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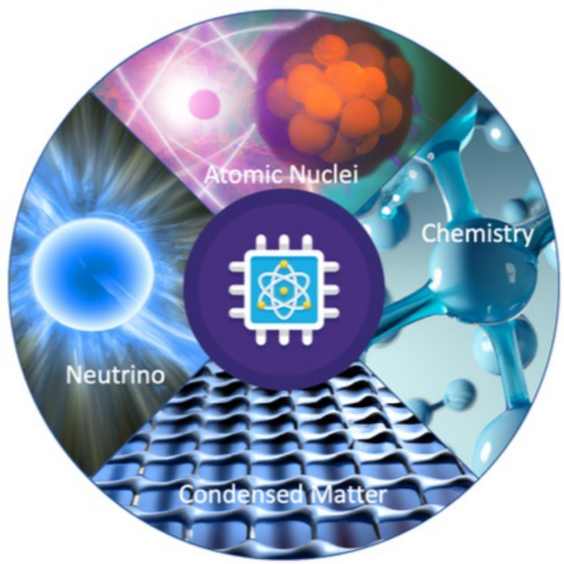
Using symmetry breaking/restoration for many-body problems on quantum devices

Denis Lacroix (IJCLab, Orsay, France)



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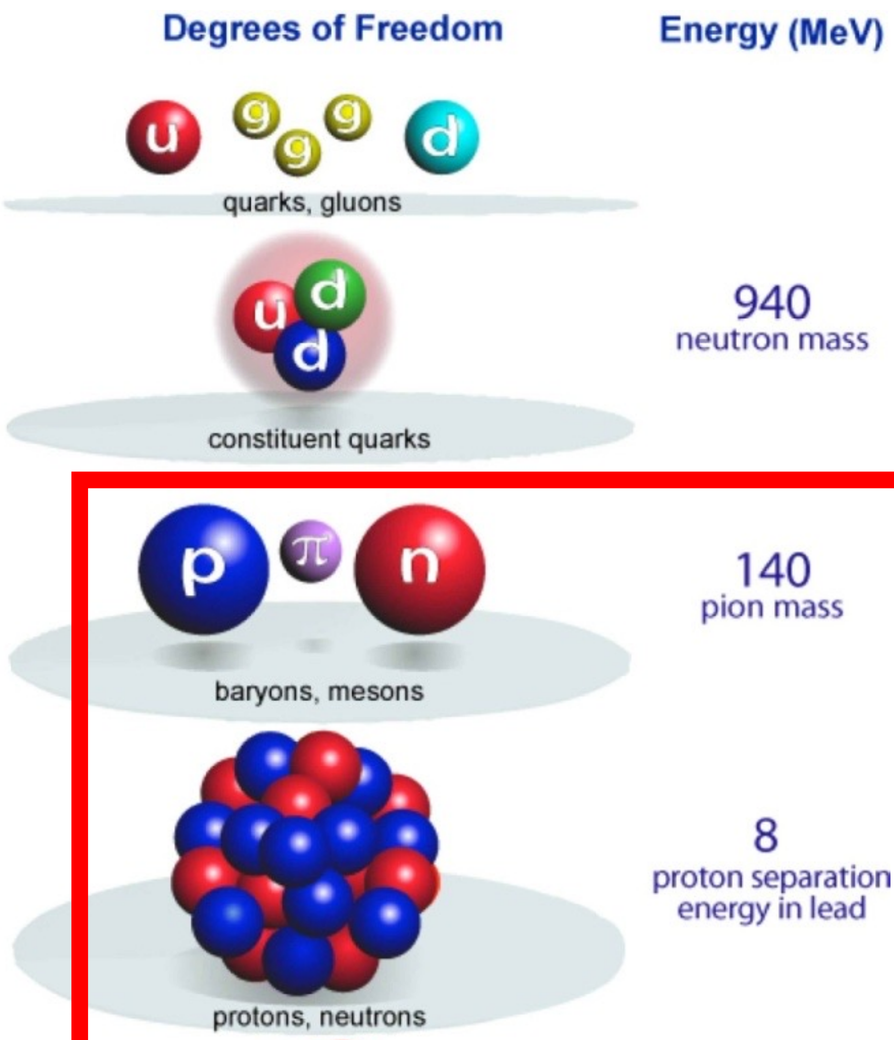
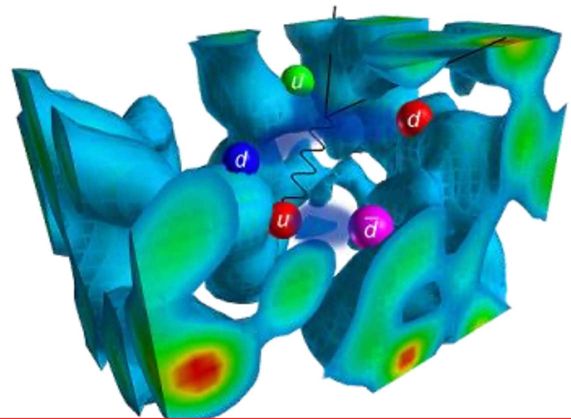
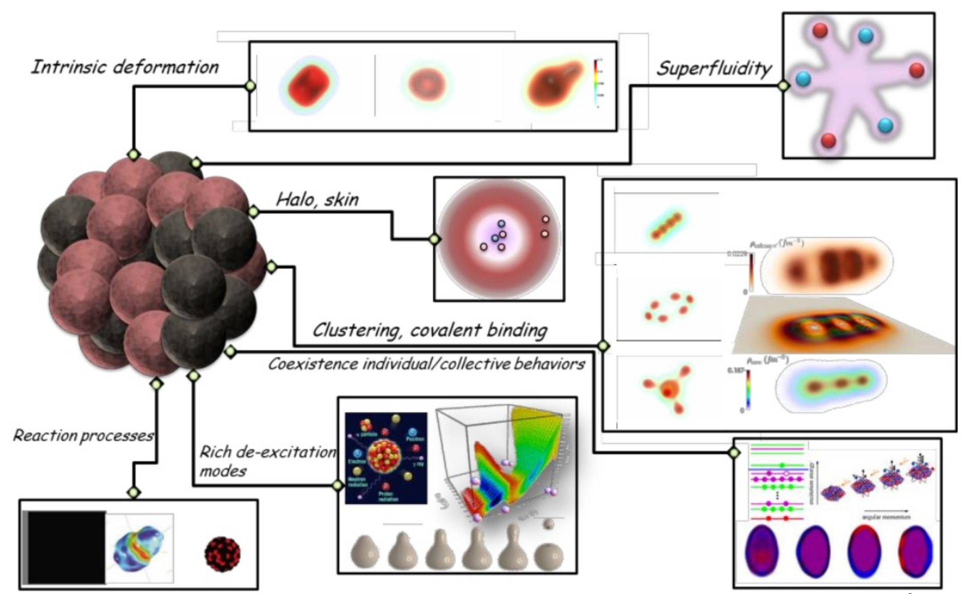
A short highlight of today's nuclear physics



From QCD



to atomic nuclei phenomena

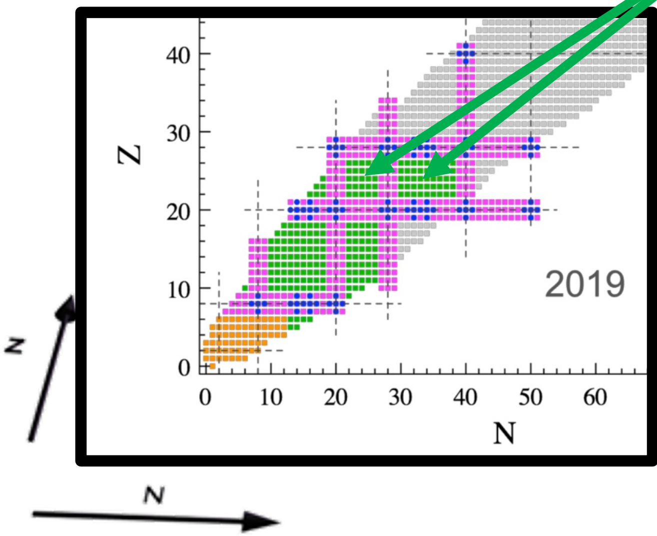


Courtesy J.P. Ebran

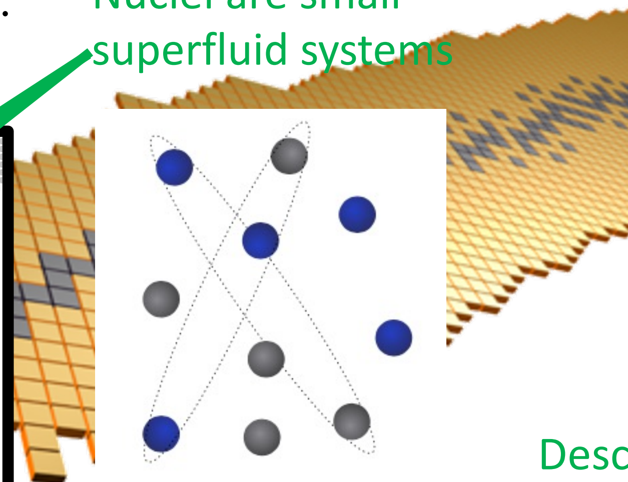
Actual tendency : Towards Full configuration-Interaction description ?

