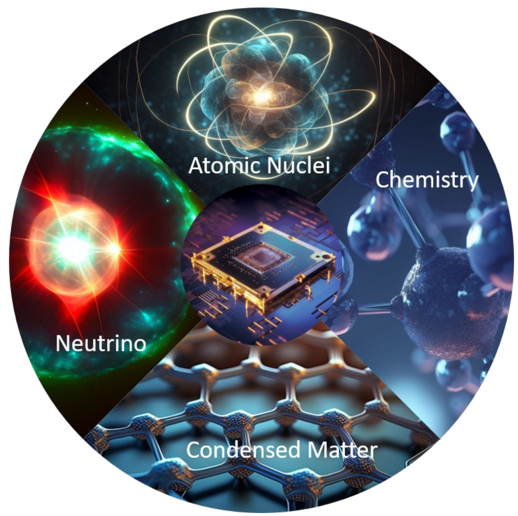
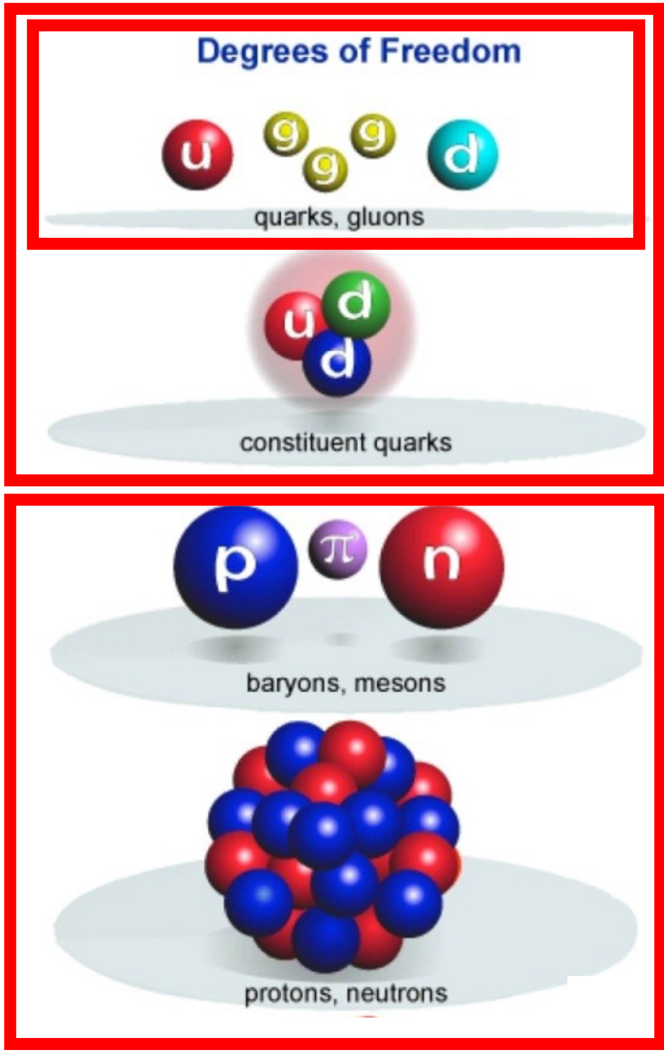
Quantum computing applied to nuclear physics

Denis Lacroix



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)



Energy (MeV)

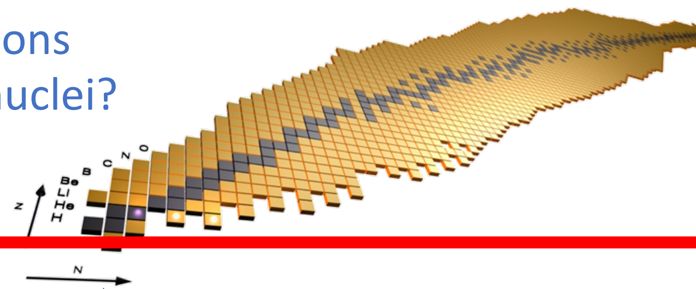
940
neutron mass

140
pion mass

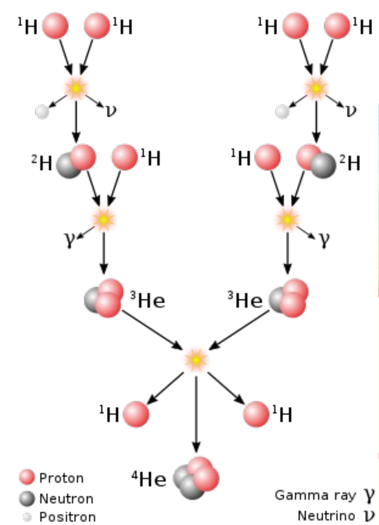
8
proton separation
energy in lead

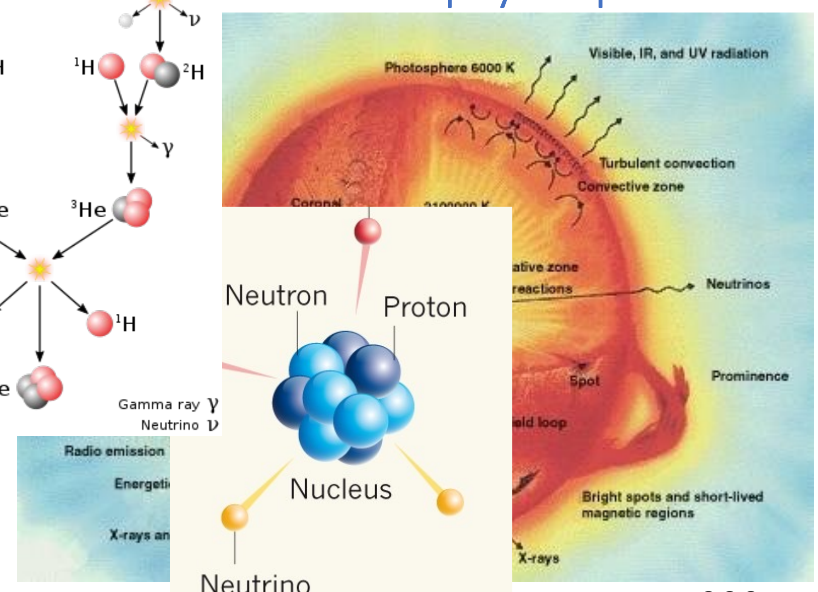
Physics beyond the standard model
From quarks to nucleons?

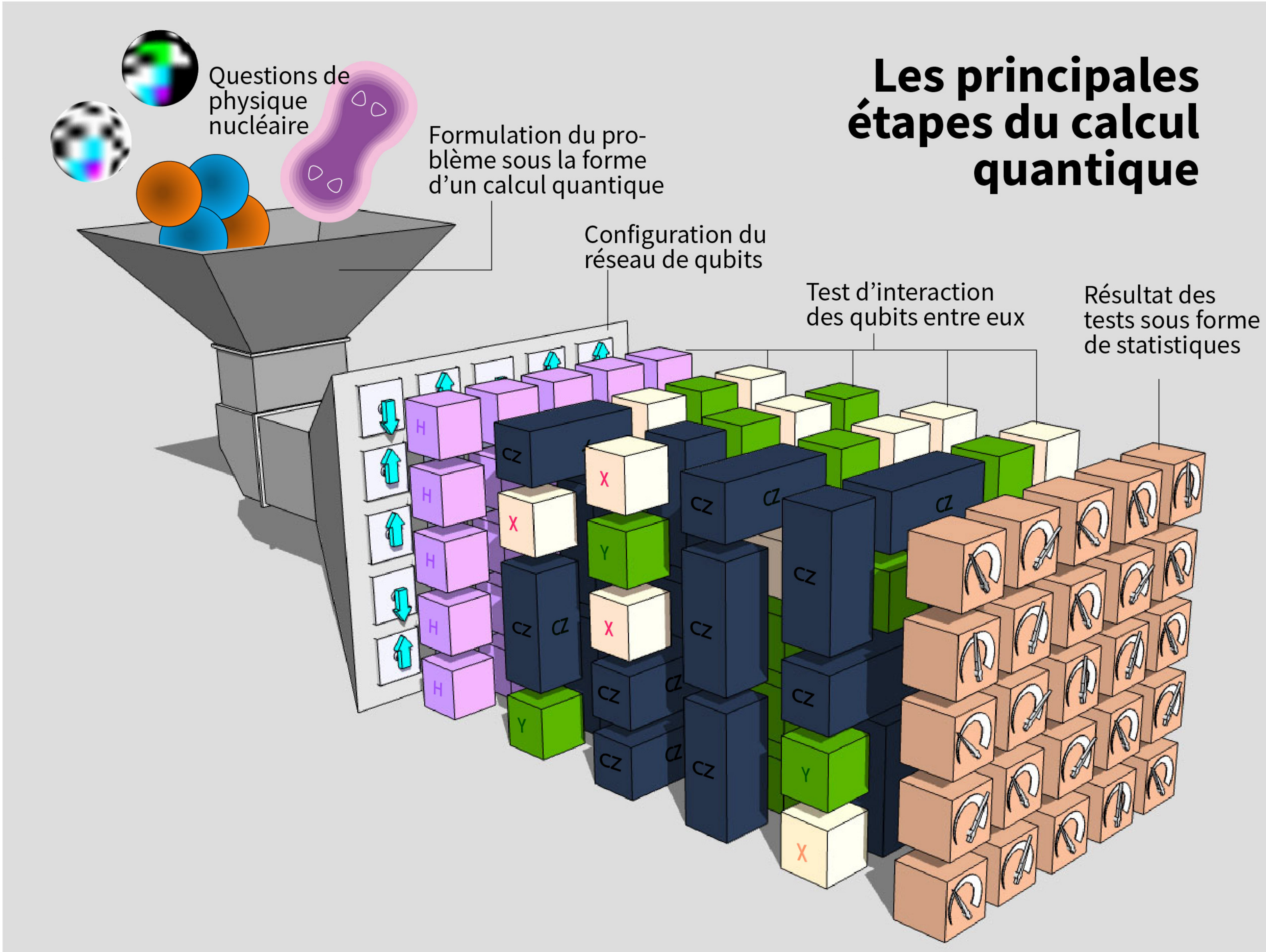
From nucleons
to atomic nuclei?



QC for simulation of specific
Astrophysics process



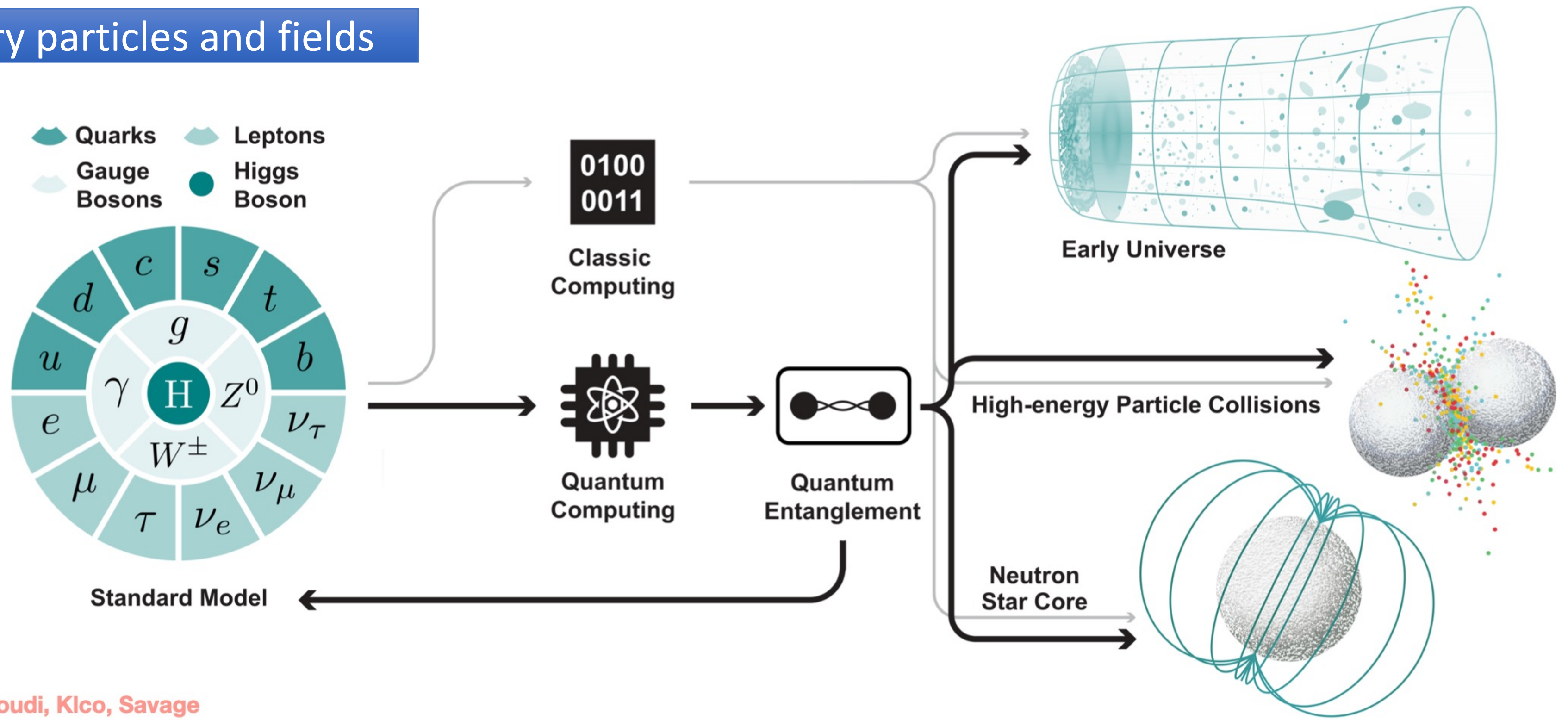




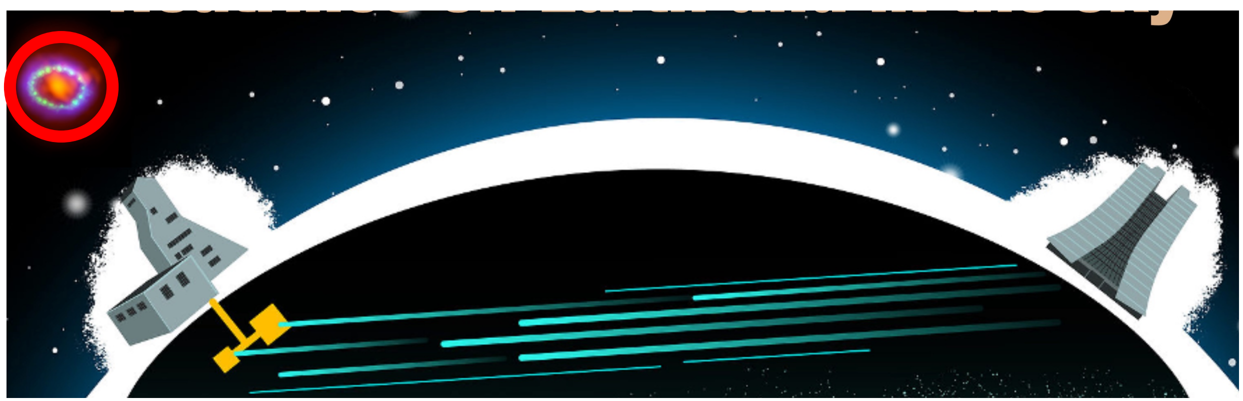
IN2P3 communication newsletter

Degrees of Freedom

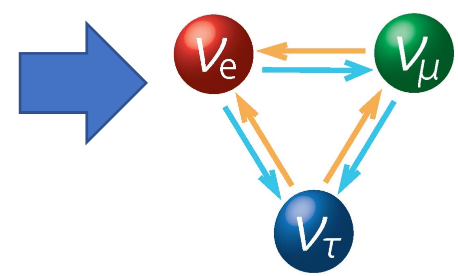
Elementary particles and fields



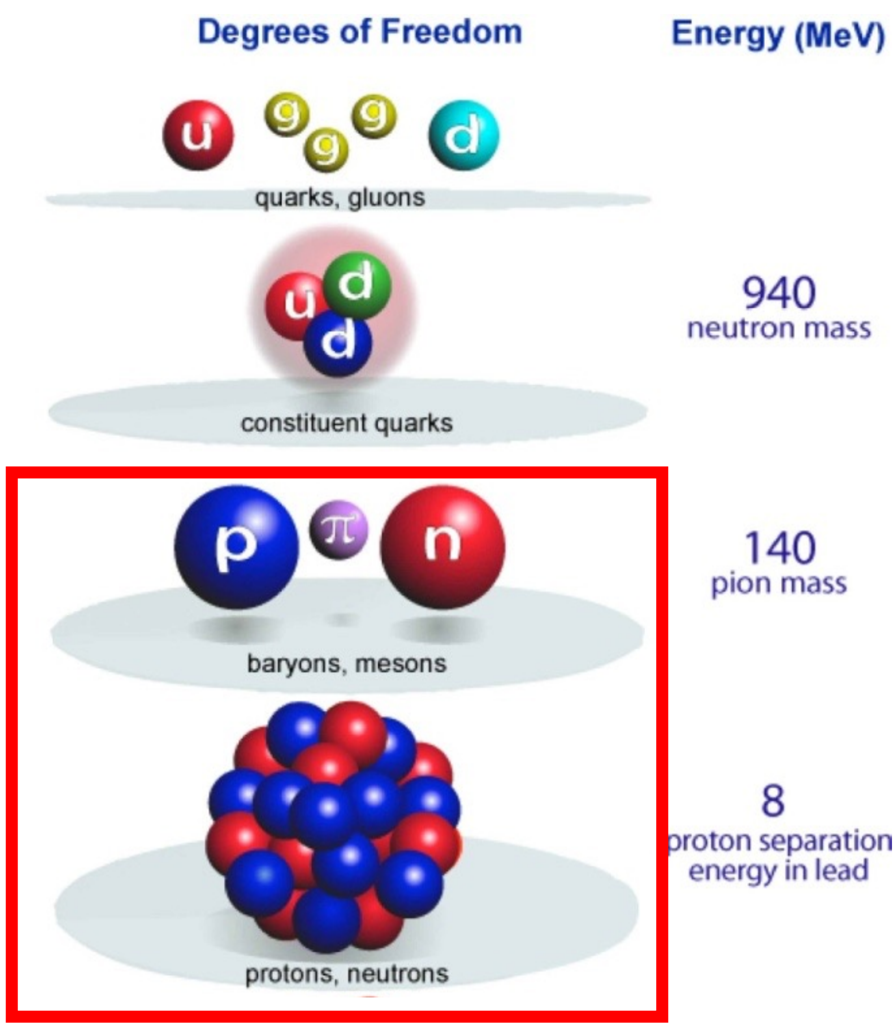
Bauer, Davoudi, Klco, Savage



Neutrino mass and oscillations



Di Meglio et al., Quantum Computing for High Energy Physics: State of the Art and Challenges, PRX Quantum (2024)



From nucleons
to atomic nuclei?

More on many-body systems treated with quantum computers

Eur. Phys. J. A (2023) 59:227
https://doi.org/10.1140/epja/s10050-023-01141-1

THE EUROPEAN PHYSICAL JOURNAL A

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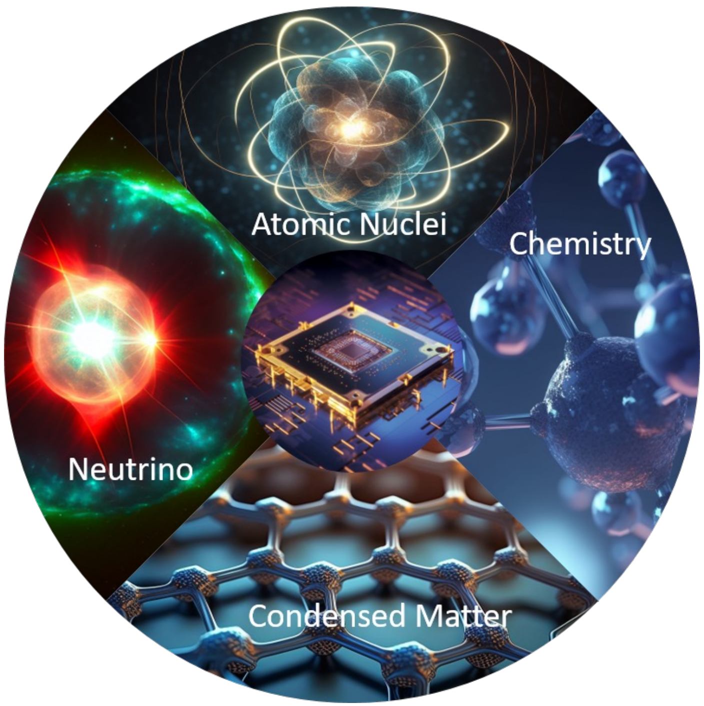
Regular Article - Theoretical Physics

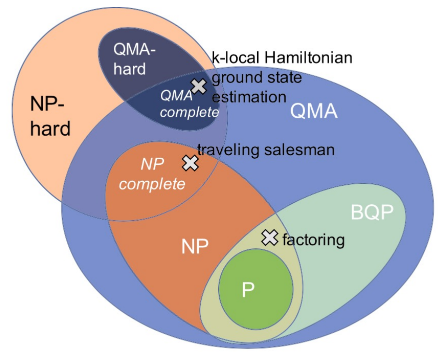
Quantum computing with and for many-body physics

Thomas Ayral[1,a], **Pauline Besserve**[1,3,b], **Denis Lacroix**[2,c], **Edgar Andres Ruiz Guzman**[2,d]

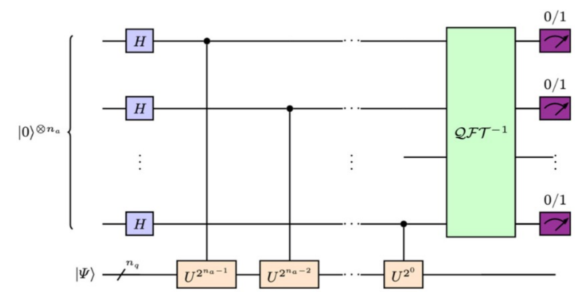
[1] Eviden Quantum Laboratory, 78340 Les Clayes-sous-Bois, France
[2] Université Paris-Saclay, CNRS/IN2P3, IJCLab, 91405 Orsay, France
[3] Centre de Physique Théorique, 91120 Palaiseau, France



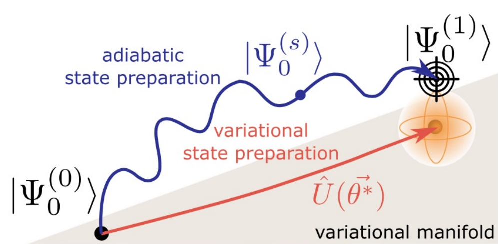
Complexity



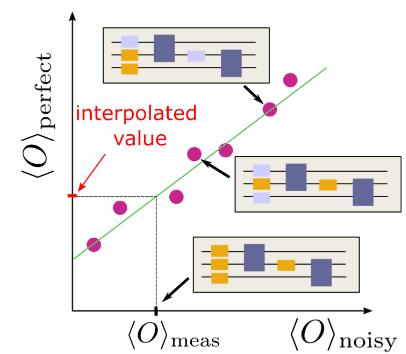
General QC



General QC

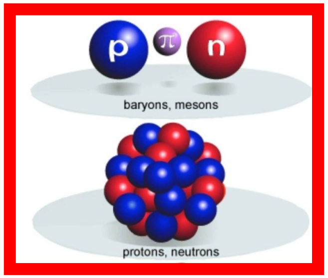


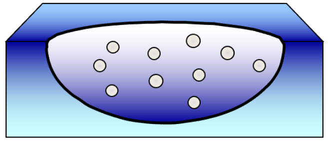
Error corrections



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

Problematic and challenges

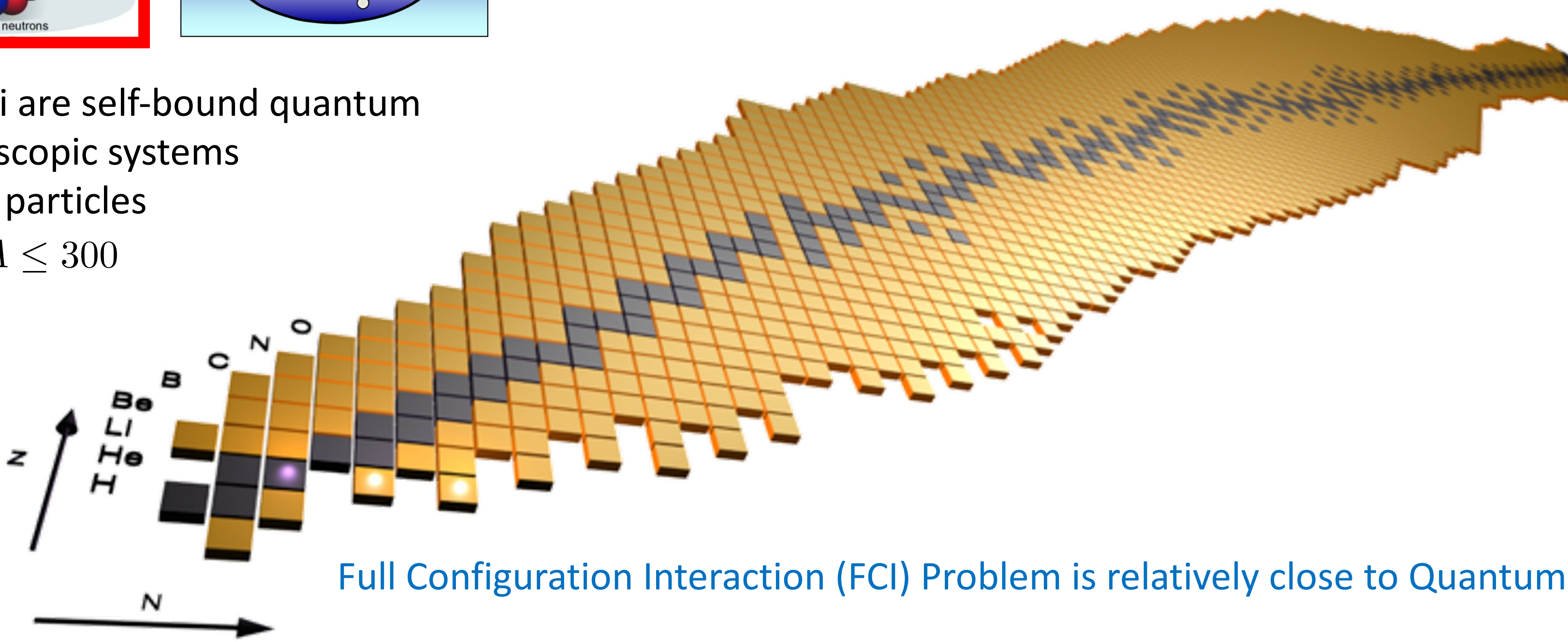




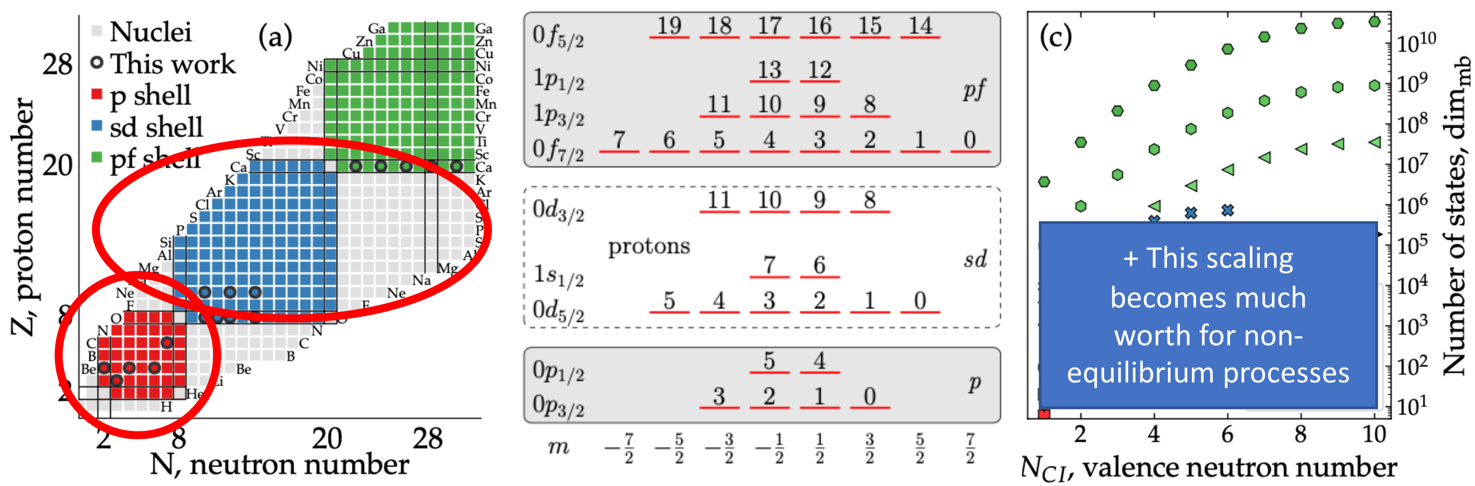
Nuclei are self-bound quantum mesoscopic systems

