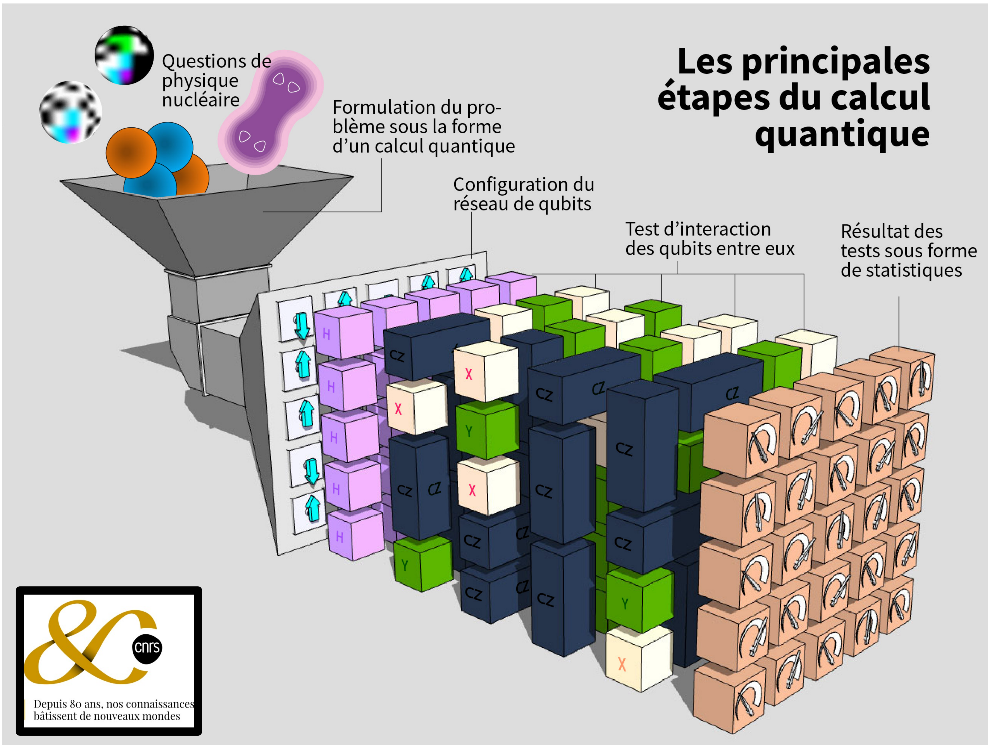
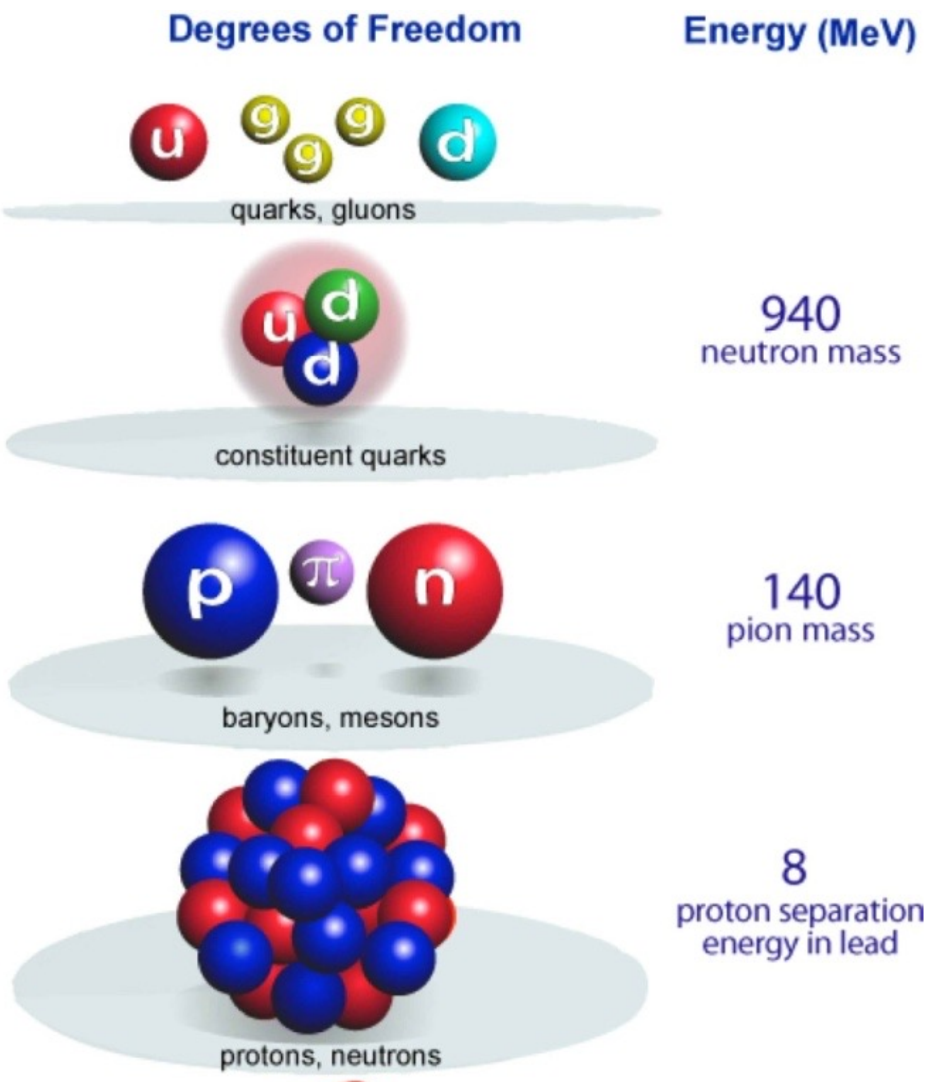
Quantum computing description of atomic nuclei: challenges and opportunities

Denis Lacroix (Paris-Saclay, IJCLab)