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

Current status

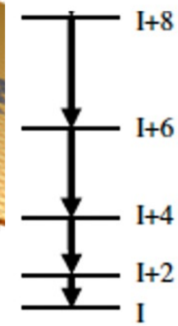


Nuclei are small superfluid systems



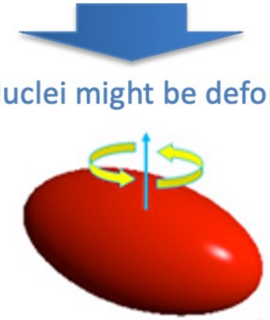
➡ Described by breaking U(1) symmetry

Nuclei do present rotational bands



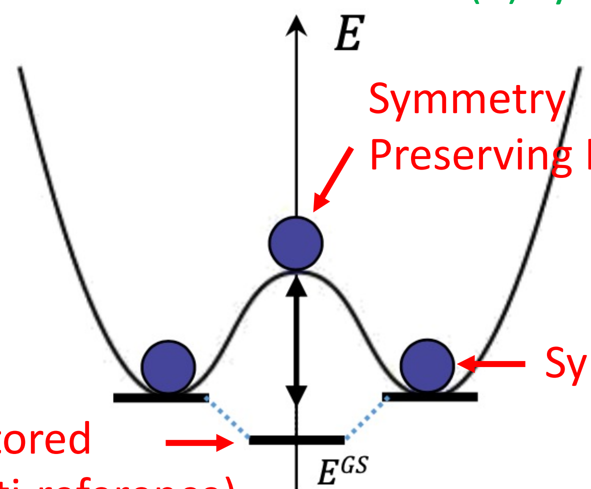
$$E_{\text{rot}} = \frac{I(I+1)}{2J}\hbar^2$$

Nuclei might be deformed



Described by breaking rotational and/or parity symmetry

➡ A specificity: atomic nuclei like to break spontaneously symmetries

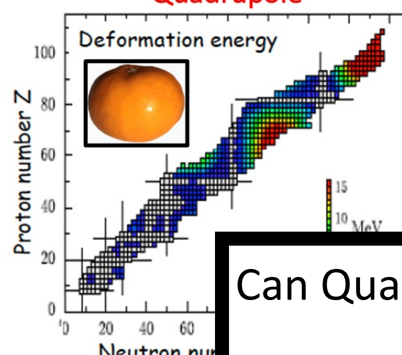


Symmetry Preserving HF state

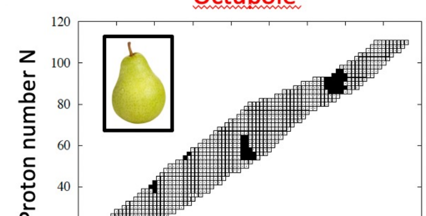
Symmetry Breaking (S

Symmetry Restored (SR) state (multi-reference)

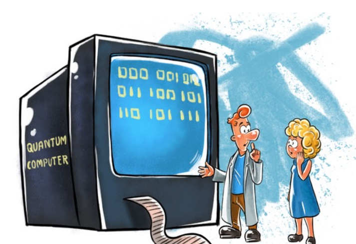
Quadrupole



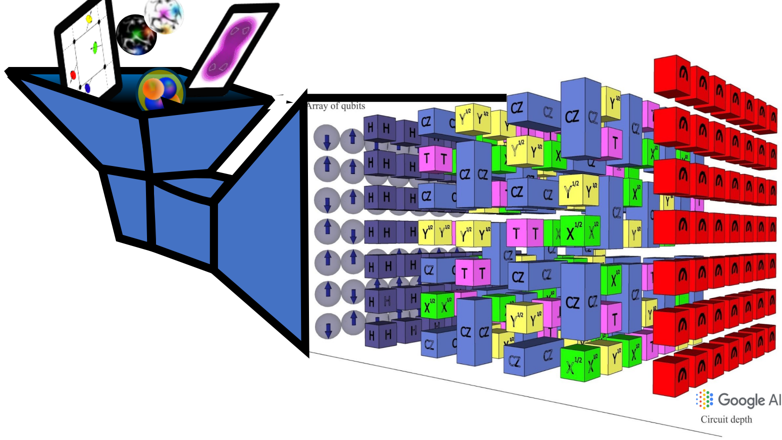
Octupole



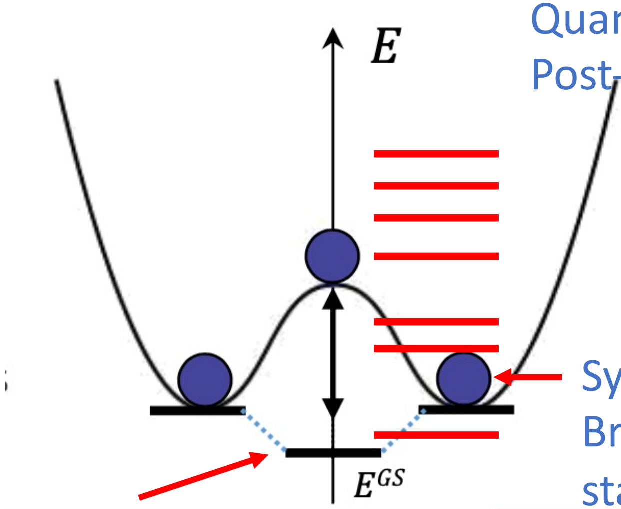
Can Quantum computers help?



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

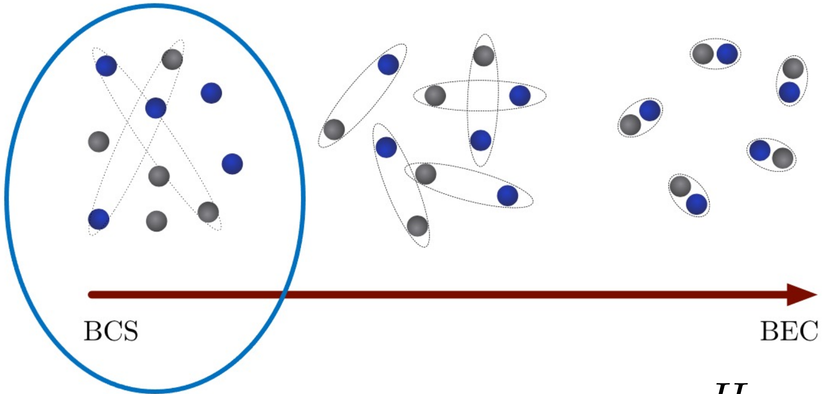
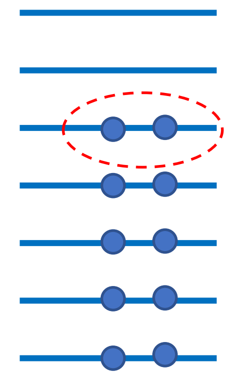


Illustration with the Richardson Hamiltonian

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

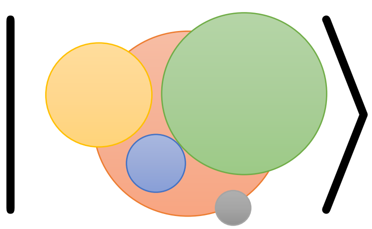


This problem is an archetype of spontaneous symmetry breaking.
An "easy" way to describe it is to break the particle number symmetry, i.e. consider wave-function that mixes different particle number

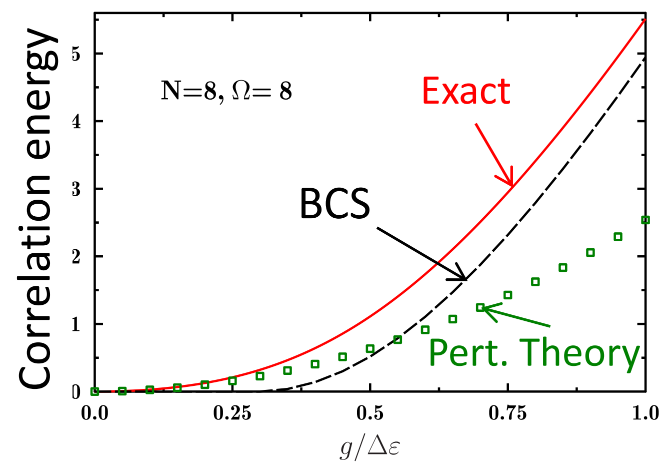
Example $|\Phi_0\rangle = \Pi_i (u_i + v_i a_i^\dagger a_{\bar{i}}^\dagger)|-\rangle$

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

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



But ultimately number of
Particle should be restored !



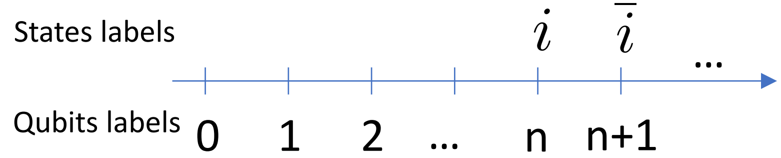
Hamiltonian and initial state

Pairing Hamiltonian

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

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

State ordering is important !

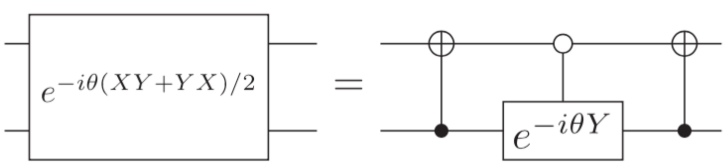


$$a_i^\dagger a_{\bar{i}}^\dagger \Rightarrow Q_n^+ Q_{n+1}^+$$

Initial (symmetry breaking) state preparation

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

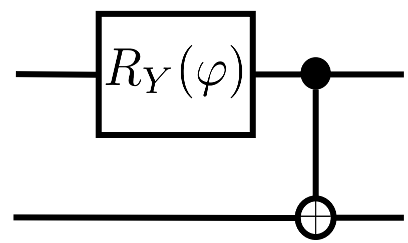
Equivalent universal gate on pairs



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

Simplified circuit (generalized Bell state)

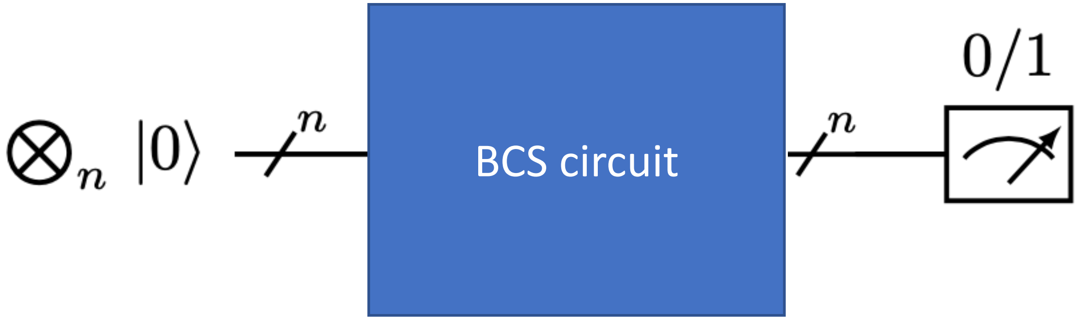
$$|\Psi\rangle = \prod_n \left[\cos\left(\frac{\varphi}{2}\right) I_n \otimes I_{n+1} + \sin\left(\frac{\varphi}{2}\right) Q_n^+ Q_{n+1}^+\right] |-\rangle$$