Nb of particles

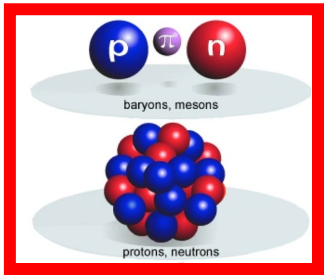
$2 \leq A \leq 300$

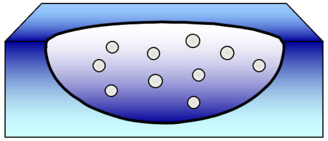


Full Configuration Interaction (FCI) Problem is relatively close to Quantum chemistry



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





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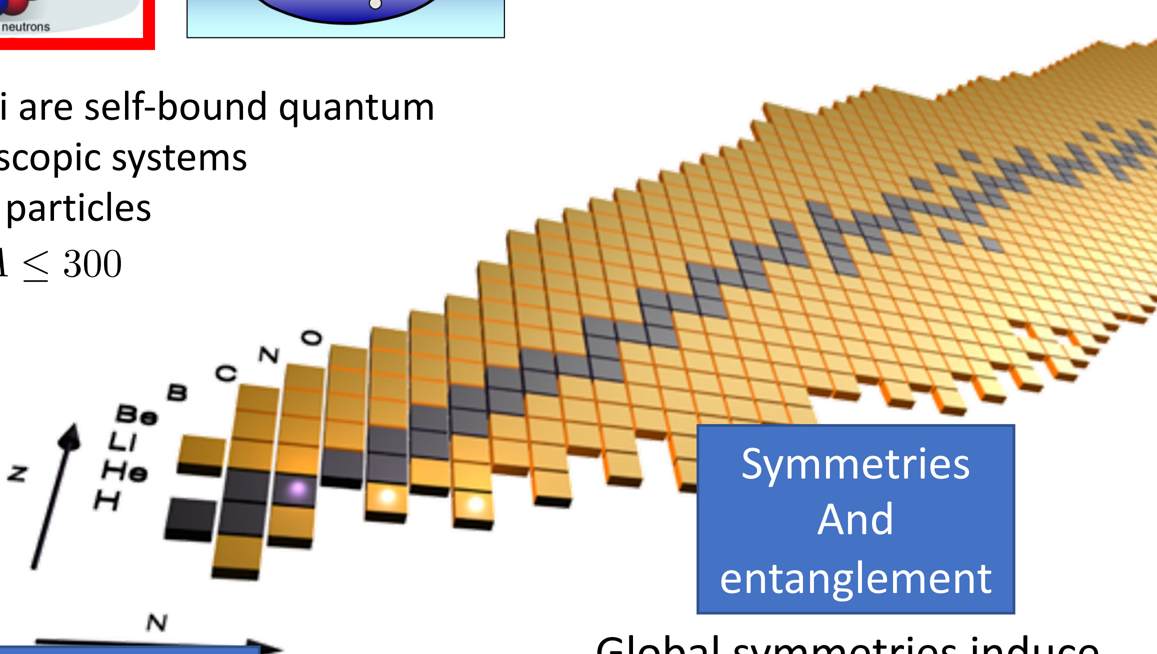
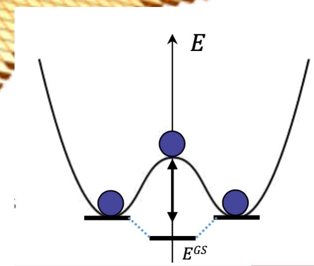
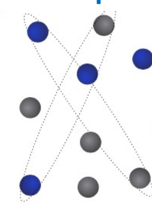




Spontaneous Broken symmetries (SB)

Small superfluid

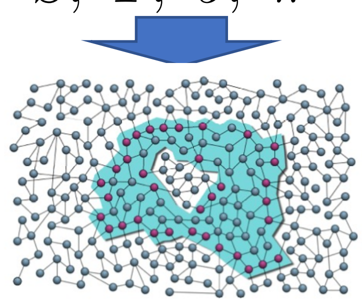


(particle number SB)

Symmetries And entanglement

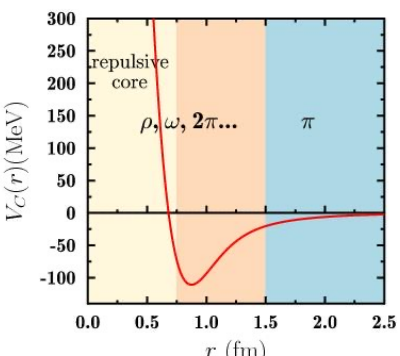
Global symmetries induce All-to-all entanglement

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



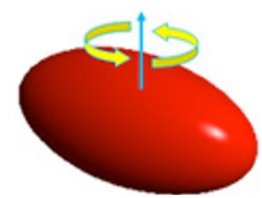
Nuclei are subject to entanglement volume law (bad candidate for Tensor Network)

Interaction



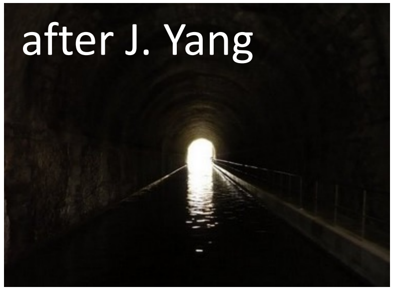
The problem is highly non-perturbative

Deformation can happen



(rotational invariance SB)

...



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

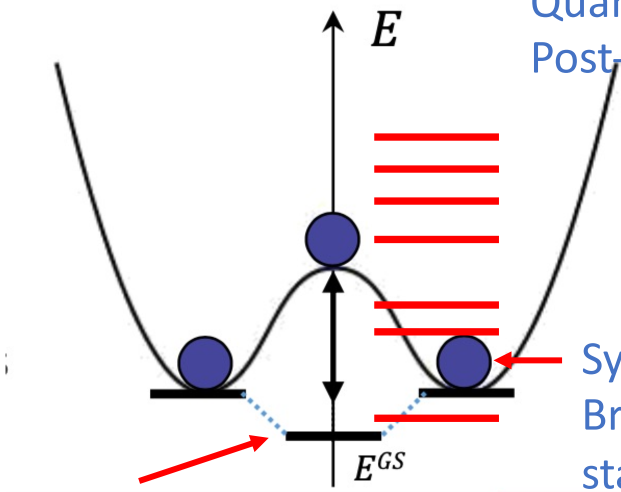
Variational optimization

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, ...)

3 Further Quantum or hybrid Quantum-Classical Post-processing



1 Symmetry Breaking (SB) state

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

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

Which symmetries ?

Many-Body	Quantum computing
Particle Number Parity Total Spin	Hamming weight Odd/Even number of 1 Permutation Invariance

Illustration with small superconductors

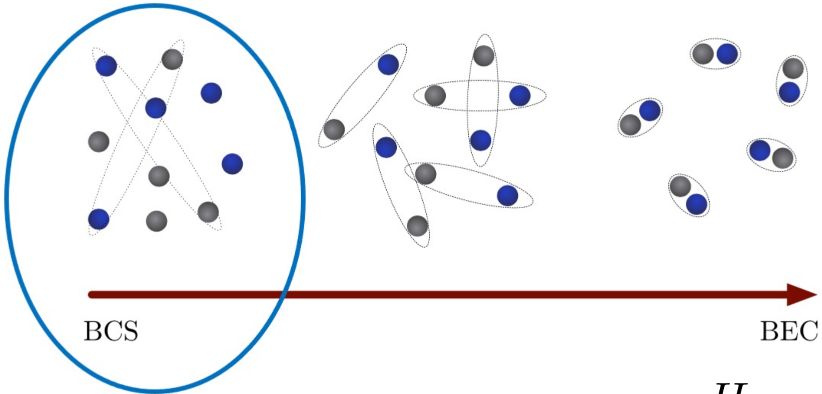
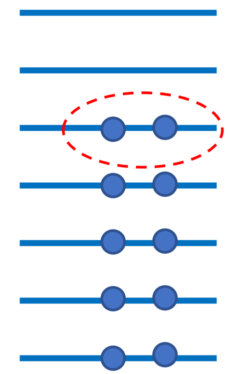


Illustration with the Richardson Hamiltonian

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

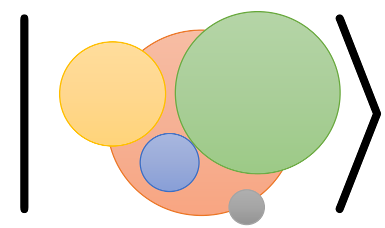


This problem is an archetype of spontaneous symmetry breaking.
An "easy" way to describe it is to break the particle number symmetry, i.e. consider wave-function that mixes different particle number

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 !

Application to the N-body pairing problem

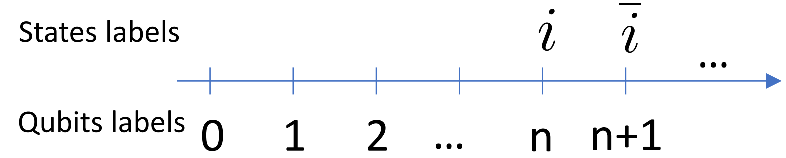
Hamiltonian and initial state

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 !

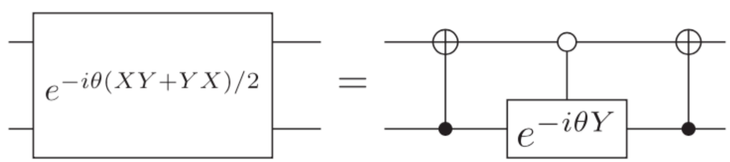


$$a_i^\dagger a_{\bar{i}}^\dagger \Rightarrow Q_n^+ Q_{n+1}^+$$

Initial (symmetry breaking) state preparation

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

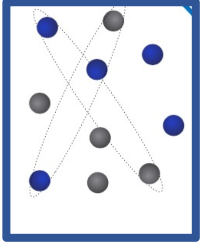
Equivalent universal gate on pairs



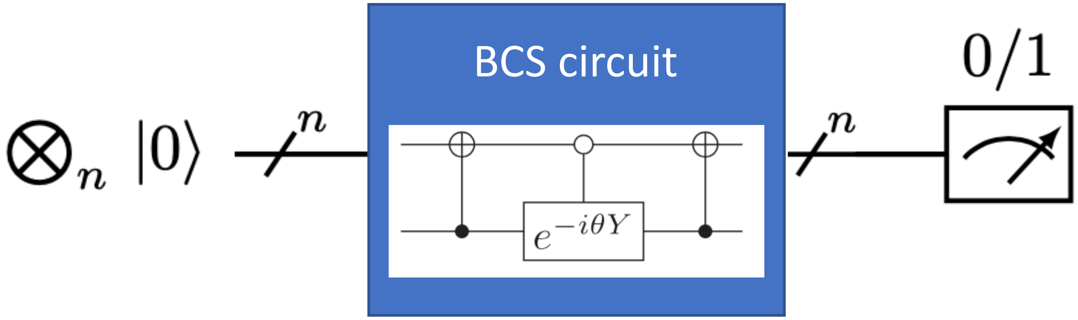
Zhang Jiang et al,
Phys. Rev. Applied 9, 044036 (2018).

Quantum computing for atomic nuclei

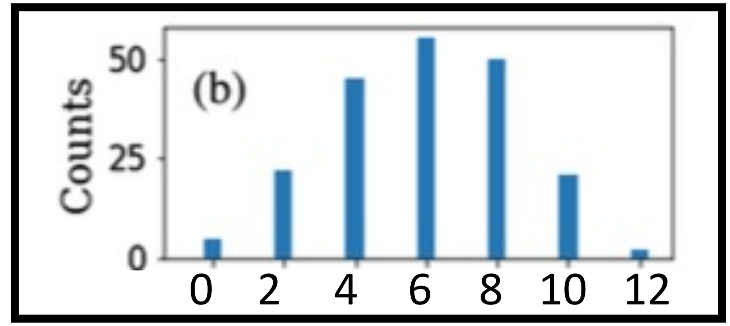
Illustration for small superfluids



Superfluidity can be described by breaking particle number

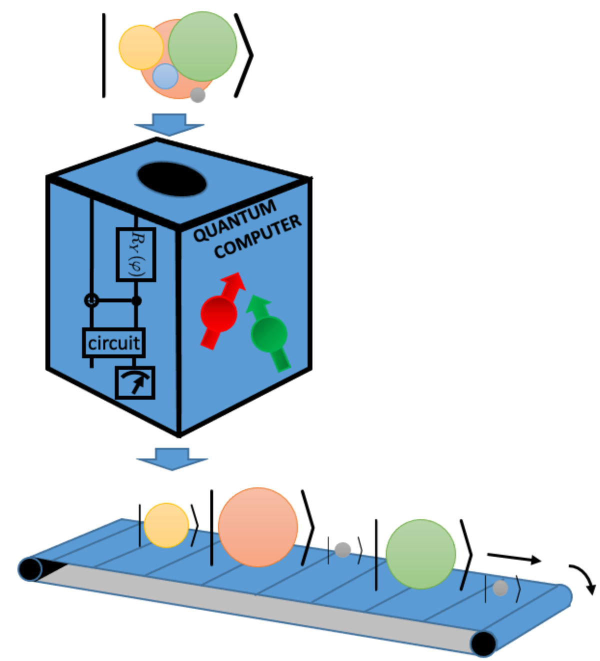


Example of mixing for 12 qubits (with qiskit)



Projection on particle number

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



For 2 qubits

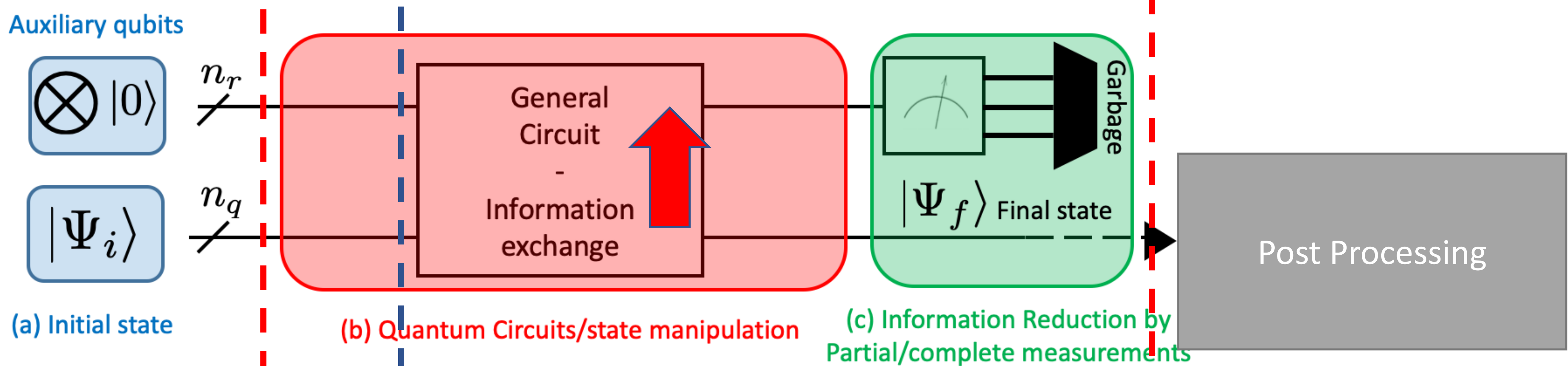
$$|\Psi\rangle = \alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle$$

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

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).

Non-destructive counting on a quantum computer



Starting point

$$|-\rangle = |0, \cdots, 0\rangle$$

Initial state

Send the information
To additional qubits
That are destroyed
after measurement

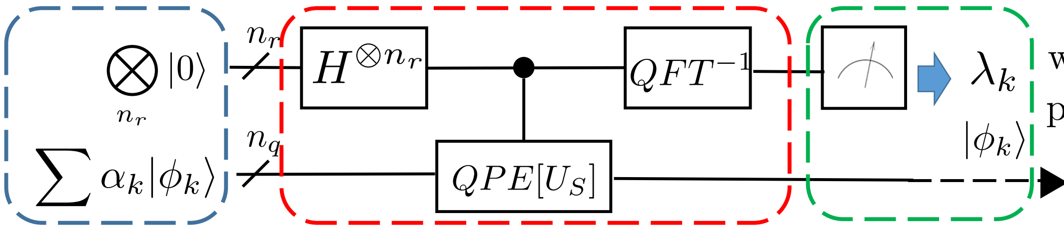
A terrific method
to do that is
quantum phase estimation

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).

Eigenvalues-Ground state and excited states



Initial configuration with symmetry breaking state

Symmetry operator eigenvalues encoding In the register qubits

Symmetry restoration through measurement

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

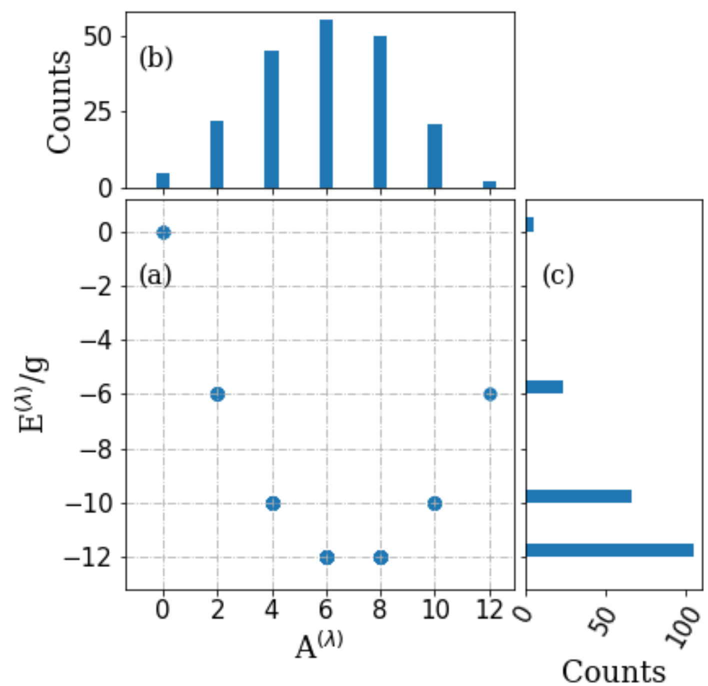
Projected BCS or with varying number Of particles

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

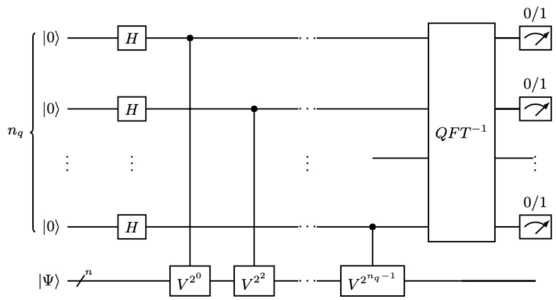
$$E/g = -\frac{1}{4}(A-\nu)(2n_q - A - \nu - 2).$$

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

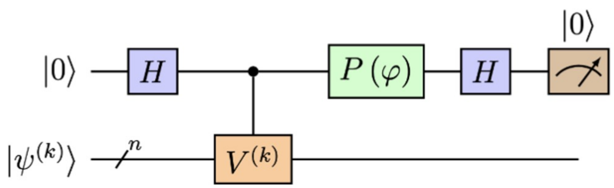
For the degenerate case, this should give the exact solution

Systematic of Phase-Estimation-based methods

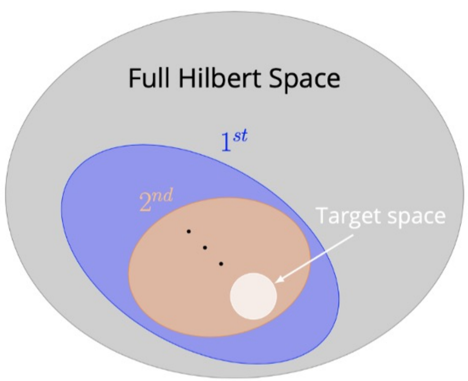
Standard Quantum Phase estimation



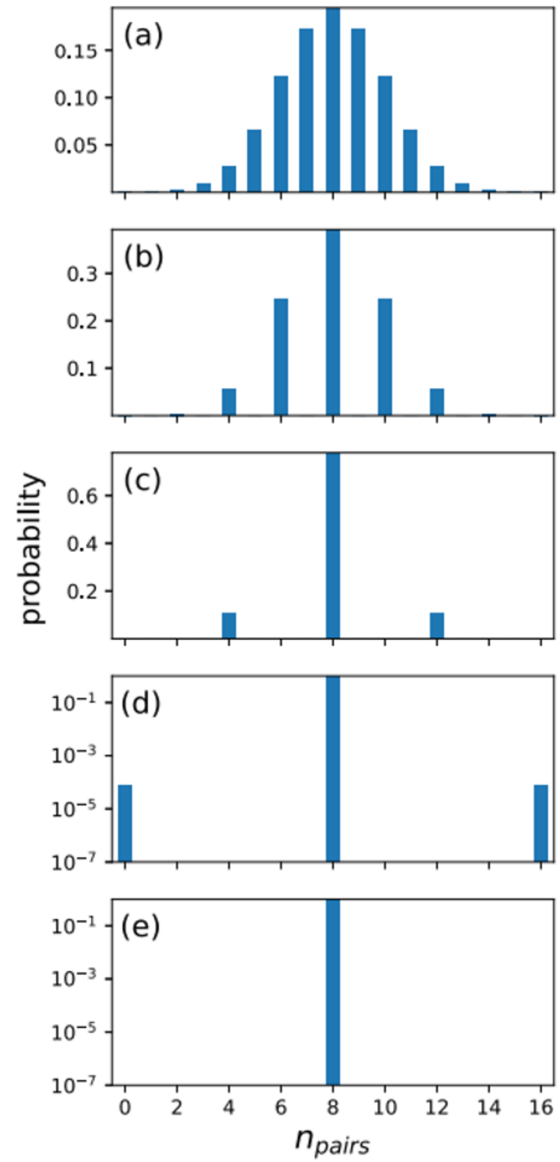
Iterative Quantum Phase estimation



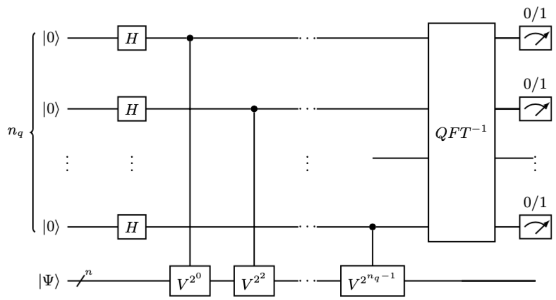
$\hat{V}^{(k)} = e^{i\phi_k \hat{N}}$ $\qquad \phi_k = \frac{\pi}{2^k}$



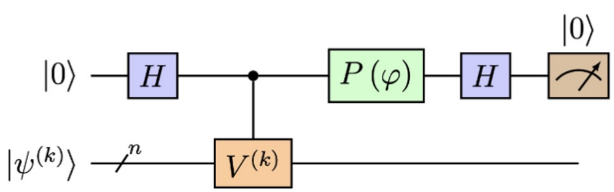
16 qubits, N = 8



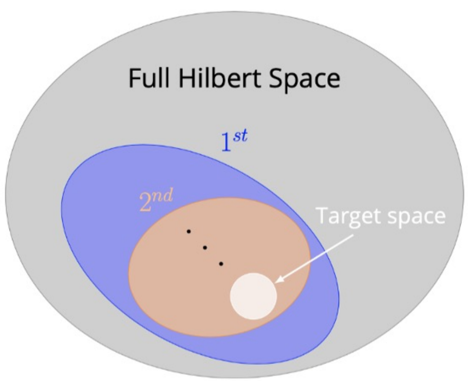
Standard Quantum Phase estimation



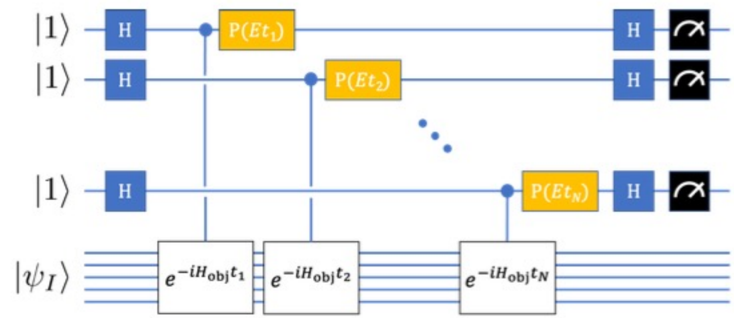
Iterative Quantum Phase estimation



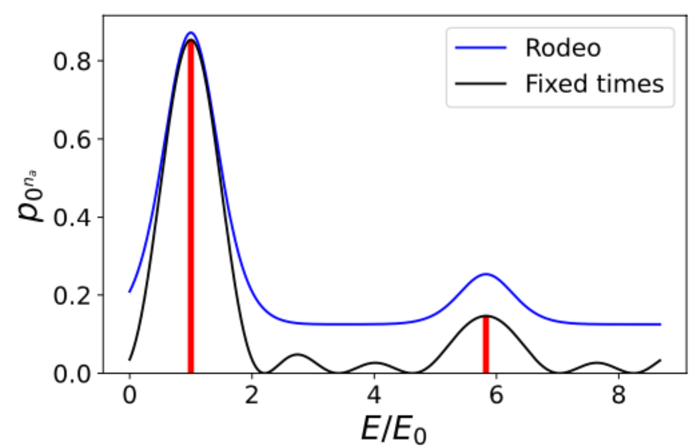
$$\hat{V}^{(k)} = e^{i\phi_k \hat{N}} \qquad \phi_k = \frac{\pi}{2^k}$$



Iterative Quantum Phase estimation + random Gaussian time (Rodeo algorithm)



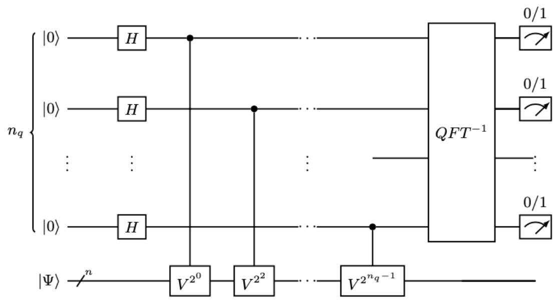
K. Choi et al., Rodeo Algorithm for Quantum Computing, Phys. Rev. Lett. 127, 040505 (2021).



