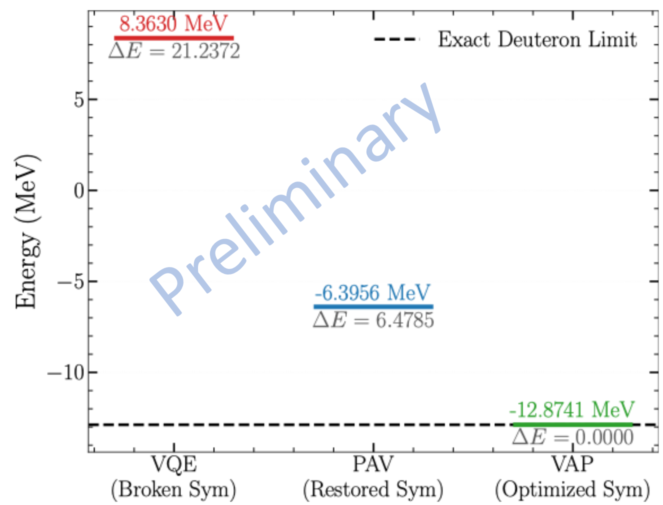
$$\hat{H} = \sum_{\langle \mathbf{l},\mathbf{l}'\rangle} \sum_{\tau s} T^{\mathbf{l}}_{\mathbf{l}'} \hat{a}^\dagger_{\mathbf{l}\tau s} \hat{a}_{\mathbf{l}'\tau s}$$ Kinetic-non local

$$+ \frac{V}{2} \sum_{\mathbf{l}} \sum_{ss'\tau\tau'} \hat{a}^\dagger_{\mathbf{l}\tau s} \hat{a}^\dagger_{\mathbf{l}\tau' s'} \hat{a}_{\mathbf{l}\tau' s'} \hat{a}_{\mathbf{l}\tau s}$$ Two-body local

$$+ W \sum_{\mathbf{l}} \sum_{\tau s} \hat{a}^\dagger_{\mathbf{l}\tau\uparrow} \hat{a}^\dagger_{\mathbf{l}\tau\downarrow} \hat{a}^\dagger_{\mathbf{l}-\tau s} \hat{a}_{\mathbf{l}-\tau s} \hat{a}_{\mathbf{l}\tau\downarrow} \hat{a}_{\mathbf{l}\tau\uparrow} .$$ Three-body local



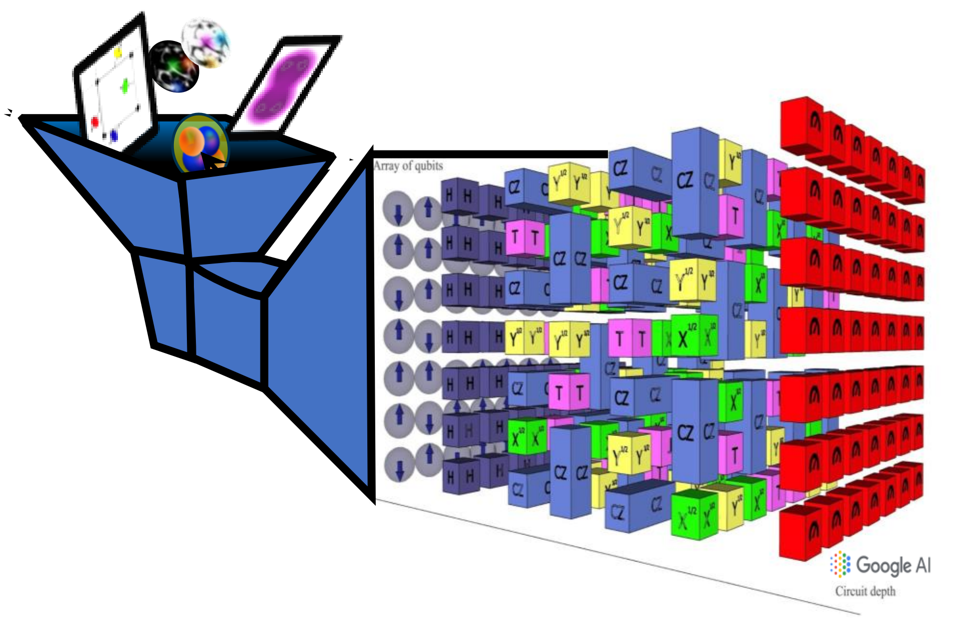
Gu, Heinz, Kiss, Papenbrock, Phys. Rev. C 113 (2026)



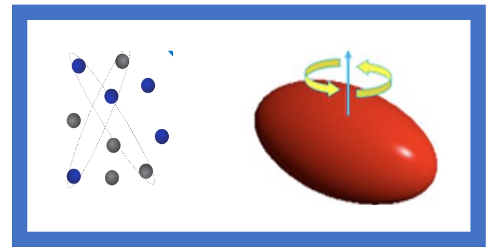
A. Singh, D. Lacroix, (*in preparation*)

The field of quantum algorithms for many-body systems is evolving rapidly.