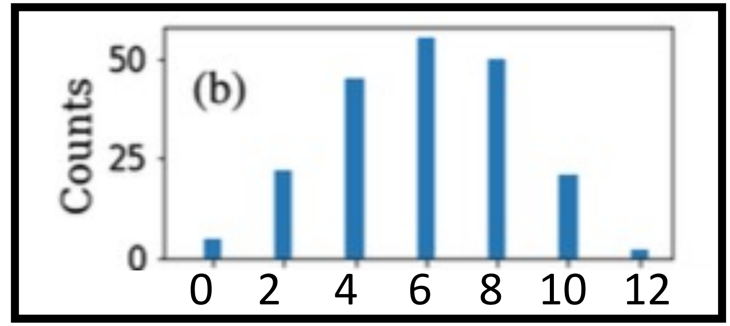
Restoration of particle number symmetry

The counting statistics problem

Direct estimate of Counting statistics

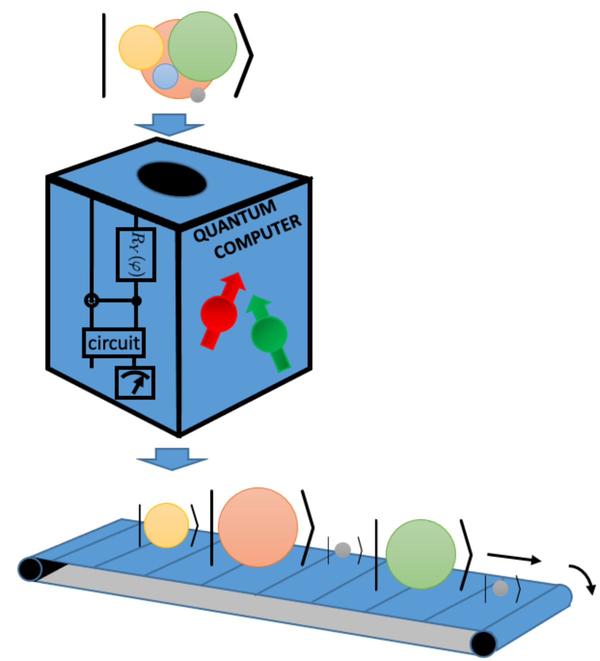


Example of mixing for 12 qubits (with qiskit)



Projection on particle number

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



For 2 qubits

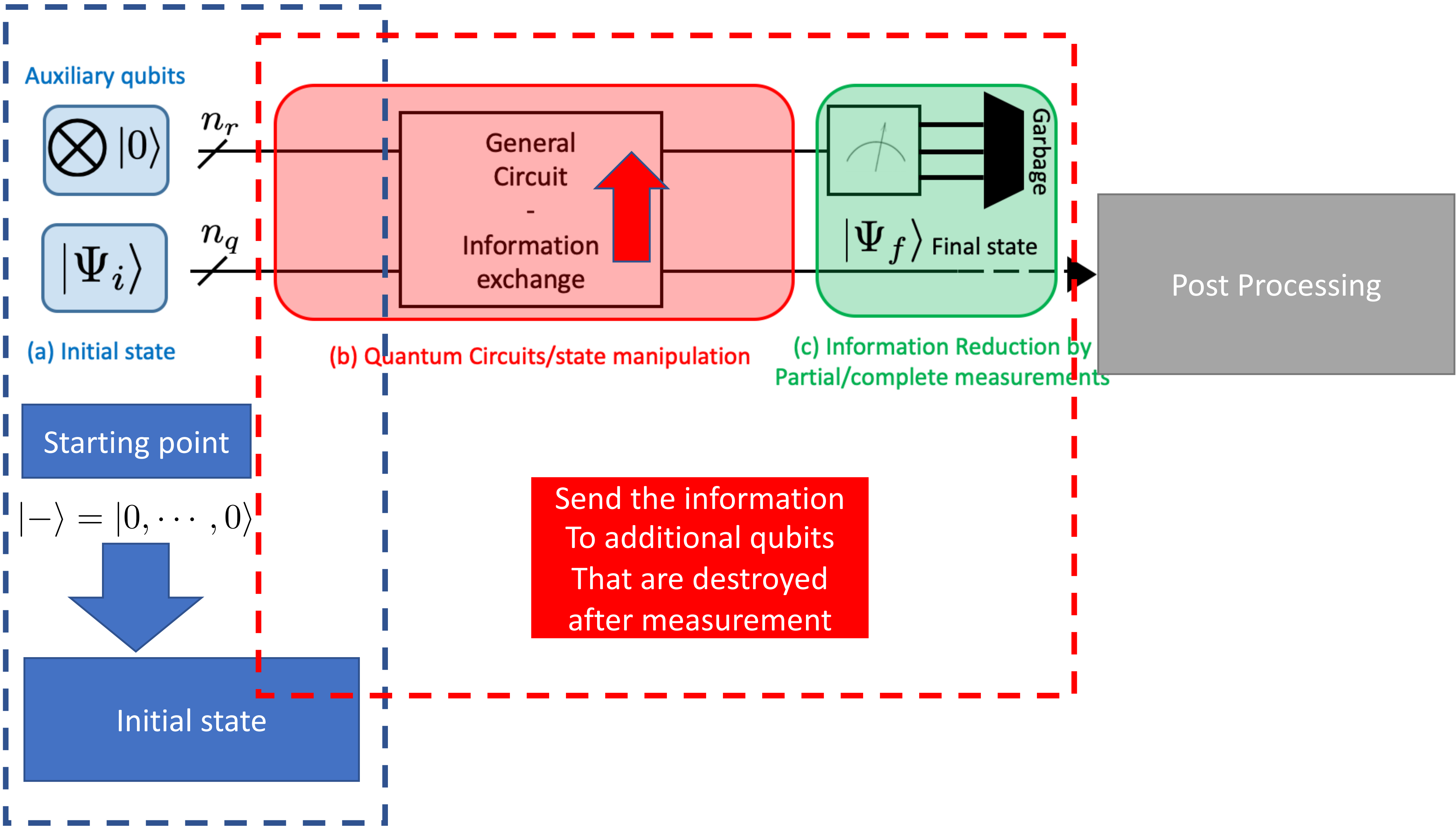
$$|\Psi\rangle = \alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle$$

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

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).

Non-destructive counting on a quantum computer



The quantum-Phase estimation (QPE) algorithm

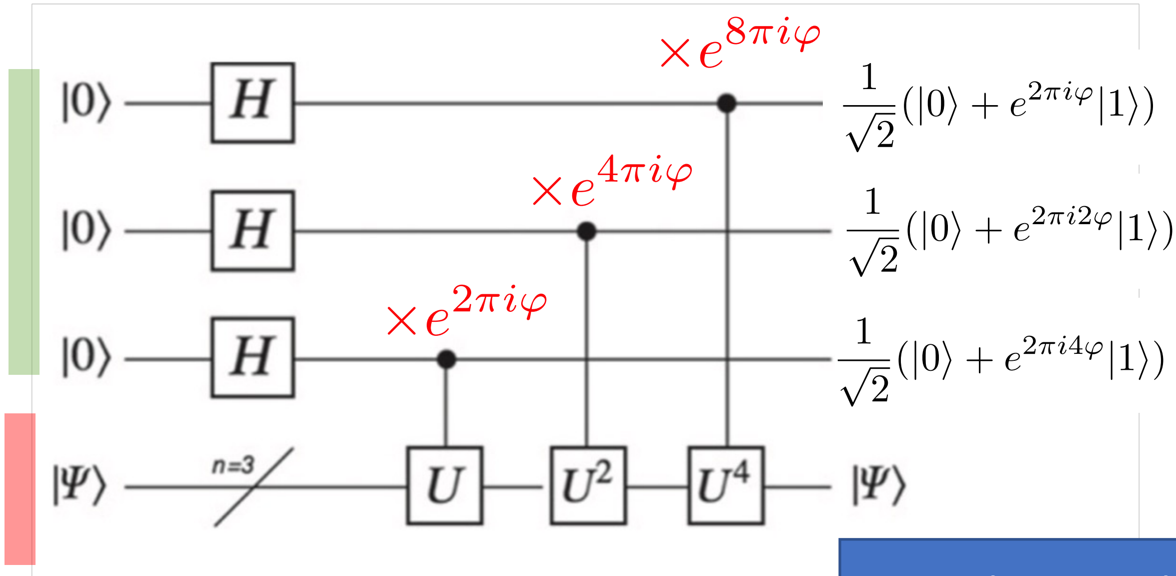
For known eigenvalue problems

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

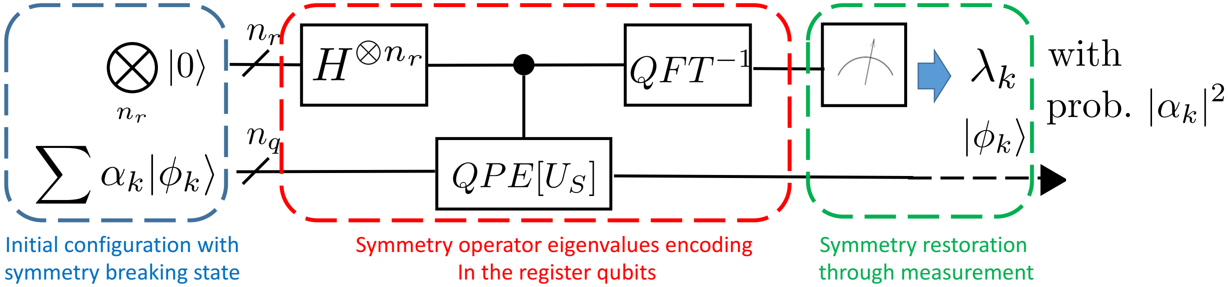
$$U = U_N = e^{2\pi i \frac{N}{2^{n_r}}} \quad \text{with} \quad N = \frac{1}{2}\sum_i (I_i - Z_i)$$

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

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

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

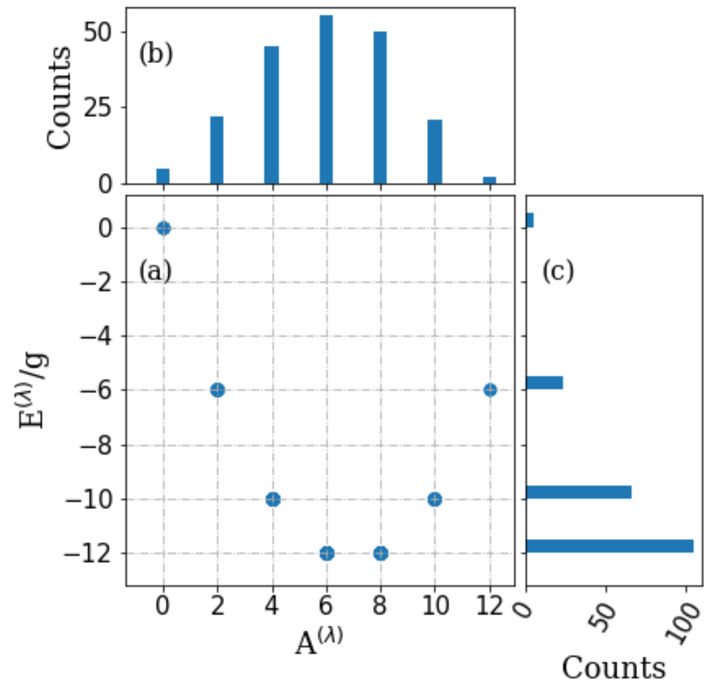
Projected BCS or with varying number Of particles