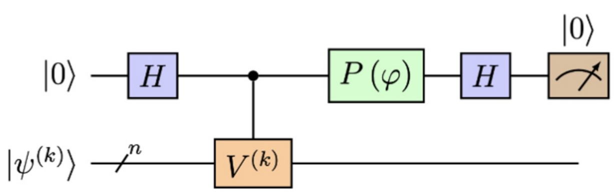
Ayral, Besserve, Lacroix, Ruiz Guzman, EPJA 59 (2023)

Systematic of QPE-based methods

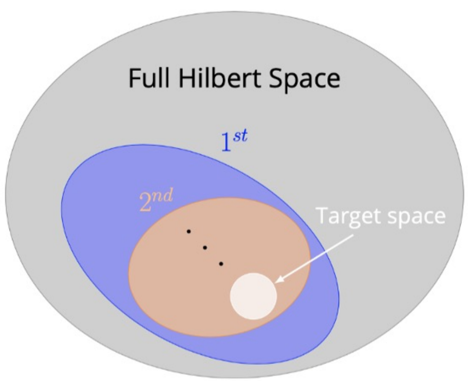
Standard Quantum Phase estimation



Iterative Quantum Phase estimation

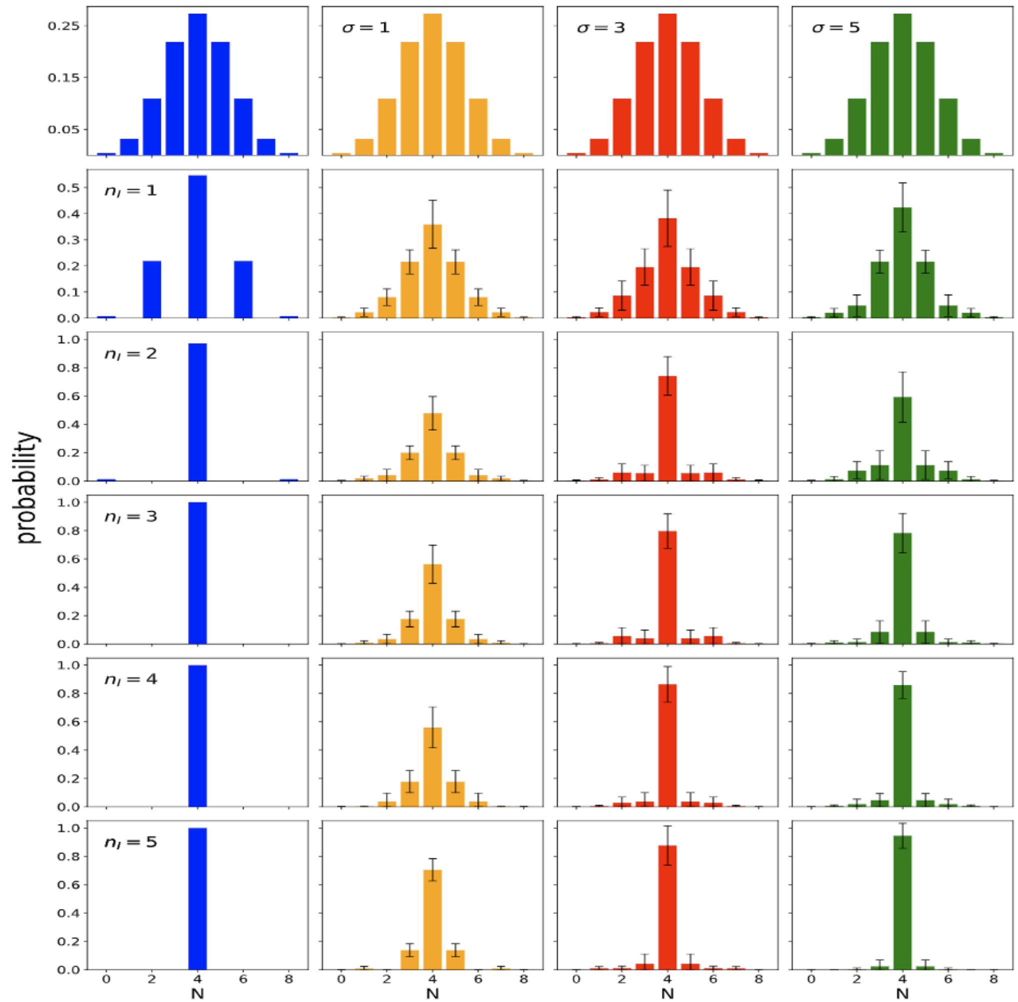


$$\hat{V}^{(k)} = e^{i\phi_k \hat{N}} \qquad \phi_k = \frac{\pi}{2^k}$$



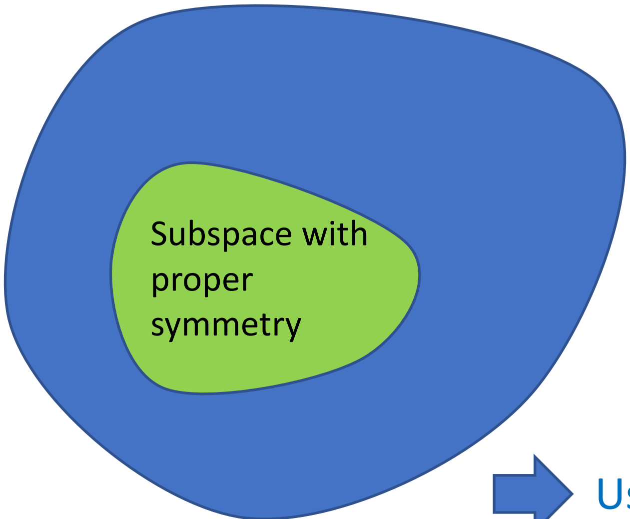
Iterative Quantum Phase estimation
+ random Gaussian time (Rodeo algorithm)

Iterative QPE   Rodeo algorithm with different resolution



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

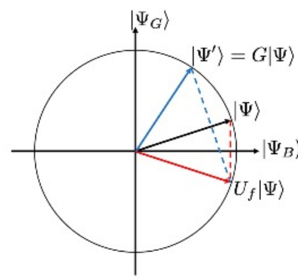
Symmetry breaking/symmetry preserving circuits and symmetry restoration on quantum computers

A quantum many-body perspective

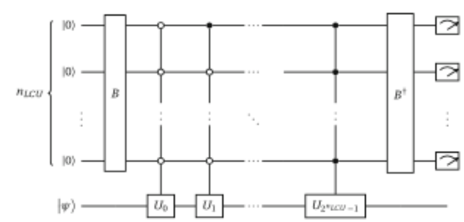
Denis Lacroix[1,a], Edgar Andres Ruiz Guzman[1,b], Pooja Siwach[2,c]

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

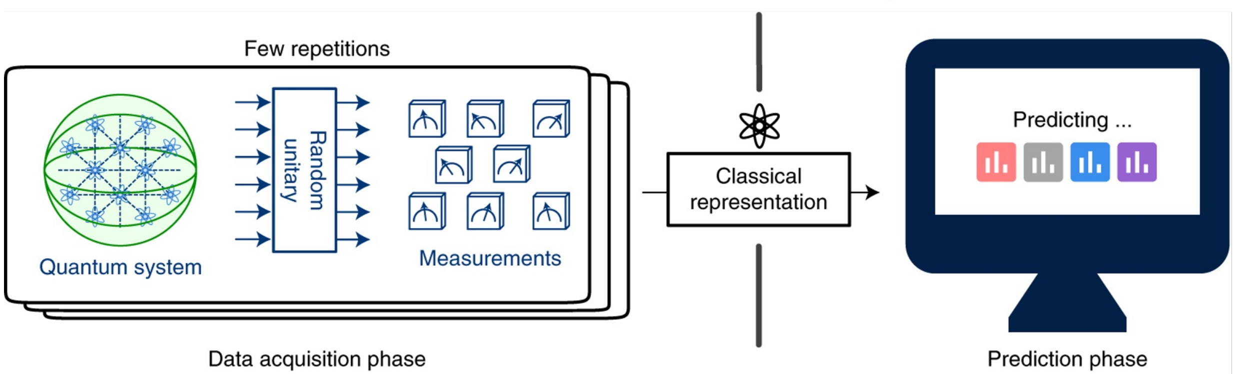
Grover and Oracle



Linear Combination of Unitaries



Use quantum tomography techniques (Classical Shadow method)



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

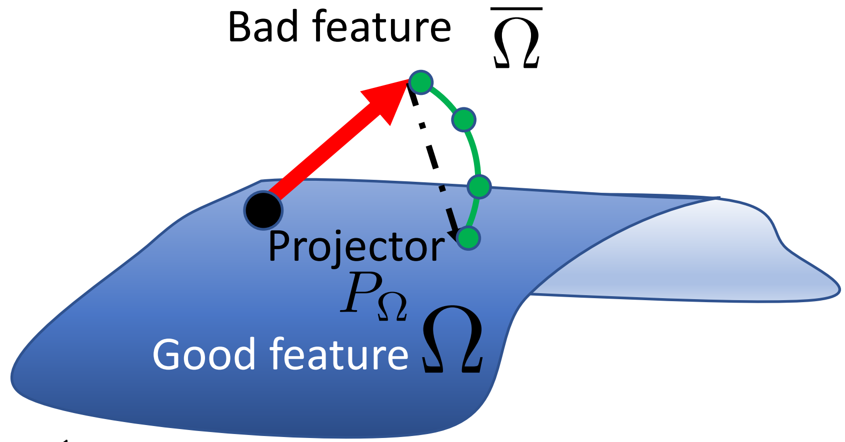
Restoring broken symmetries using quantum search "oracles"
Edgar Andres Ruiz Guzman and Denis Lacroix
Phys. Rev. C **107**, 034310 (2023) - Published 16 March 2023

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

Grover Classification operator (Oracles)

$$\hat{U}_f |k\rangle = (-1)^x \text{ with } x \begin{cases} 0 & if \ |k\rangle \in \bar{\Omega} \\ 1 & if \ |k\rangle \in \Omega \end{cases}$$

Lov K. Grover, Phys. Rev. Lett. **79**, 325 (1997)



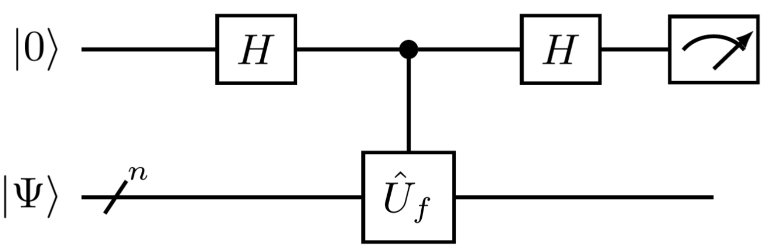
We (physicists) are more familiar with projectors

$$P_\Omega \Rightarrow U_f = +1 P_\Omega - 1(1 - P_\Omega) = 2P_\Omega - 1$$

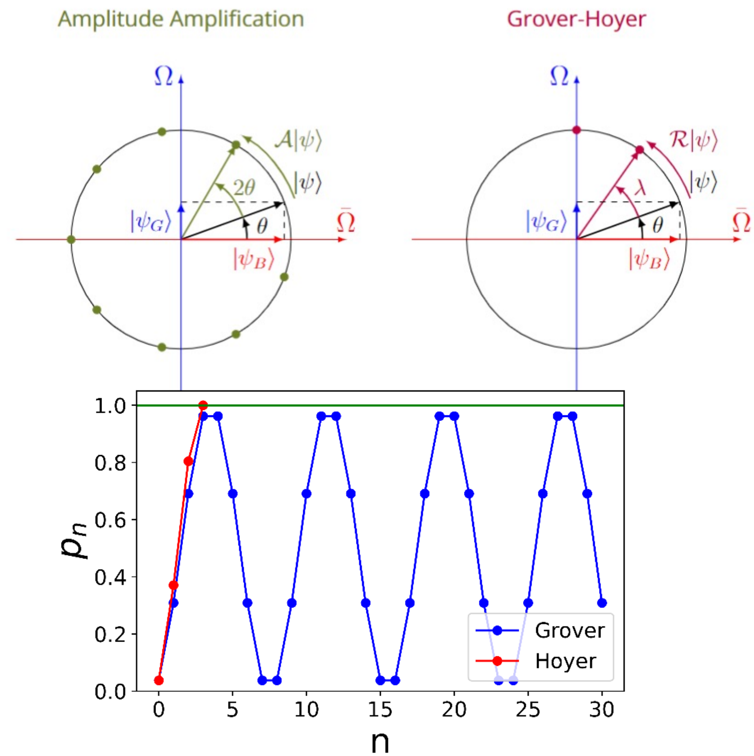
Methods based on projectors

Oracle + Hadamard test

Grover technique



$$\frac{1}{2}\{|0\rangle \otimes [I + \hat{U}_f]|\Psi\rangle + |1\rangle \otimes [I - \hat{U}_f]|\Psi\rangle\} = |0\rangle|\Psi_B\rangle + |1\rangle|\Psi_G\rangle$$



E. A. Ruiz Guzman and D. Lacroix, Phys. Rev. **C 107**, 034310 (2023)

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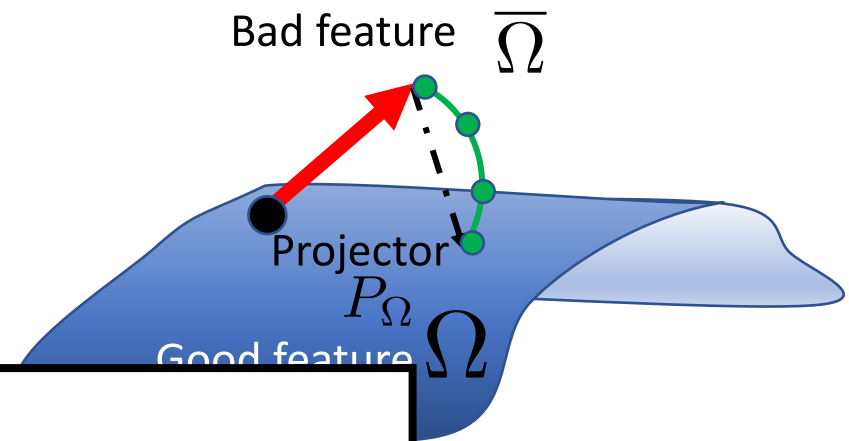
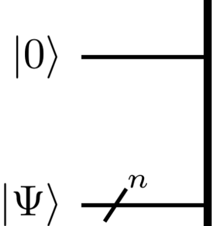


We (physi

P_Ω

Methods

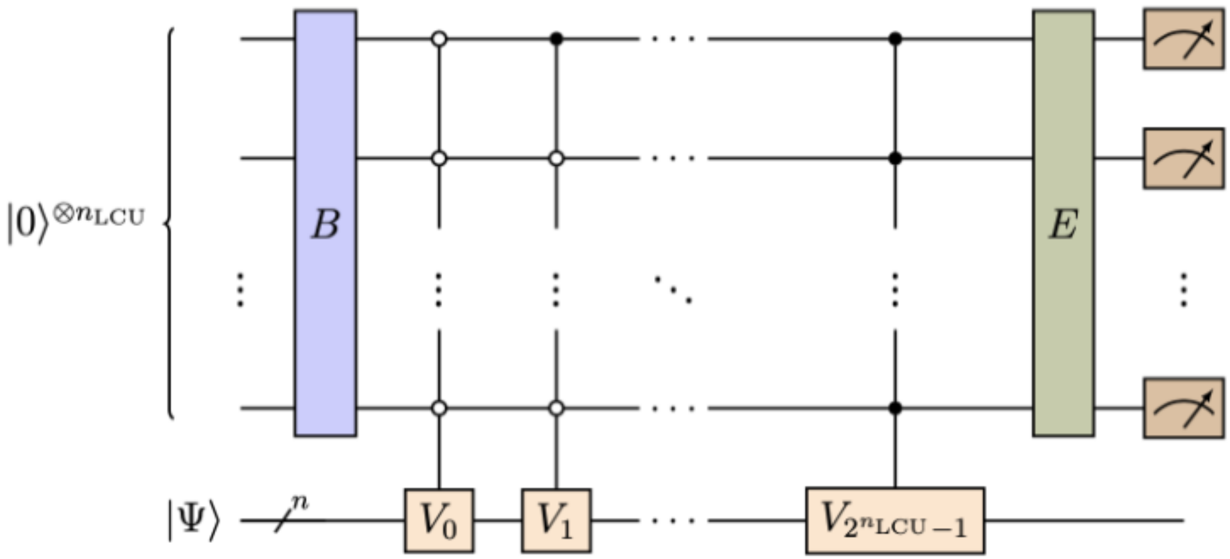
Oracle + H

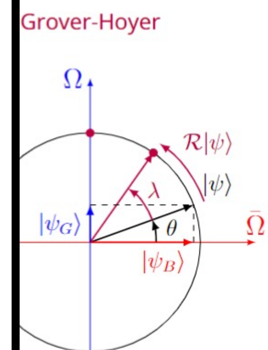


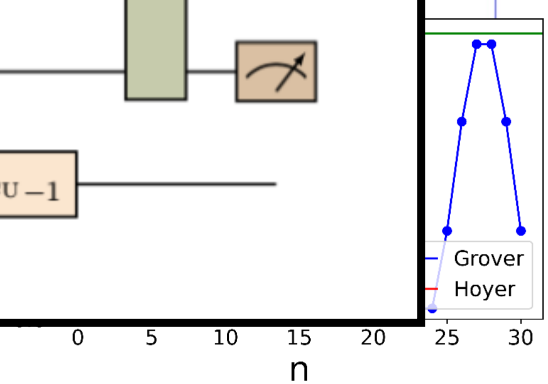
$\frac{1}{2}\{|0\rangle \otimes [I + \hat{U}$

Practical implementation of projectors

$$P_N = \frac{1}{n+1}\sum_{k=0}^{n} e^{\frac{2\pi i k(\hat{N}-N)}{n+1}}$$ = sum of unitary operators







E. A. Ruiz Guzman and D. Lacroix, Phys. Rev. **C 107**, 034310 (2023)

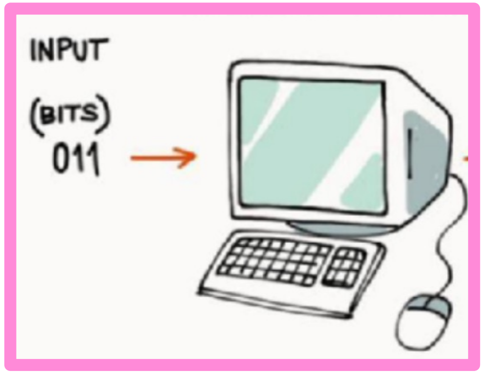
Hybrid Quantum-classical methods to perform symmetry projection

Using the classical computing knowledge

QPU

Bad state preparation

CPU



Good state reconstruction

Simple illustration with particle number

$$P_N = \frac{1}{2\pi}\int_0^{2\pi} e^{-i\varphi(\hat{N}-N)}$$

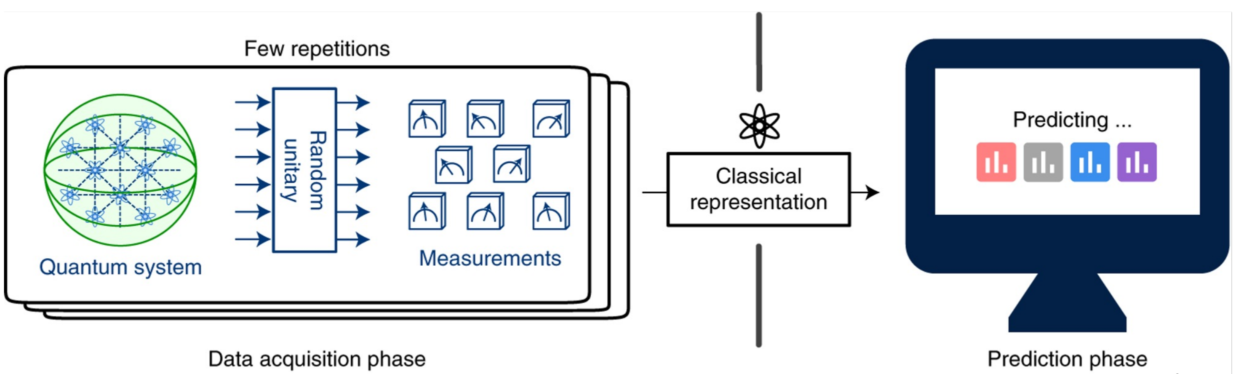
QPU

$$\langle \hat{O} \rangle_{SR} = \frac{\int_0^{2\pi} e^{i\varphi N} \langle \hat{O} e^{-i\varphi \hat{N}} \rangle_{SB}}{\int_0^{2\pi} e^{i\varphi N} \langle e^{-i\varphi \hat{N}} \rangle_{SB}}$$

CPU

“Professional” version

Use quantum tomography techniques
(Classical Shadow method)



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

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

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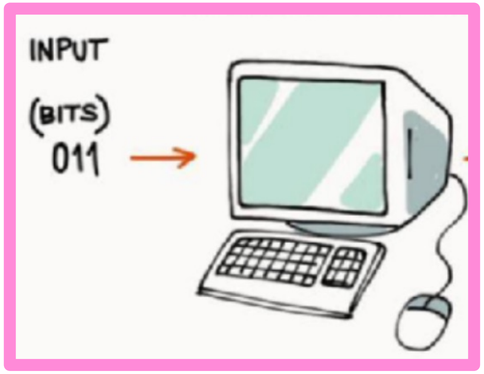

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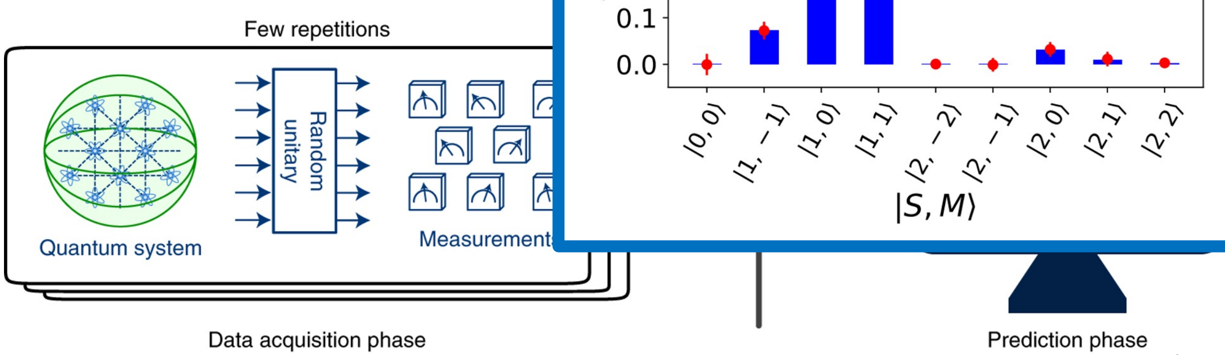
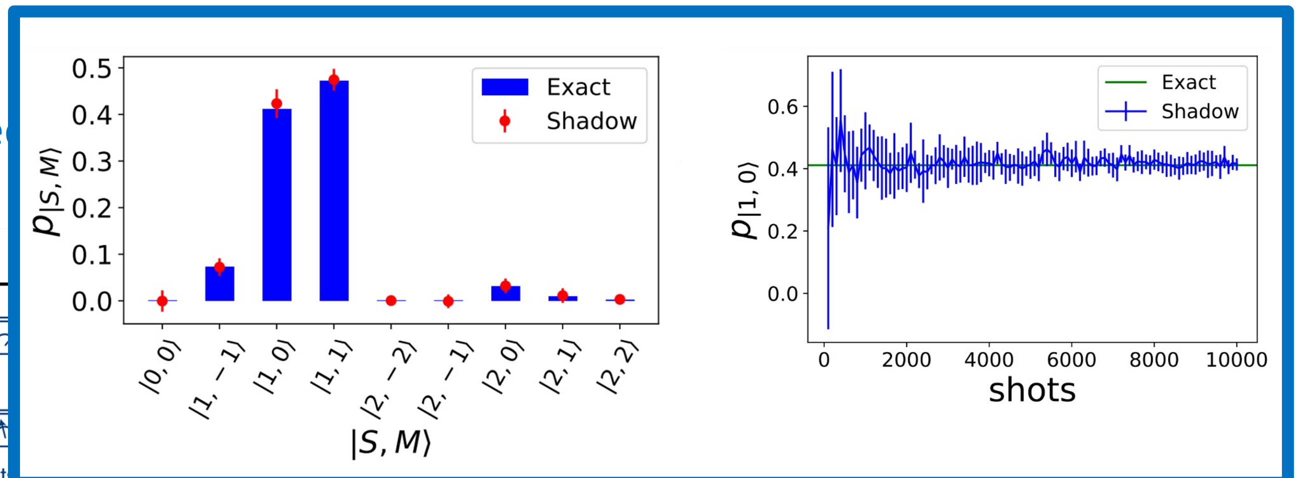
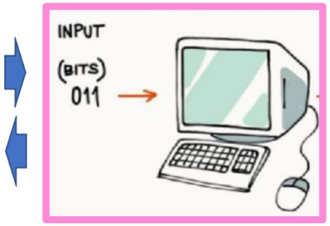




H.-Y. Huang, R. Kueng and J. Preskill; Nat. Phys. 16, 1050 (2020)

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

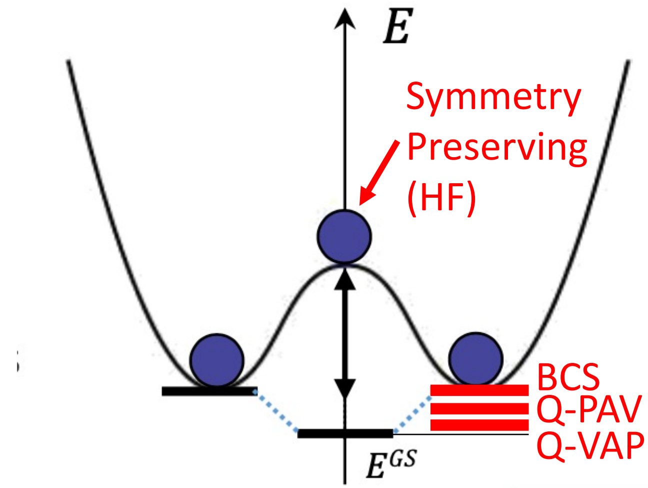
Classical optimization



Coming back to our superconducting problem

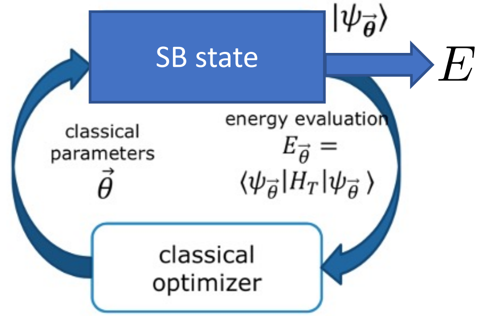
Combining projection with variational method

Pair occupation are now encoded

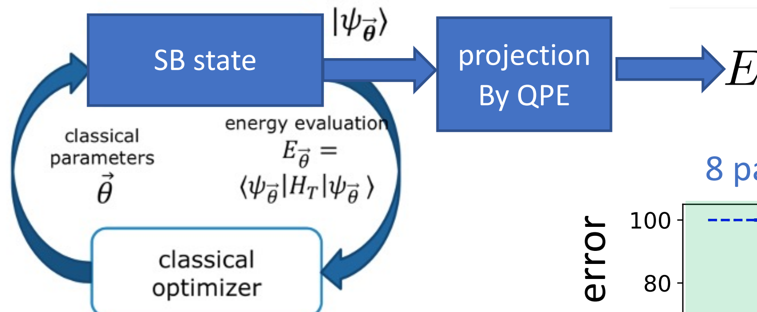


Quantum-Classical optimizers

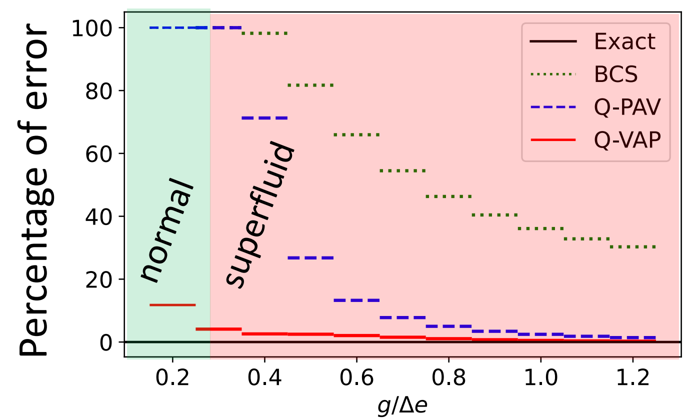
- Standard BCS theory



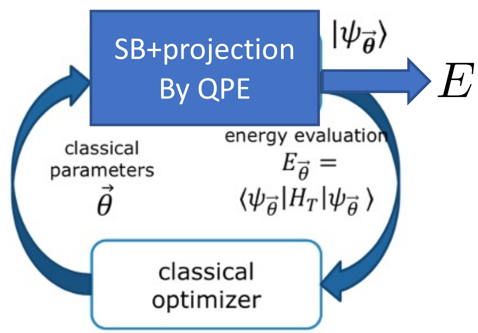
- Project after optimization
  Q-PAV: Quantum Projection After Variation