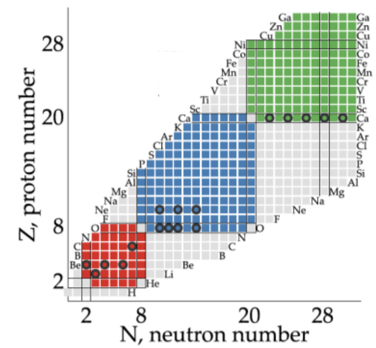
Experimental quantum computing platforms are improving constantly.



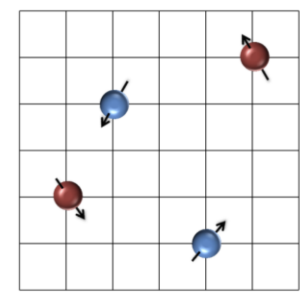
Symmetry problem



Traditional shell-model



Lattice pionless EFT



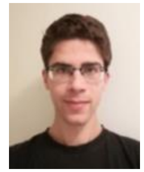
Special Thanks to

PhD students/postdocs


E. A. Ruiz Guzman


Y. Beaujeault-Taudiere


J. Zhang


S. Aychet Claisse


C. de Correc


R. Bocquet


A.Singh

Collaborators

LPSC Grenoble Laboratoire de Physique Subatomique et de Cosmologie

THE UNIVERSITY of WISCONSIN MADISON

UNIVERSITÀ DI TRENTO

CERN

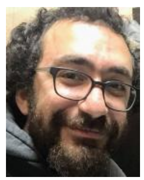
IBM Quantum

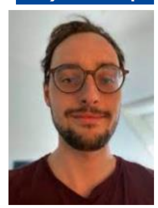
cea

Arizona State University


M. Mangin Brinet


B. Balantekin


A. Roggero


O. Kiss


F. Tavernelli


F. Tacchino


Vittorio Somà


P. Siwach

ÉCOLE POLYTECHNIQUE IP PARIS

QSL Quantum Software Lab

EVIDEN an atos business

ALICE & BOB

ICGM Institut Charles Gerhardt Montpellier

UNIVERSIDAD D SEVILLA 1505

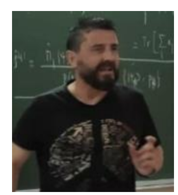

T. Ayral

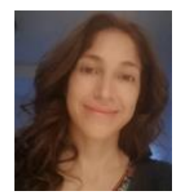

P. Besserve

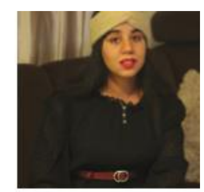