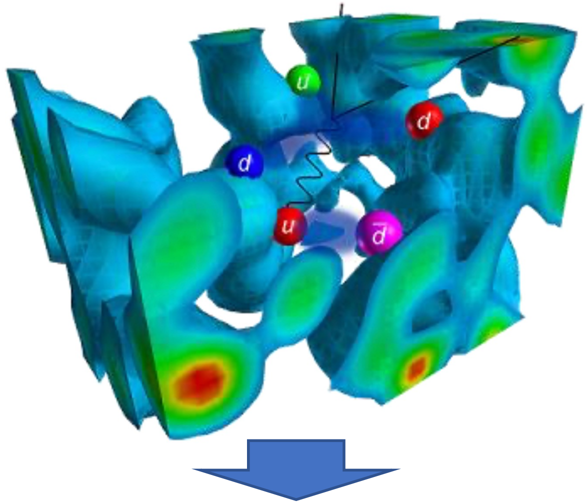


QC2I project

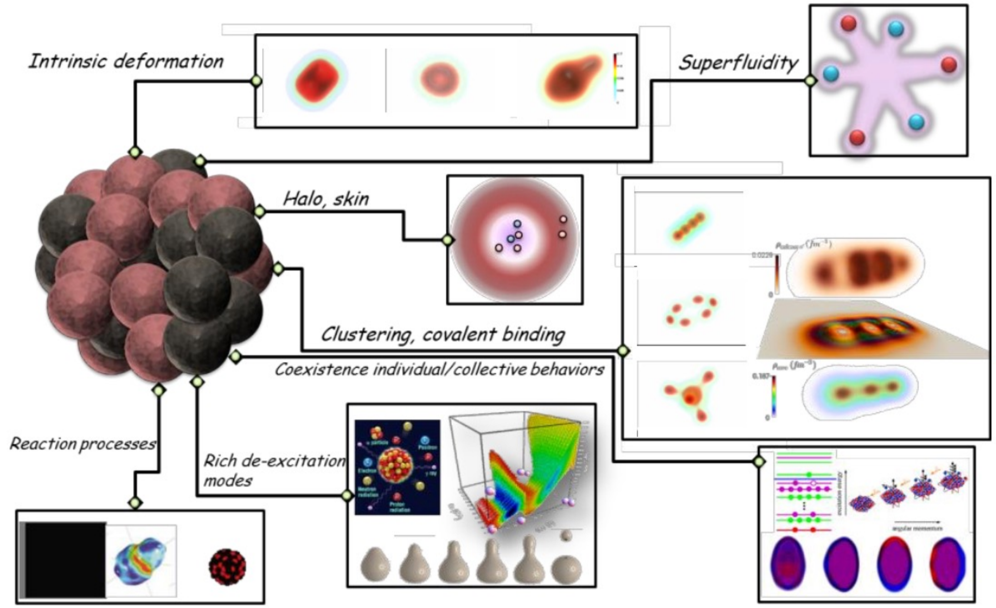
https://qc.pages.in2p3.fr/web/

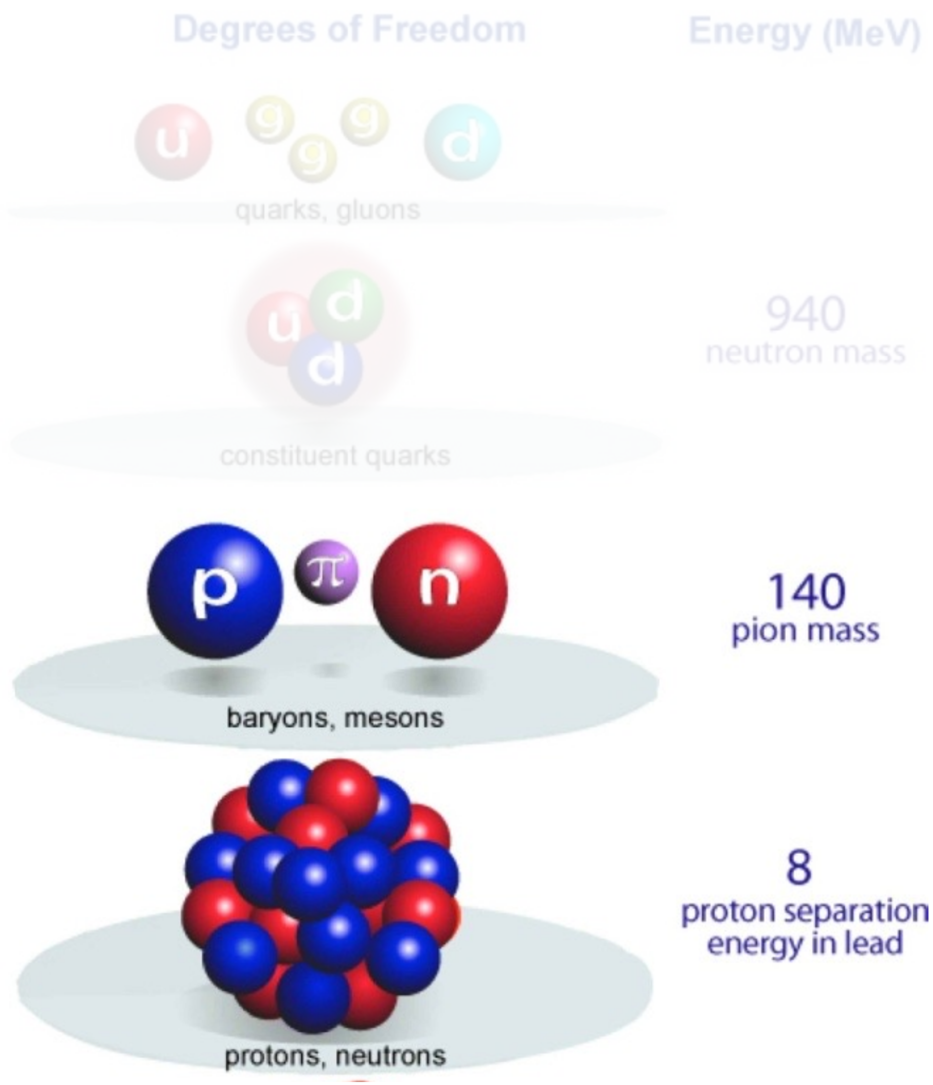


From QCD



to atomic nuclei phenomena

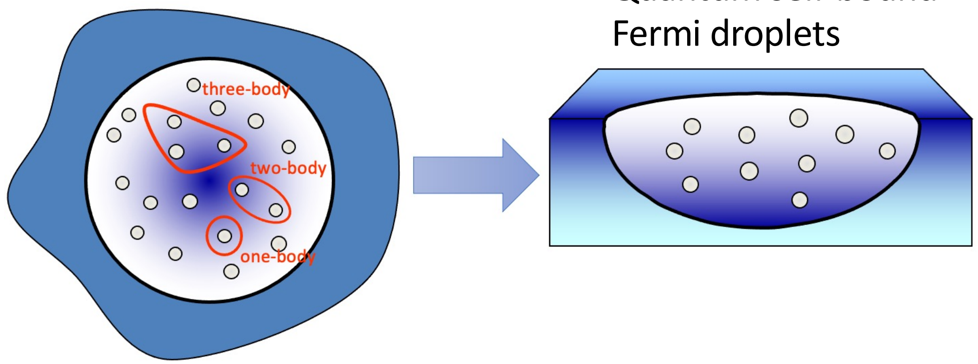




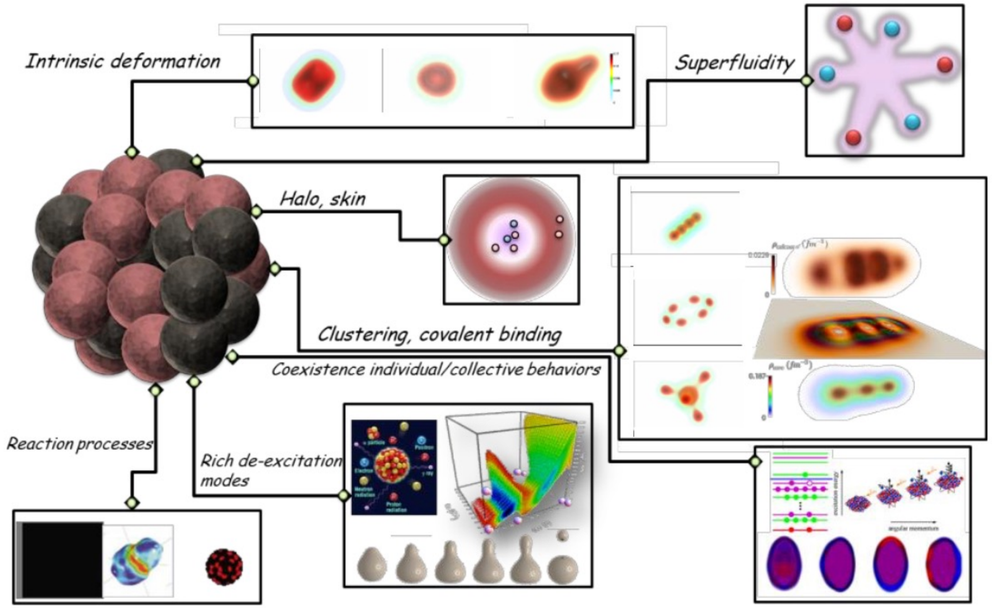
Some phenomenology

Strongly interacting fermions

Quantum self-bound
Fermi droplets

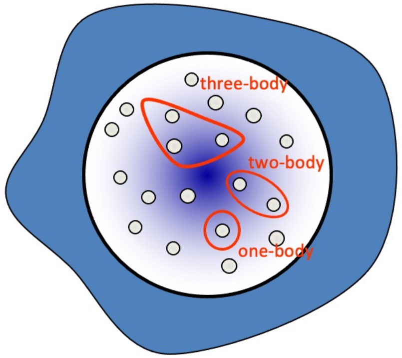


to atomic nuclei phenomena



Actual tendency : Towards Full Configuration-Interaction (ab-initio) description ?

Strongly interacting fermions

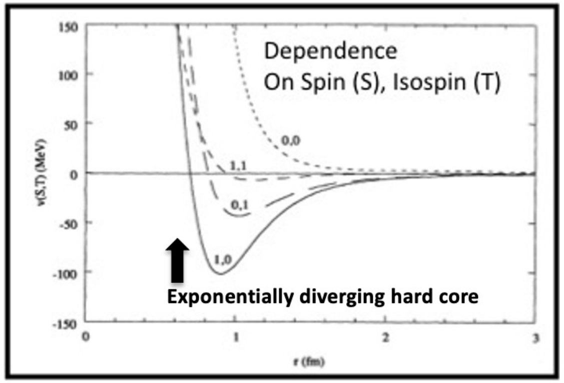


- Start from the full Hamiltonian
- Obtain the energy spectra

$$\phi_{\rm nucleon} \equiv \phi(\mathbf{r}, \sigma, \tau)$$

$\sigma = \uparrow, \downarrow$ spin

$\tau = n, p$ isospin

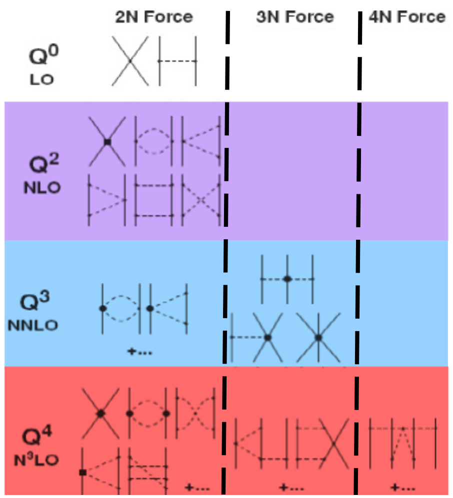


Wiringa, Rev. Mod. Phys. 1993

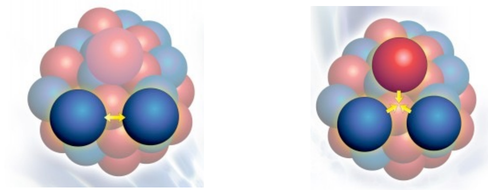
+ Coulomb field

Challenges

- The interaction is highly non-perturbative
- Starting from 2005: new generations of interactions were Developed getting rid of the short-range part



- Still the strong interaction is rather elusive: emergence of 3-body (and more generally multi-body) interaction

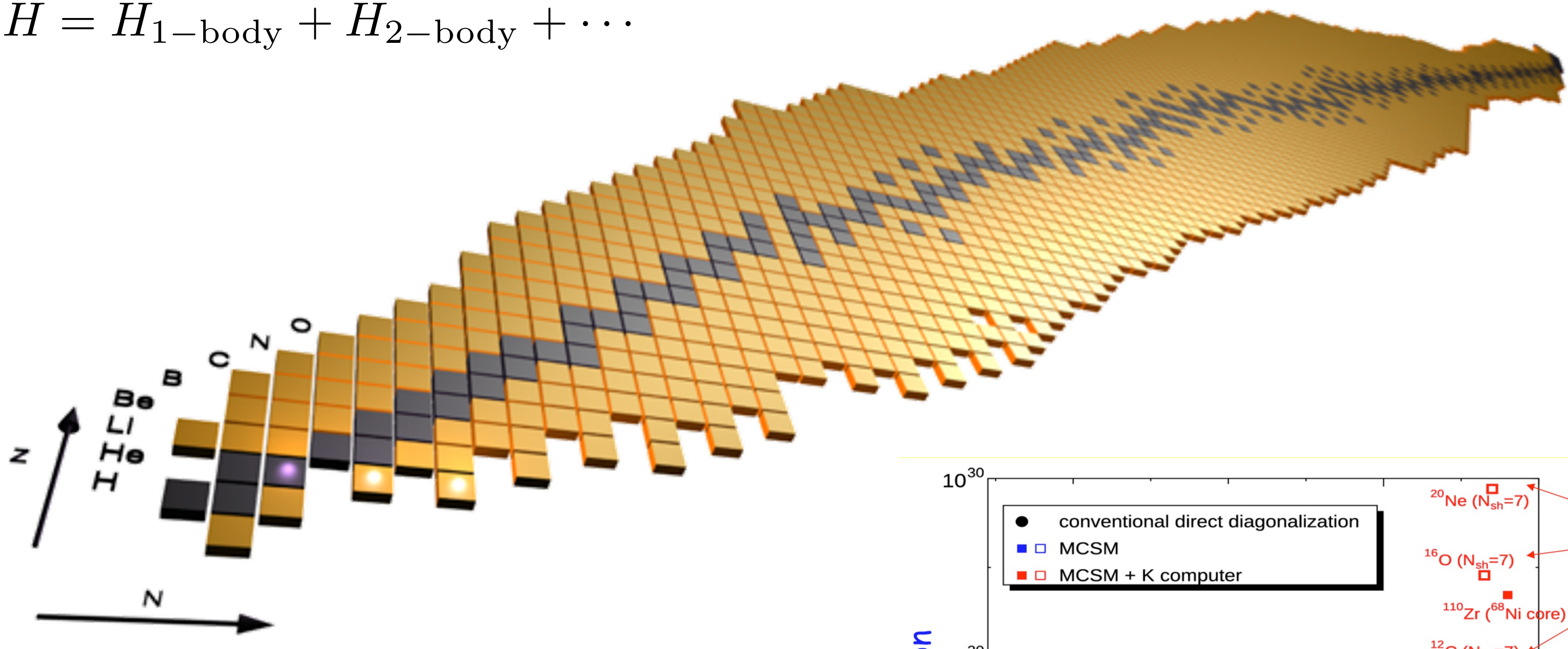


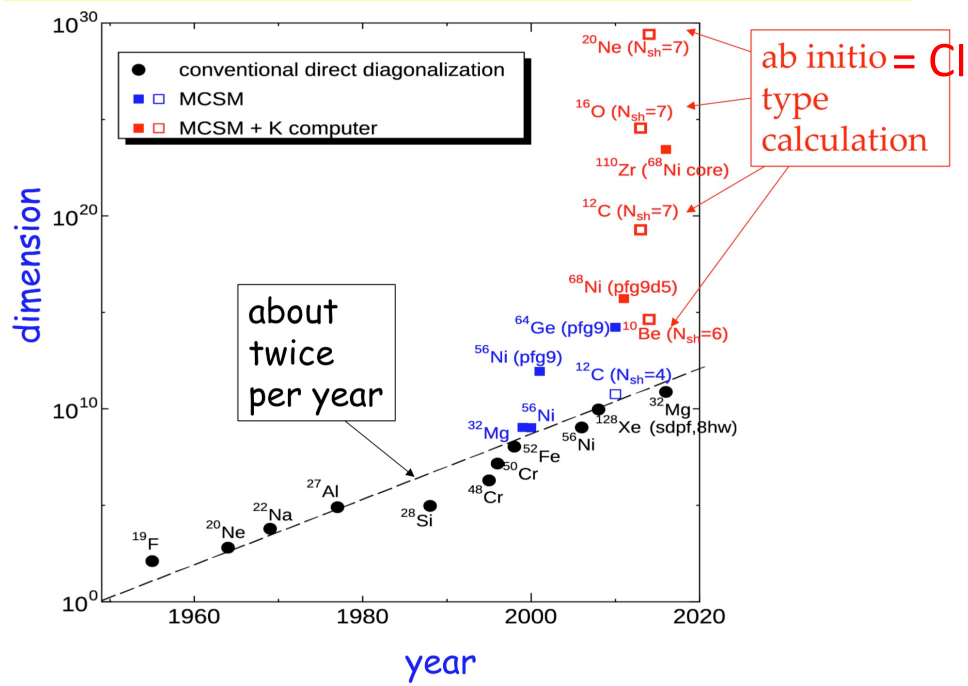
- So far, we can assume that we have a starting Hamiltonian

$$H = H_{1-\rm body} + H_{2-\rm body} + \cdots$$

Actual tendency : Towards Full configuration-Interaction description ?

$$H = H_{1-\text{body}} + H_{2-\text{body}} + \cdots$$





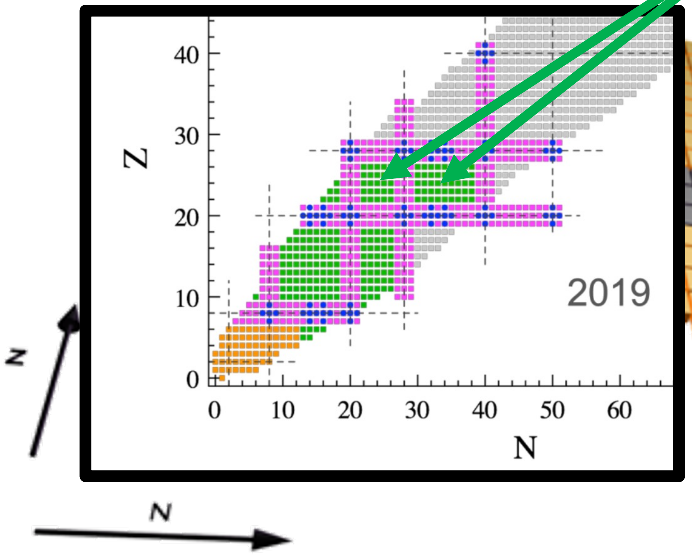
➡ Atomic nuclei are mesoscopic systems (particle Number ranges from 2 to 300+).
When mass increases we have an exponential growth of the Hilbert space