8 particles on 8 equidistant levels



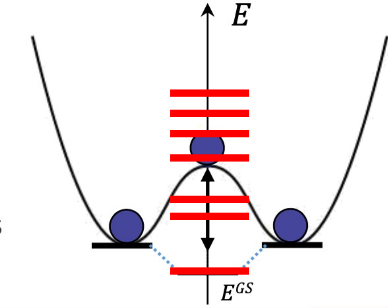
- The optimization is made on the Symmetry restored state.
  Q-VAP: Quantum Variation After Projection

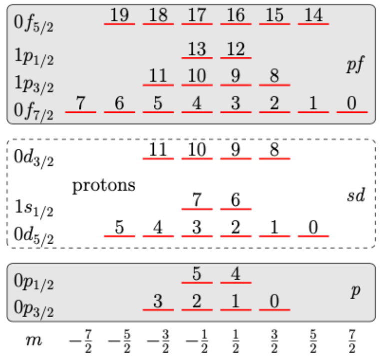


Ruiz Guzman and Lacroix, PRC 105 (2022)

Spectral methods

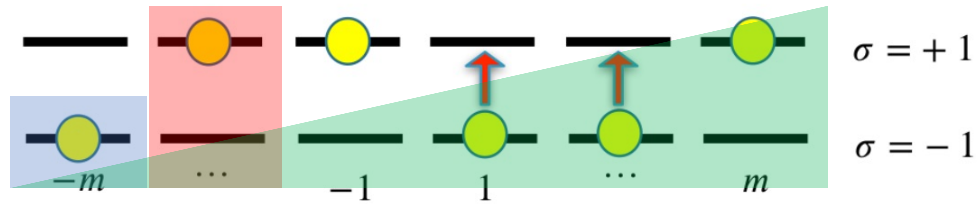
Getting excited states





Today's challenges:

- -Identify pilot applications,
- -Reduce the Quantum resources
- -Develop novel quantum algorithms

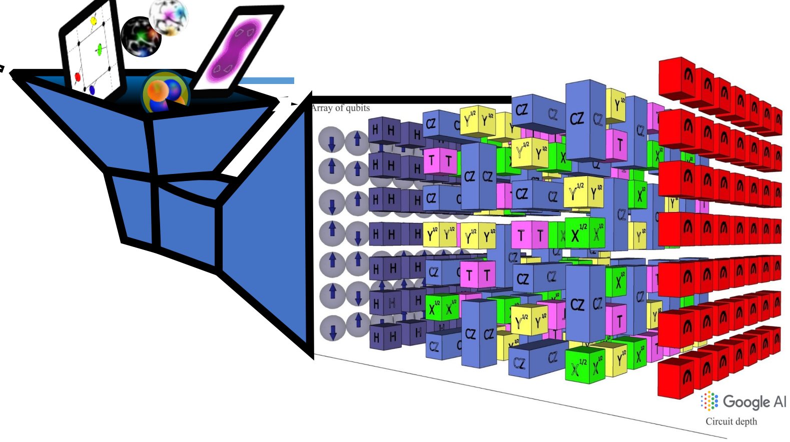


q = Number of qubits

Fermions-to-qubit: Jordan-Wigner	SU(2) encoding	J-scheme (compact) +parity encoding
1 level = 1 qubit	2 levels = 1 qubit	$\vert J, M\rangle \rightarrow \vert[M]\rangle$
$q = 2N$	$q = N$	Use first quantization
		$q = \lceil \log_2 N \rceil$

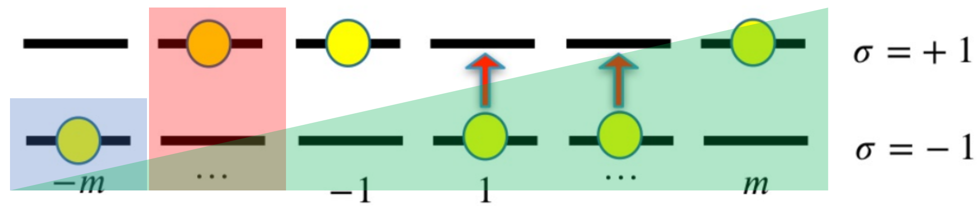
$$\begin{cases} X_\alpha = |1_\alpha\rangle\langle 0_\alpha| + |0_\alpha\rangle\langle 1_\alpha|, \\ Y_\alpha = i|1_\alpha\rangle\langle 0_\alpha| - i|0_\alpha\rangle\langle 1_\alpha|, \\ Z_\alpha = |0_\alpha\rangle\langle 0_\alpha| - |1_\alpha\rangle\langle 1_\alpha| \end{cases}$$

$$H = \frac{\varepsilon}{2}\sum_{\alpha=1}^{N} Z_\alpha + \frac{V}{4}\sum_{\alpha\neq\beta}^{N}(X_\alpha X_\beta - Y_\alpha Y_\beta),$$



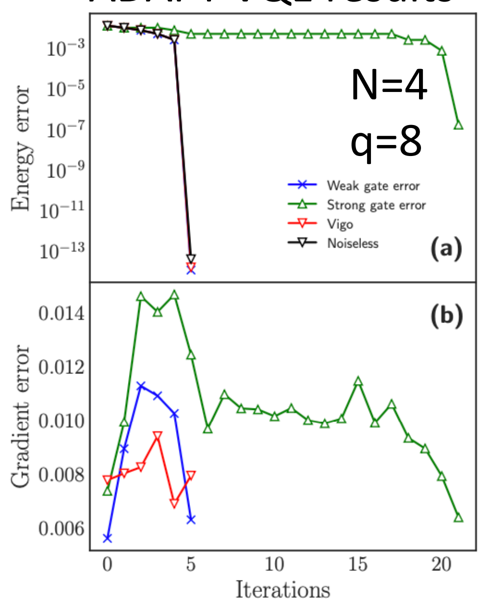
q = Number of qubits

Encoding the Lipkin model on a quantum register



Fermions-to-qubit: Jordan Wigner

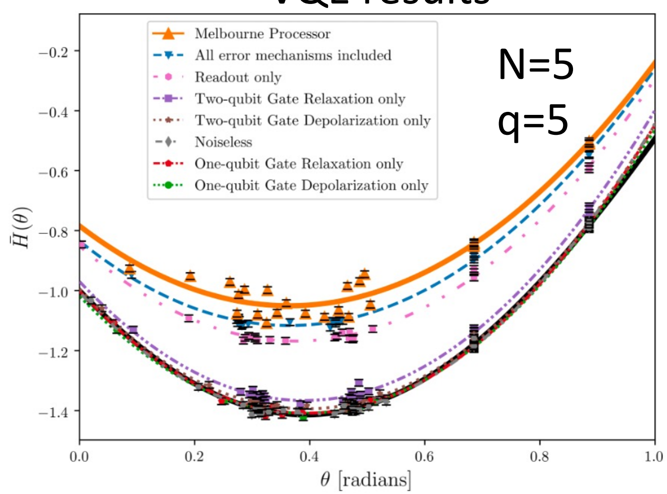
ADAPT-VQE results



J. Romero et al, PRC 105 (2022)

SU(2) encoding

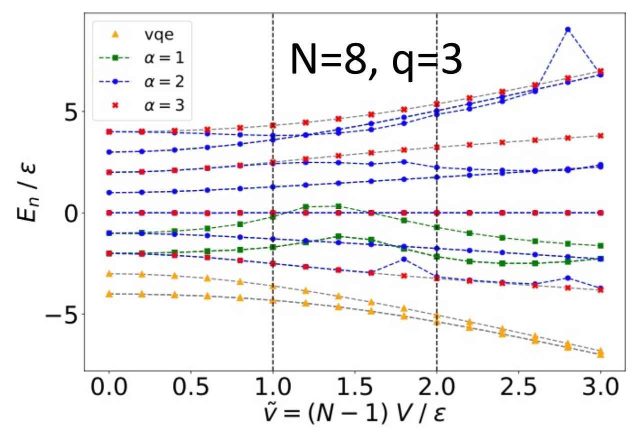
VQE results



M. Cervia et al, PRC 104 (2021)

J-scheme (compact) +parity encoding

QEOM-technique



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

A few Achievements in WP 4.1

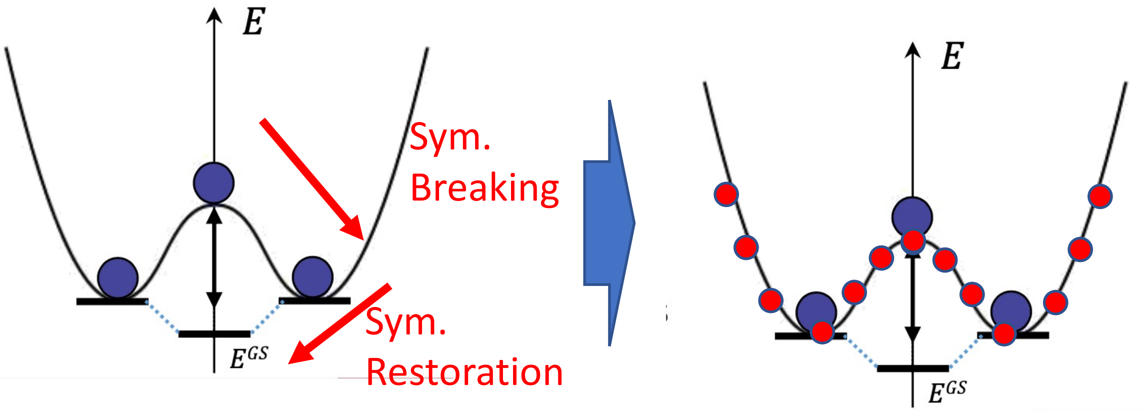
Ansatz/Hybrid Algorithms

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 †
S/IN2P3, IJCLab, 91405 Orsay, France

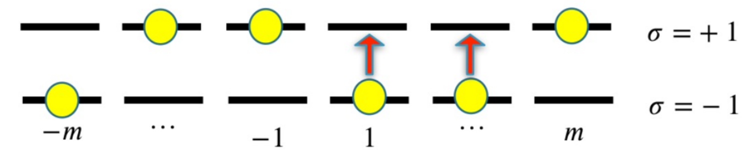


Quantum Generator Coordinate Method

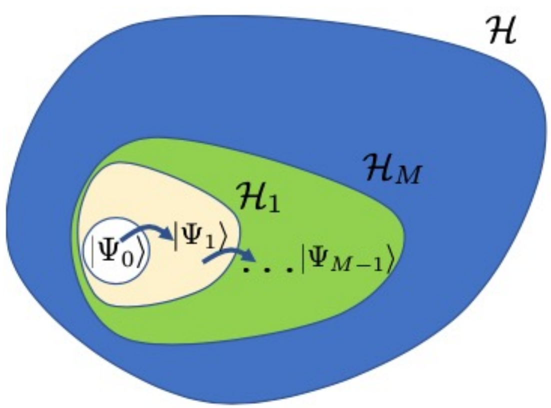
$$|\Psi\rangle = \int_{\mathbf{q}} f(\mathbf{q})|\Phi(\mathbf{q})\rangle d\mathbf{q}$$

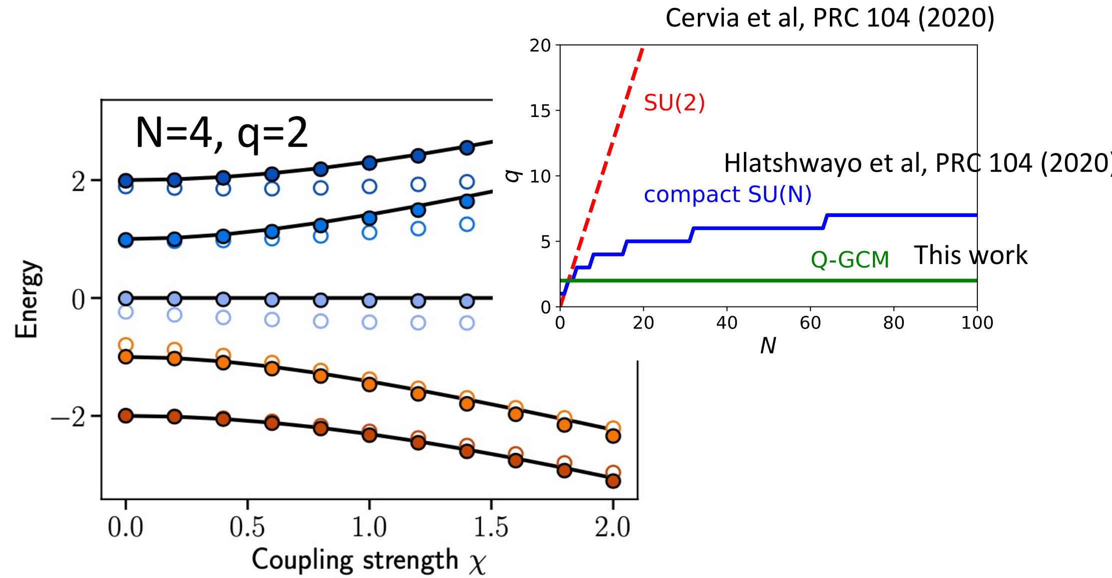
$$\int_{\mathbf{q}'} d\mathbf{q}' \left[\mathcal{H}(\mathbf{q},\mathbf{q}') - E\mathcal{N}(\mathbf{q},\mathbf{q}')\right] f(\mathbf{q}') = 0$$

Application



Quantum Subspace expansion





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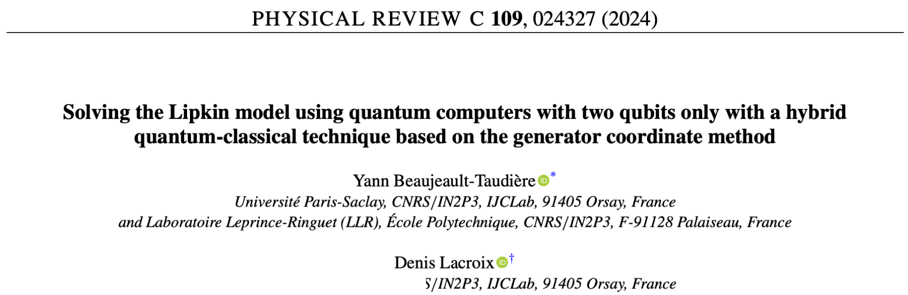
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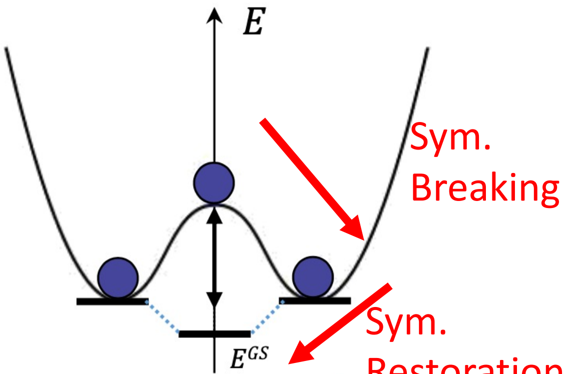

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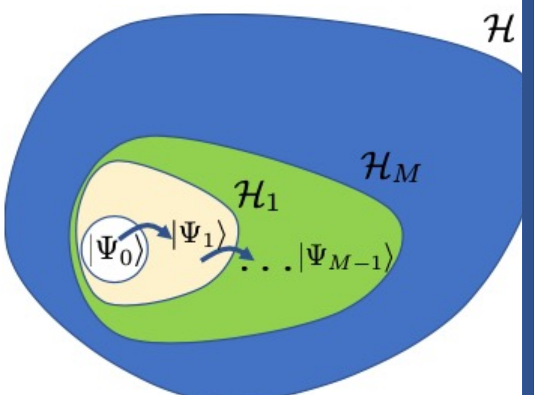
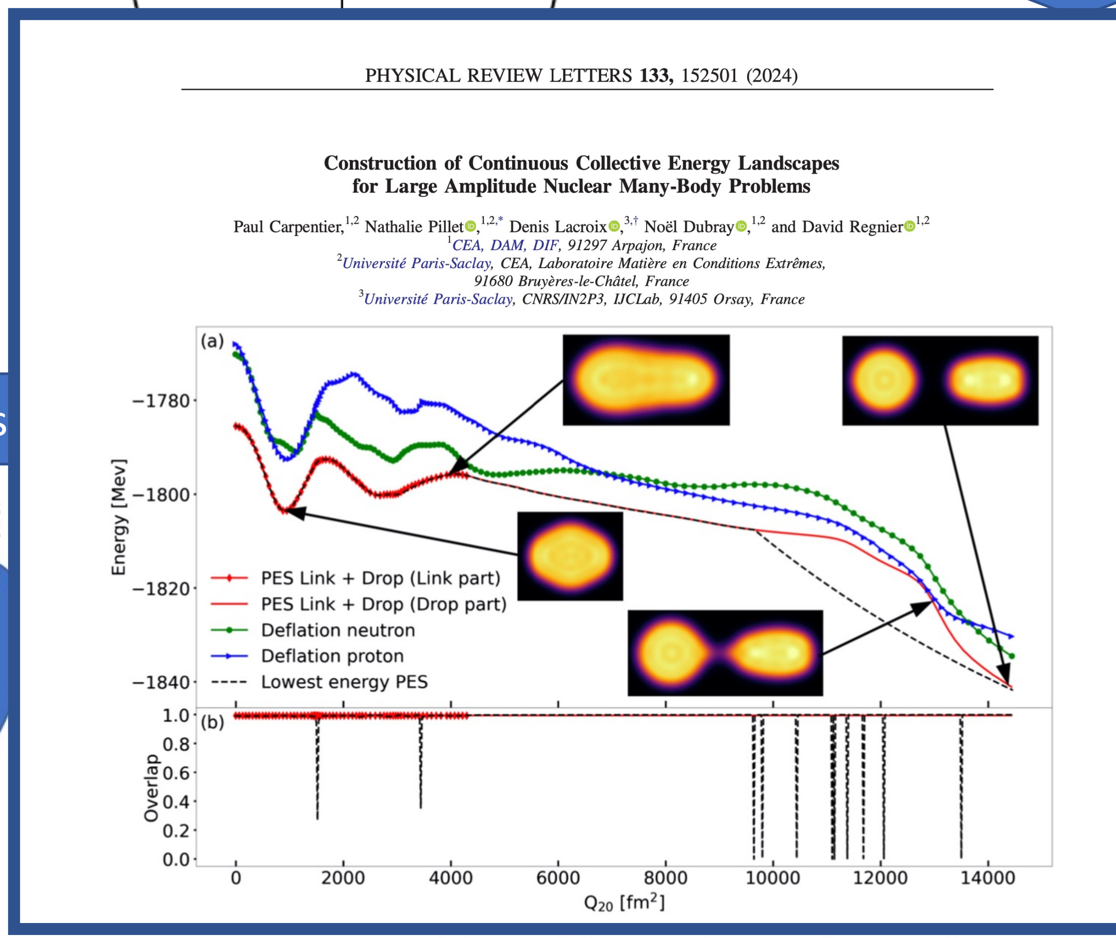
$\mathbf{q}, \mathbf{q}')]\, f(\mathbf{q}') = 0$

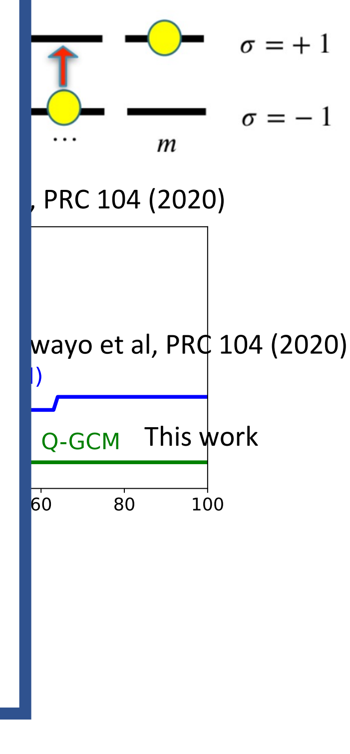
Quantum Subspace expans




PHYSICAL REVIEW LETTERS **133**, 152501 (2024)

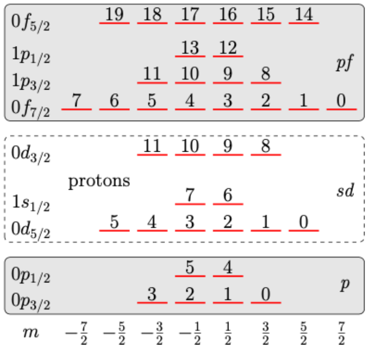
Construction of Continuous Collective Energy Landscapes for Large Amplitude Nuclear Many-Body Problems

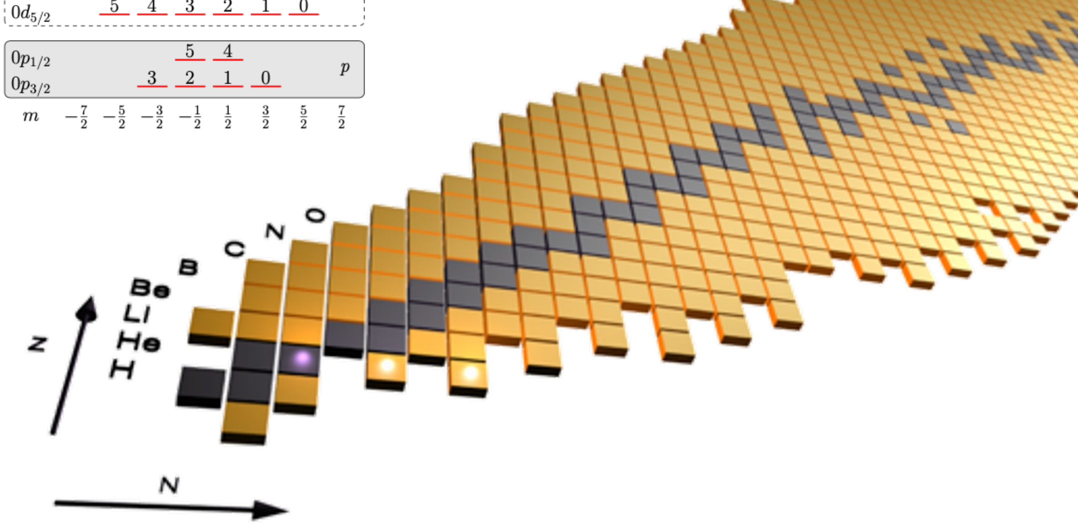
Paul Carpentier,[1,2] Nathalie Pillet,[1,2,*] Denis Lacroix,[3,†] Noël Dubray,[1,2] and David Regnier[1,2]
[1]*CEA, DAM, DIF, 91297 Arpajon, France*
[2]*Université Paris-Saclay, CEA, Laboratoire Matière en Conditions Extrêmes, 91680 Bruyères-le-Châtel, France*
[3]*Université Paris-Saclay, CNRS/IN2P3, IJCLab, 91405 Orsay, France*



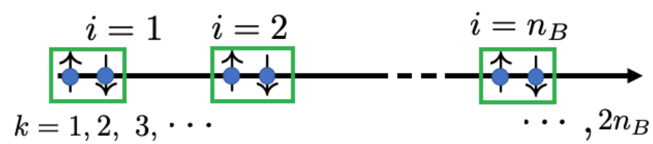
Getting closer to realistic problems

Is the breaking of symmetries always a good idea?

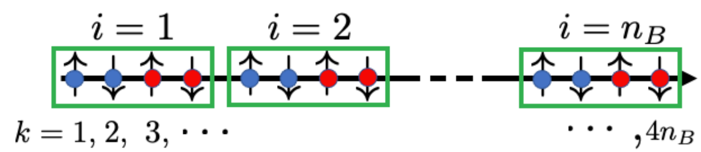




Most tests up to know were made on Particles with spins (s).



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).

And try to control symmetry breaking

Iterative construction of the ansatz

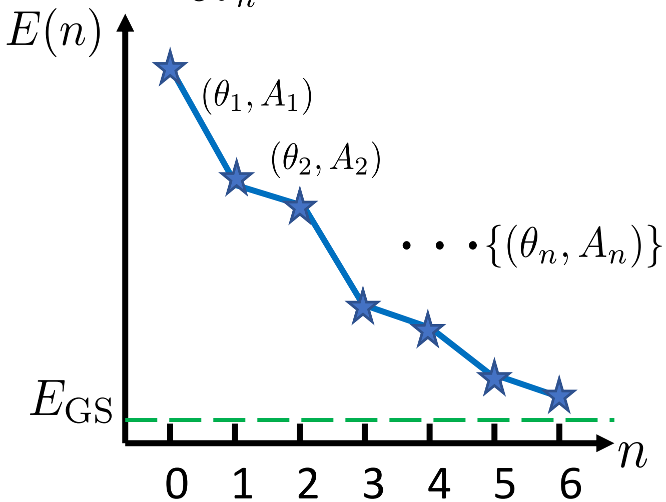
Grimsley, et al, Nat. Commun. 10 (2019)

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

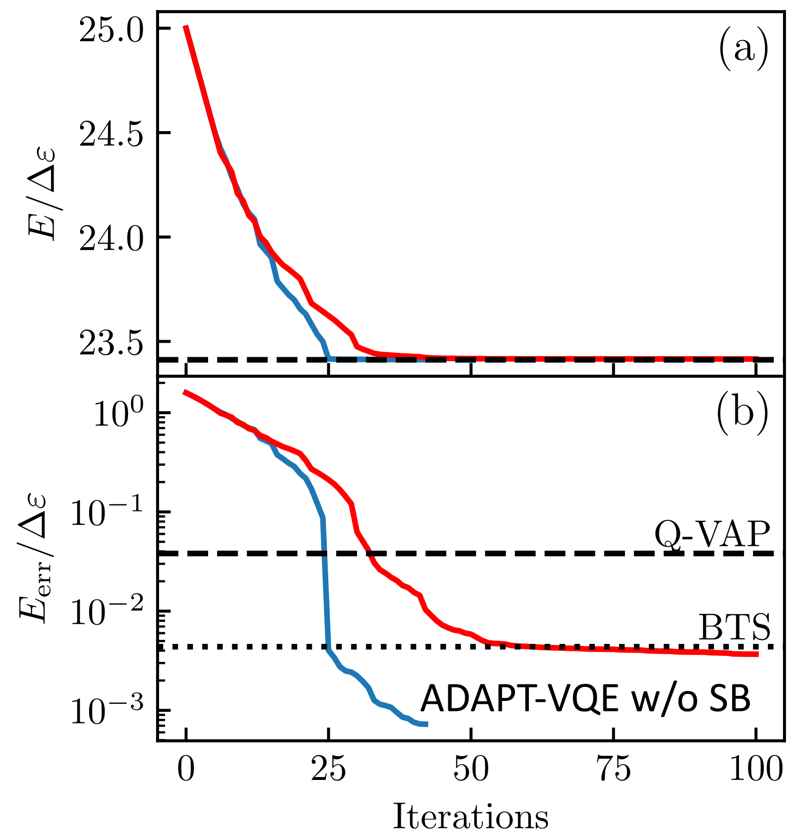
$$|n\rangle = e^{i\theta_n A_n}|n-1\rangle = \prod_{k=1}^{n} e^{i\theta_k A_k}|0\rangle \qquad A_n \in \{O_1, \cdots, O_\Omega\}$$

Such that

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

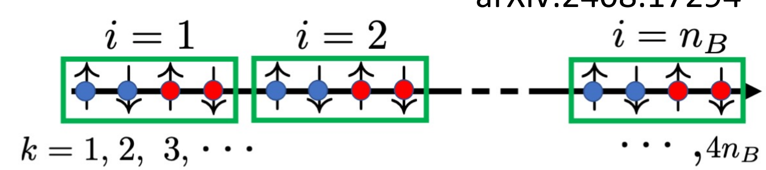


ADAPT-VQE applied to the Superfluid problems: only spins



J. Zhang, D. Lacroix, and Y. Beaujeault-Taudière, PRC (in press) arXiv:2408.17294

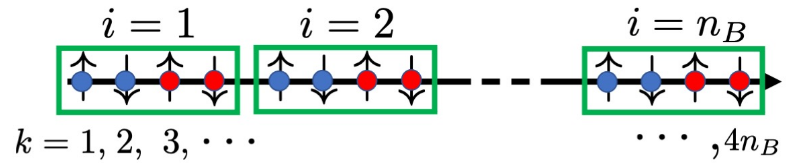
Extension to spin and isospin



Is breaking symmetries always a good idea?