C. Bertrand


F. Jamet


B. Senjean


Jesus pascual Casado

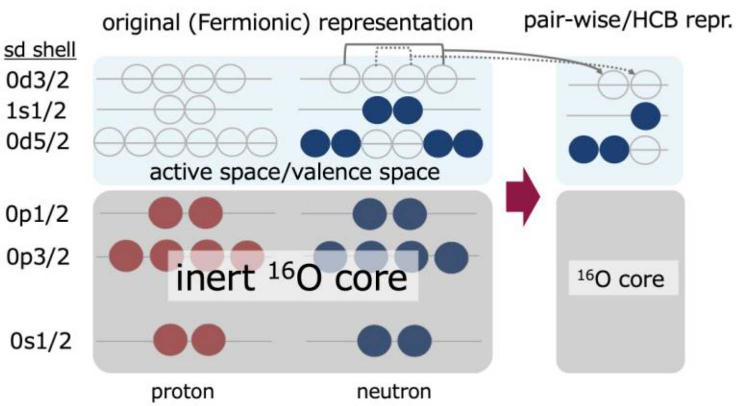

Laura Oliveira Atencio

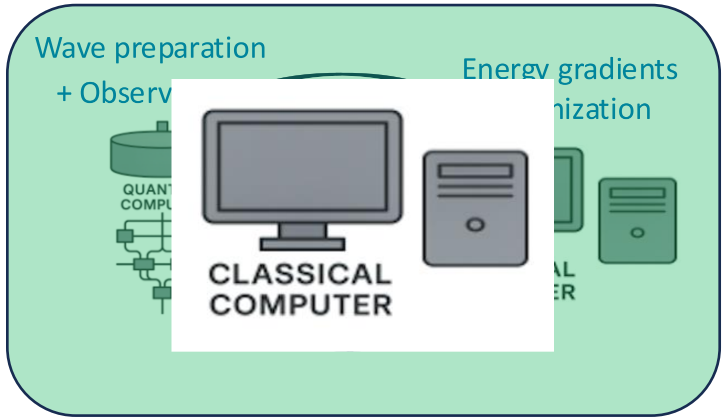

S. Baid

Additional discussions
(applications to real quantum computers)

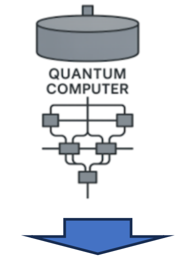
Simplified Shell Model applications on real quantum computers

Hard-core Boson mapping





After optimal solution Is found



Build the Approximate GS Compute observable

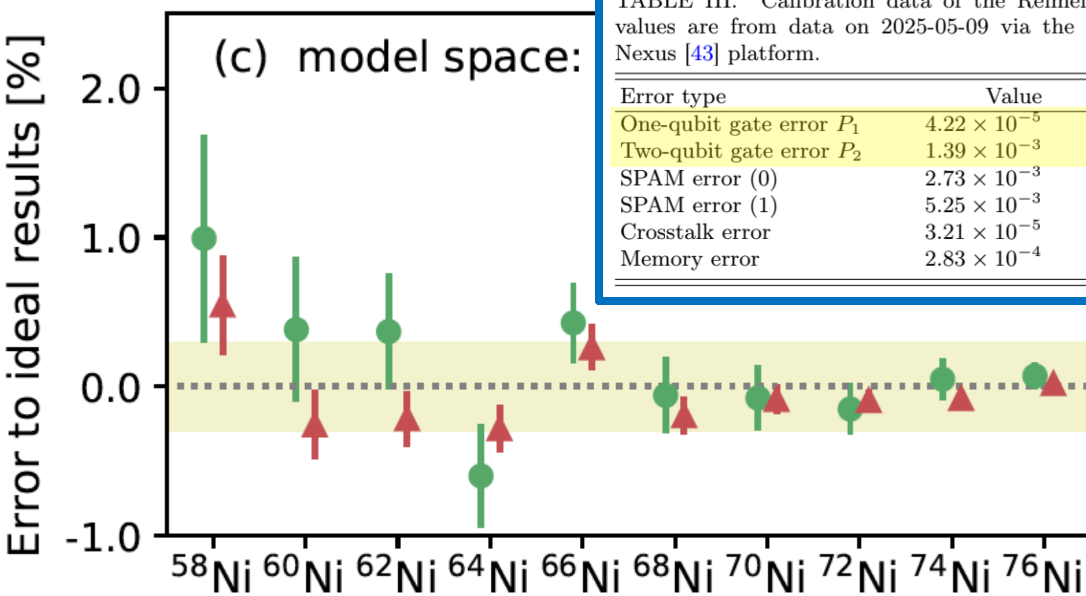
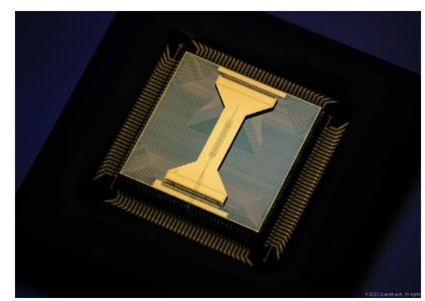


TABLE III. Calibration data of the Reimei device. The values are from data on 2025-05-09 via the Quantinuum's Nexus [43] platform.

Error type	Value	Uncertainty
One-qubit gate error P_1	4.22×10^{-5}	5.23×10^{-6}
Two-qubit gate error P_2	1.39×10^{-3}	5.92×10^{-5}
SPAM error (0)	2.73×10^{-3}	1.57×10^{-4}
SPAM error (1)	5.25×10^{-3}	2.18×10^{-4}
Crosstalk error	3.21×10^{-5}	1.89×10^{-6}
Memory error	2.83×10^{-4}	2.32×10^{-5}

RIKEN-Quantinuum's Reimei device (trapped Ion)



Sota Yoshida, Takeshi Sato, Takumi Ogata, Masaaki Kimura, Phys. Rev. Res. (2026)