In *pf* shell :
^{56}Ni **1,087,455,228**
In *pf-sdg* space :
^{78}Ni **210,046,691,518**

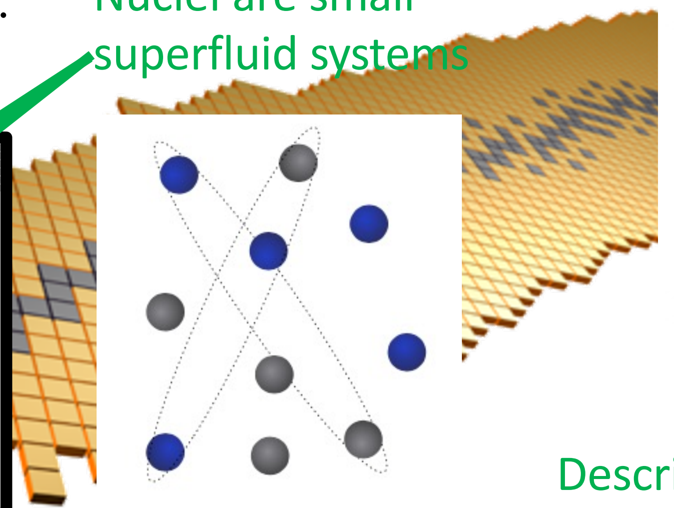
Actual tendency : Towards Full configuration-Interaction description ?

$$H = H_{1-\text{body}} + H_{2-\text{body}} + \cdots$$

Current status

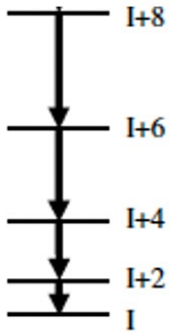


Nuclei are small superfluid systems



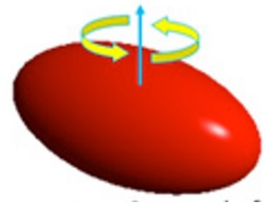
➡ Described by breaking U(1) symmetry

Nuclei do present rotational bands



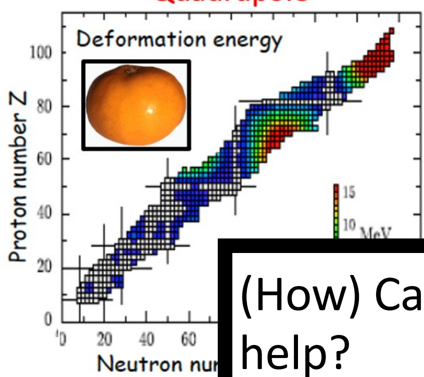
$$E_{\text{rot}} = \frac{I(I+1)}{2J}\hbar^2$$

Nuclei might be deformed

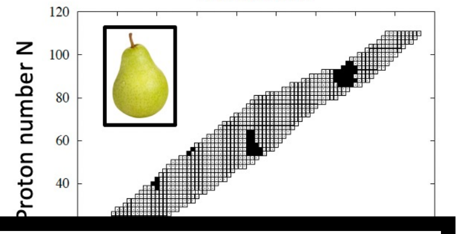


Described by breaking rotational and/or parity symmetry

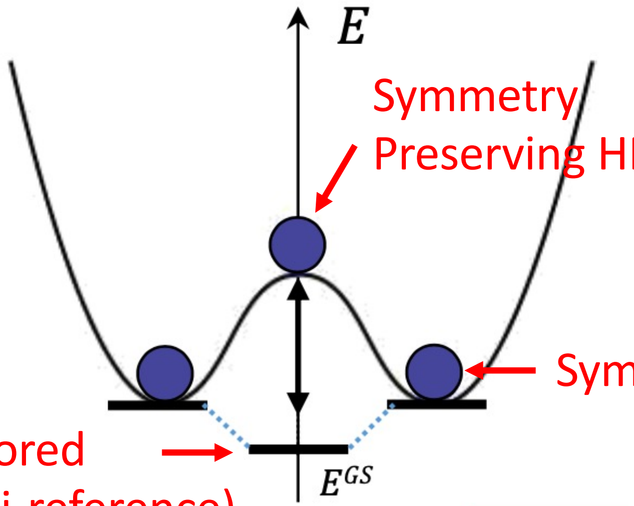
Quadrupole



Octupole



➡ A specificity: atomic nuclei like to break spontaneously symmetries

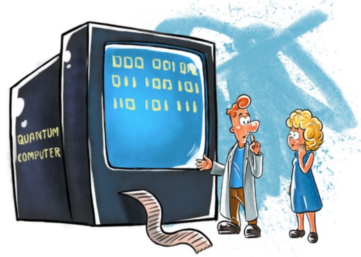


Symmetry Preserving HF state

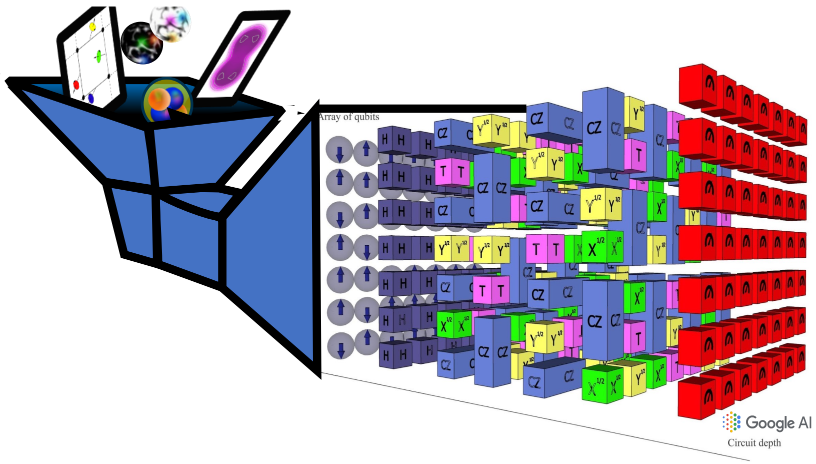
Symmetry Breaking (S

Symmetry Restored (SR) state (multi-reference)

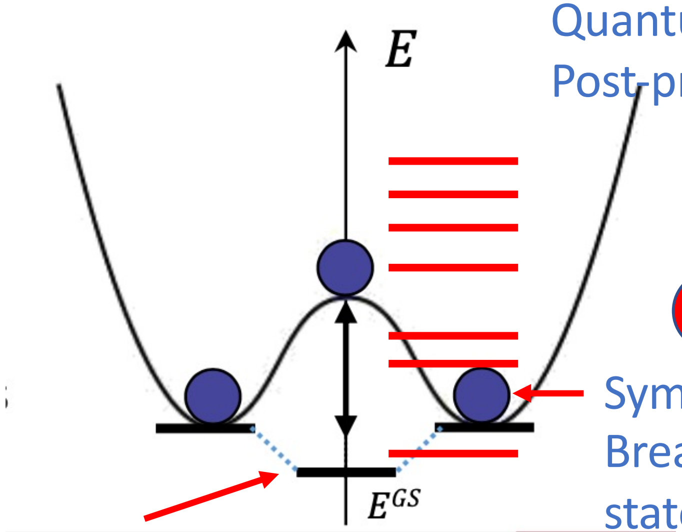
(How) Can Quantum computers help?



What we have started to do



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, …)

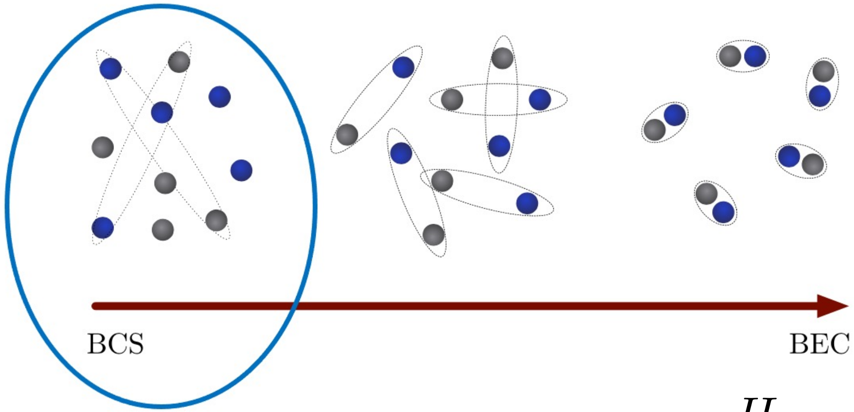
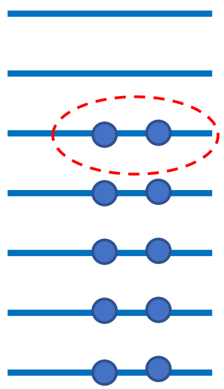


Illustration with small superconductors

Illustration with the Richardson Hamiltonian

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

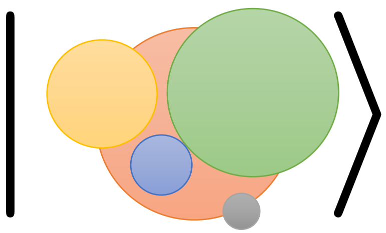


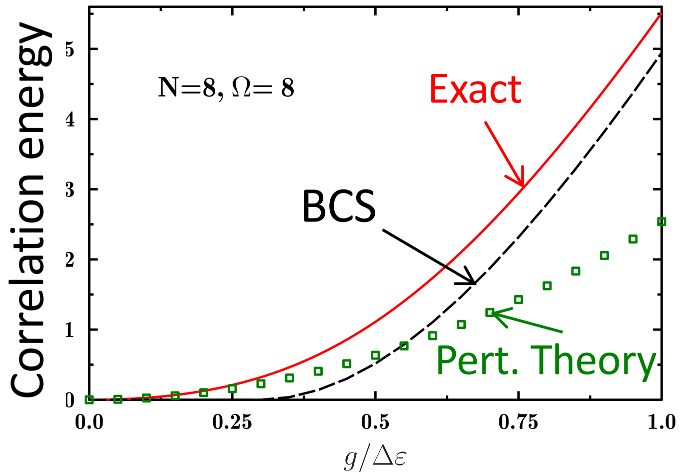
This problem is an archetype of spontaneous symmetry breaking.
An "easy" way to describe it is to break the particle number symmetry, i.e. consider wave-function that mixes different particle number

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

The particle number - U(1) symmetry)
is broken





But ultimately number of
Particle should be restored !

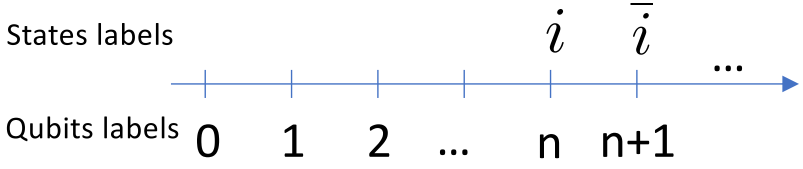
Hamiltonian and initial state

Pairing Hamiltonian

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

Jordan-Wigner transfo: $\frac{1}{2}(I_i - Z_i)$

State ordering is important !



$$a_i^\dagger a_{\bar{i}}^\dagger \Rightarrow Q_n^+ Q_{n+1}^+$$

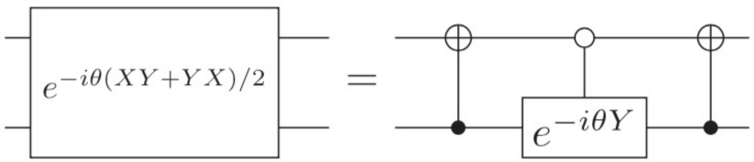
Initial (symmetry breaking) state preparation

$$|\Psi\rangle = \exp\left\{ -\sum_{i>0} \varphi_i \left(a_i^\dagger a_{\bar{i}}^\dagger - a_{\bar{i}} a_i \right) \right\} |0\rangle \quad \xrightarrow{\varphi_i = \varphi} \quad |\Psi\rangle = \prod_{n>0} e^{i\varphi(X_n Y_{n+1} + Y_n X_{n+1})/2} |-\rangle$$

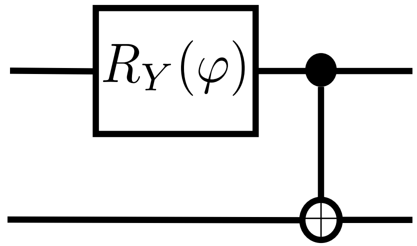
Simplified circuit (generalized Bell state)

$$|\Psi\rangle = \prod_n \left[\cos\left(\frac{\varphi}{2}\right) I_n \otimes I_{n+1} + \sin\left(\frac{\varphi}{2}\right) Q_n^+ Q_{n+1}^+ \right] |-\rangle$$