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



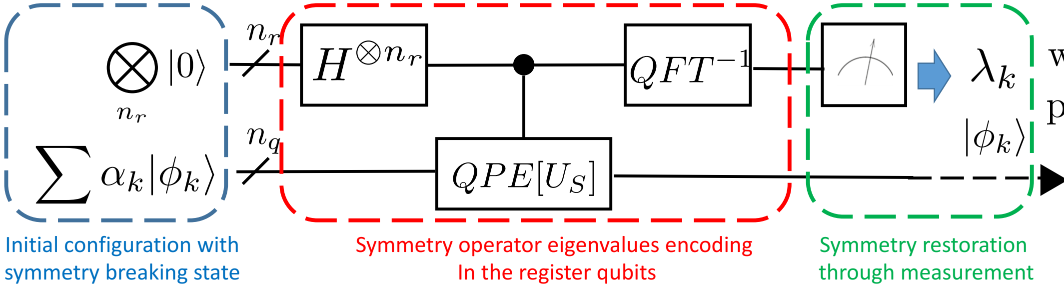
Exact solution

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

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

For the degenerate case, this should give the exact solution

Eigenvalues-Ground state and excited states



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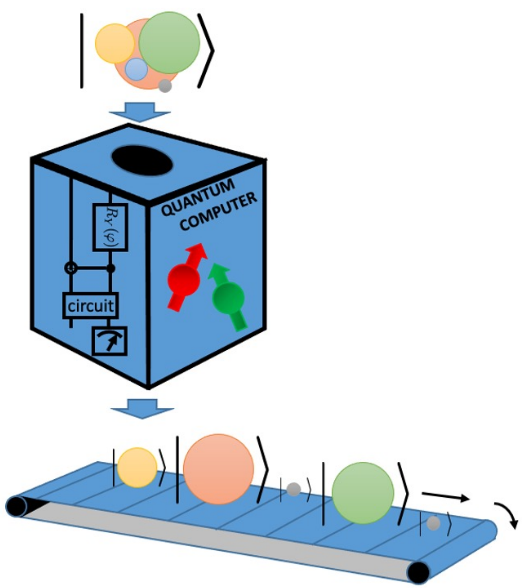
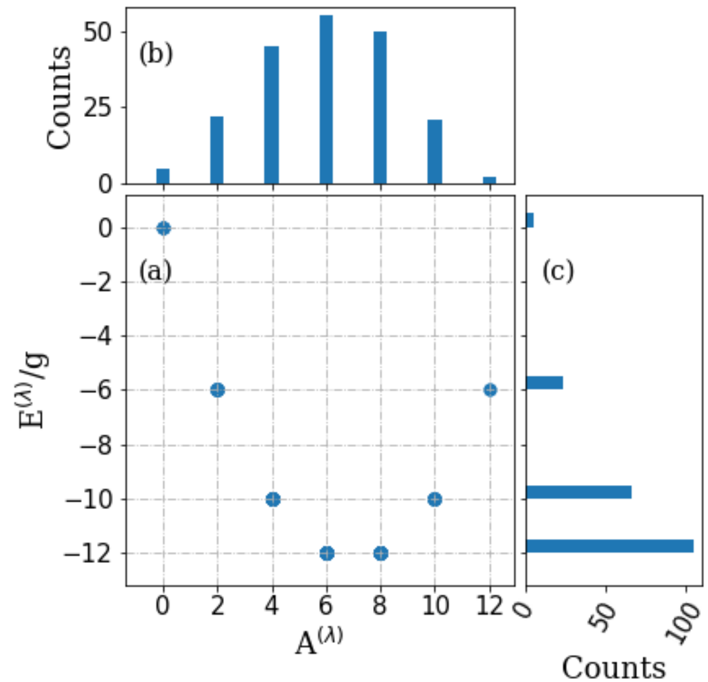


6 pairs



Exact solution

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

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

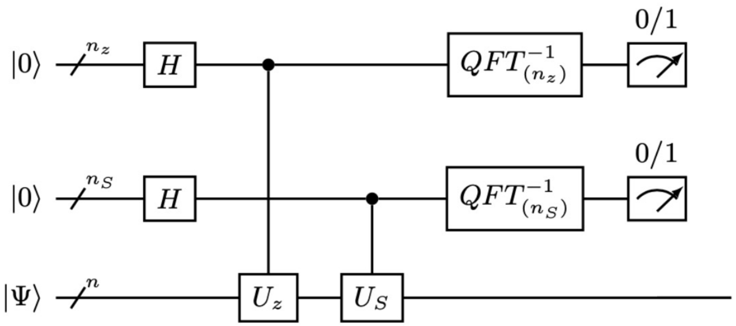
Examples

- 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).

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

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



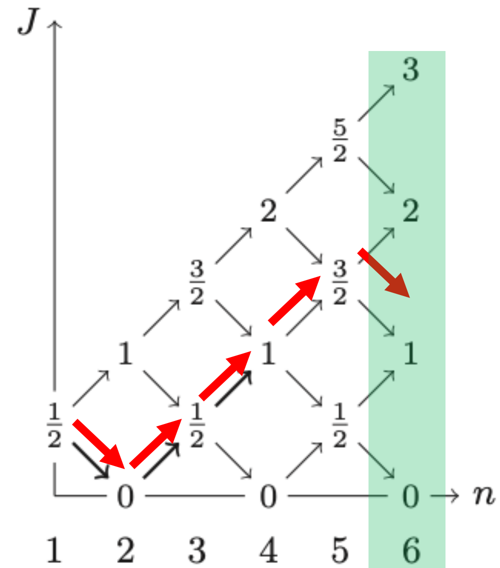
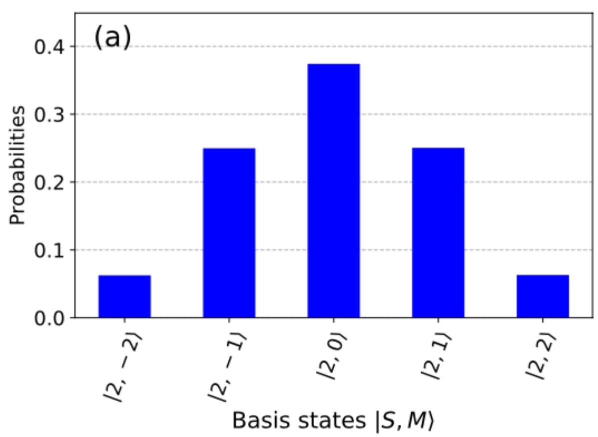
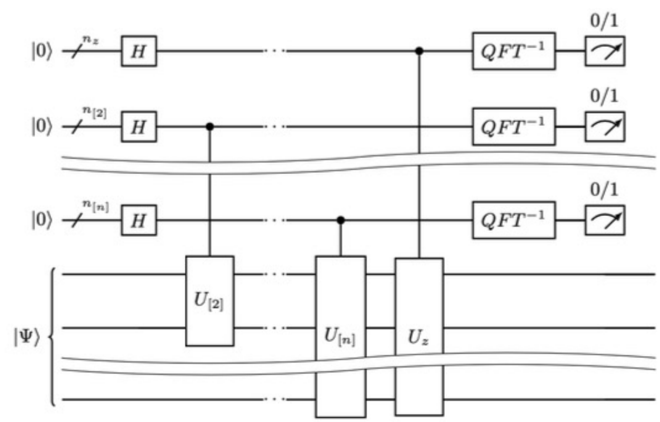


Illustration $\quad |\Psi\rangle = \bigotimes_n H|0\rangle$



The full basis can eventually be constructed



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

Coming back to our superconducting problem

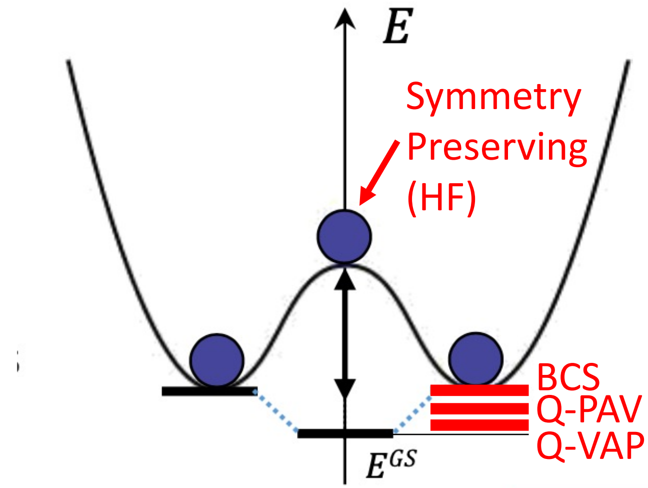
Combining projection with variational method