Extension to the proton-neutron pairing Hamiltonian problem

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



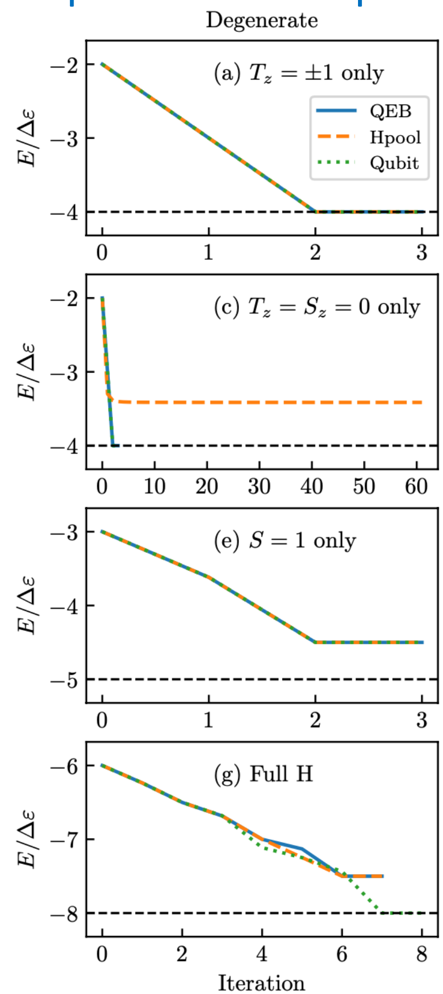
Different Hamiltonian limit

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

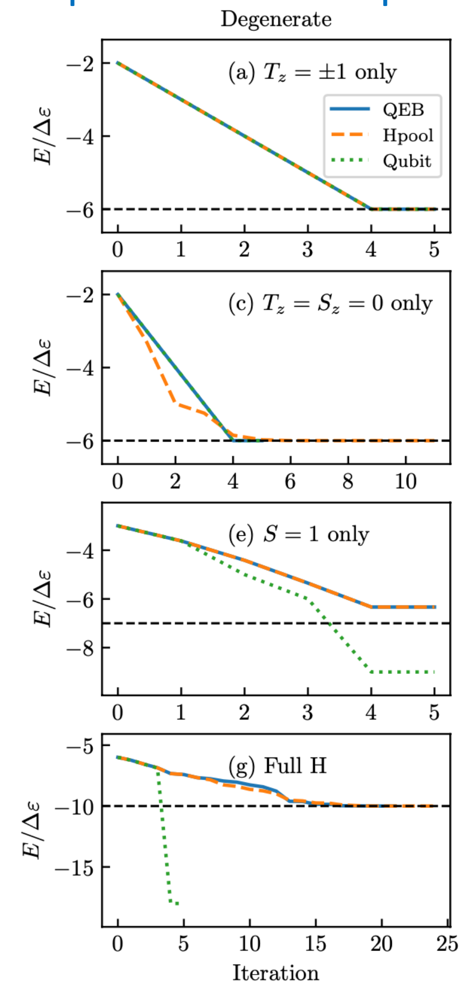
Different operator pool in ADAPT-VQE breaking or not symmetries

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

4 particles on 8 qubits



4 particles on 12 qubits



J. Zhang, DL, and Y. Beaujeault-Taudière, PRC (in press) arXiv:2408.17294

Is breaking symmetries always a good idea?

Extension to the proton-neutron pairing Hamiltonian problem

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

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

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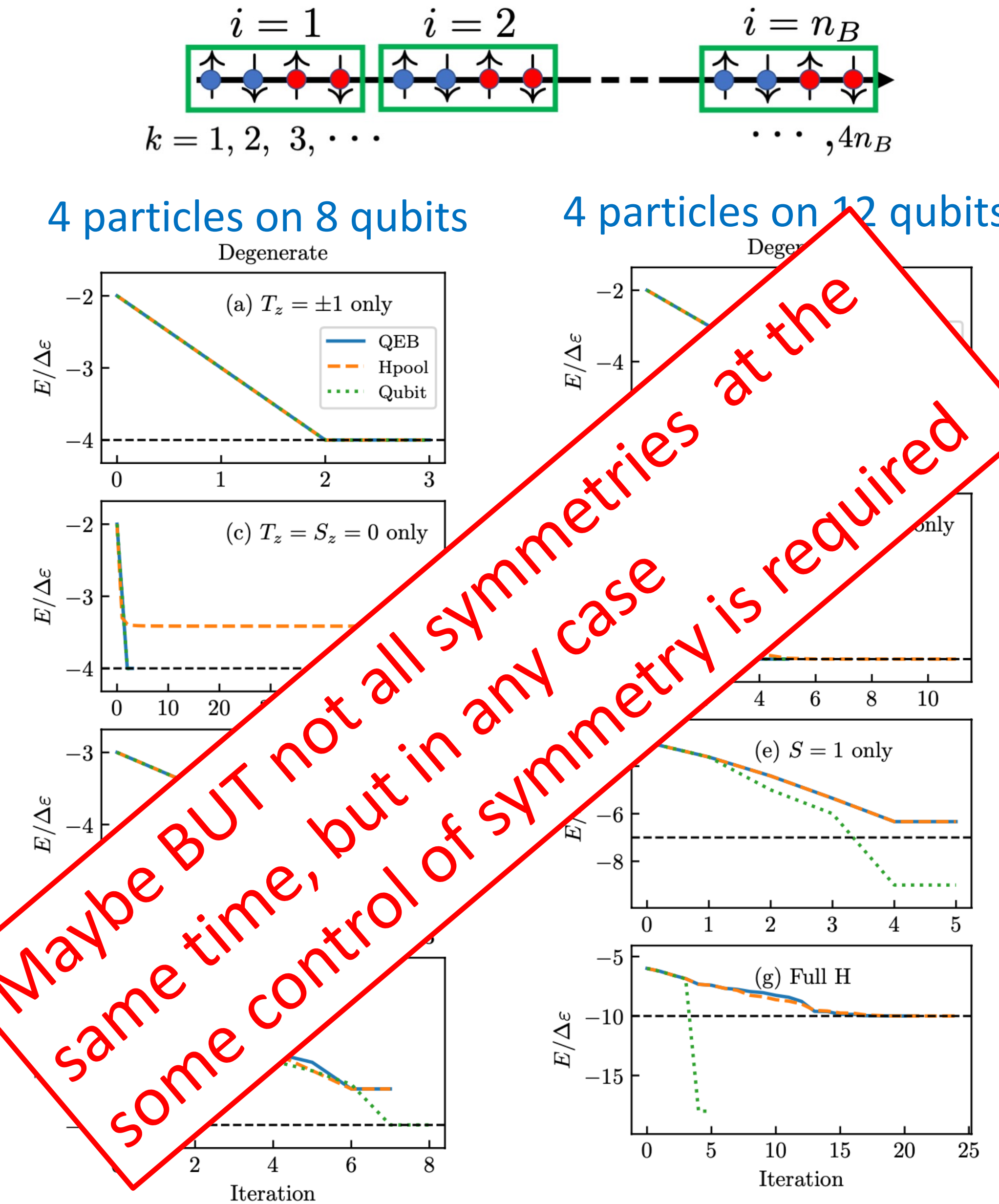


Maybe BUT not all symmetries at the same time, but in any case some control of symmetry is required

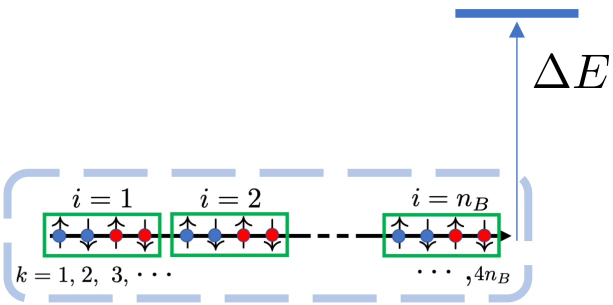
J. Zhang, DL, and Y. Beaujeault-Taudière, PRC (in press) arXiv:2408.17294

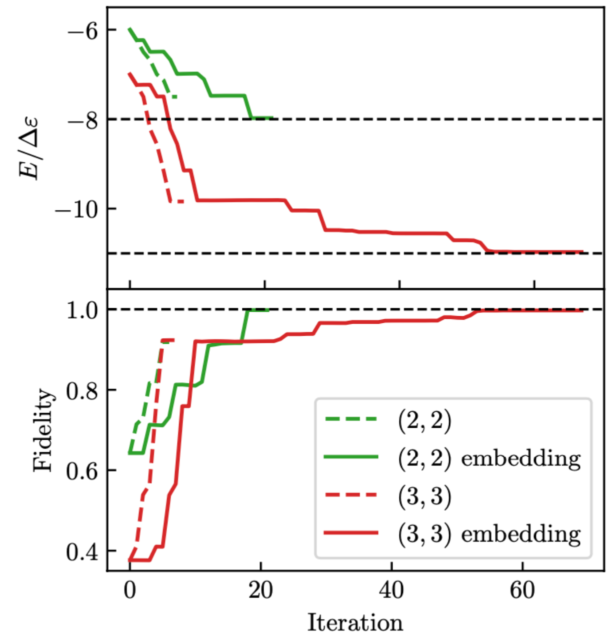
Specific methods to improving convergence

Going closer to nuclei: adding isospin

Embedding

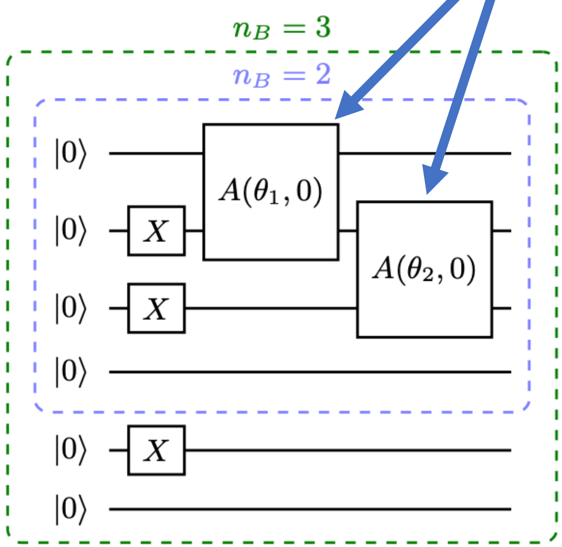
Fictitious set of qubits

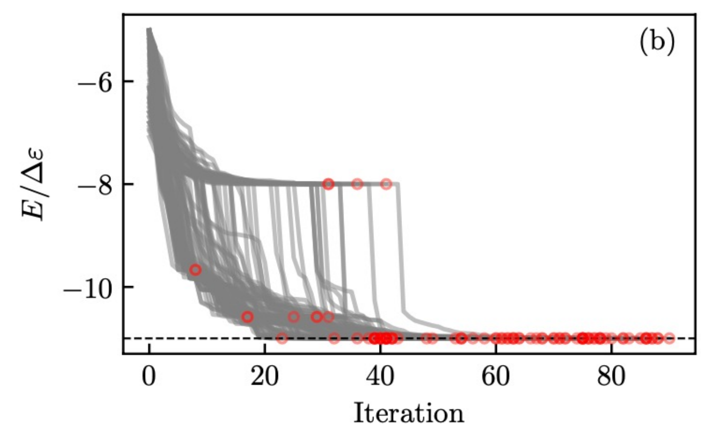




Initial condition Randomization

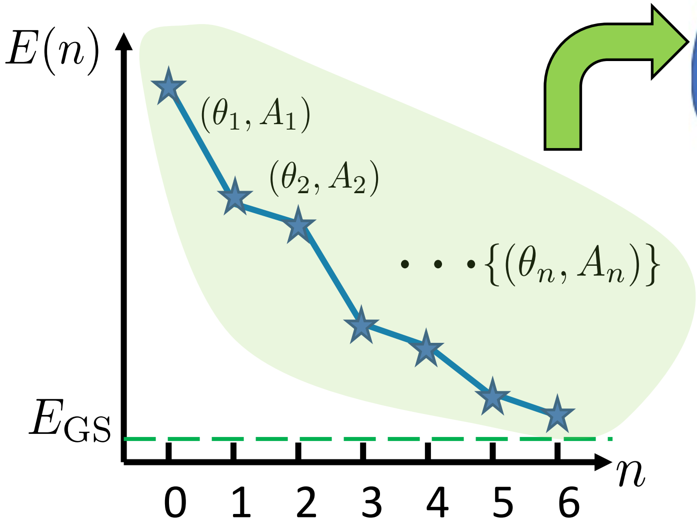
Initial random entangler

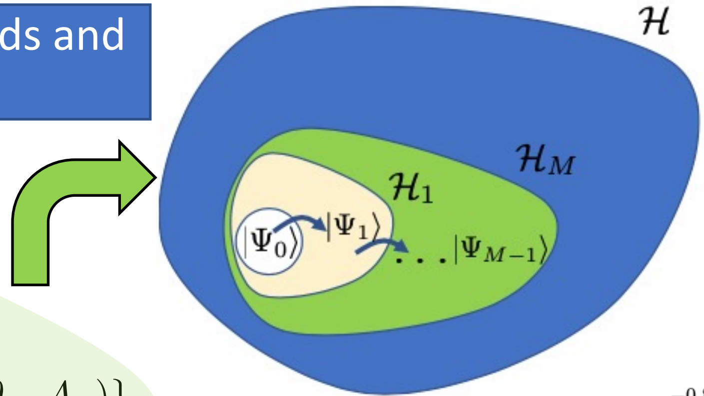




J. Zhang, DL, and Y. Beaujeault-Taudière, PRC (in press) arXiv:2408.17294

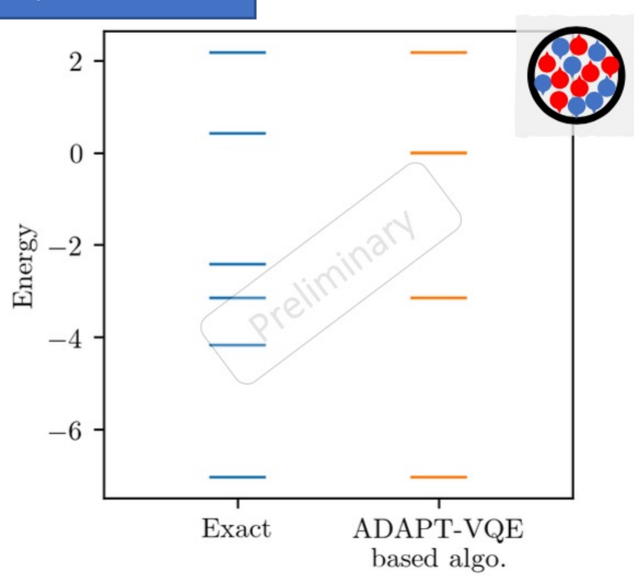
Combining adaptative methods and configuiration mixing



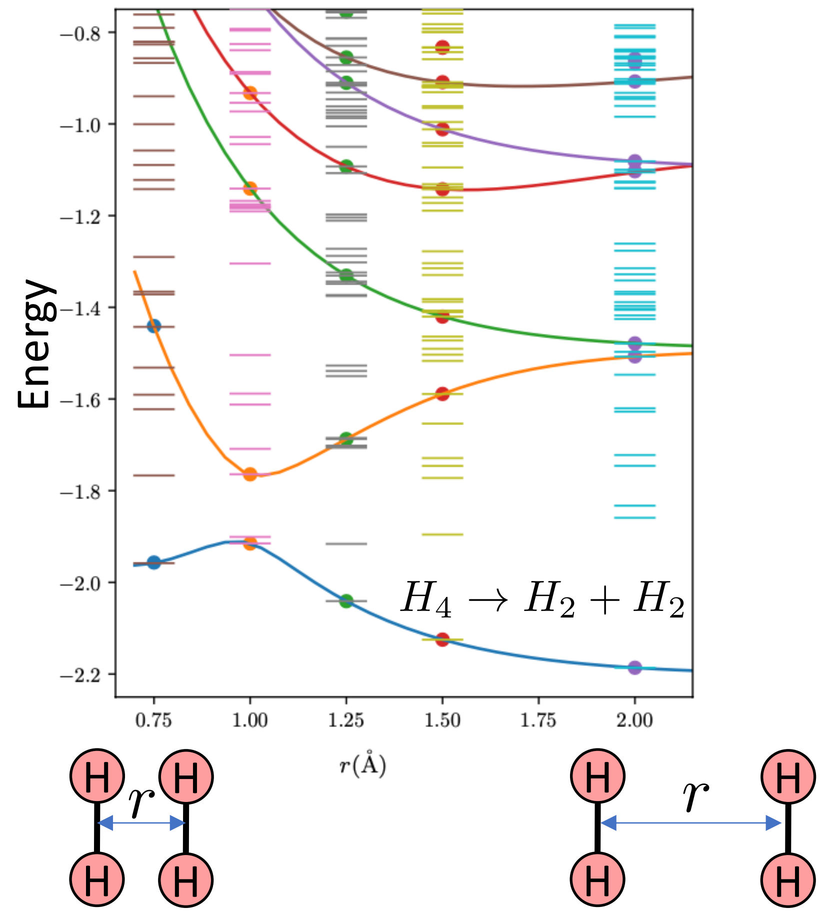


Preliminary results

np-pairing

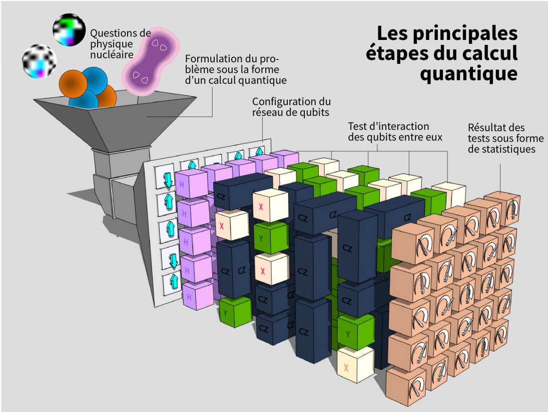


molecule dissociation



J. Zhang, PhD thesis Univ. Paris-Saclay (2025)

Conclusions and outlook



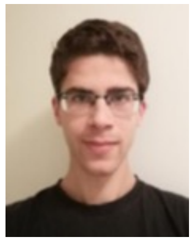
In the Indico, more on:
- -Symmetry and entanglement
- -Phase-estimation
- -Excited states with quantum Krylov
- -Green's function computed with QC.
- -Neutrino oscillations

Thanks to my Collaborators

IJCLab Irène Joliot-Curie Laboratoire de Physique des 2 Infinis — université PARIS-SACLAY — cnrs

E. A. Ruiz Guzman
Now at

J. Zhang



S. Aychet Claisse

Y. Beaujeault-Taudiere

WESTERN MICHIGAN UNIVERSITY — Lawrence Livermore National Laboratory

M. O. Hlatshwayo
Now at

UKRI National Quantum Computing Centre

P. Siwach

IBM Quantum

EVIDEN an atos business

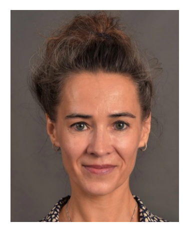
T. Ayral

P. Besserve
Now at
Edimbourg

LPSC Grenoble Laboratoire de Physique Subatomique et de Cosmologie

M. Mangin Brinet

WESTERN MICHIGAN UNIVERSITY



E. Litivinova

UNIVERSITÀ DI TRENTO

A. Roggero

Thank you!

More topics

-- For online version –

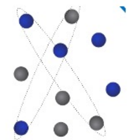
Symmetry breaking, entanglement and Ansatz

A few Achievements in WP 4.1

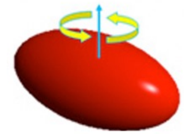
Symmetries and entanglement

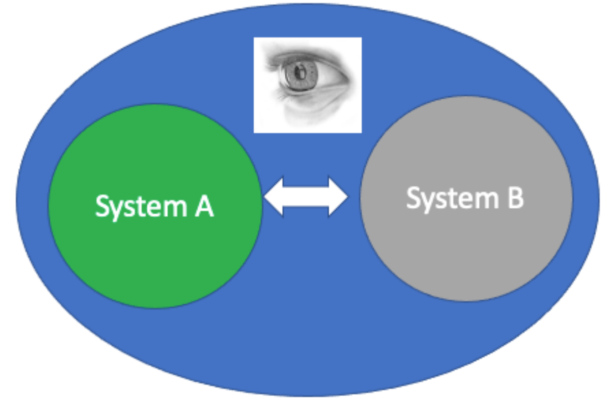
Spontaneous Broken symmetries (SB)

Particle number



Total spins

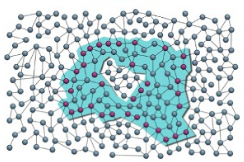




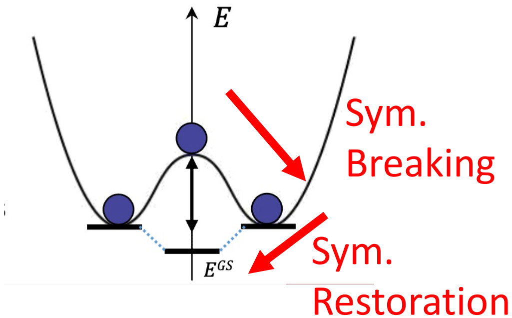
Symmetries And entanglement

Global symmetries induce All-to-all entanglement

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



Global symmetries leads to global entanglement



$$|K,n\rangle$$

$$|0_n\rangle \otimes |K,n-1\rangle \qquad |1_n\rangle \otimes |K-1,n-1\rangle$$

$$|1_{n-1}1_n\rangle \otimes |K-2,n-2\rangle \quad |1_{n-1}0_n\rangle \otimes |K-1,n-2\rangle \quad |0_{n-1}1_n\rangle \otimes |K-1,n-2\rangle \quad |0_{n-1}0_n\rangle \otimes |K,n-2\rangle$$

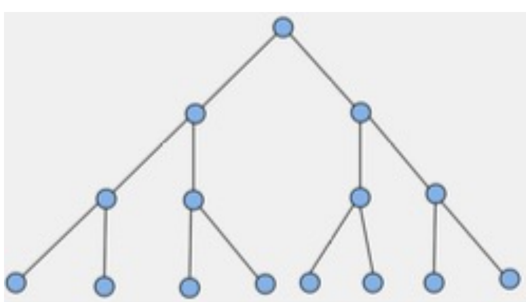
...

→ Many symmetry-preserving states are states made from Binary Tree states (BTS)

→ Key role of permutation invariance

$$|K,n\rangle = \sum_{l=0}^{K} \sqrt{\lambda_l^A} |l,k\rangle_A \otimes |K-l,n-k\rangle_{\bar{A}}$$

$$S_A = -\sum_{l=0}^{K} \lambda_l^A \log_2 \lambda_l^A$$



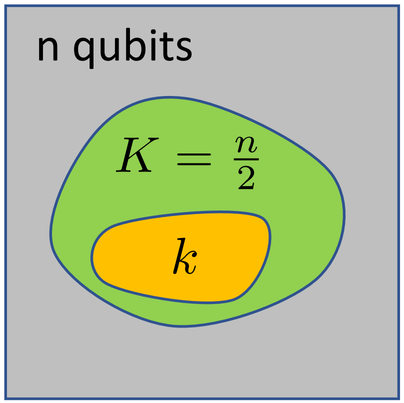
A few Achievements in WP 4.1

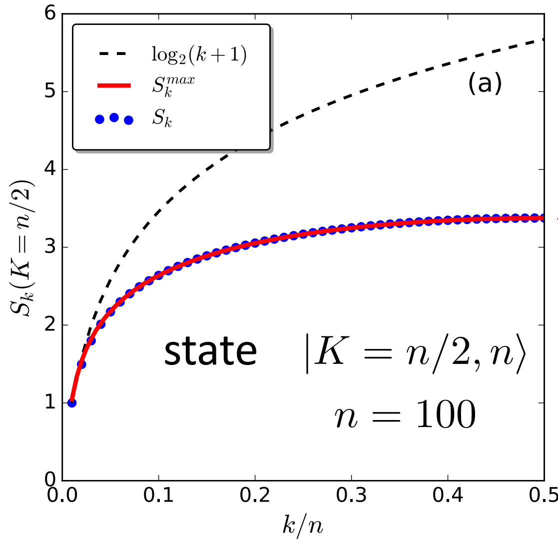
Ansatz/entanglement

PHYSICAL REVIEW C **110**, 034310 (2024)

Entanglement in selected binary tree states: Dicke or total spin states or particle-number-projected BCS states

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





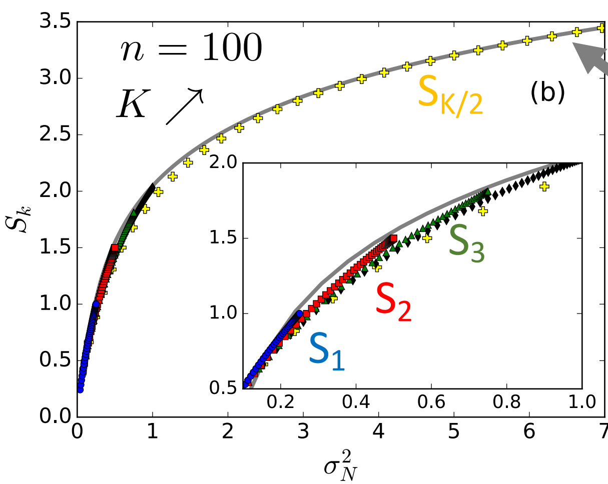
$$S_k^{\max} = \frac{1}{2}\log_2\left[\frac{\pi e}{2}\right] + \frac{1}{2}\log_2 k\left[\frac{n-k}{n-1}\right]$$

$$P(1-P) \leq \frac{1}{4}$$

$$\tilde{S}_k = \frac{1}{2}\log_2\left[2\pi e P(1-P)\right] + \frac{1}{2}\log_2 k\left[\frac{n-k}{n-1}\right]$$

with $P = k/K$

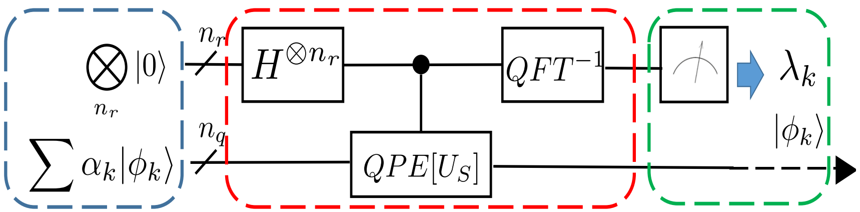
$$\tilde{S}_k = \frac{1}{2}\log_2(2\pi e \sigma_N^2)$$

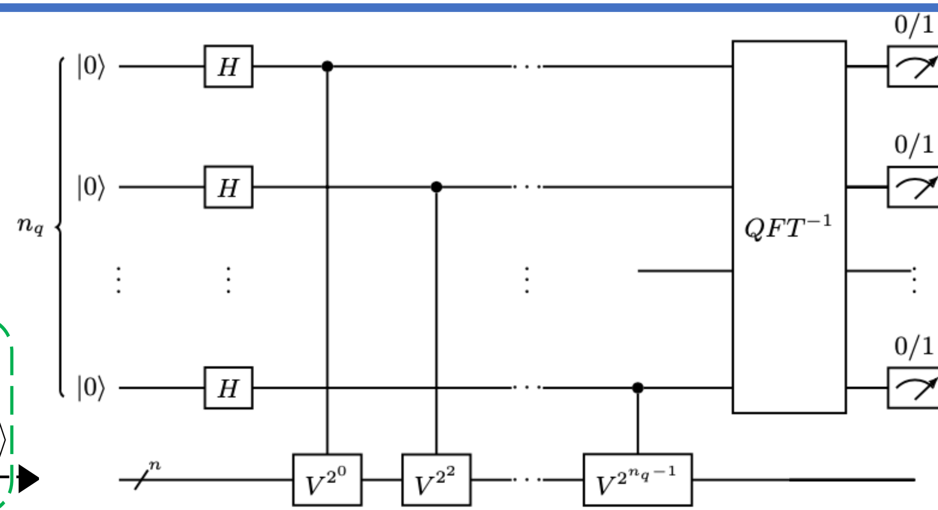


More on Phase Estimation

Illustration of the QPE method with projected state

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

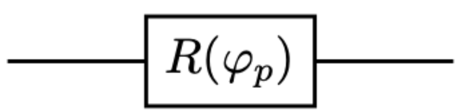
$$U(\tau) = e^{-i\tau H}$$

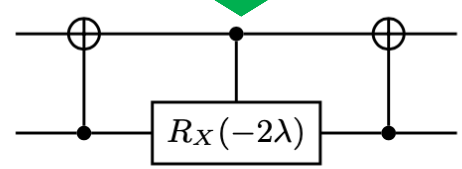
$$U(\tau) = \prod U(\Delta\tau) \longrightarrow \prod U_\varepsilon(\Delta\tau)U_g(\Delta\tau)$$

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

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

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





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 $\lambda_k = a m_k$, $a = \text{cst}$
- 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).