Equivalent universal gate on pairs



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

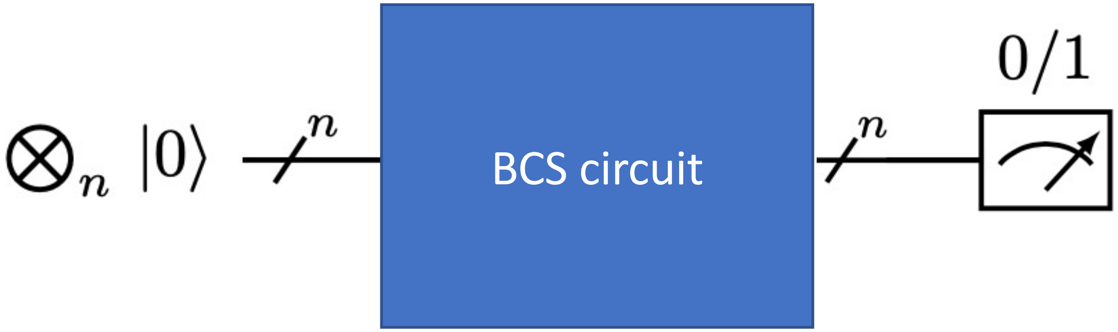


All calculations here are done with IBM qiskit toolkit

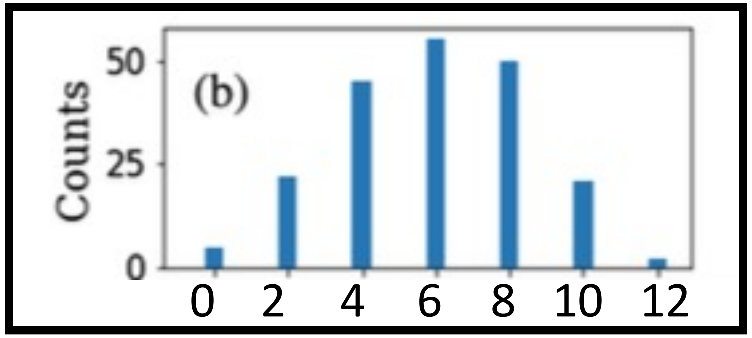
Restoration of particle number symmetry

The counting statistics problem

Direct estimate of Counting statistics

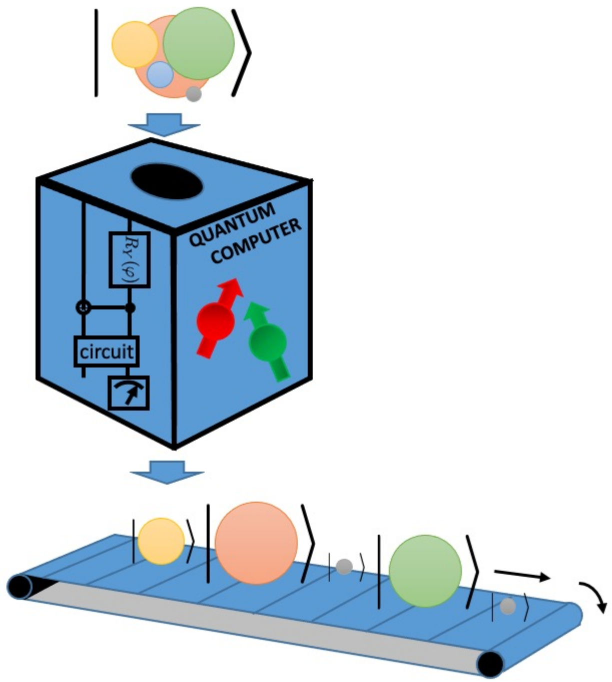


Example of mixing for 12 qubits (with qiskit)



Projection on particle number

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



For 2 qubits

$$|\Psi\rangle = \alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle$$

$$|N=0\rangle \qquad \propto |N=1\rangle \qquad |N=2\rangle$$

A possible way to perform the projection is to use
The Quantum-Phase-Estimation method with *N* itself

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

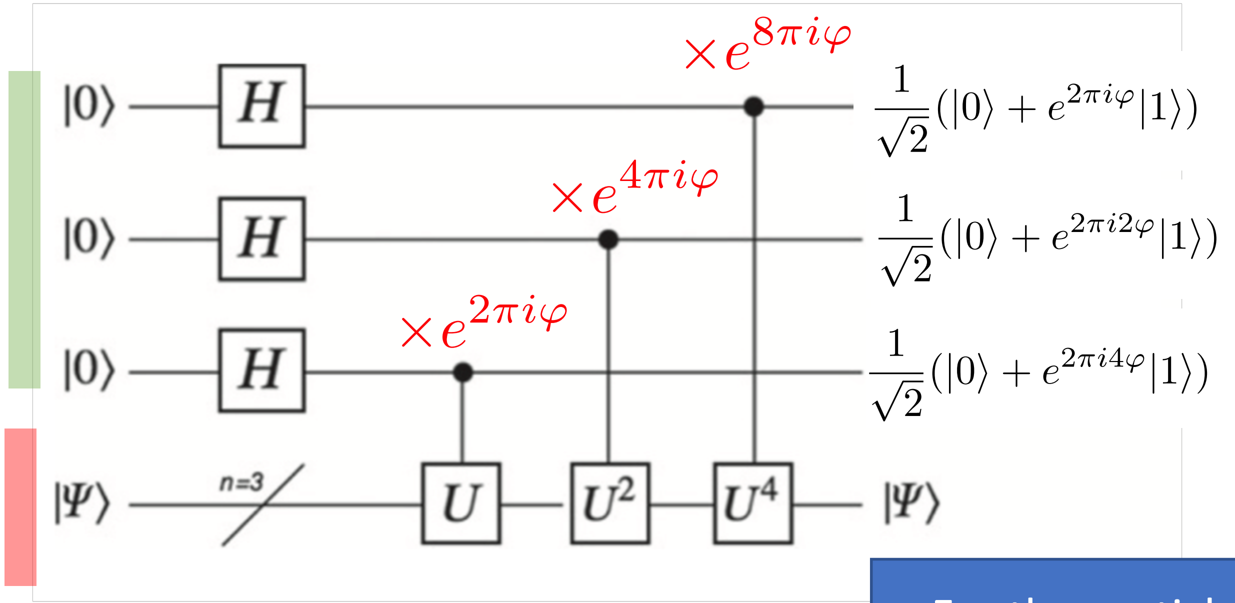
For known eigenvalue problems

Assume a unitary operator U

Assume an eigenstate $|\Psi\rangle$ Such that $U|\Psi\rangle = e^{2\pi i\varphi}|\Psi\rangle$

nr Register qubits

Working qubits



QFT $^{-1}$

$$|2^{n_r}\varphi\rangle \otimes |\Psi\rangle$$

General Case

$$|\Psi\rangle = \sum_k \alpha_k|\phi_k\rangle \xrightarrow{\text{QPE}} \sum_k \alpha_k|\theta_k 2^{n_r}\rangle \otimes |\phi_k\rangle$$

register eigenstate

For the particle number projection

$$U = U_N = e^{2\pi i \frac{N}{2^{n_r}}} \quad \text{with} \quad N = \frac{1}{2}\sum_i (I_i - Z_i)$$

Assume eigenvalues $\{0, 1, \cdots, A\}$

Constraint: $0 \leq \frac{A}{2^{n_r}} < 1$ then $\frac{A}{2^{n_r}} = 0.a_1 \cdots a_{n_r - 1}$

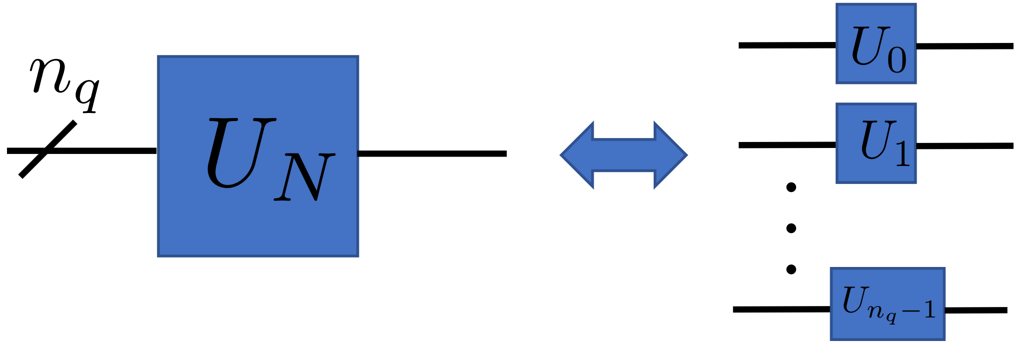
If I measure given binary number in the ancillary qubit. After measurement, I have the projection on the associated particle number component

Practical details

$$U_N = \prod_j U_j$$

$$U_i = |0_i\rangle\langle 0_i| + \exp(i\pi/2^{n_0-1})|1_i\rangle\langle 1_i|$$

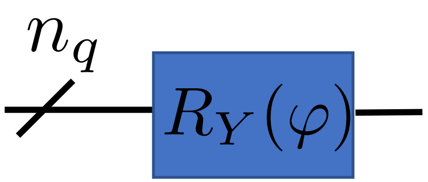
$$U_i = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/2^{n_0-1}} \end{bmatrix}$$



Example: Qubit counting statistics

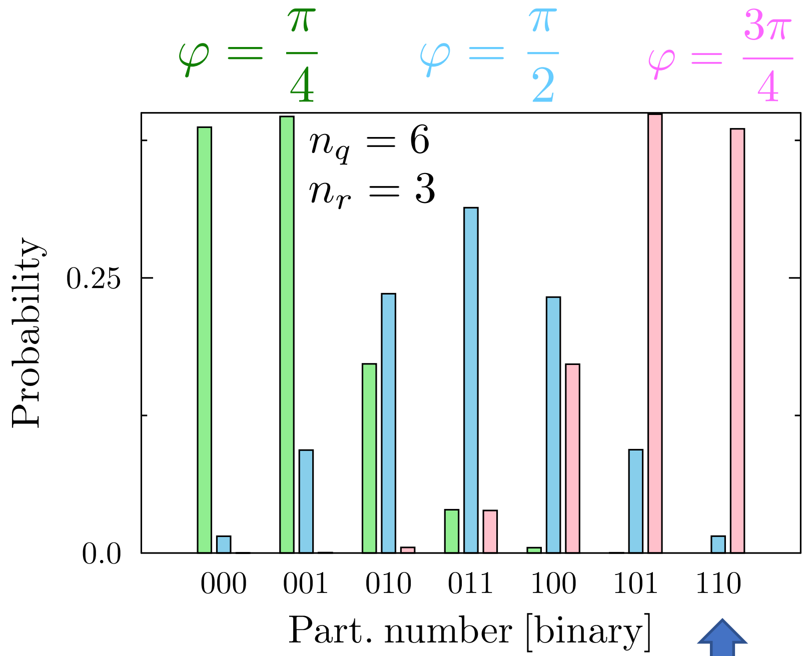
Initial state

$\bigotimes |0_j\rangle$



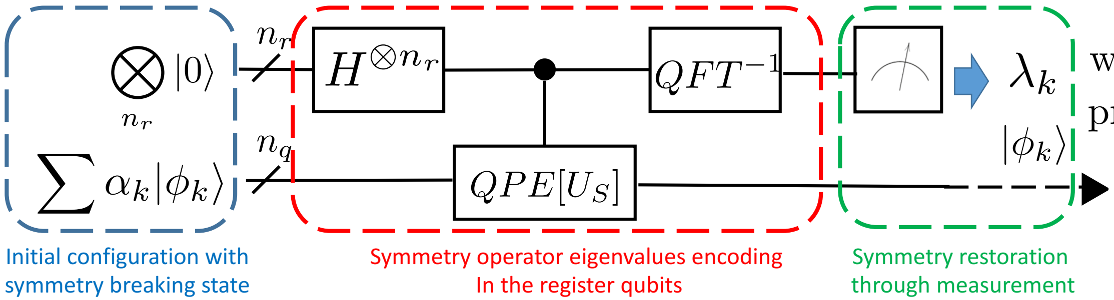
$\bigotimes [\cos(\varphi/2)|0_j\rangle + \sin(\varphi/2)|1_j\rangle]$

$$P(A) = C_{n_q}^A p^A (1-p)^{n_q-A}$$
$$p = \sin^2(\varphi/2)$$



$$6/2^4 = 1/2 + 1/4 + 0/8 \equiv [110]$$

Eigenvalues-Ground state and excited states



Measurement

Example of an event:

$$|011\cdots010\rangle^{(\lambda)} \otimes |\phi_{A^{(\lambda)}}\rangle$$

$$= A^{(\lambda)}$$

BCS/HFB state

$$|\Psi\rangle = \prod_n \left[\cos\left(\frac{\varphi}{2}\right) I_n \otimes I_{n+1} + \sin\left(\frac{\varphi}{2}\right) Q_n^+ Q_{n+1}^+\right] |-\rangle$$