Possible optimization schemes

Pair occupation are now encoded

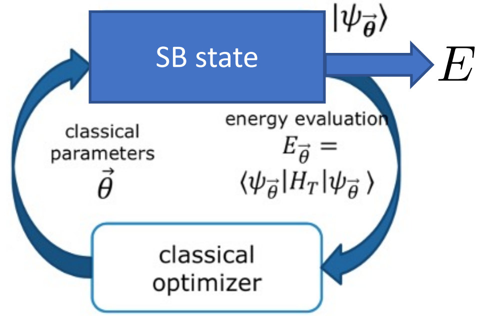
Variational
Symmetry-Breaking ansatz

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

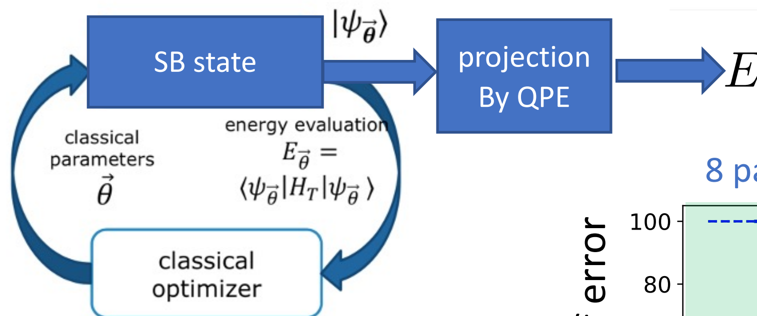


Quantum-Classical optimizers

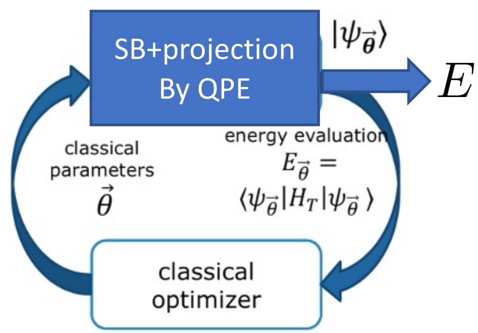
- Standard BCS theory



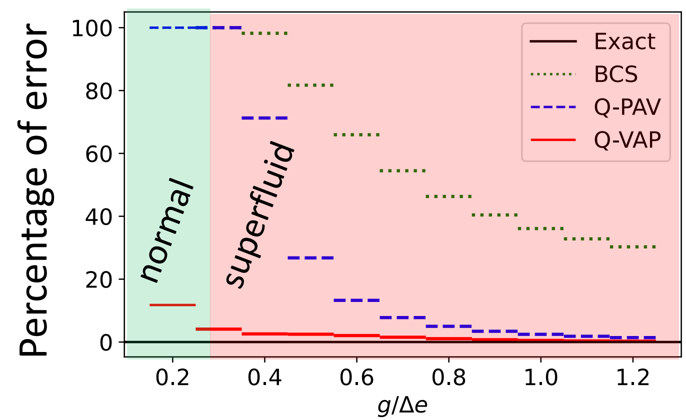
- Project after optimization
  Q-PAV: Quantum Projection After Variation



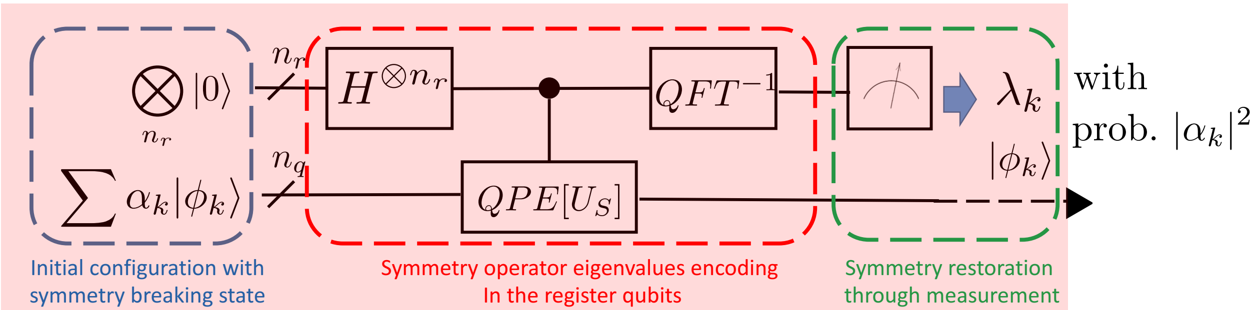
- The optimization is made on the Symmetry restored state.
  Q-VAP: Quantum Variation After Projection



8 particles on 8 equidistant levels



Complete strategy



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

➡ Post-processing to get excited states:
Quantum Phase Estimation

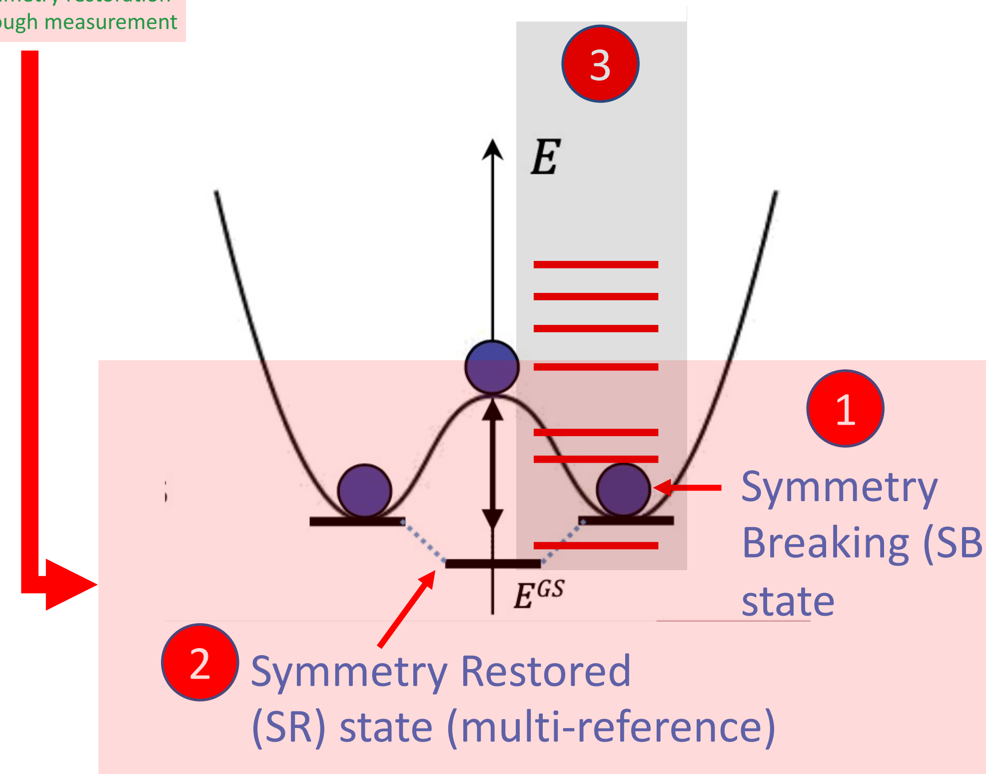
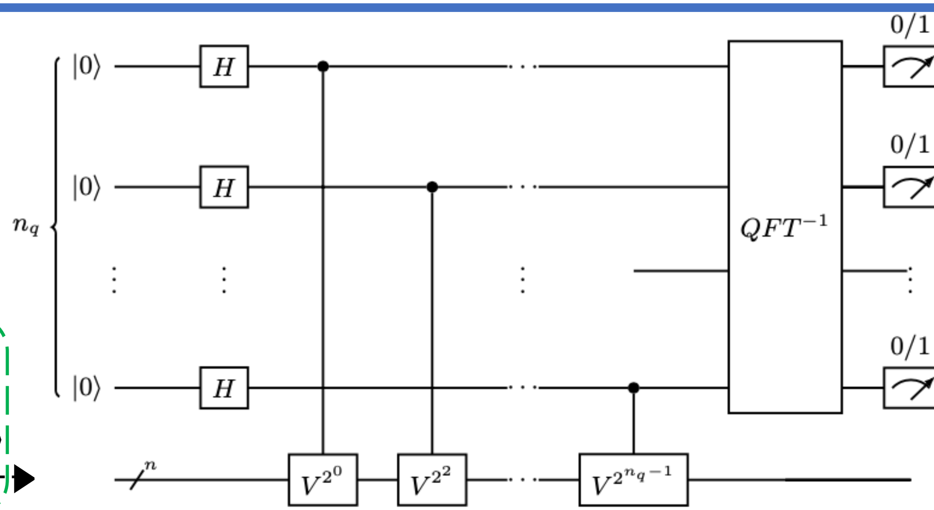
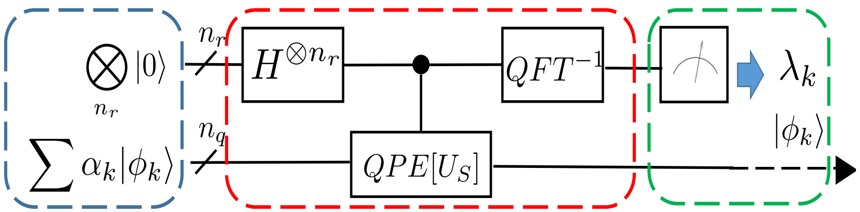


Illustration of the QPE method with projected state



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

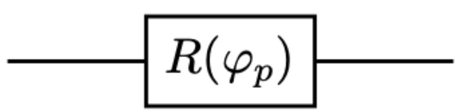
$$U(\tau) = e^{-i\tau H}$$

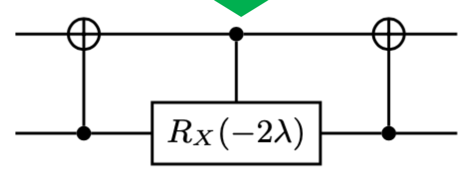
$$U(\tau) = \prod U(\Delta\tau) \longrightarrow \prod U_\varepsilon(\Delta\tau)U_g(\Delta\tau)$$