A focus on neutrino oscillation physics simulated on quantum computers

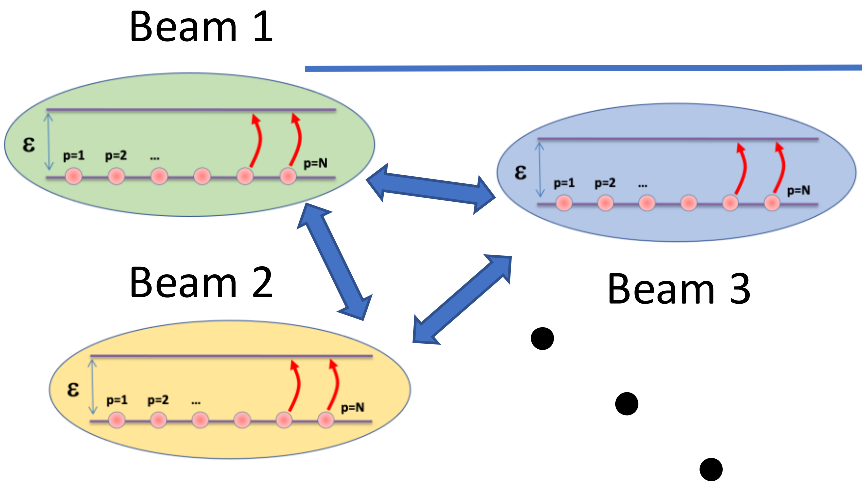


Illustration of the Hamiltonian (2 flavor approx)

Oscillation
$$H_\nu = \frac{1}{N}\sum_{i=0}^{N-1} \sin(2\theta_\nu)X_i - \cos(2\theta_\nu)Z_i$$

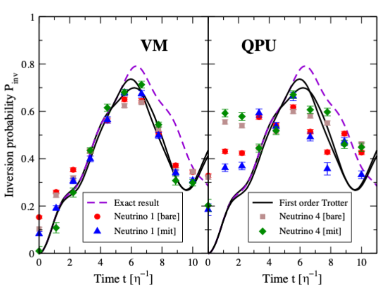
Coupling
$$H_{\nu\nu} = \sum_{i<j}^{N-1} G_{i,j}[X_iX_j + Y_iY_j + Z_iZ_j].$$

4 neutrinos
IBM-Vigo QPU

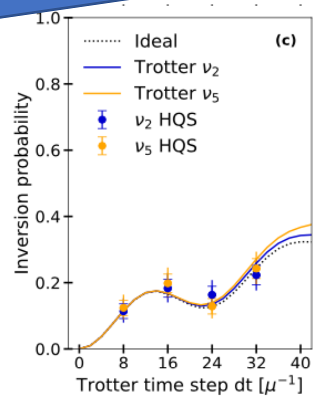
4 & 8 neutrinos
HQD-H1
Trapped Ion device

12 neutrinos
Quantinuum's H1-1
20 qubit trapped-ion

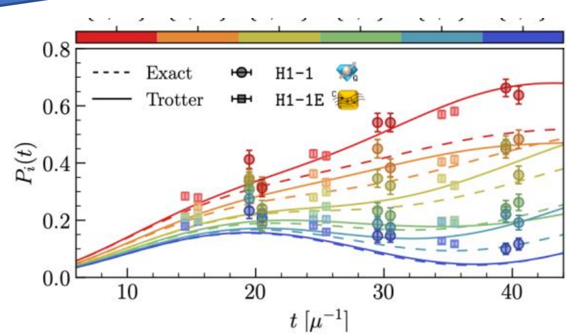
12 neutrinos / qutrits
H1-1 & ibm_torino



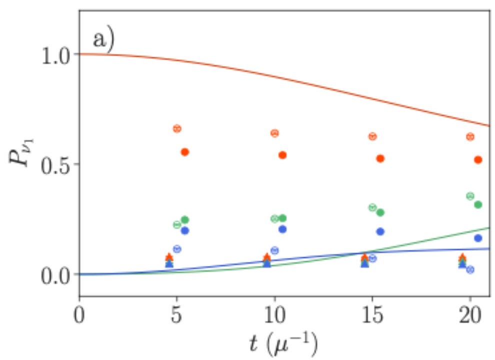
Hall et al, PRD 104 (2021)



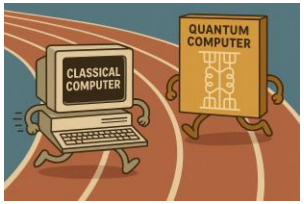
Amitrano,et al, PRD 107, (2023)



Illa et al, PRL 130 (2023)