Measurement

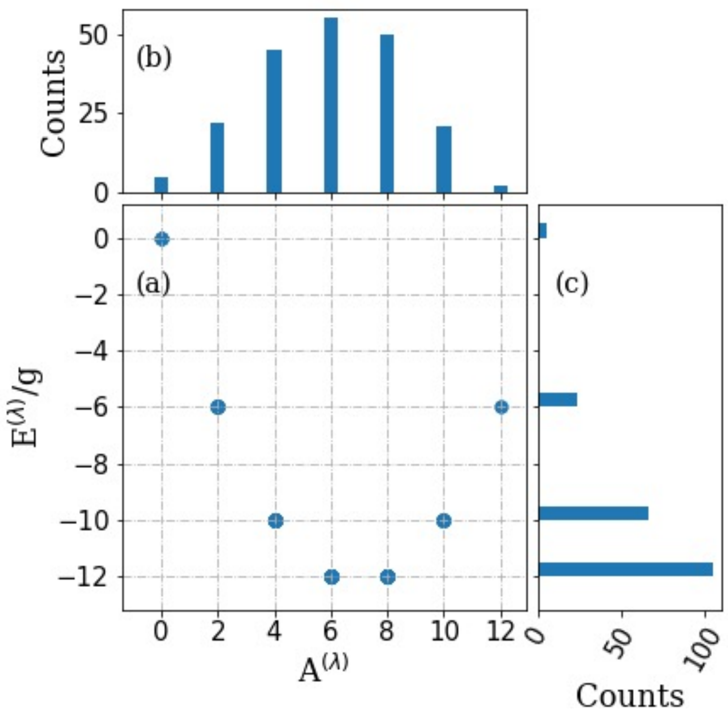
Projected BCS or with varying number Of particles

Degenerate case

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

$$\langle \phi_{A^{(\lambda)}} | H | \phi_{A^{(\lambda)}} \rangle$$

6 pairs



Exact solution

$$E/g = -\frac{1}{4}(A - \nu)(2n_q - A - \nu - 2).$$

H was encoded on the full Fock space with $A < n_q$

For the degenerate case, this should give the exact solution

Use the QPE approach for operators with known eigenvalues to obtain entangled states

Hypothesis:

- Assume a hermitian operator *S* acting on *nq* qubits
- Assume that *S* has discrete eigenvalues $\{\lambda_0 \leq \cdots \leq \lambda_M\}$ with $\lambda_k = a m_k$, $a = \mathrm{cst}$
- Define the operator

$$U_S = \exp\left\{2\pi i \left[\frac{S - \gamma_0}{a 2^{n_0}}\right]\right\}$$

- Eigenvalues of U_S are given by $e^{2\pi i \theta_k}$ with $\theta_k = (m_k - m_0)/2^{n_0}$

If $(m_k - m_0) < 2^{n_0}$ ⇒ $\theta_k < 1$

and θ_k is exactly written as a binary fraction

⇒ It is then optimal for the QPE use.
An optimal choice for the number of register qubits is $n_r = n_0$

and $n_r - 1 \leq \ln(m_k - m_0)/\ln 2 < n_r$.

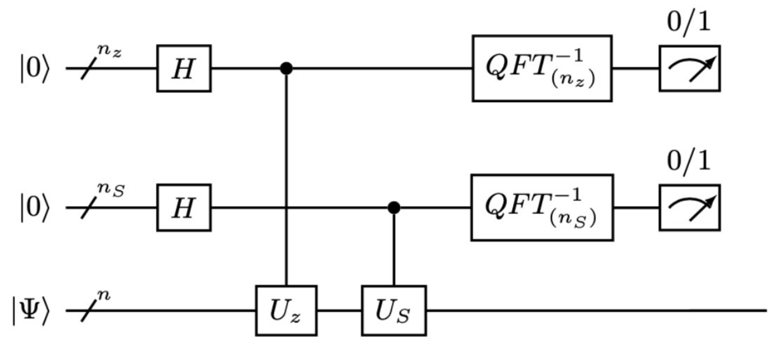
Examples

- parity
- Part. number
- $J_z = \hbar m$
- $J^2 = \hbar^2 j(j+1)$

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

Projection on $\mathbf{S}^2$ and S_z components

$$|\Psi\rangle = \sum_{s_i \in \{0,1\}} \Psi_{s_1,\cdots,s_N} |s_1,\cdots,s_n\rangle. \quad \Rightarrow \quad |\Psi\rangle = \sum_{S,M} \sum_{g=1}^{d_{S,M}} c^g_{S,M} |S,M\rangle_g.$$



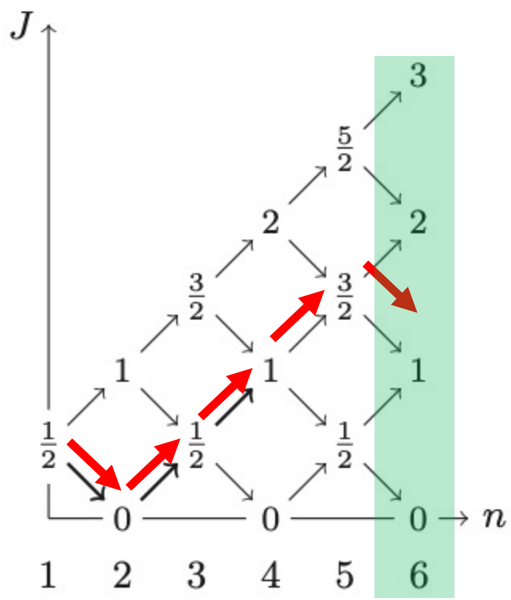
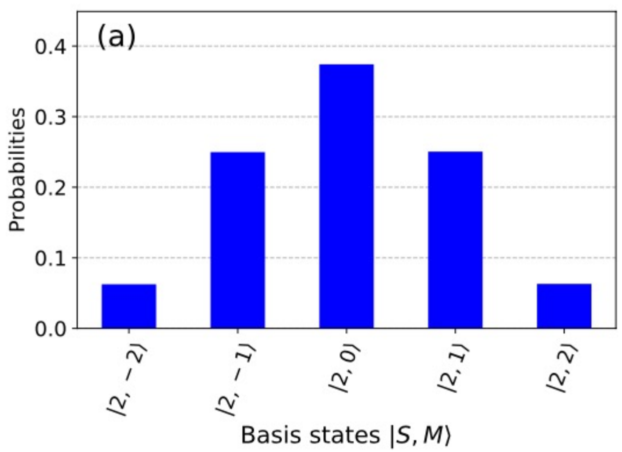
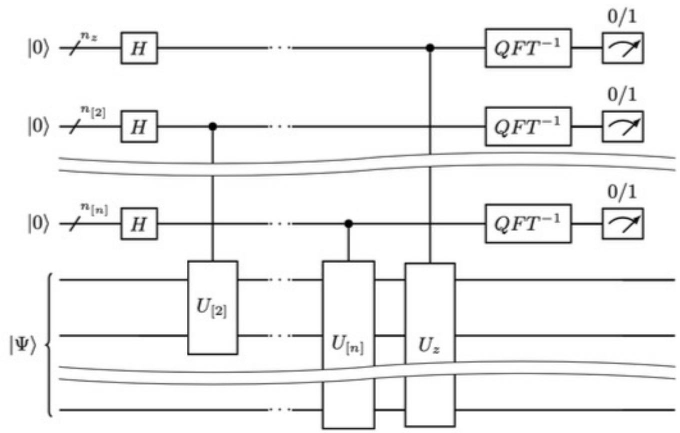


Illustration $|\Psi\rangle = \bigotimes_n H|0\rangle$



The full basis can eventually be constructed



P. Siwach and DL, arXiv:2106.10867

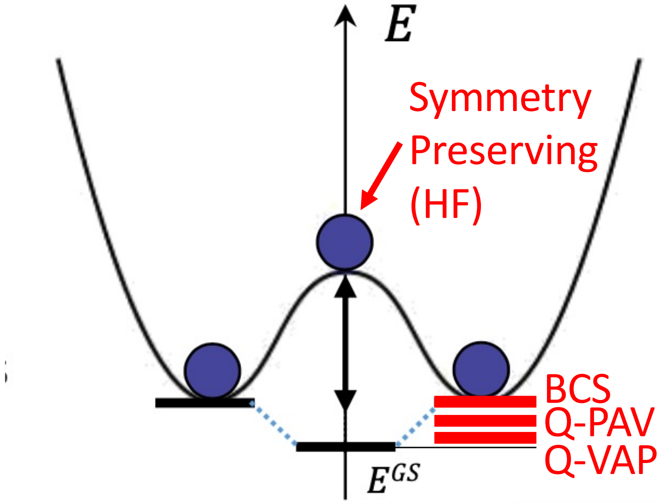
Coming back to our superconducting problem

Combining projection with variational method

Possible optimization schemes

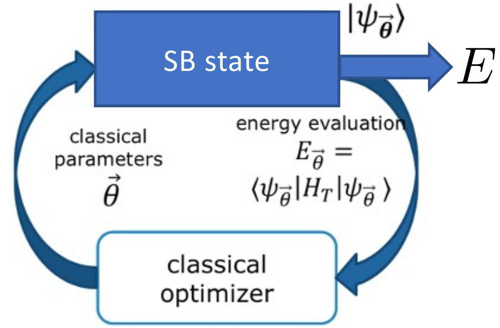
Pair occupation are now encoded

Variational
Symmetry-Breaking ansatz $|\Psi(\{\theta_p\})\rangle = \bigotimes_{p=1}^{N-1} [\sin(\theta_p)|0_p\rangle + \cos(\theta_p)|1_p\rangle]$

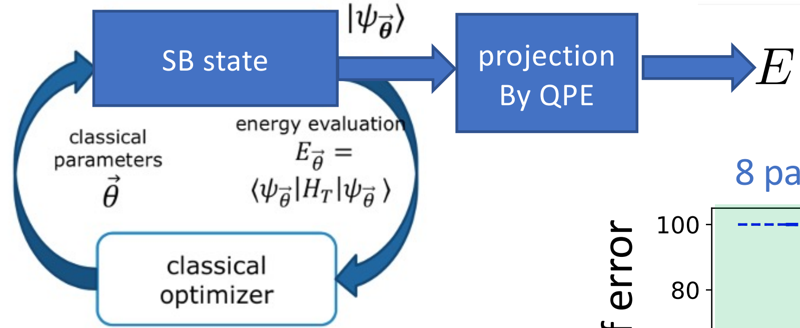


Quantum-Classical optimizers

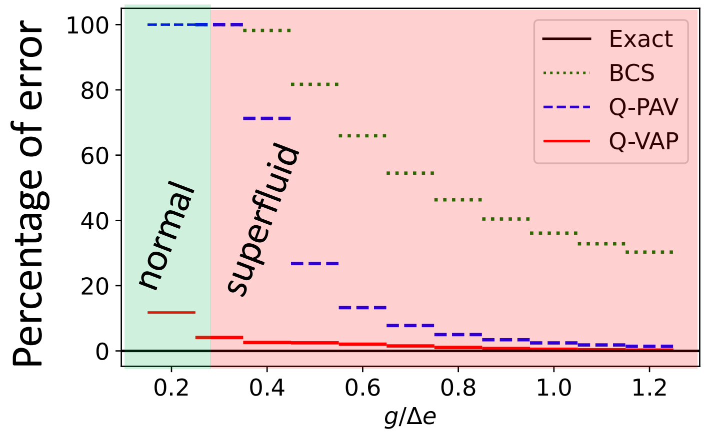
→ Standard BCS theory



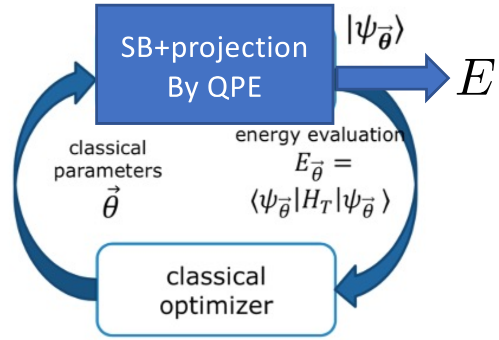
→ Project after optimization
Q-PAV: Quantum Projection After Variation