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

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

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





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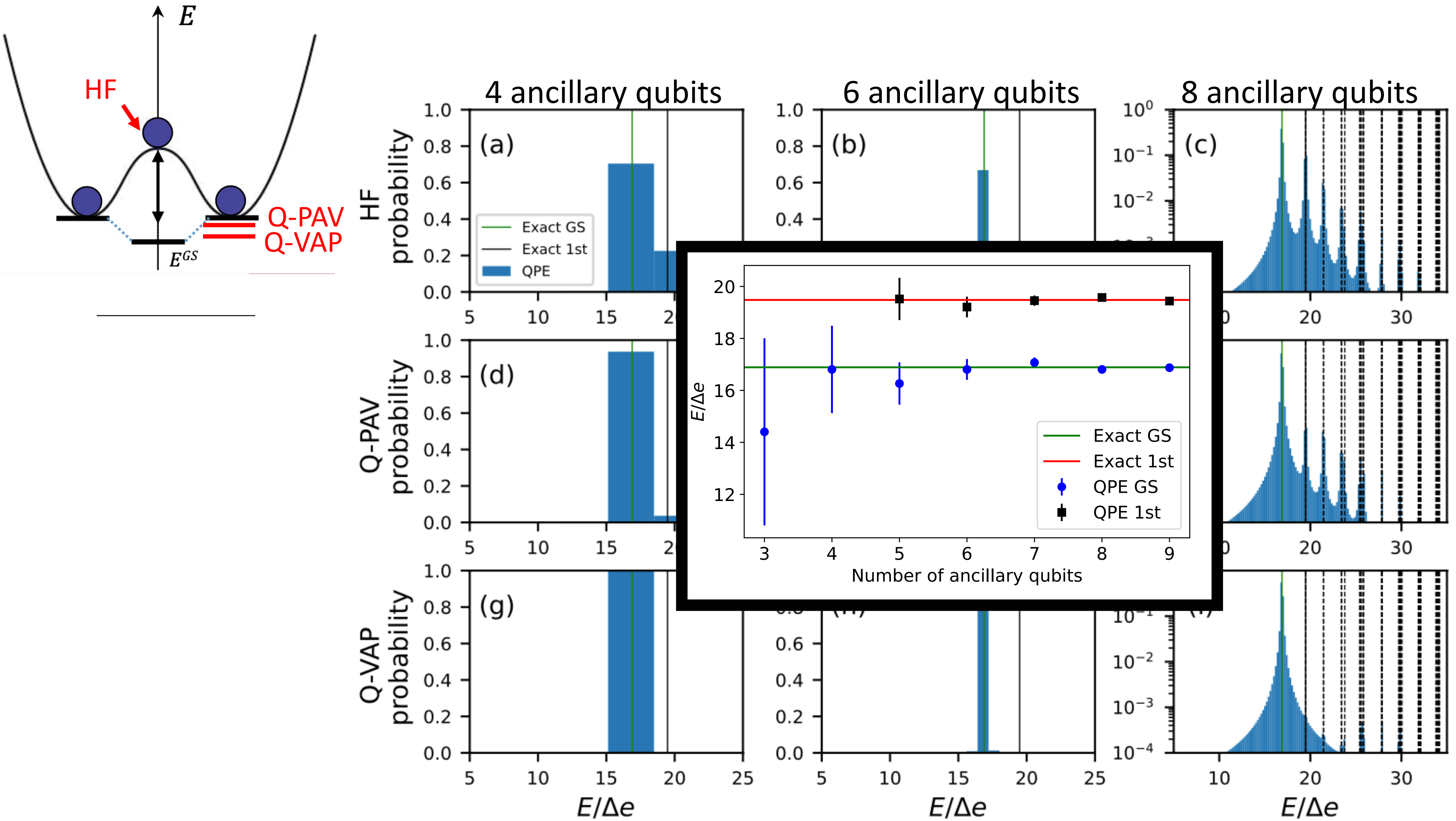
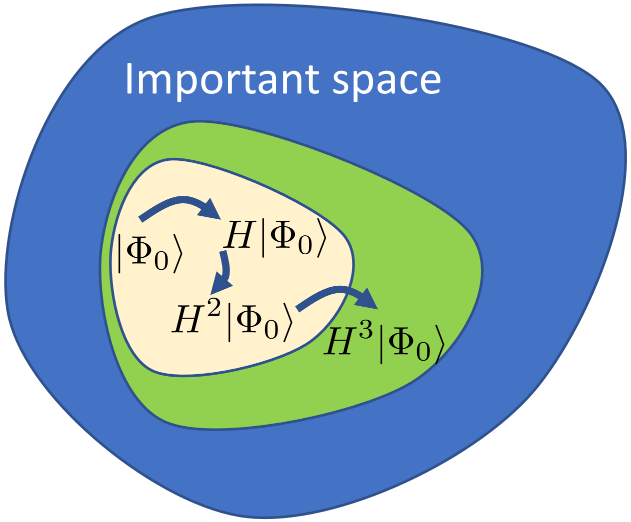


Approximate method : Krylov Based methods

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

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

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

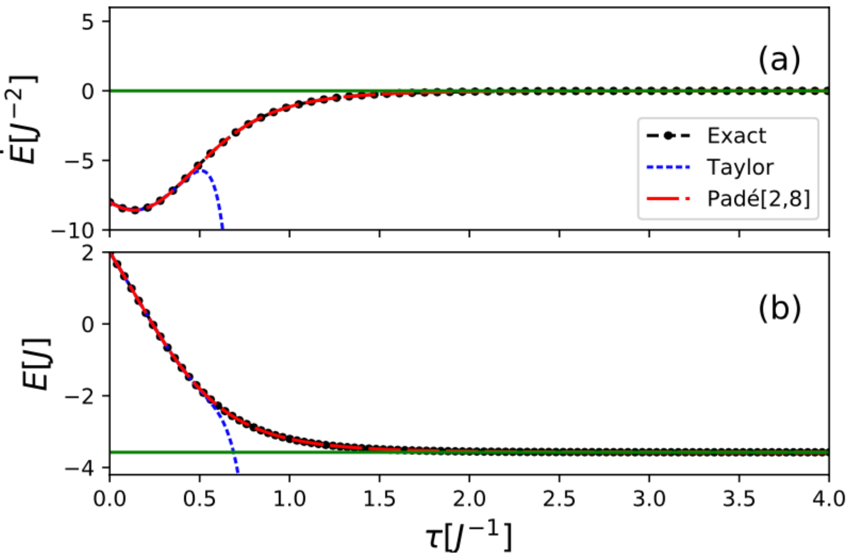
$$\langle H^K \rangle_0 = i^K \left. \frac{d^K F(t)}{dt^K} \right|_{t=0}$$

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

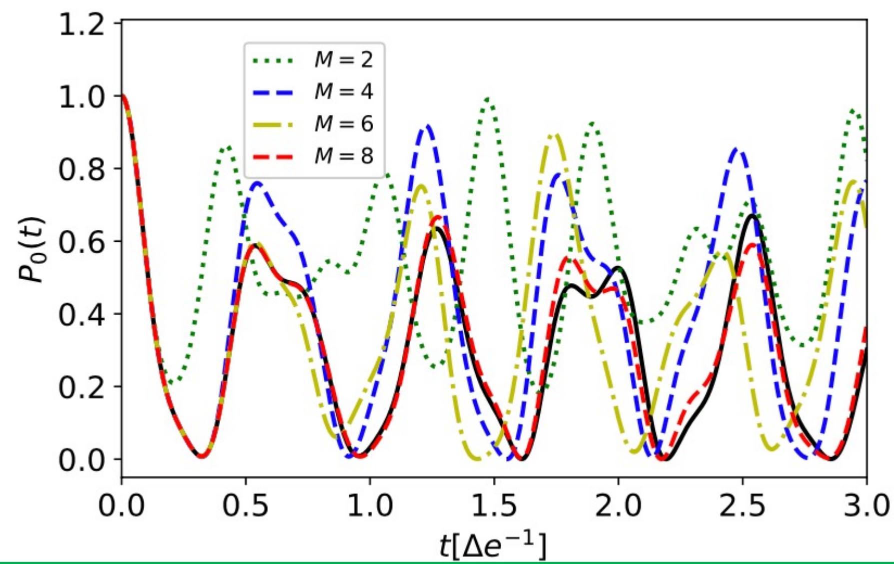
Solve the eigenvalue problem on the classical computer

$F(t) = \langle \Phi$

$F(t) = 1$

$\langle H^K$

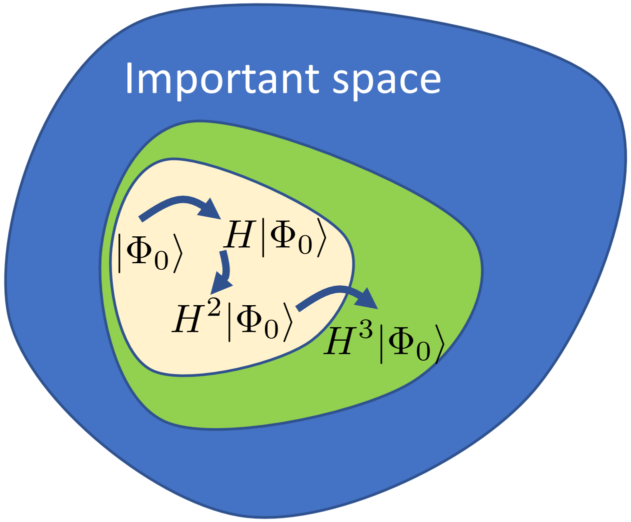
Approximate real-time dynamics



Ruiz-Guzman and Lacroix, arXiv:2104.08181v2

Approximate method : Krylov Based methods

Highly Truncated Hilbert space

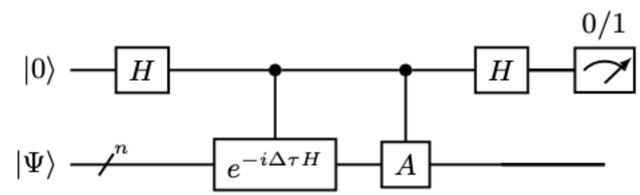


$$\{|\Psi\rangle,\ H|\Psi\rangle, \cdots,\ H^{M-1}|\Psi\rangle\} \equiv \{|\Phi_i\rangle\}_{i=0,M-1}$$

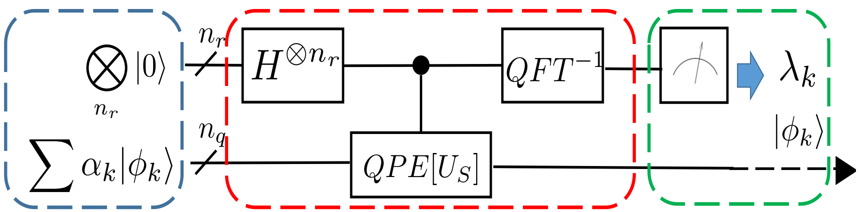
$$\{|\Psi\rangle,\ e^{-i\tau_1 H}|\Psi\rangle, \cdots,\ e^{-i\tau_{M-1} H}|\Psi\rangle\}$$

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

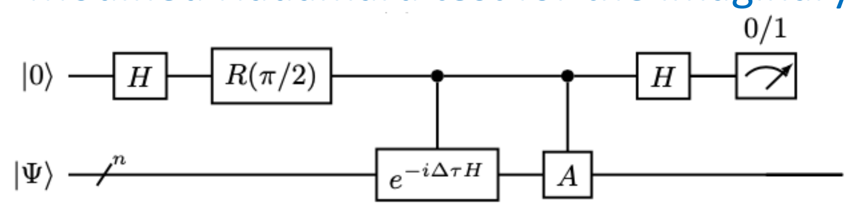
Hadamard test for the real part of *O* and *H*