The quantum-Phase estimation (QPE) algorithm

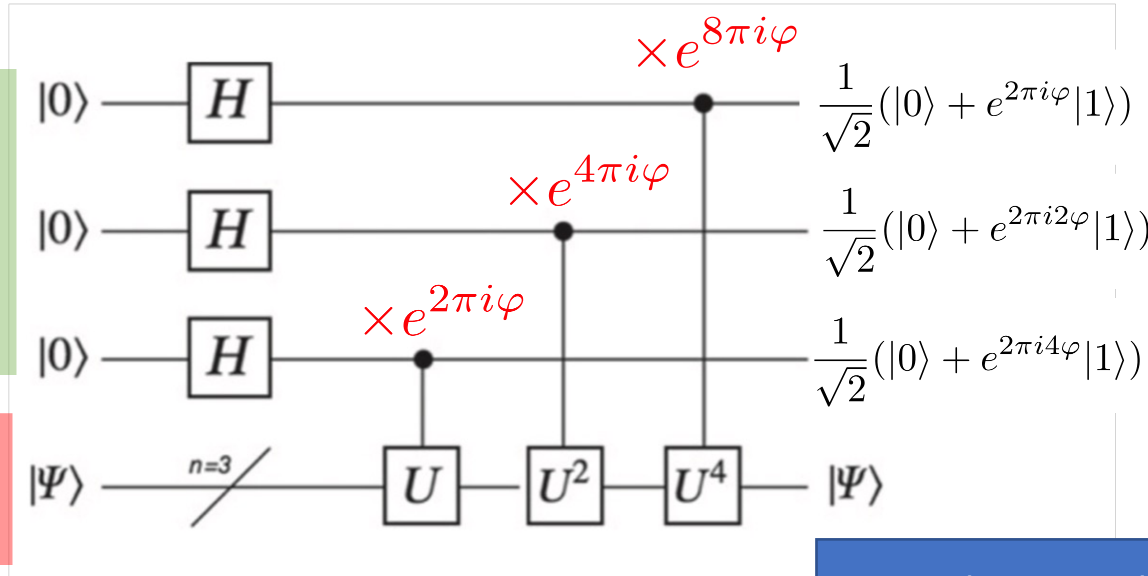
For known eigenvalue problems

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: $0 \le \frac{A}{2^{n_r}} < 1$ 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

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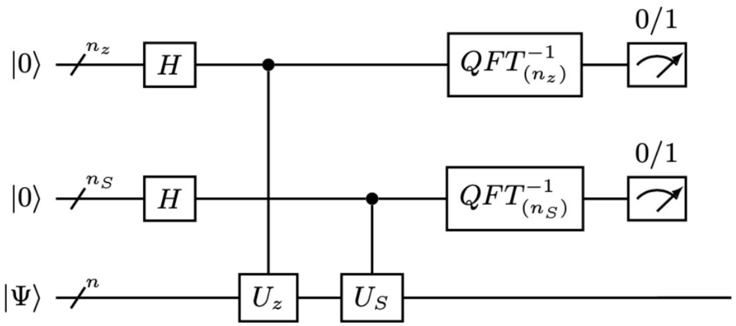
D. Lacroix, *"Symmetry-Assisted Preparation of Entangled Many-Body States on a Quantum Computer"*, PRL 125, 230502 (2020).

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

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



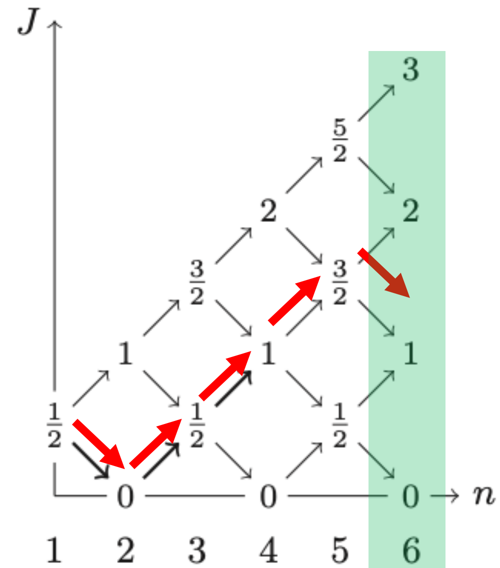
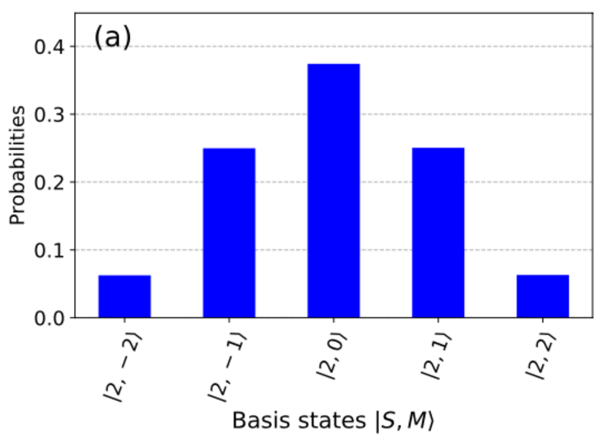
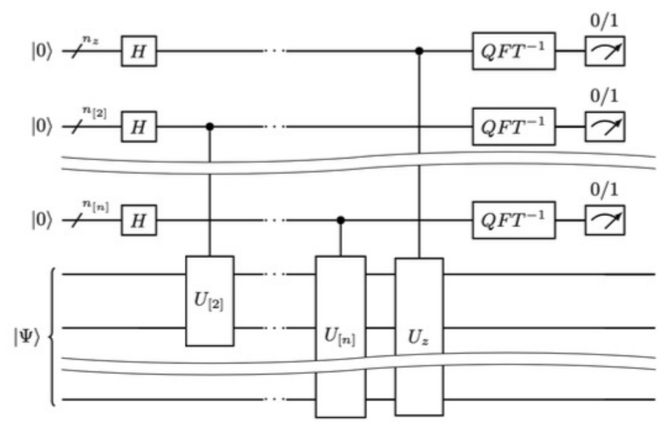


Illustration $|\Psi\rangle = \bigotimes_n H|0\rangle$

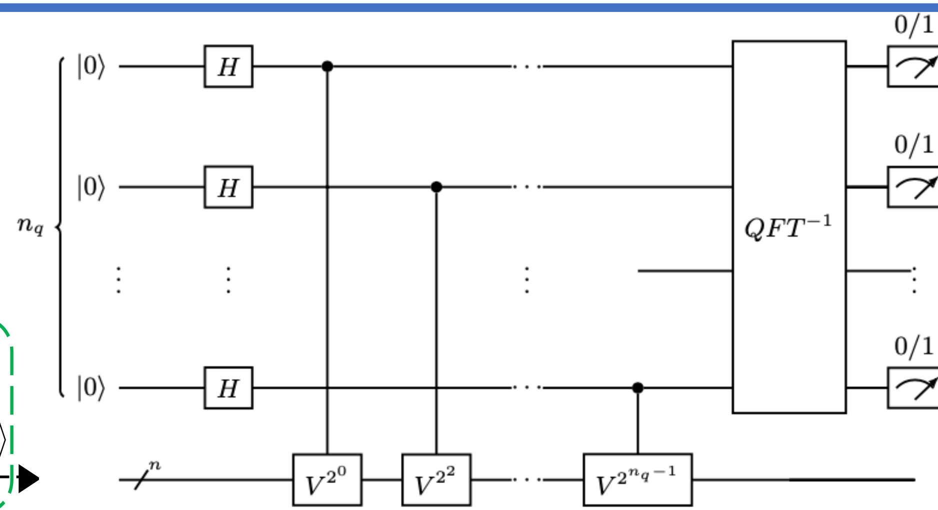


The full basis can eventually be constructed

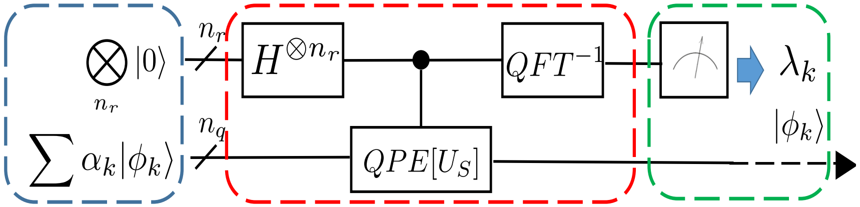


P. Siwach and DL, Phys. Rev. A 104, 062435 (2021)

Illustration of the QPE method for energy with projected state



Initial state preparation



Some technical details

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

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

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

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

For the propagator, we used the Trotter-Suzuki method

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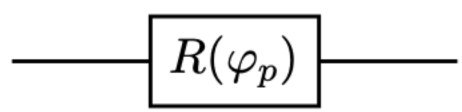


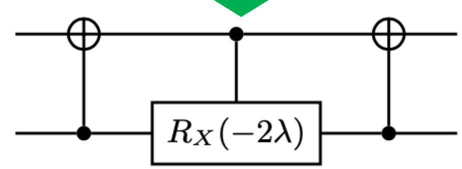
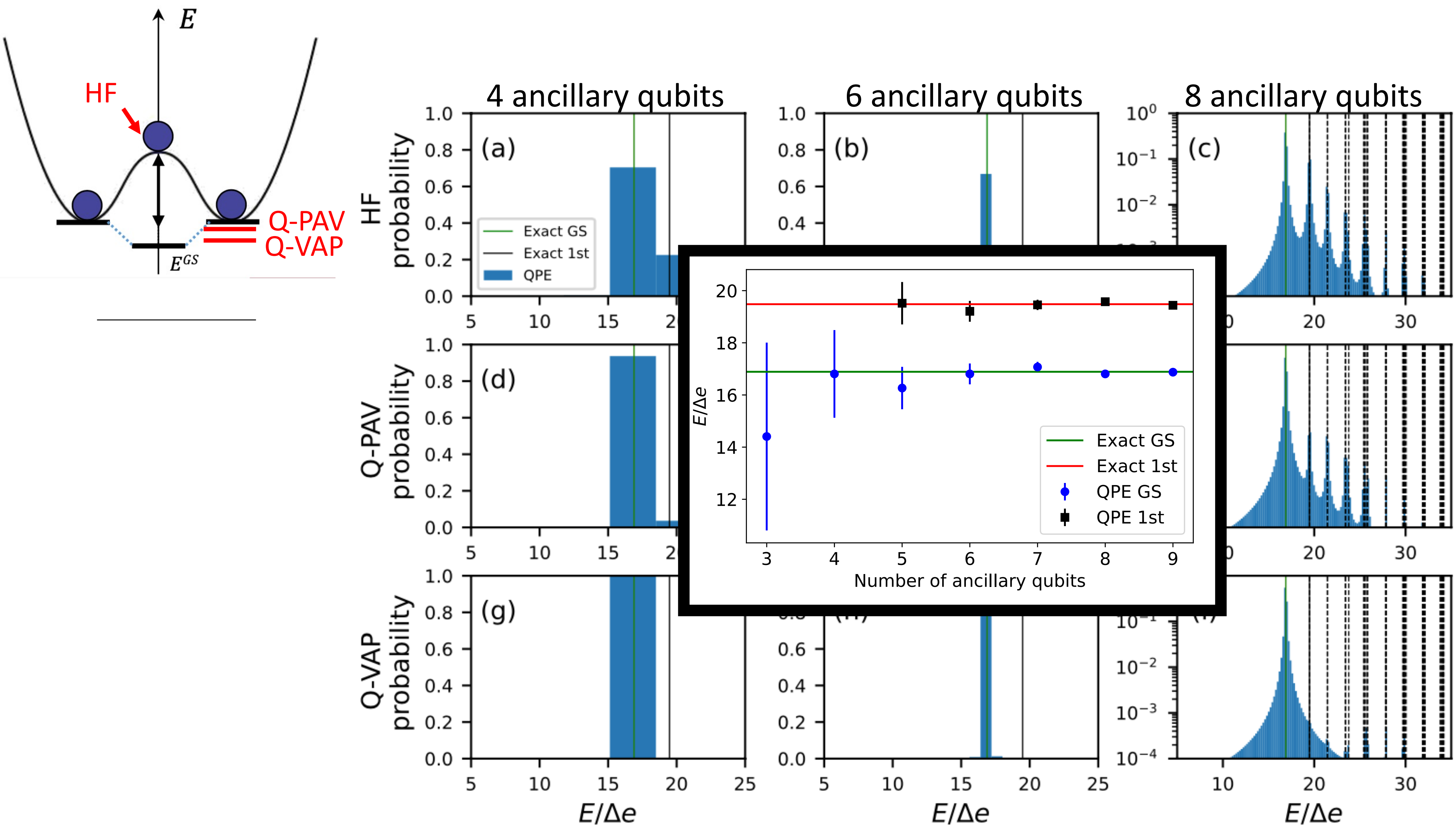
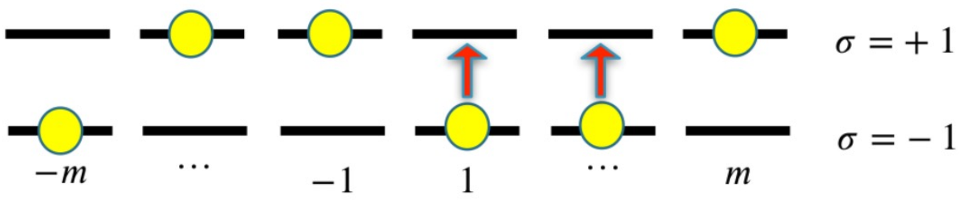


Illustration of the QPE method with projected state



More on symmetry and Lipkin model

Symmetry dilemma: in general using symmetries to solve a problem is a good idea



Lipkin model

$$H = \epsilon J_0 - \frac{1}{2} V (J_+^2 + J_-^2)$$

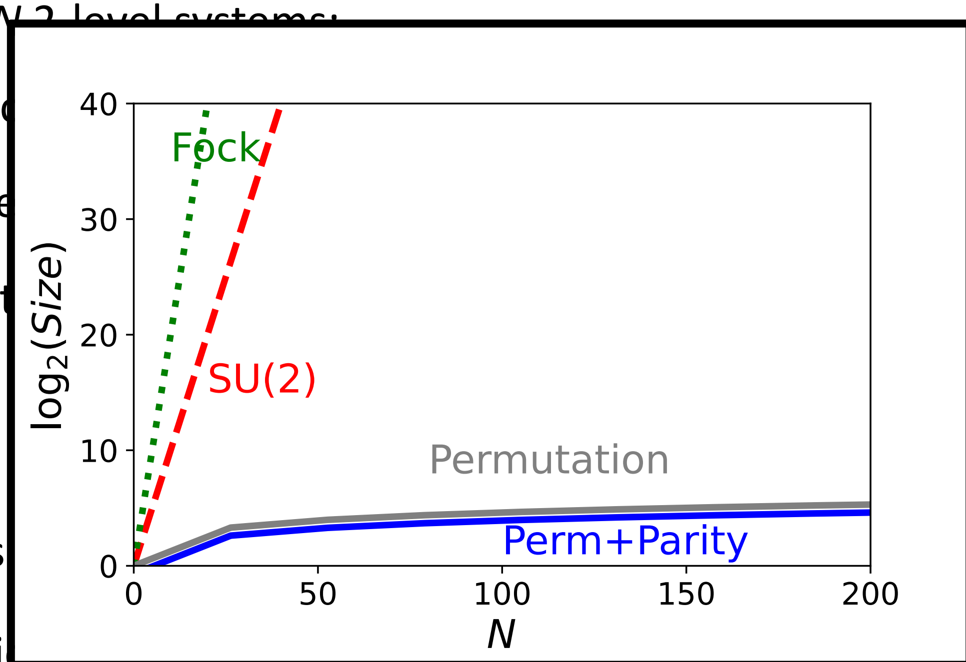
$$J_0 = \frac{1}{2} \sum_{\sigma,m} \sigma c^\dagger_{\sigma,m} c_{\sigma,m}$$ Counts difference of particle number

$$J_+ = J_-^\dagger = \sum_m c^\dagger_{1,m} c_{-1,m}$$ Make jumps between Lower and upper level

Conservation laws and symmetries

For a set of N 2-level systems:

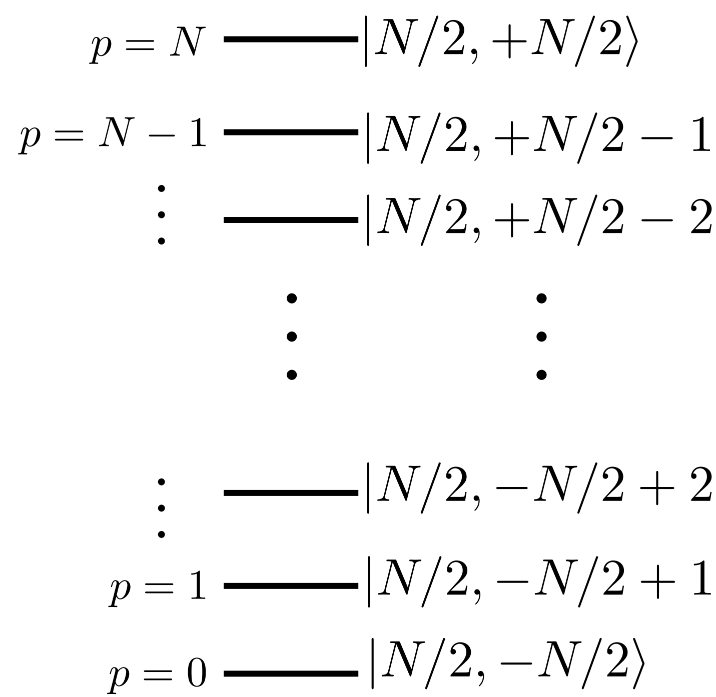
- Full Fo
- Particle
- Permut



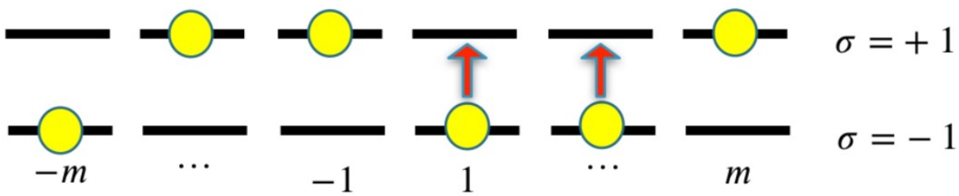
p denotes ... el

Permutati ... total angular momentum $\mathbf{J^2}$ → $(N+1)$ states $|J, M\rangle$

- Parity (odd/even M) → $(N+1)/2$



Symmetry dilemma: in general using symmetries to solve a problem is a good idea



Lipkin model

$$H = \epsilon J_0 - \frac{1}{2}V(J_+^2 + J_-^2)$$

$$J_0 = \frac{1}{2}\sum_{\sigma,m} \sigma c^\dagger_{\sigma,m} c_{\sigma,m}$$ Counts difference of particle number

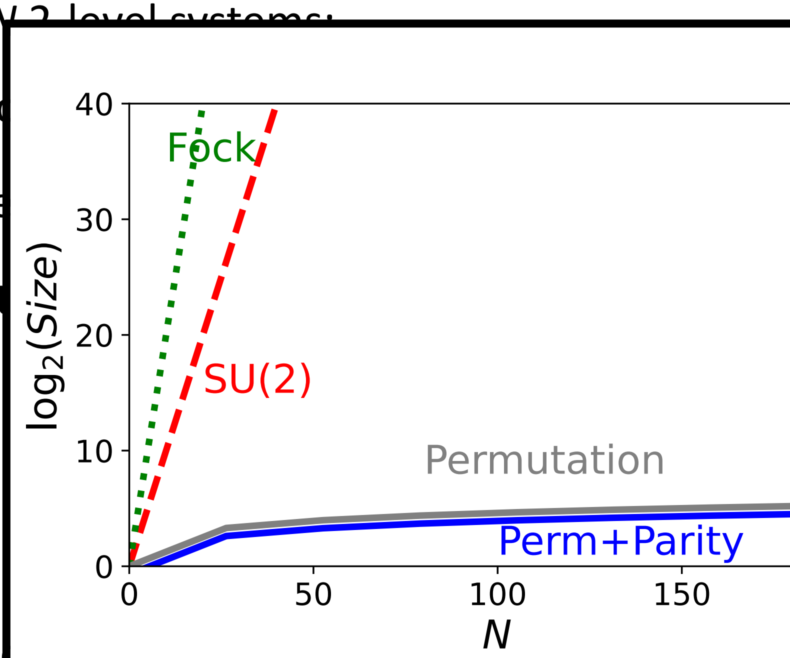
$$J_+ = J_-^\dagger = \sum_m c^\dagger_{1,m} c_{-1,m}$$ Make jumps between Lower and upper level

Conservation laws and symmetries

For a set of N 2-level systems:

- Full Fo
- Particle
- Permut

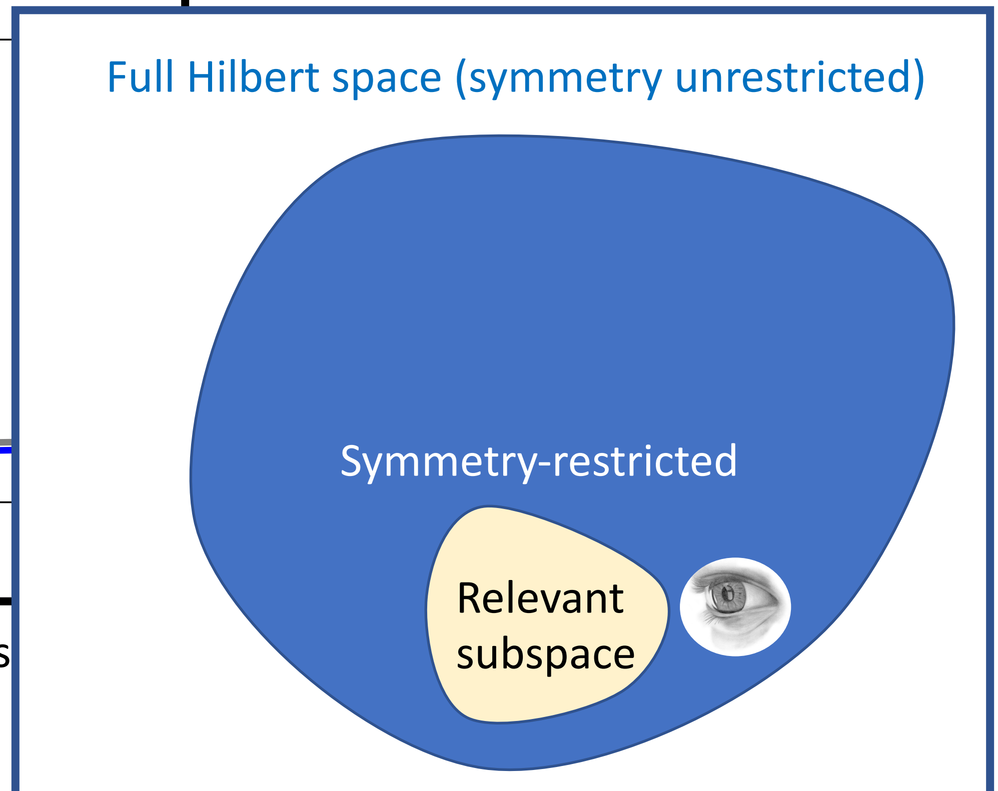
p denotes



Permutati

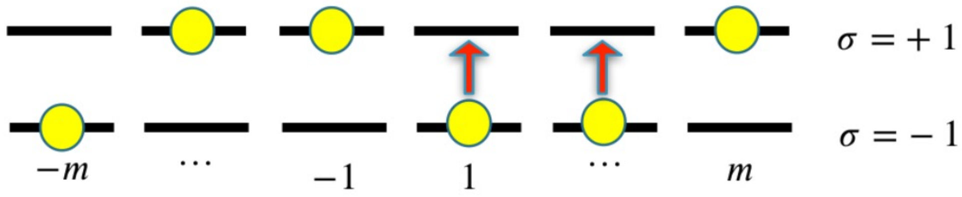
total angular momentum $\mathbf{J}^2$ → $(N+1)$ states

- Parity (odd/even M) → $(N+1)/2$



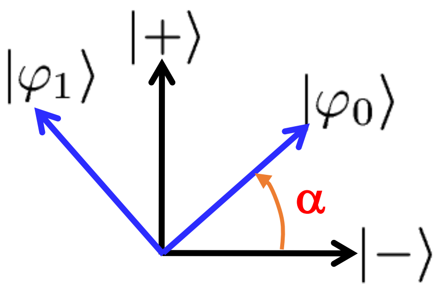
Symmetry dilemma: in general using symmetries to solve a problem is a good idea

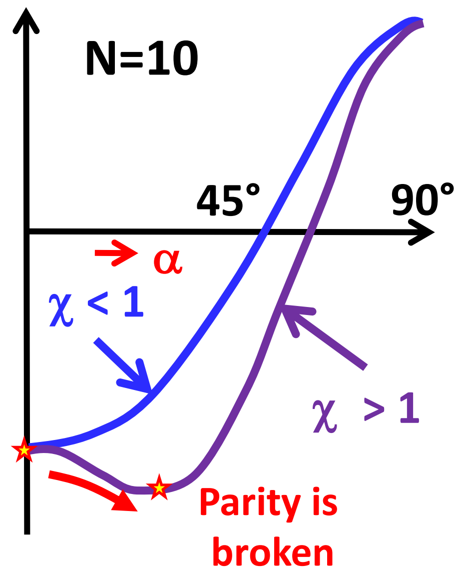
But not always…

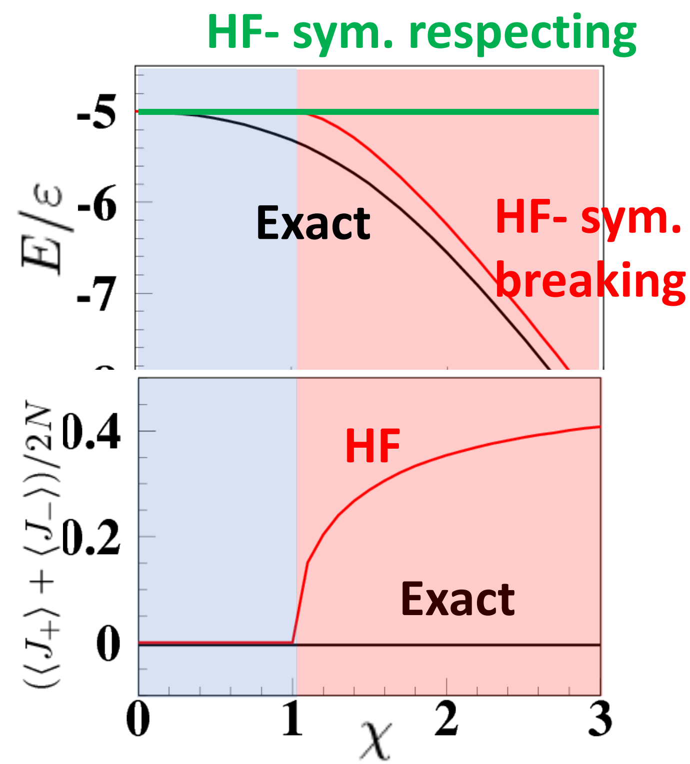


Mean-field and quantum phase transition

Hartree-Fock solution







Symmetry preserving ansatz

Symmetry breaking ansatz

(+) Require less qubits

(-) Lead to more compact encoding

(-) requires more operations to prepare states

(+) Ansatz might be more predictive at low cost

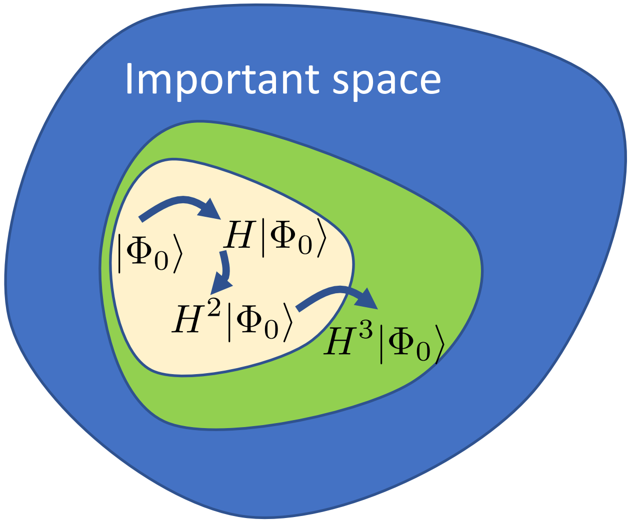
(+) Less operations to prepare the ansatz

(-) Symmetries should be restored, ultimately !