8 particles on 8 equidistant levels

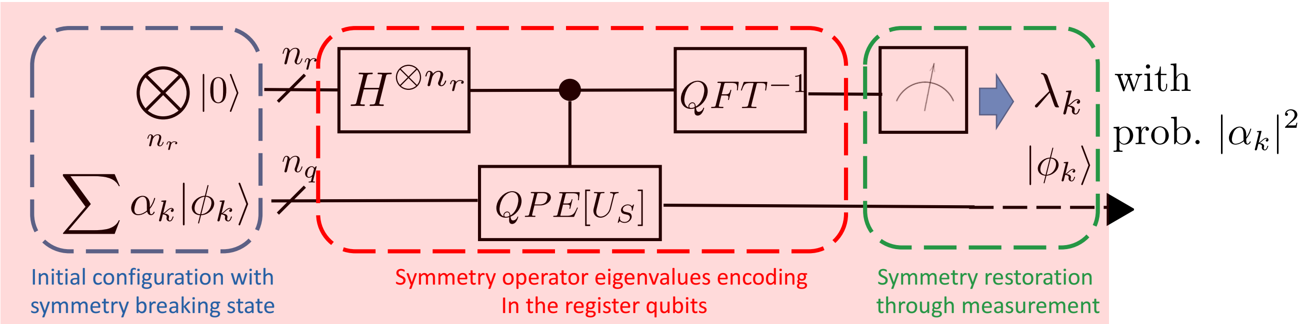


→ The optimization is made on the Symmetry restored state.
Q-VAP: Quantum Variation After Projection



Post-processing of projected states

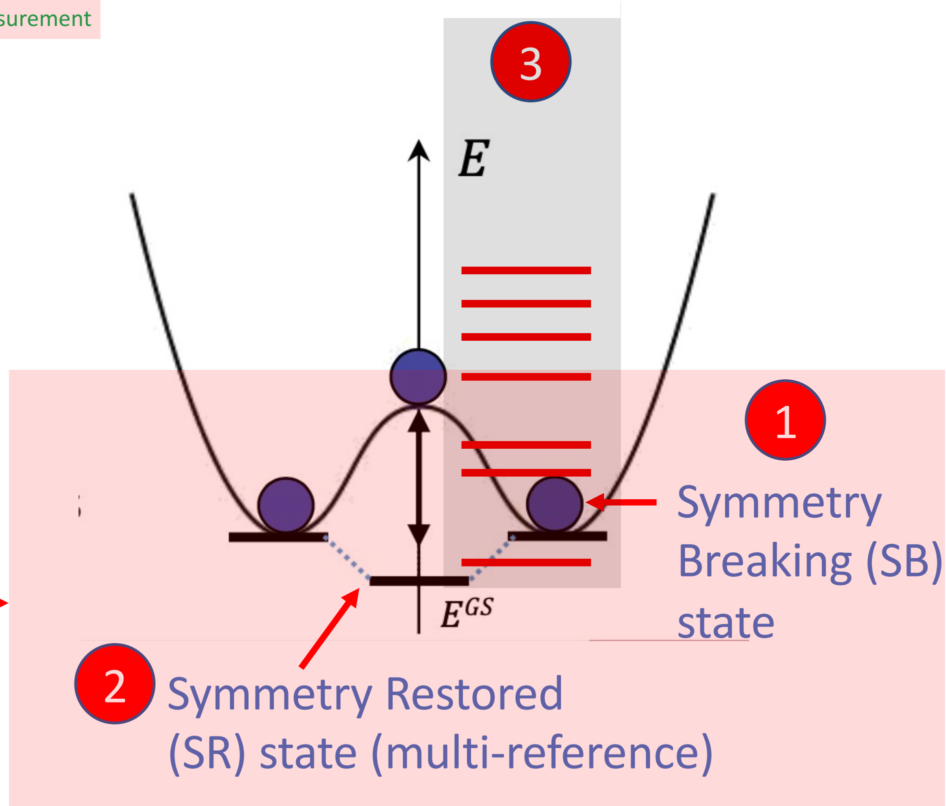
Complete strategy



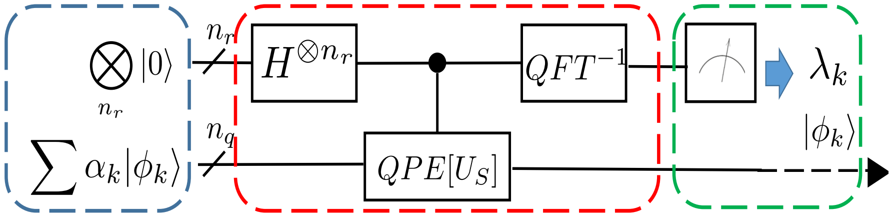
Initial state preparation
(HF, BCS, P-VAP, Q-VAP)

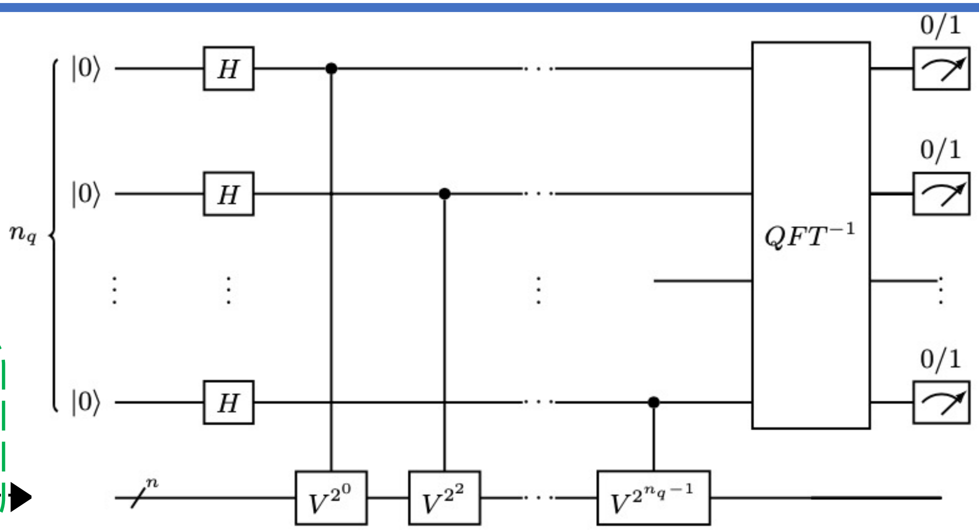
➡ Purely quantum method:
Quantum Phase Estimation

➡ Hybrid Quantum-Classical
Quantum Krylov method



Initial state preparation





Some technical details

$$V = \exp\left\{-2\pi i \left(\frac{H - E_{\min}}{E_{\max} - E_{\min}}\right)\right\}$$

For the propagator, we used the Trotter-Suzuki method

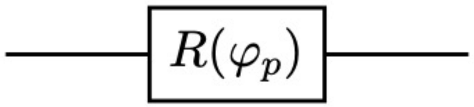
$$U(\tau) = e^{-i\tau H}$$

$$U(\tau) = \prod U(\Delta\tau) \longrightarrow \prod U_\varepsilon(\Delta\tau) U_g(\Delta\tau)$$

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

$$\prod_p \begin{pmatrix} 1 & 0 \\ 0 & \exp\left(-2i\tilde{\varepsilon}_p \Delta t\right) \end{pmatrix} \qquad \prod_{p>q} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\lambda_{pq}) & i\sin(\lambda_{pq}) & 0 \\ 0 & i\sin(\lambda_{pq}) & \cos(\lambda_{pq}) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

with $\lambda_{pq} = g\Delta t$



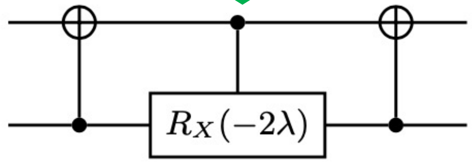
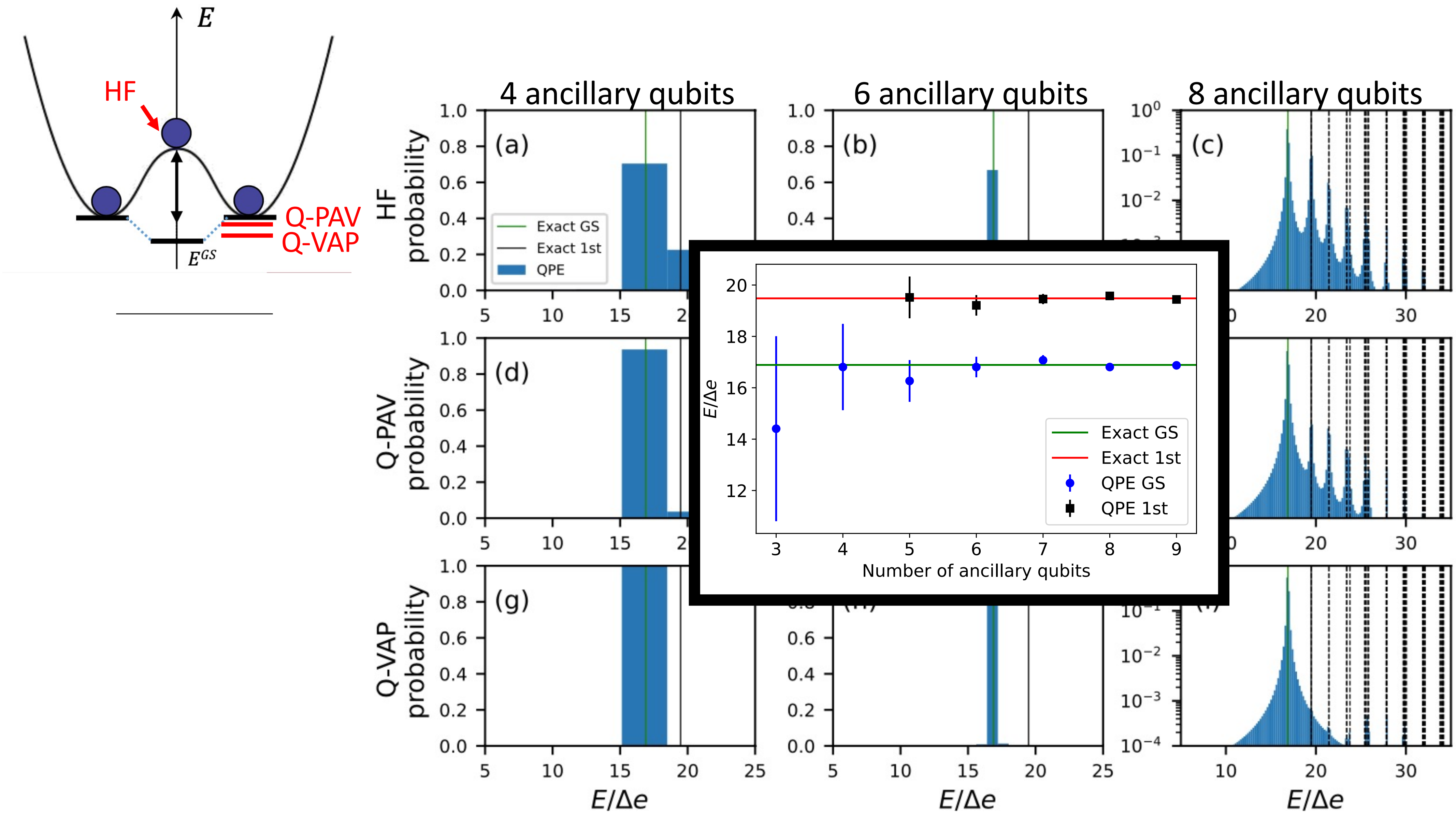
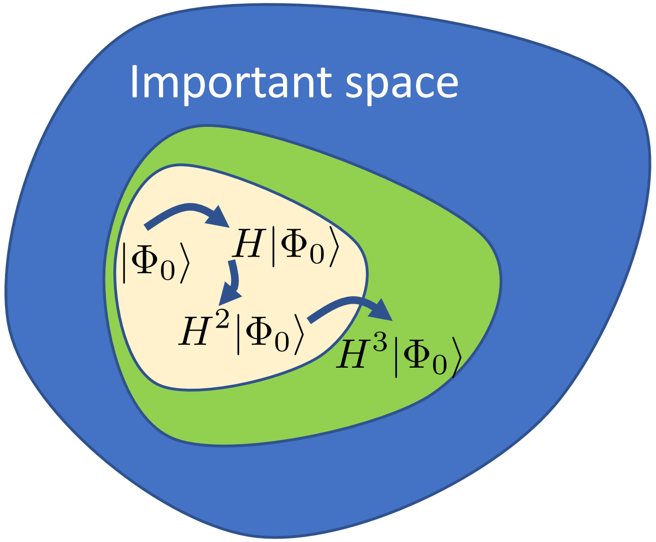