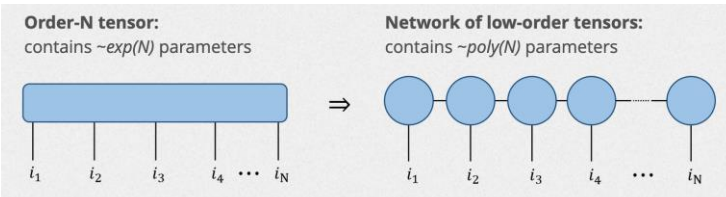


Turro et al,
PRD D 111 (2025)

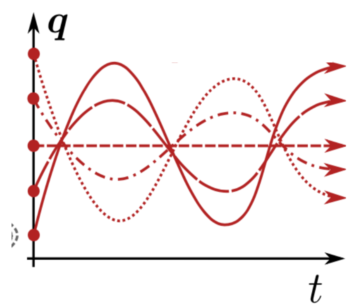


A focus on neutrino oscillation physics simulated on quantum computers

Matrix Product State



Phase-Space approach



Lacroix et al, Phys Rev. D106 (2022), Phys Rev D110 (2024).
Mangin Brinet, DL, Phys. Rev. D 113 (2026)
De Correc et al, APS Open science 1, (2026)

200 qubits → 300 qutrits → 2000 qubits

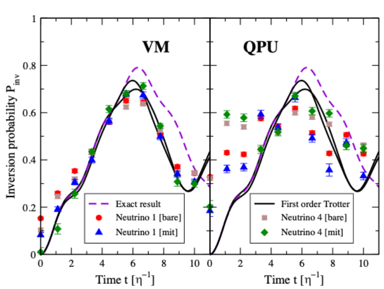
4 neutrinos
IBM-Vigo QPU

4 & 8 neutrinos
HQD-H1
Trapped Ion device

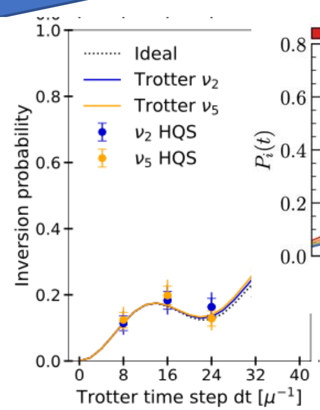
12 neutrinos
Quantinuum's H1-1

12 neutrinos / qutrits
H1-1 & ibm_torino

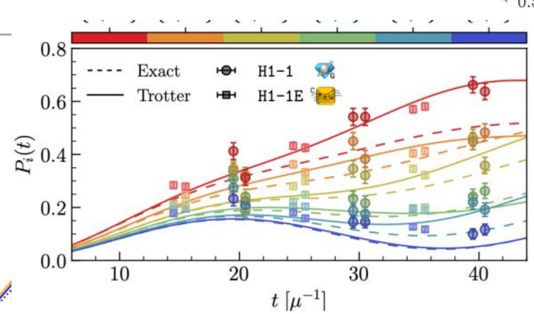
>100 neutrinos
IBM machines



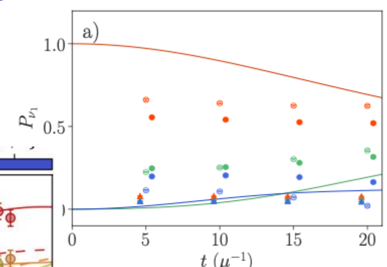
Hall, PRD 104 (2021)



Amitrano, PRD 107 (2023)

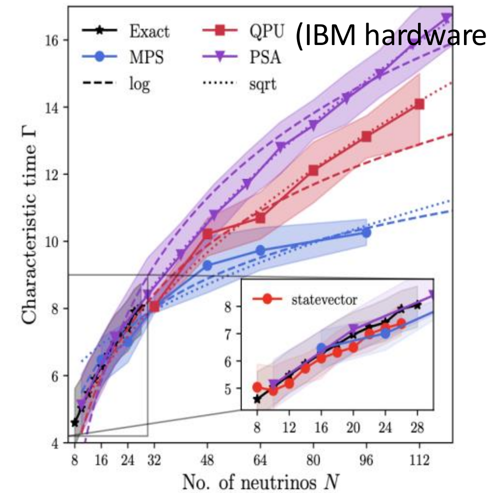


Illa, PRL 130 (2023)



Turro, PRD 111 (2025)

Neutrino thermalization time



Kiss, Tavernelli, Tacchino, Lacroix, Roggero, nature com., arxiv:2510.24841