More on Excited states using Quantum Krylov method

Approximate method : Krylov Based methods

Hilbert space



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

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 strategy

Compute overlap and Hamiltonian matrix elements on the quantum computer

Solve the eigenvalue problem on the classical computer

Our first attempt: use the generating function of H

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

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

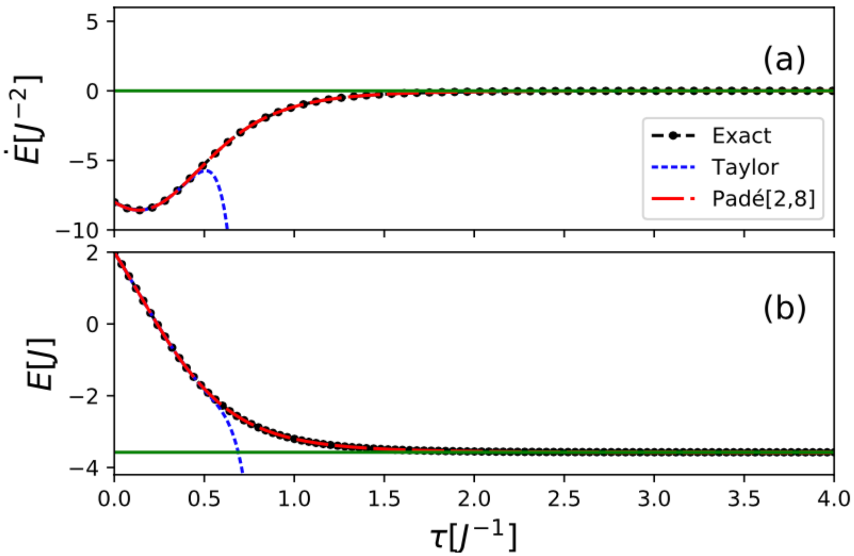
$$\langle H^K \rangle_0 = i^K \left. \frac{d^K F(t)}{dt^K} \right|_{t=0}$$

Ruiz-Guzman and Lacroix, arXiv:2104.08181v2

Approximate method : Krylov Based methods

Hilbert space

Fermi-Hubbard model – Imaginary time
(t-expansion + Padé extrapolation)



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

Diagonalize in the non-orthogonal subspace

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

eigenvalue problem

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

Compute overlap and Hamiltonian matrix elements on the quantum computer

Solve the eigenvalue problem on the classical computer

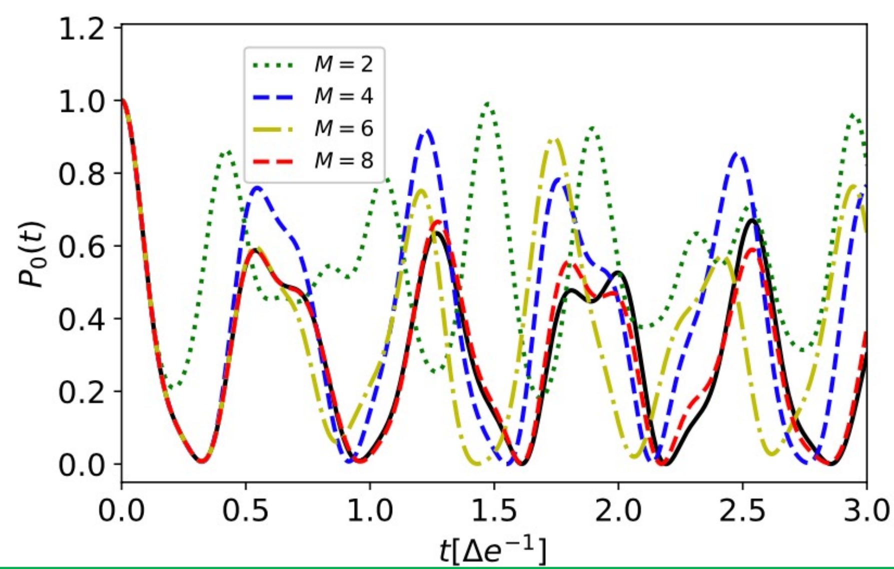
at

$$F(t) = \langle \Phi$$

$$F(t) = 1$$

$$\langle H^K$$

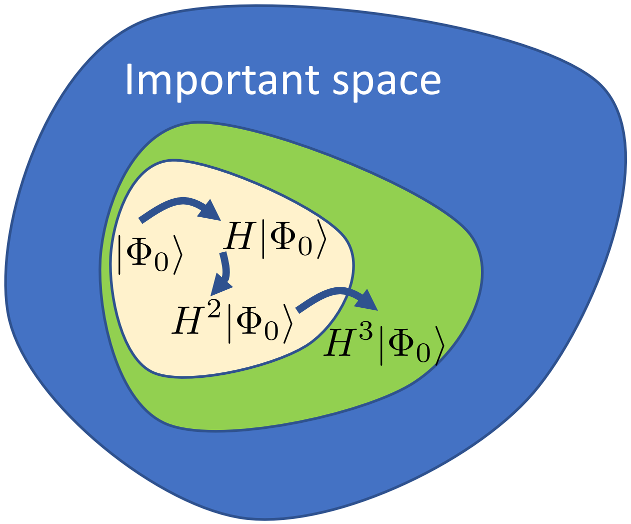
Approximate real-time dynamics



Ruiz-Guzman and Lacroix, arXiv:2104.08181v2

Approximate method : Krylov Based methods

Highly Truncated Hilbert space

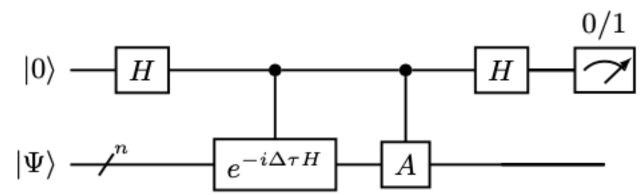


$$\{|\Psi\rangle,\ H|\Psi\rangle, \cdots,\ H^{M-1}|\Psi\rangle\} \equiv \{|\Phi_i\rangle\}_{i=0,M-1}$$

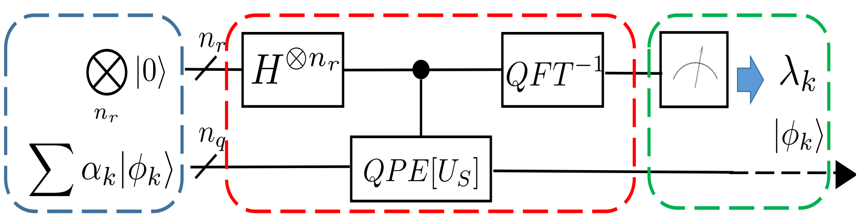
$$\{|\Psi\rangle,\ e^{-i\tau_1 H}|\Psi\rangle, \cdots,\ e^{-i\tau_{M-1} H}|\Psi\rangle\}$$

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

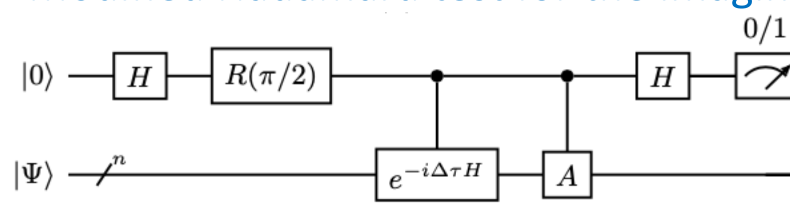
Hadamard test for the real part of *O* and *H*



Initial state preparation

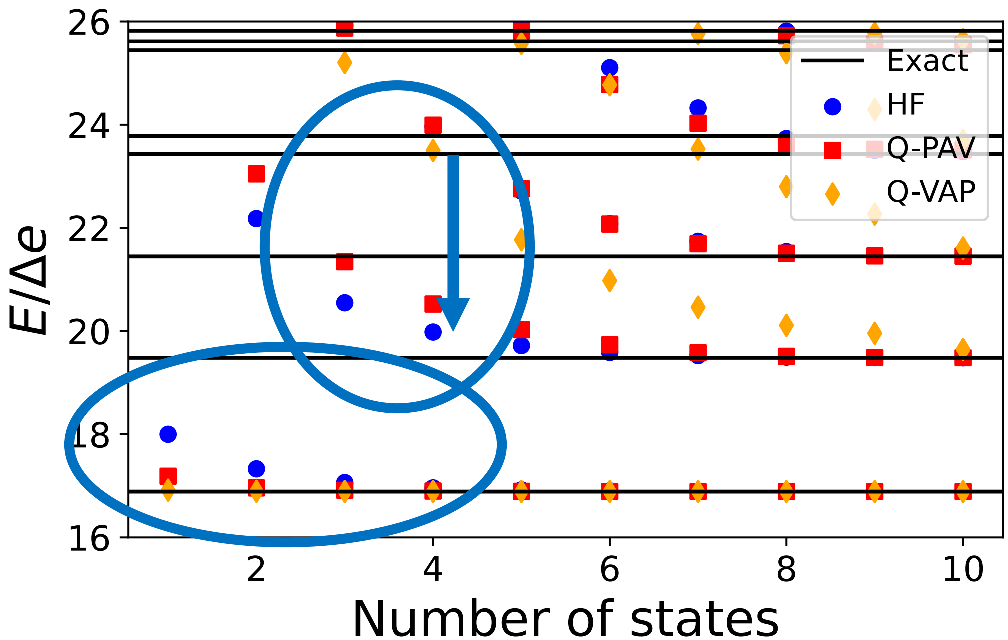


Modified Hadamard test for the imaginary part



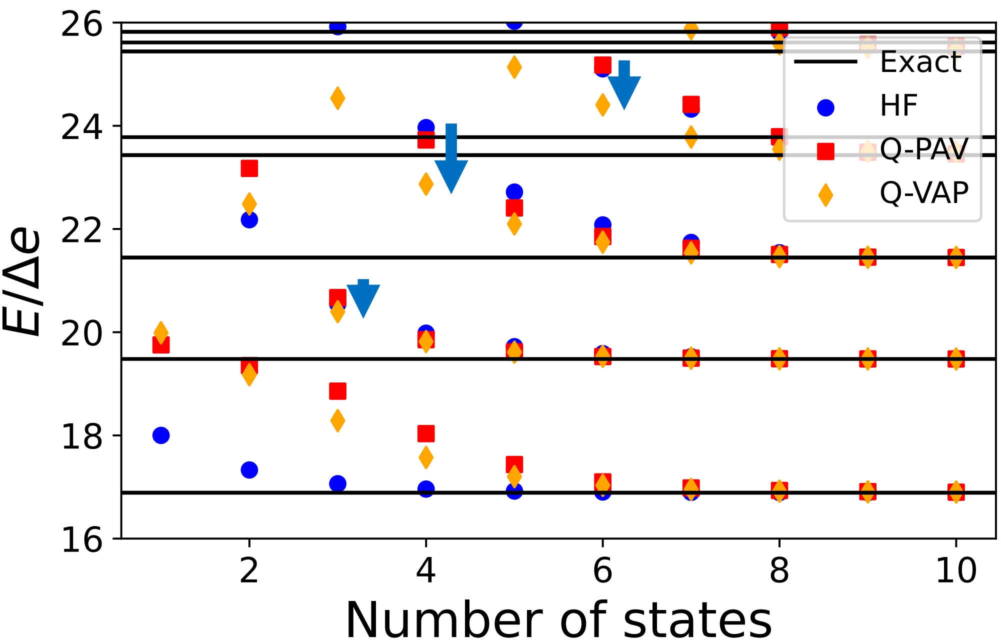
Diagonalization on a classical computer

Comparison QPE vs Quantum Krylov



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

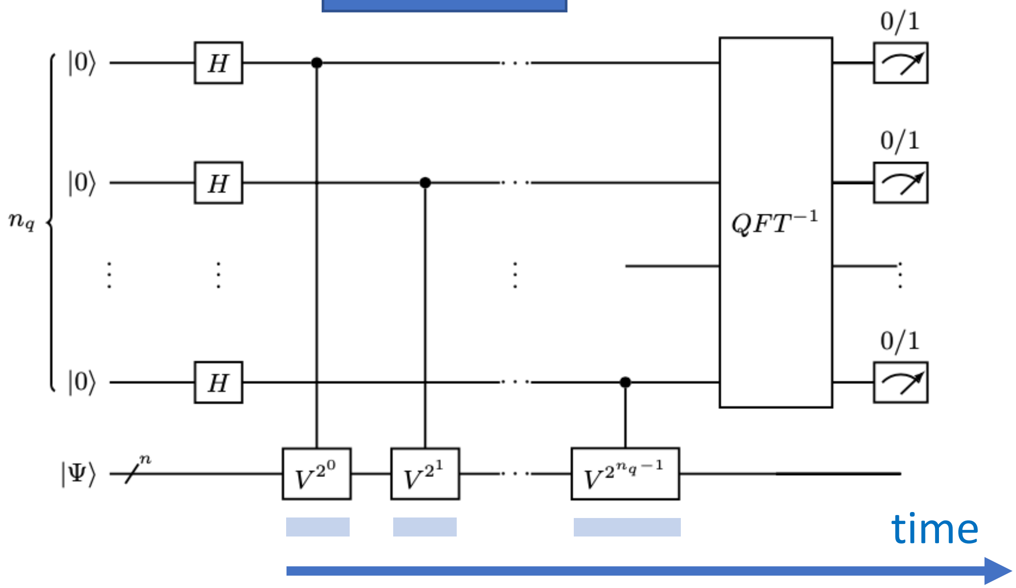
$$|\Psi\rangle = \bigotimes_p [\sin(\theta_p)|0_p\rangle + \cos(\theta_p)|1_p\rangle]$$

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

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

Comparison QPE vs Quantum Krylov after Q-VAP

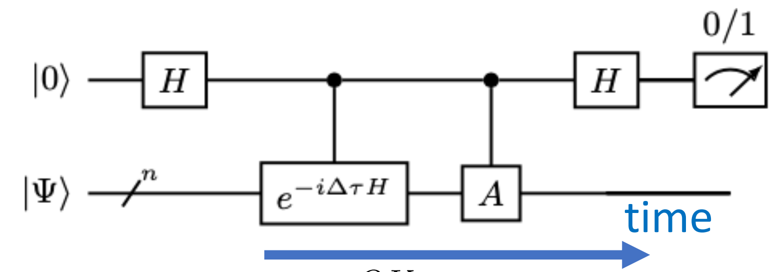
QPE



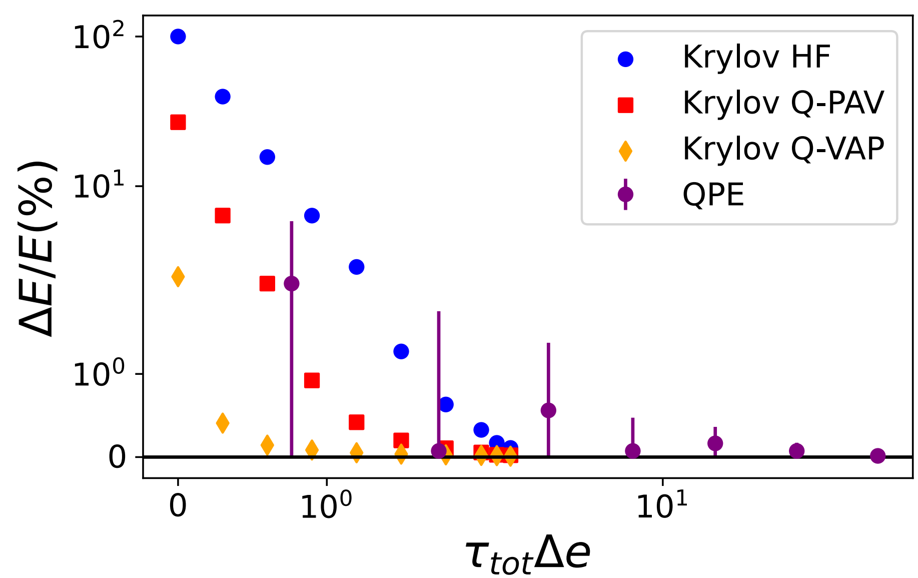
$$\tau_{\mathrm{QPE}} + 2\tau_{\mathrm{QPE}} + \cdots + 2^{n_q-1}\tau_{\mathrm{QPE}}$$

$$\tau_{\mathrm{tot}}^{\mathrm{QPE}}(n_q) = (2^{n_q} - 1)\,\tau_{\mathrm{QPE}}$$

Quantum Krylov



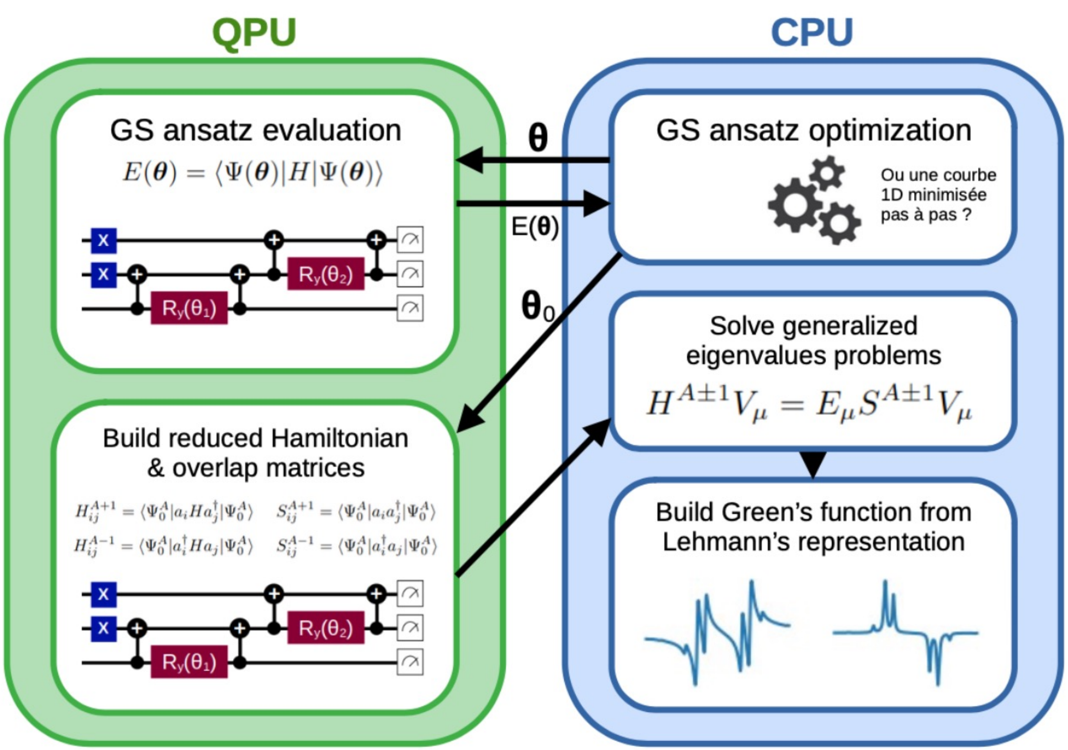
$$\tau_{\mathrm{tot}}^{QK}(M)$$



Green’s function

Ongoing projects

Computing one-body Green's function with Hybrid quantum-classical methods



Dhawan, Zgid, Motta, J. Chem. Theory and Comp. 20, 4629 (2024)

Green's function matrix elements

$$G_{ij}(t,t') = \langle \Psi_0 | \mathrm{T}[a^\dagger_j(t) a_i(t')] | \Psi_0 \rangle$$

Lehman representation

$$G_{ij}(\omega) = \frac{\langle \Psi^N_0 | a_i | \Psi^{N+1}_k \rangle \langle \Psi^{N+1}_k | a^\dagger_j | \Psi^N_0 \rangle}{\omega - (E^{N+1}_k - E^N_0) + i\eta} + \sum_k \frac{\langle \Psi^N_0 | a^\dagger_j | \Psi^{N-1}_k \rangle \langle \Psi^{N-1}_k | a_i | \Psi^N_0 \rangle}{\omega - (E^N_0 - E^{N-1}_k) - i\eta}.$$

Strategy

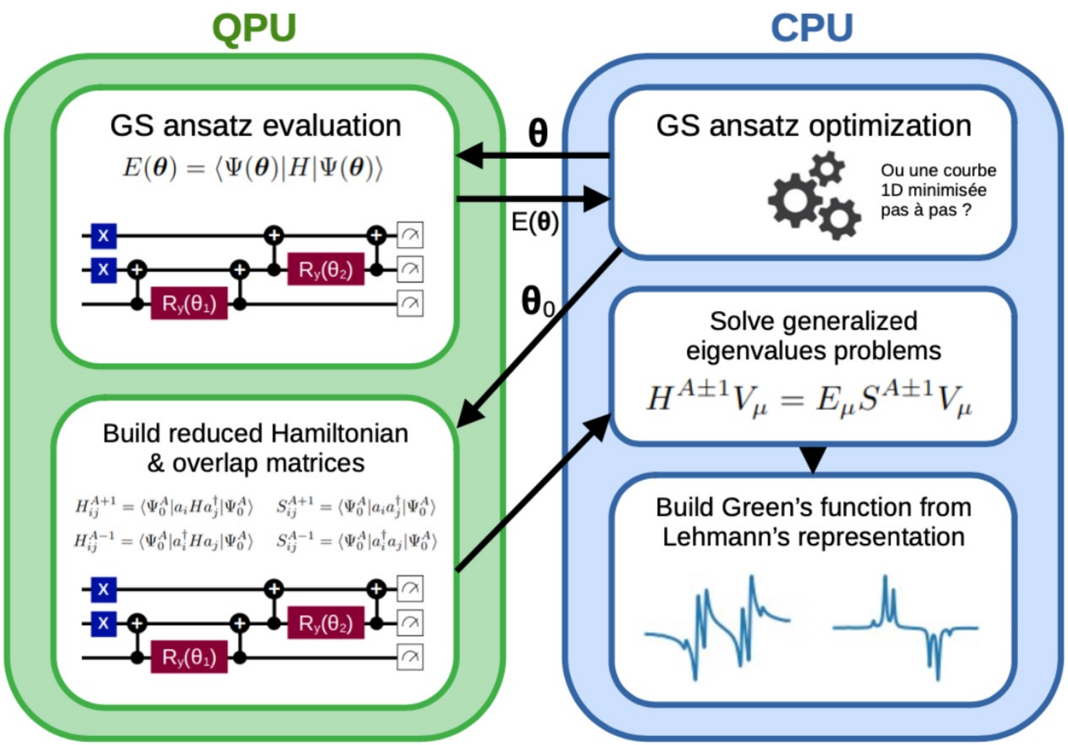
- Design and optimize an accurate Ansatz for the ground state for N particles
- Use two separate Quantum Space Expansion For (N+1) and (N-1) particles

Aychet-Claisse, Lacroix, Somà, Zhang, in preparation

A few Achievements in WP 4.1

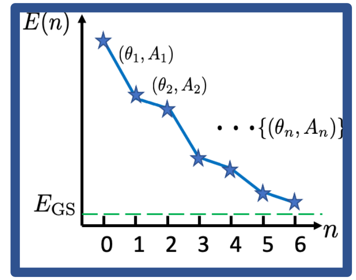
Ongoing projects

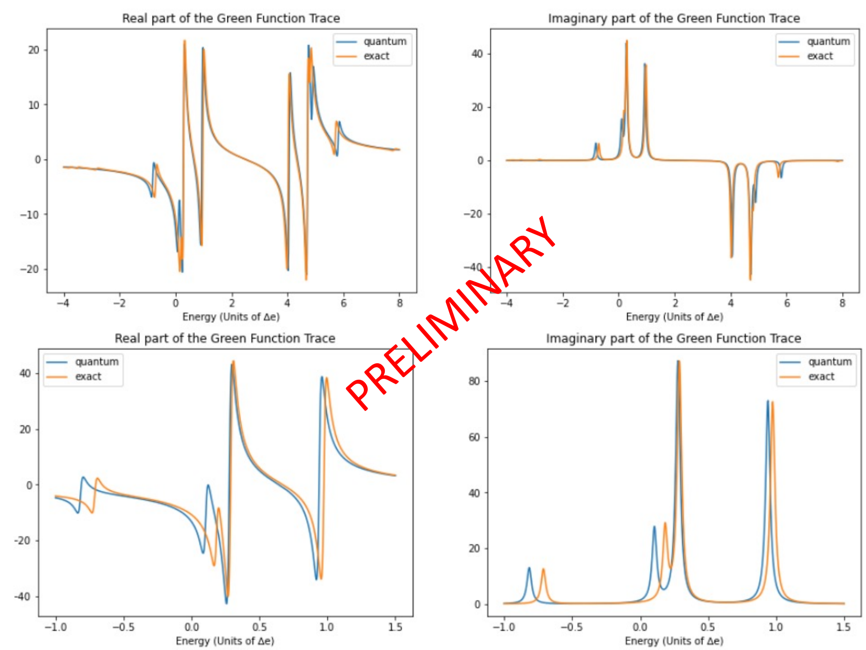
Computing one-body Green's function with Hybrid quantum-classical methods