Illustration of the QPE method with projected state



Hilbert space



Our strategy

Compute overlap and Hamiltonian matrix elements on the quantum computer

Solve the eigenvalue problem on the classical computer

$$\{|\Psi\rangle,\ H|\Psi\rangle, \cdots,\ H^{M-1}|\Psi\rangle\} \equiv \{|\Phi_i\rangle\}_{i=0,M-1}$$

Diagonalize in the non-orthogonal subspace

$$O_{ij} = \langle \Phi_i | \Phi_j \rangle \qquad H_{ij} = \langle \Phi_i | H | \Phi_j \rangle$$

Generalized eigenvalue problem

$$|\xi_\alpha\rangle = \sum_n c_n(\alpha)|\Psi_n\rangle \Rightarrow \sum_n c_n(\alpha) H_{in} = E_\alpha \sum_n c_n(\alpha) O_{in}$$

Our first attempt: use the generating function of H

$$F(t) = \langle \Phi_0 | e^{-itH} | \Phi_0 \rangle$$

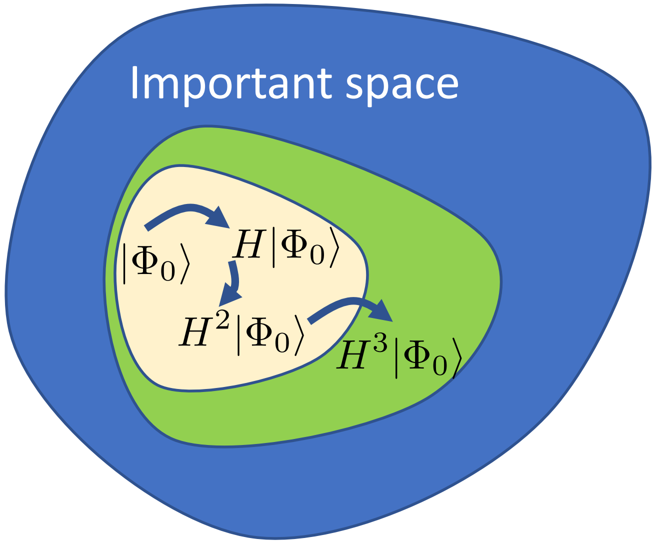
$$F(t) = 1 - it\langle H \rangle_0 + \frac{(-it)^2}{2}\langle H^2 \rangle_0 + \cdots$$

$$\langle H^K \rangle_0 = i^K \left. \frac{d^K F(t)}{dt^K} \right|_{t=0}$$

E. A. Ruiz-Guzman and DL, arXiv:2104.08181

Quantum Krylov method

Highly Truncated Hilbert space

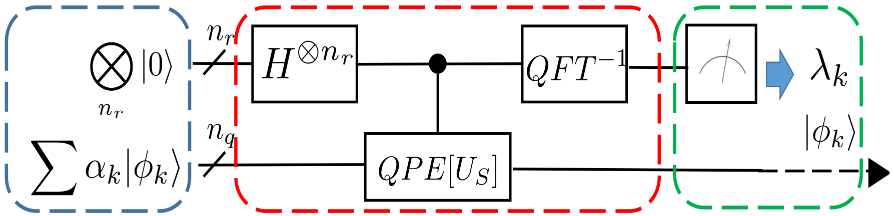


$$\{|\Psi\rangle,\ H|\Psi\rangle, \cdots,\ H^{M-1}|\Psi\rangle\} \equiv \{|\Phi_i\rangle\}_{i=0,M-1}$$

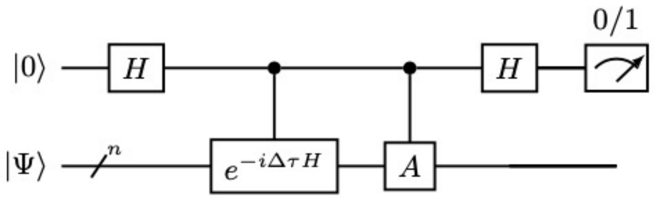
$$\{|\Psi\rangle,\ e^{-i\tau_1 H}|\Psi\rangle, \cdots,\ e^{-i\tau_{M-1} H}|\Psi\rangle\}$$

$$O_{ij} = \langle\Phi_i|\Phi_j\rangle = \langle\Psi|e^{-i(\tau_j-\tau_i)H}|\Psi\rangle \qquad H_{ij} = \langle\Psi|He^{-i(\tau_j-\tau_i)H}|\Psi\rangle$$

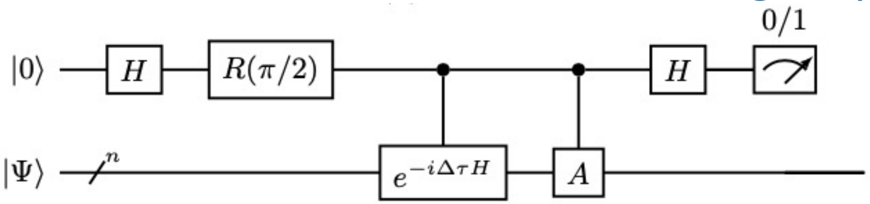
Initial state preparation



Hadamard test for the real part of *O* and *H*

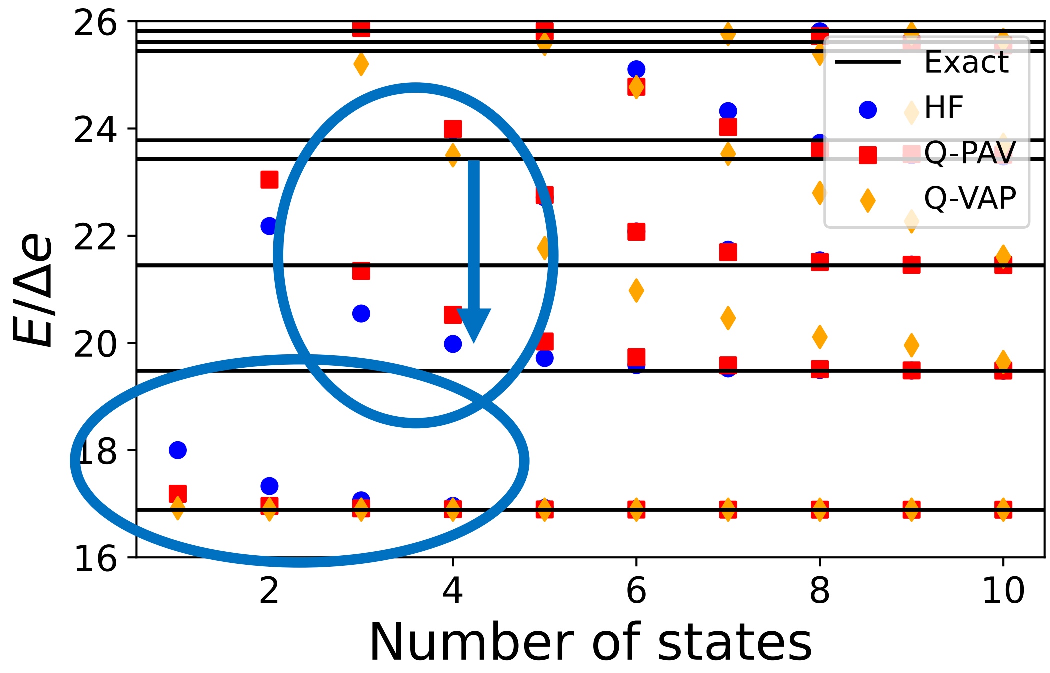


Modified Hadamard test for the imaginary part

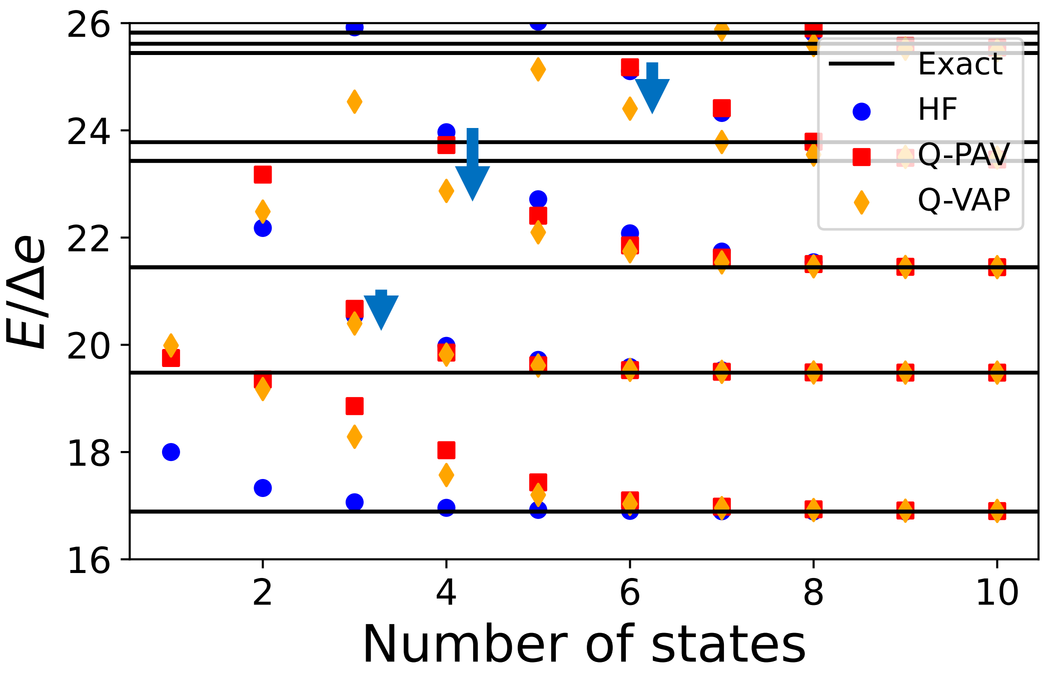


Diagonalization on a classical computer

Comparison QPE vs Quantum Kr



- The combination of Q-VAP + Quantum Krylov Is very good for the Ground state
- But Q-VAP + Quantum Krylov is worth than others for excited states



A possible solution

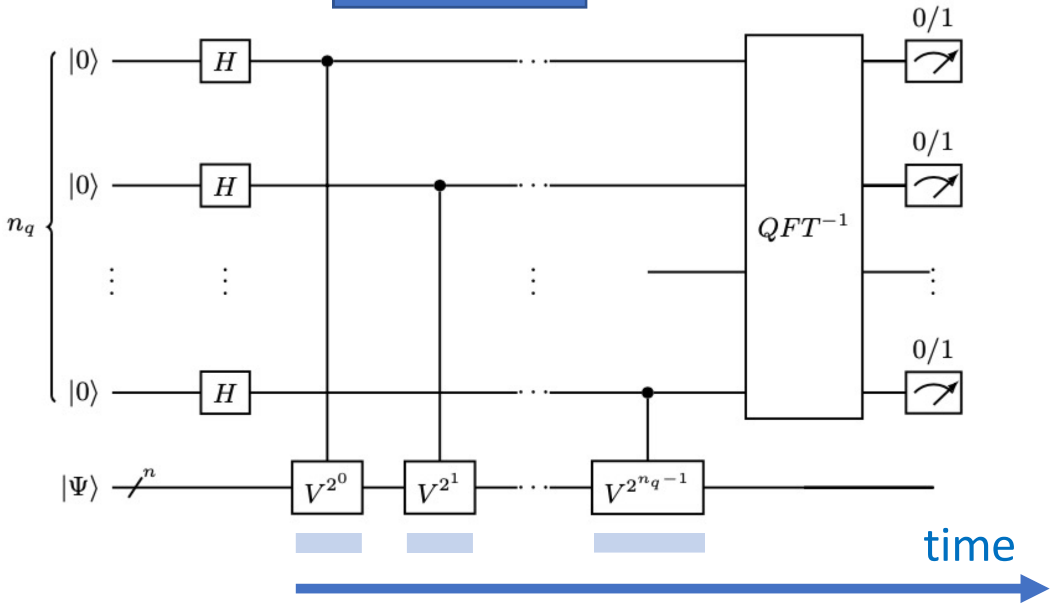
$$|\Psi\rangle = \bigotimes_p [\sin(\theta_p)|0_p\rangle + \cos(\theta_p)|1_p\rangle]$$

$$|\Psi'\rangle = [-\cos(\theta_i)|0_i\rangle + \sin(\theta_i)|1_i\rangle] \bigotimes_{p\neq i} [\sin(\theta_p)|0_p\rangle + \cos(\theta_p)|1_p\rangle]$$