Initial state preparation

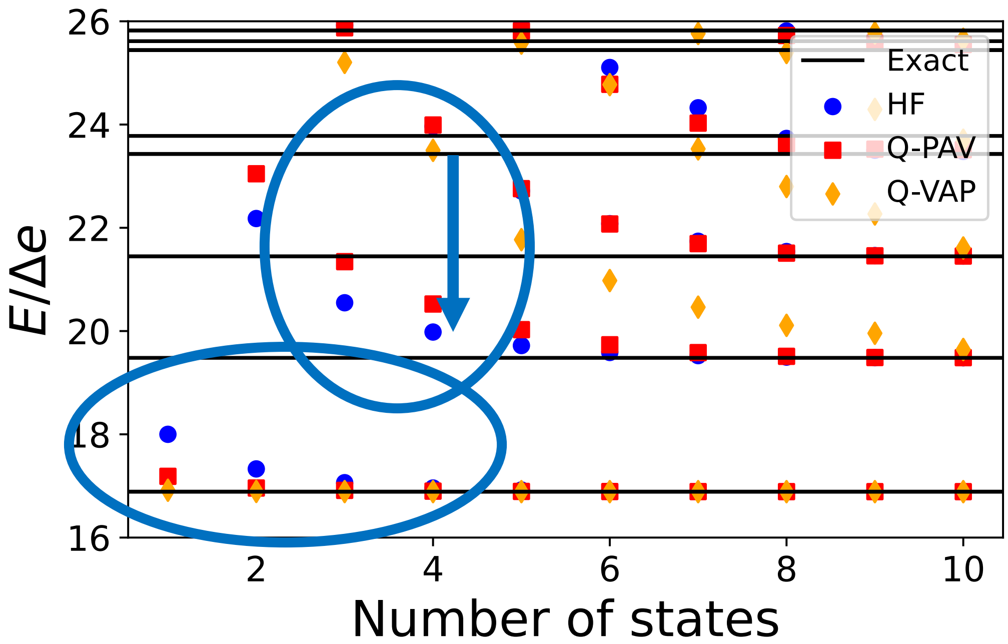


Modified Hadamard test for the imaginary part

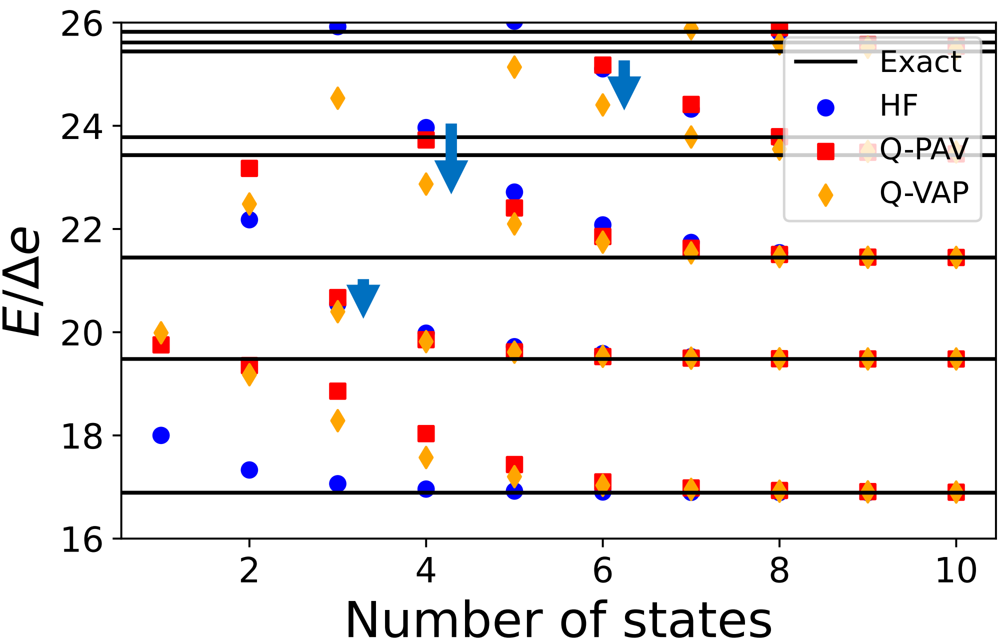


Diagonalization on a classical computer

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

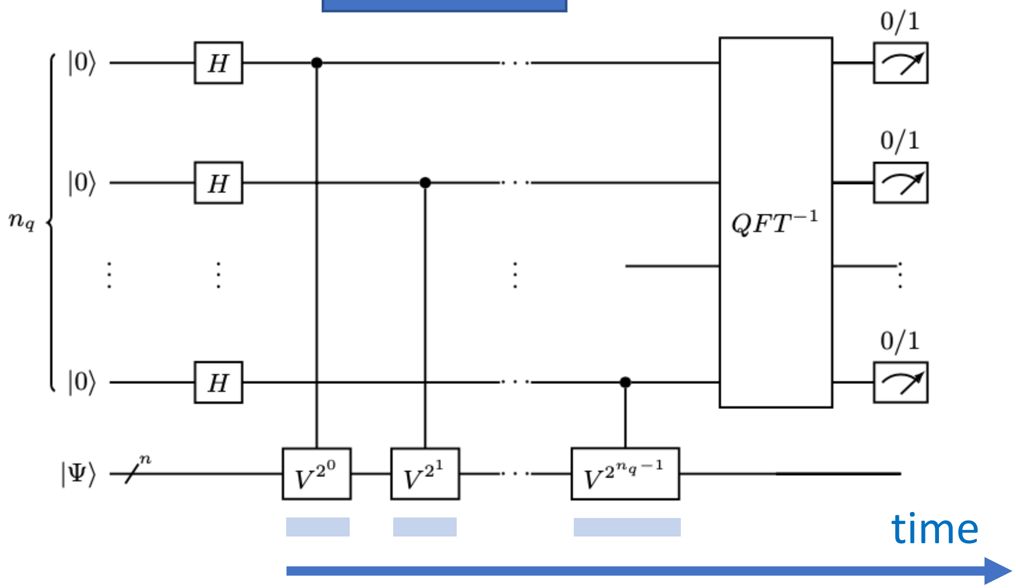
$$|\Psi\rangle = \bigotimes_p \left[\sin(\theta_p)|0_p\rangle + \cos(\theta_p)|1_p\rangle\right]$$

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

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

Comparison QPE vs Quantum Krylov after Q-VAP

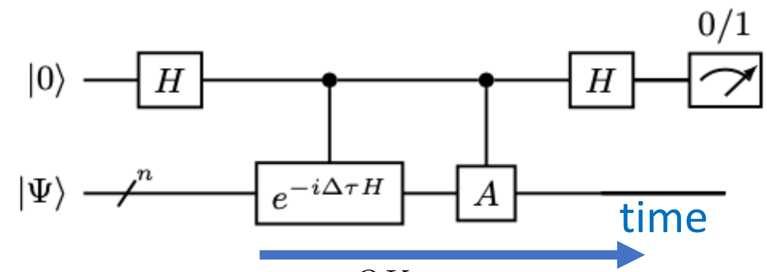
QPE



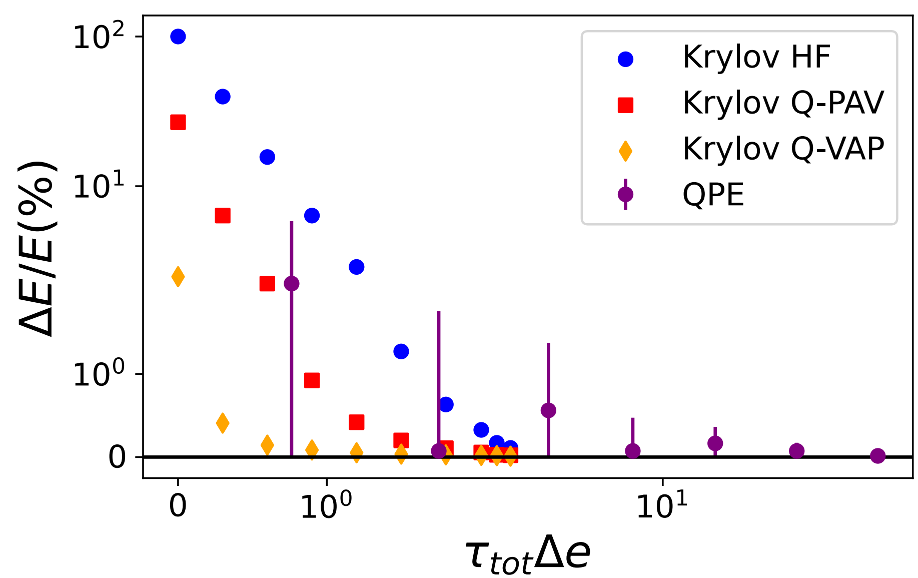
$$\tau_{\mathrm{QPE}} + 2\tau_{\mathrm{QPE}} + \cdots + 2^{n_q-1}\tau_{\mathrm{QPE}}$$

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

Quantum Krylov

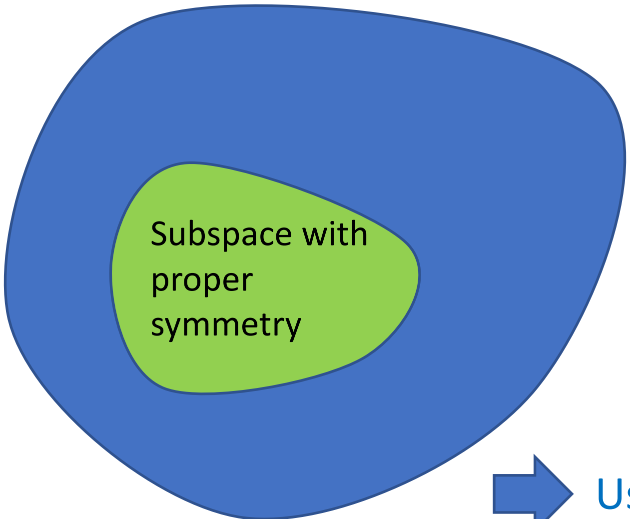


$$\tau_{\mathrm{tot}}^{QK}(M)$$



Exploration of different methods for the symmetry problems

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

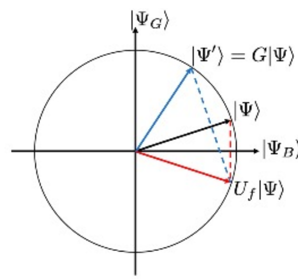
Symmetry breaking/symmetry preserving circuits and symmetry restoration on quantum computers

A quantum many-body perspective

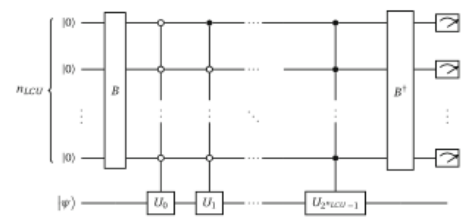
Denis Lacroix[1,a], Edgar Andres Ruiz Guzman[1,b], Pooja Siwach[2,c]