Dhawan, Zgid, Motta, J. Chem. Theory and Comp. 20, 4629 (2024)

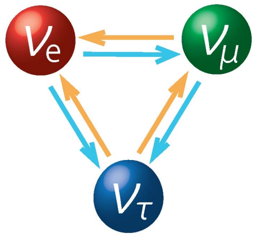
Initial state Prep. with ADAPT-VQE

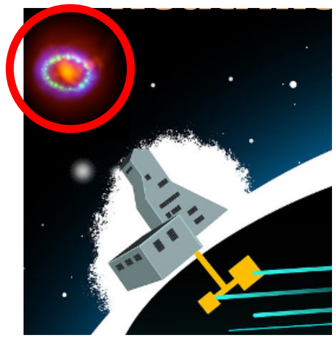


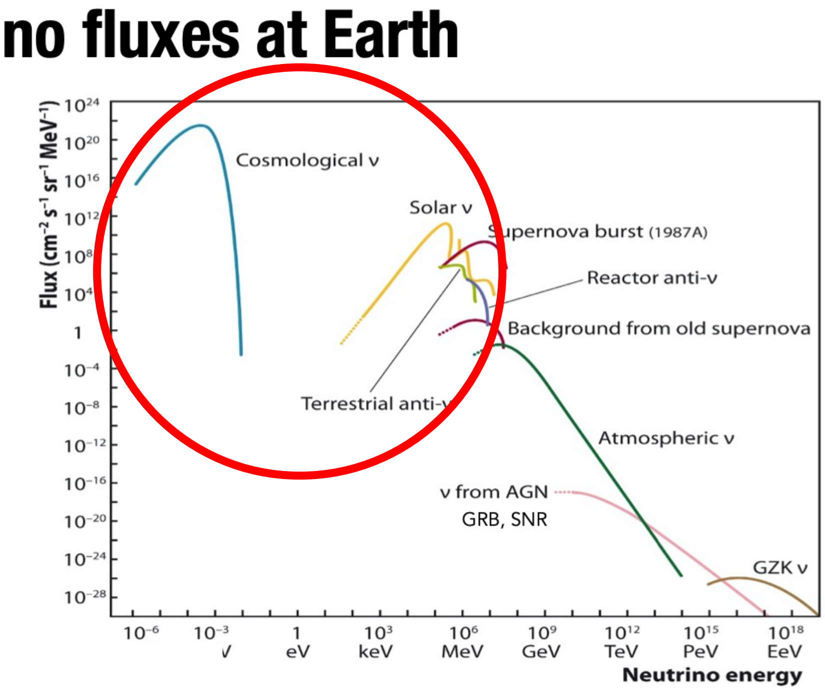


Aychet-Claisse, Lacroix, Somà, Zhang, in preparation

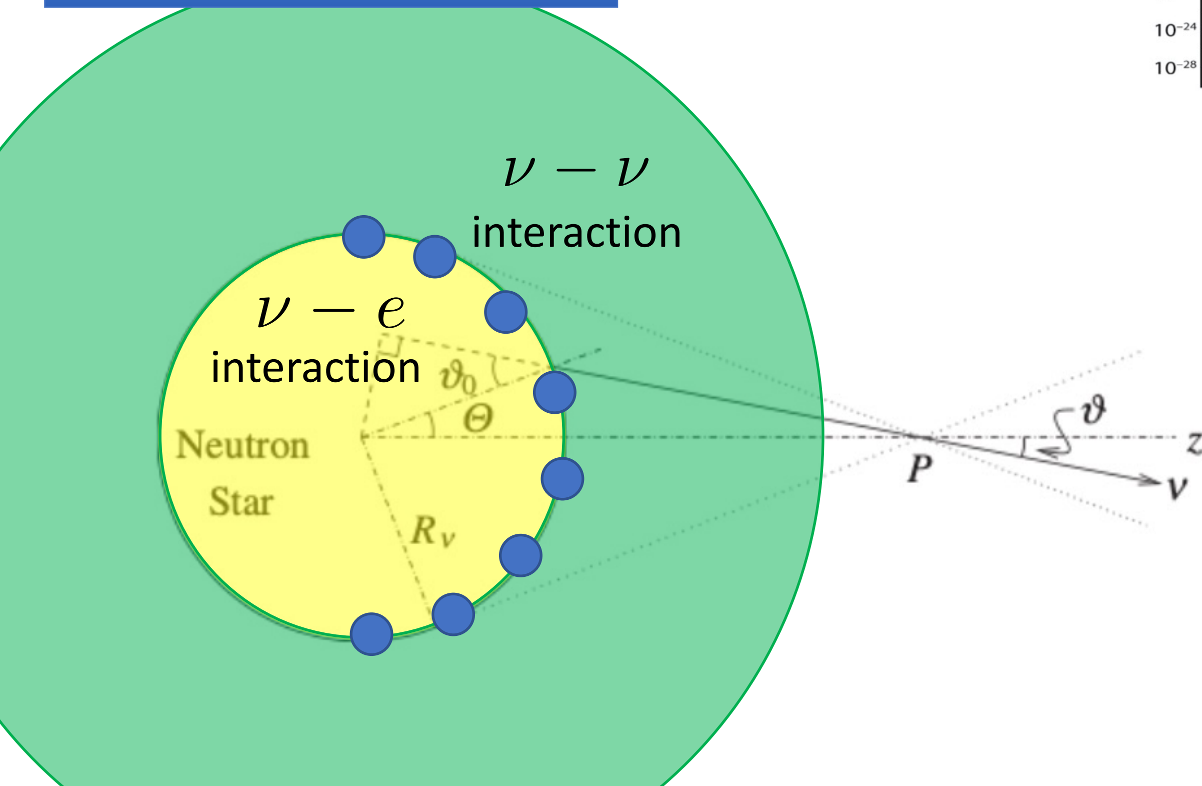
-- More on Neutrinos treated on quantum computers --



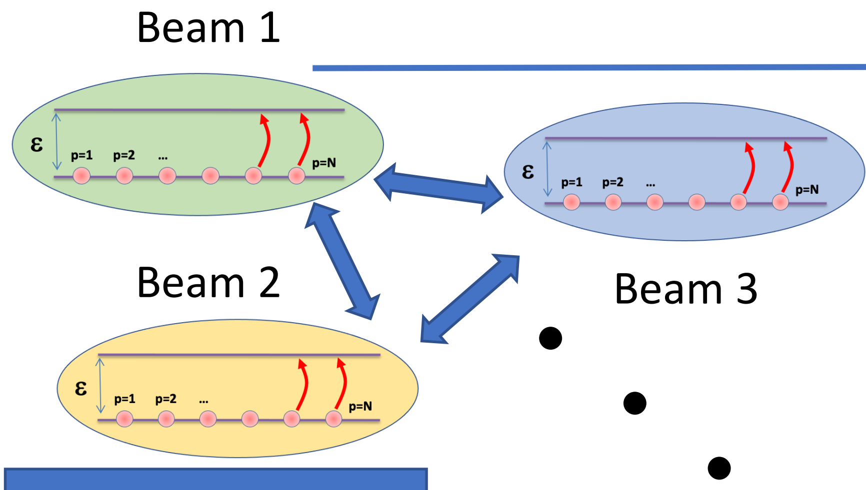




Where is the complexity?



The problem is mapped to a many-body open quantum system problem equivalent to interacting qubits or qutrits.



Trotterization

Illustration of the Hamiltonian (2 flavor approx)

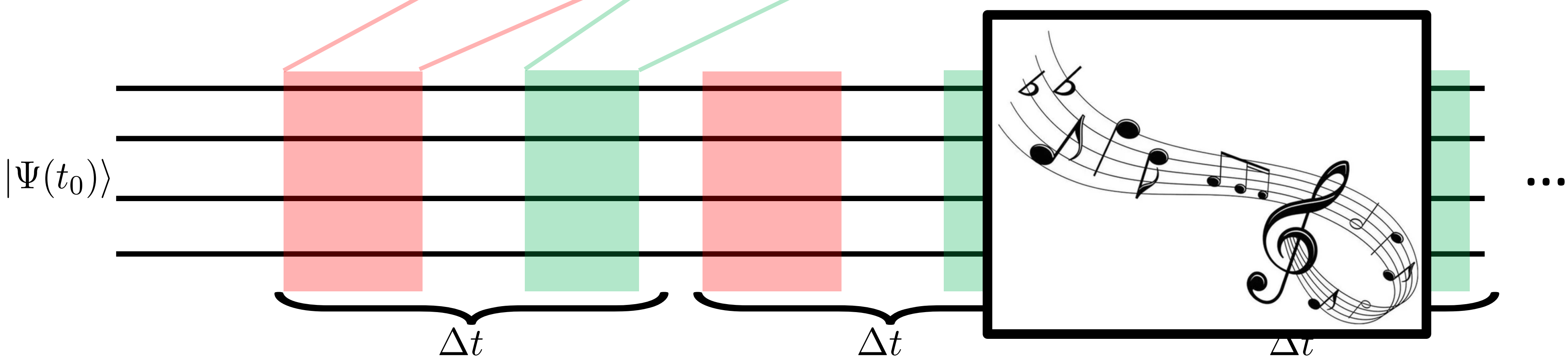
Oscillation $$H_\nu = \frac{1}{N}\sum_{i=0}^{N-1} \sin(2\theta_\nu)X_i - \cos(2\theta_\nu)Z_i$$

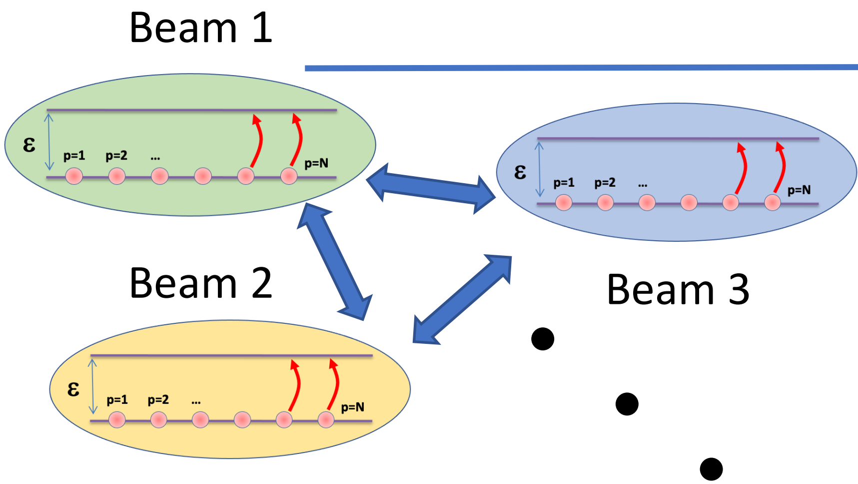
Coupling $$H_{\nu\nu} = \sum_{i<j}^{N-1} G_{i,j}[X_iX_j + Y_iY_j + Z_iZ_j].$$

1. Decomposition of *H* into elementary blocks
2. Use a transformation (Trotter-Suzuki)

Example : $e^{i\Delta t H_1/\hbar} = e^{-i\Delta t H_1/\hbar} e^{-i\Delta t H_2/\hbar}$

3. Transforms to circuit





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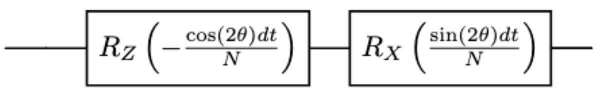
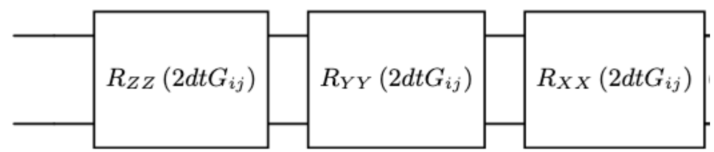
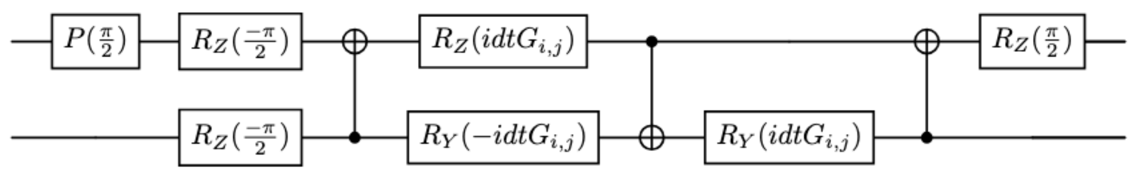


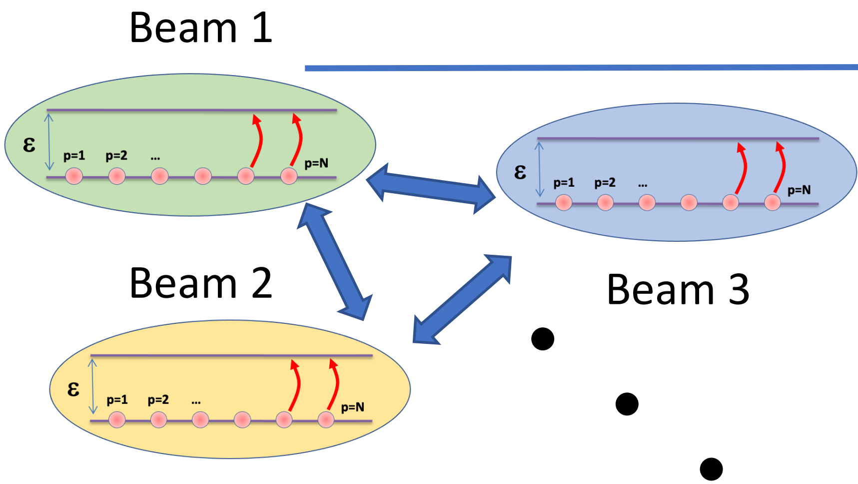
$$H_{\nu\nu} = \sum_{i<j}^{N-1} G_{i,j}[X_iX_j + Y_iY_j + Z_iZ_j].$$



or with optimization



A focus on neutrino oscillation physics simulated on quantum computers



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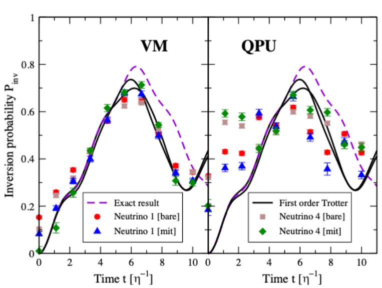
Coupling
$$H_{\nu\nu} = \sum_{i<j}^{N-1} G_{i,j}[X_i X_j + Y_i Y_j + Z_i Z_j].$$

4 neutrinos
IBM-Vigo QPU

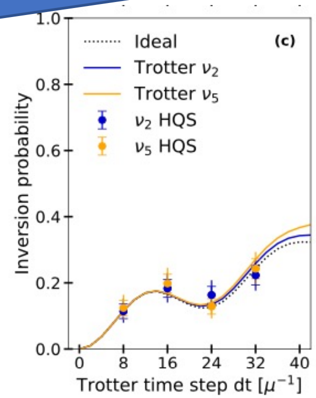
4 & 8 neutrinos
HQD-H1
Trapped Ion device

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

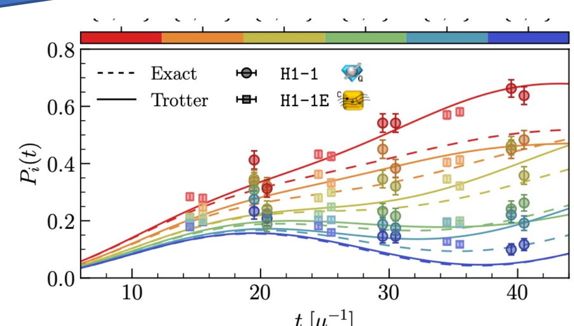
12 neutrinos / qutrits
H1-1 & ibm_torino



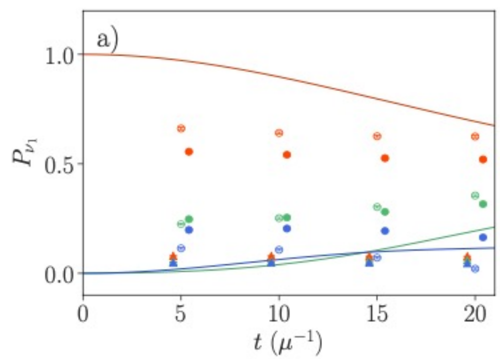
Hall et al, PRD 104 (2021)



Amitrano,et al, PRD 107, (2023)



Illa et al, PRL 130 (2023)

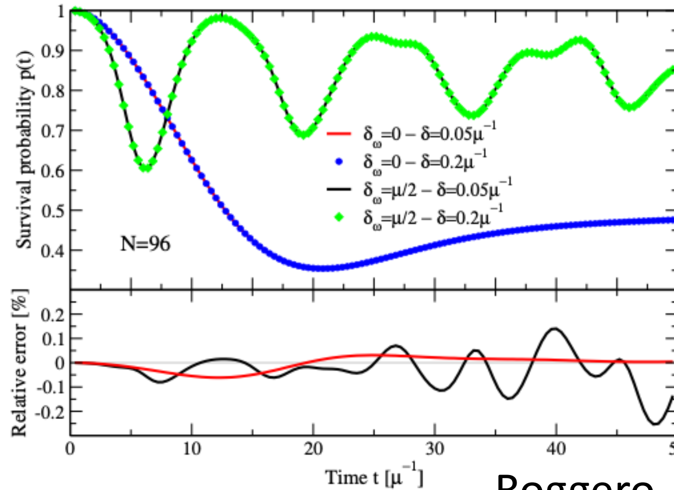


Turro et al,
arxiv:2407.13914

A focus on neutrino oscillation physics
Is also pushing the limit of classical simulation

Tensor network

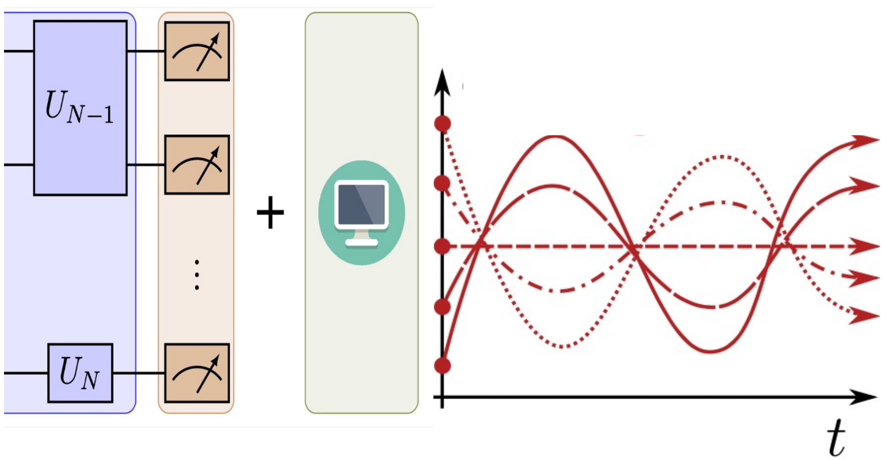
Using MPS layers to simulate neutrino evolution



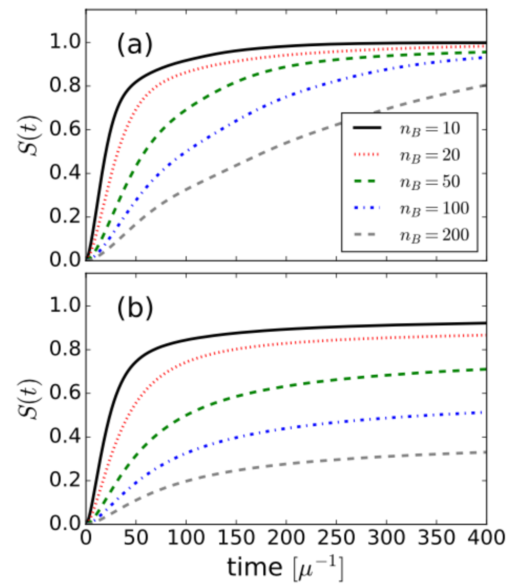
Up to ~100 neutrinos

Roggero, Phys. Rev. D 104 (2021)
Cervia et al, Phys. Rev. D 105 (2022)

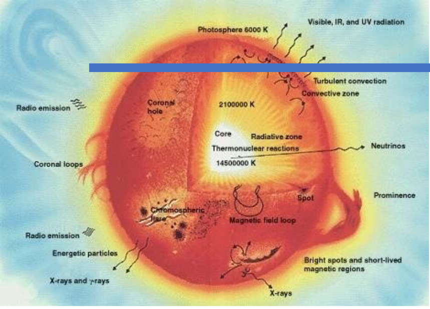
Phase-space methods



Lacroix et al, 2409.20215, PRD *in press*



Several hundreds of neutrinos

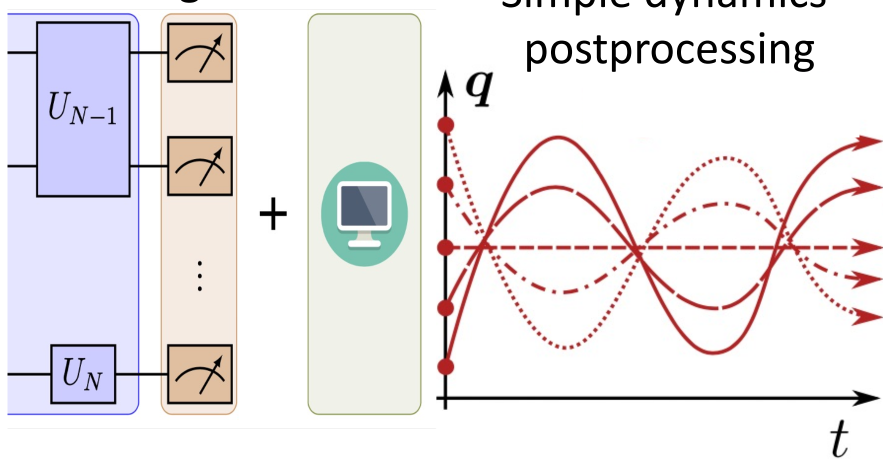


A few Achievements in WP 4.1

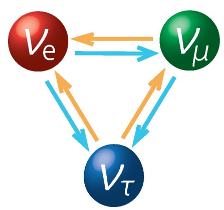
Using quantum computers as generator of events

Sampling of initial configurations

Simple dynamics postprocessing



Application to neutrino oscillations



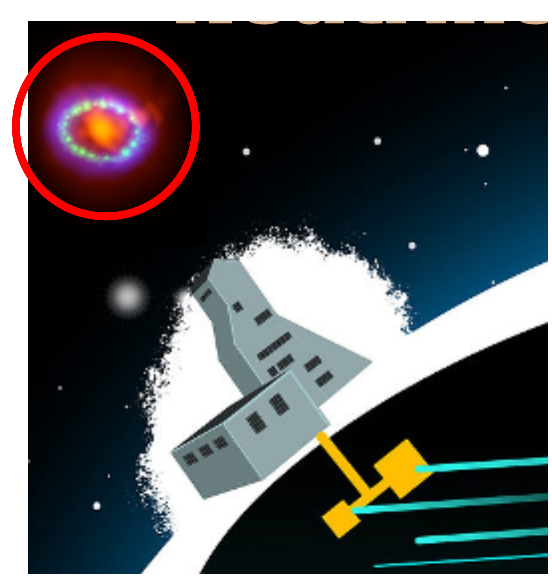
PHYSICAL REVIEW D **VOL..XX,** 000000 (XXXX)

Phase-space methods for neutrino oscillations: Extension to multibeams

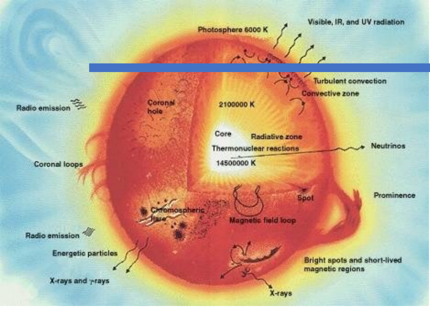
Denis Lacroix,[1,*] Angel Bauge,[1] Bulent Yilmaz,[2] Mariane Mangin-Brinet,[3] Alessandro Roggero,[4,5] and A. Baha Balantekin[6]

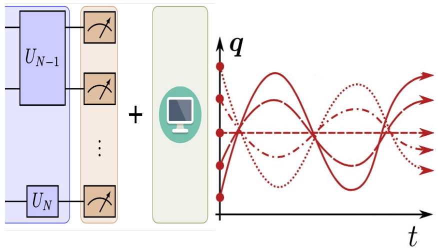
[1]*Université Paris-Saclay, CNRS/IN2P3, IJCLab, 91405 Orsay, France*
[2]*Physics Department, Faculty of Sciences, Ankara University, 06100 Ankara, Turkey*
[3]*Laboratoire de Physique Subatomique et de Cosmologie, CNRS/IN2P3, 38026 Grenoble, France*
[4]*Dipartimento di Fisica, University of Trento, via Sommarive 14, I–38123, Povo, Trento, Italy*
[5]*INFN-TIFPA Trento Institute of Fundamental Physics and Applications, Trento, Italy*
[6]*Department of Physics, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA*

(Received 2 October 2024; accepted 23 October 2024)



Using quantum computers as generator of events





PHYSICAL REVIEW D **110**, 103027 (2024)

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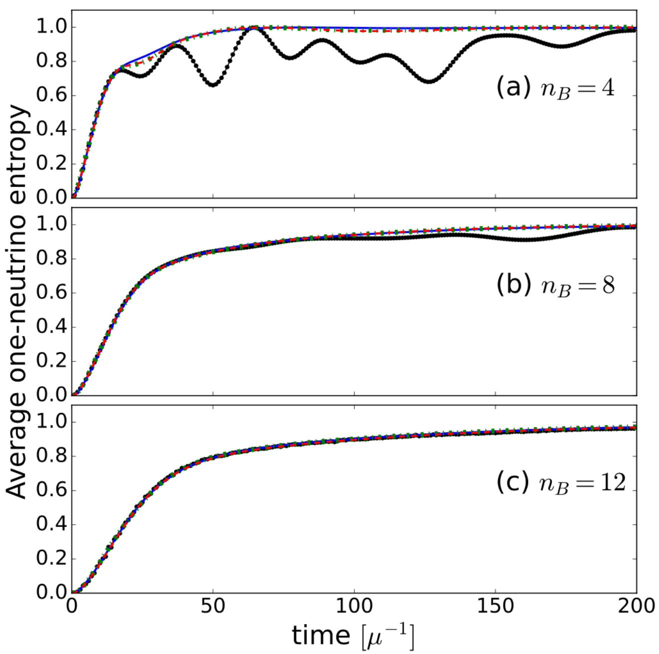
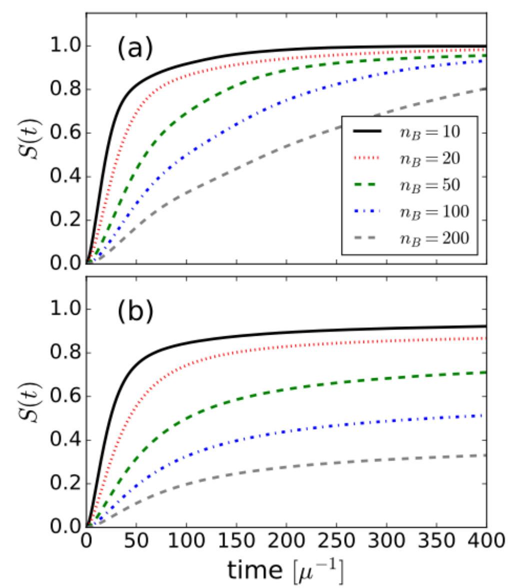
Comparison exact (black) and approximate



Possible to simulate 200+ entangled qubits on a laptop



For comparison
Tensor Network
(90 neutrinos max)