$$\langle\Psi'|\Psi\rangle = 0$$

Comparison QPE vs Quantum Krylov after Q-VAP

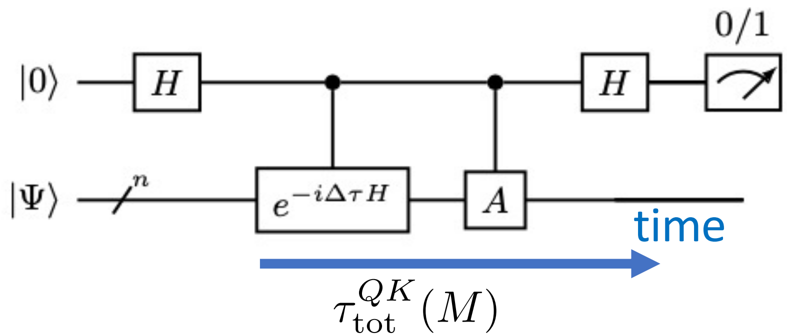
QPE

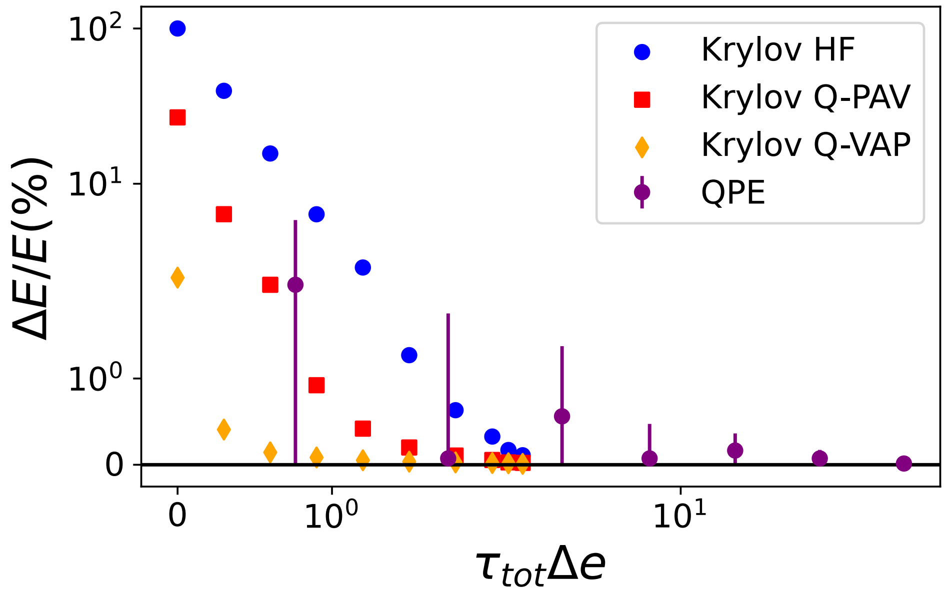


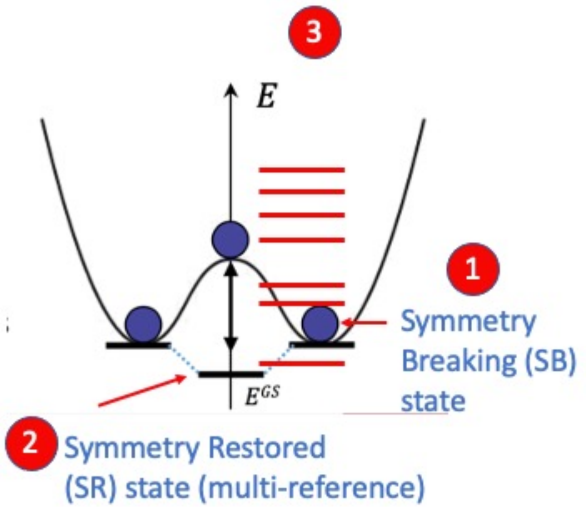
$$\tau_{\text{QPE}} + 2\tau_{\text{QPE}} + \cdots + 2^{n_q-1}\tau_{\text{QPE}}$$

$$\tau_{\text{tot}}^{\text{QPE}}(n_q) = \left(2^{n_q} - 1\right)\tau_{\text{QPE}}$$

Quantum Krylov





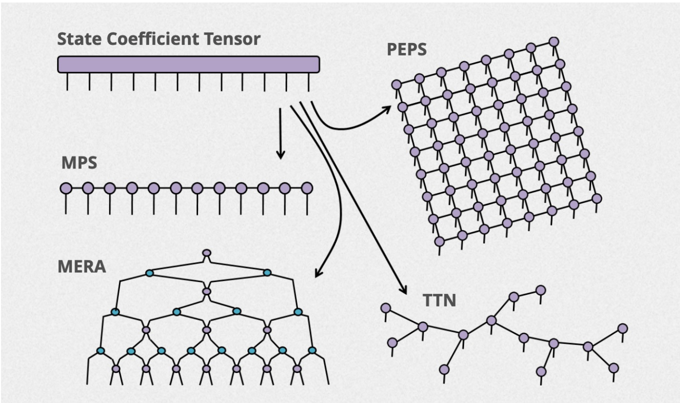


- We are starting to explore many-body techniques for quantum computing
- We made a focus on symmetry-breaking and symmetry restoration
- Interesting results on Q-VAP + CI techniques

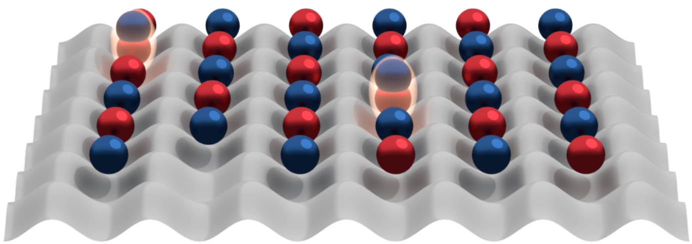
E. A. Ruiz Guzman and DL, in preparation

Ongoing/starting projects

More Systematic exploration of quantum ansatz

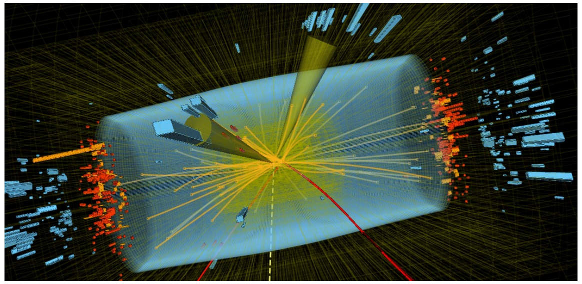


Atomic nuclei on lattices



J. Zhang thesis

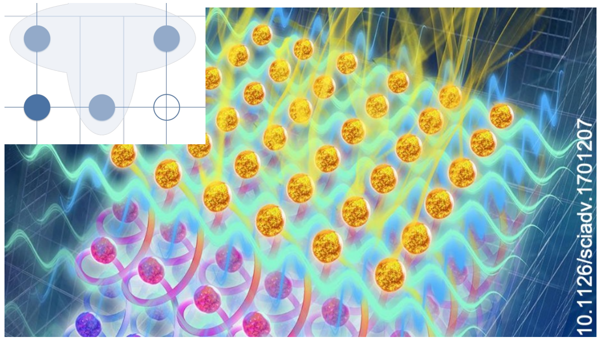
Quantum Machine Learning



Y. Beaujeault-Taudiere (postdoc)

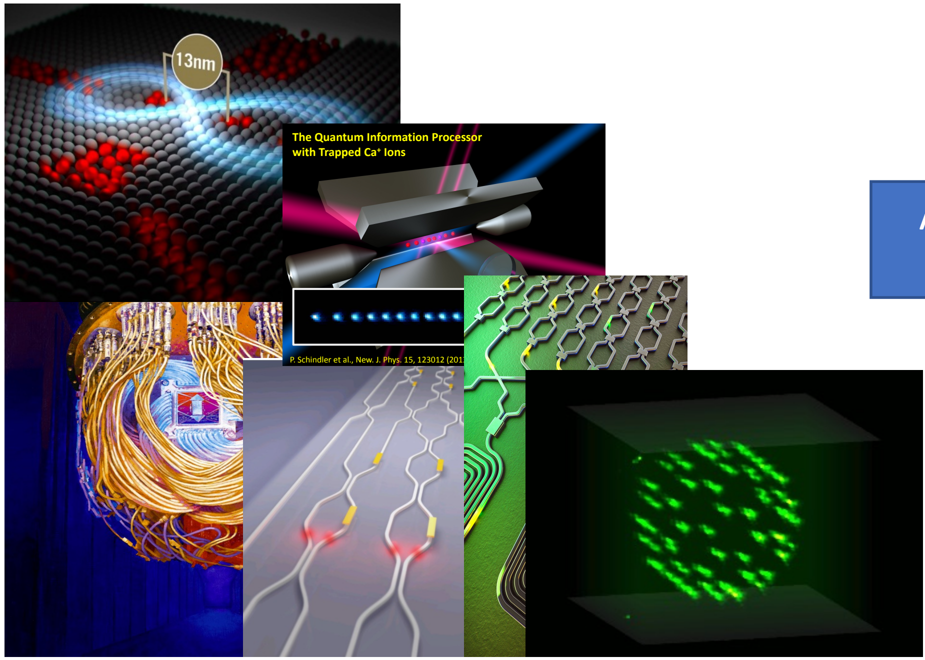
Few initiated applications in the world in the two infinities field

Lattice gauge theories



Zohar, Kolck, Savage, …

E. Zohar, J. I. Cirac, B. Reznik, Phys. Rev. Lett. **110**, 125304 (2013)
E. Zohar, J. I. Cirac, B. Reznik, Phys. Rev. A **88** 023617 (2013)
E. Zohar, J. I. Cirac, B. Reznik, Rep. Prog. Phys. **79**, 014401 (2016)
D. González Cuadra, **E. Zohar**, J. I. Cirac, New J. Phys. **19** 063038 (2017)

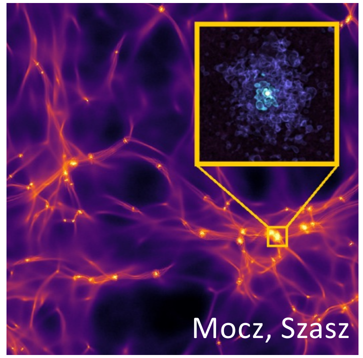


N-body problem

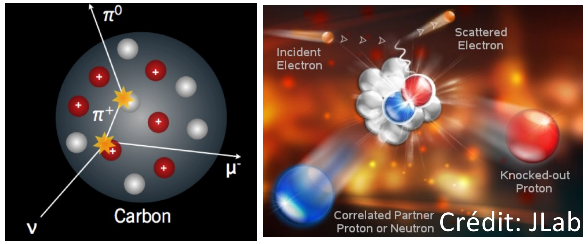
N-body nuclear systems

Dumitrescu, Hagen, Carlson, Papenbrock…

Dark matter

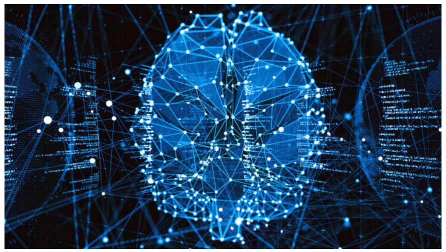


Dynamics: e, ν scattering

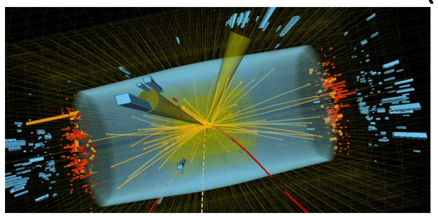


Roggero, Carlson, …

Applications to data mining (event classification)



CMS-detector (with LLR)



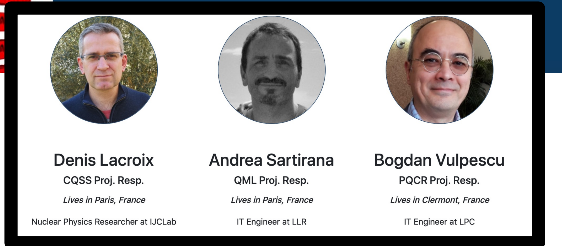
https://qc.pages.in2p3.fr/web/

Some advertising

QC2I is a computing project supported by IN2P3, the French national nuclear and particle physics institute. Its goal is to explore the possible applications of the emerging quantum computing technologies to particles and nuclear physics problems as well as astrophysics. The main tasks are:

- to identify, within IN2P3, scientists/engineers/technicians who are interested in using quantum technologies,
- to facilitate the access and training on quantum computers,
- to identify milestones applications for nuclear/particle physics and astrophysics,
- to design dedicated algorithms and proof of principle applications.

The project action has three main directions: **Prepare the Quantum Computing Revolution** (PQCR), **Quantum Machine Learning** (QML), **Complex Quantum Systems Simulation** (CQSS)



Thank You