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

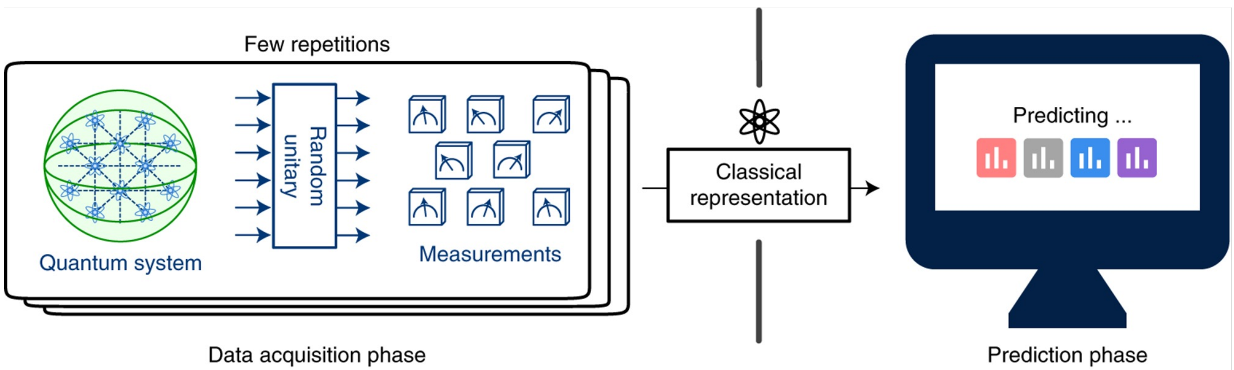
Grover and Oracle



Linear Combination of Unitaries



Use quantum tomography techniques (Classical Shadow method)



Restoring broken symmetries using quantum search "oracles"

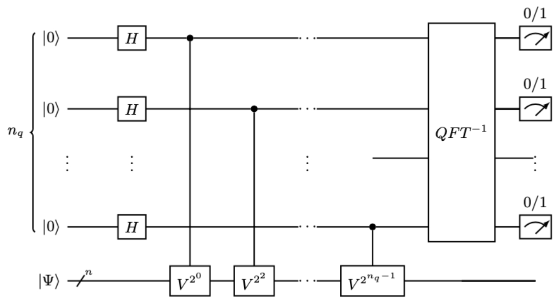
Edgar Andres Ruiz Guzman and Denis Lacroix

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

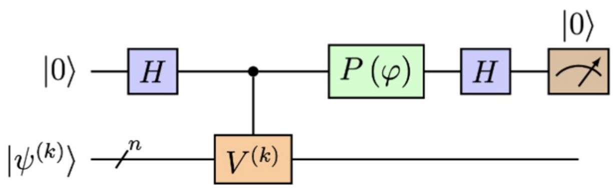
E.A. Ruiz Guzman, PhD thesis, in preparation

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

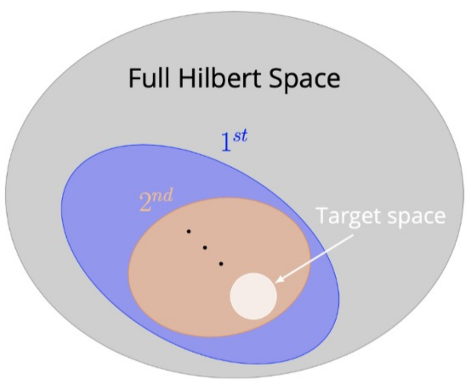
Standard Quantum Phase estimation



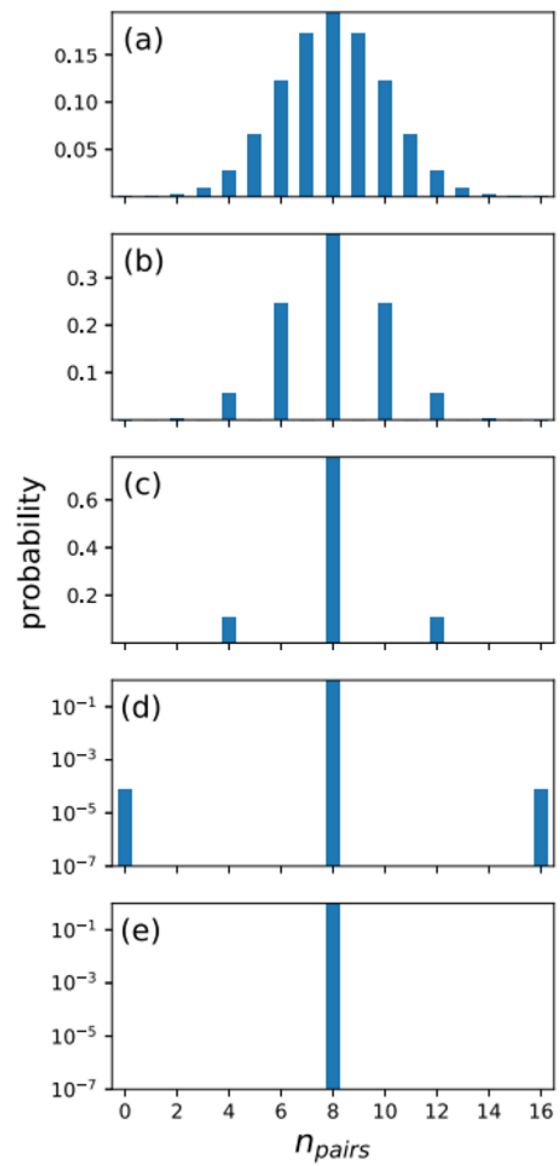
Iterative Quantum Phase estimation



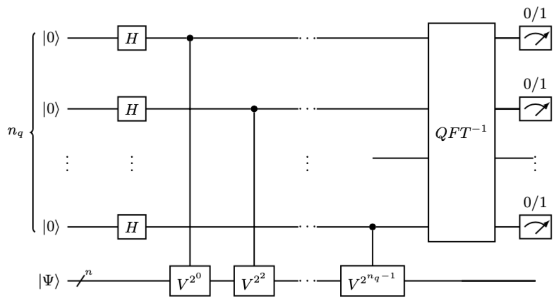
$$\hat{V}^{(k)} = e^{i\phi_k \hat{N}} \qquad \phi_k = \frac{\pi}{2^k}$$



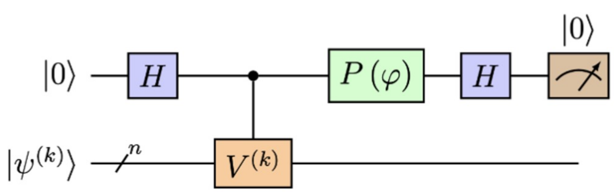
16 qubits, N = 8



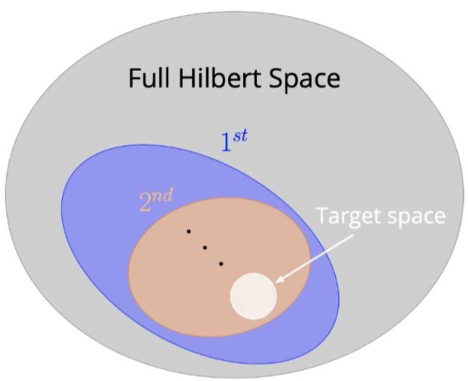
Standard Quantum Phase estimation



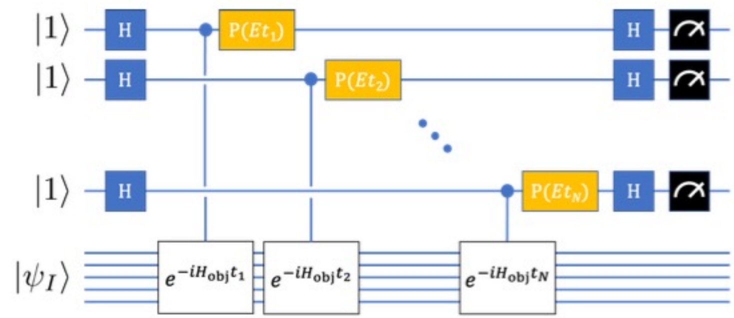
Iterative Quantum Phase estimation



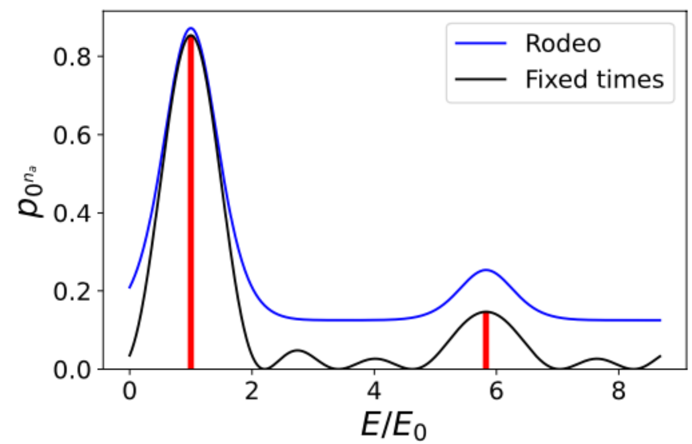
$\hat{V}^{(k)} = e^{i\phi_k \hat{N}}$ $\phi_k = \frac{\pi}{2^k}$



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



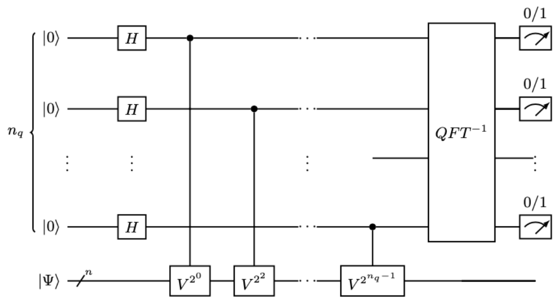
K. Choi et al., Rodeo Algorithm for Quantum Computing, Phys. Rev. Lett. 127, 040505 (2021).



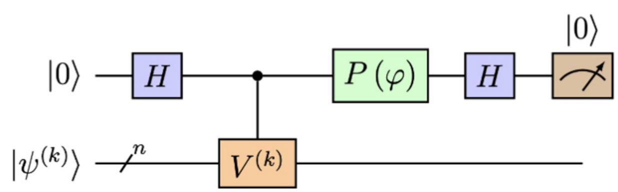
Ayral, Besserve, Lacroix, Ruiz Guzman, arxiv:2303.04850

Systematic of QPE-based methods

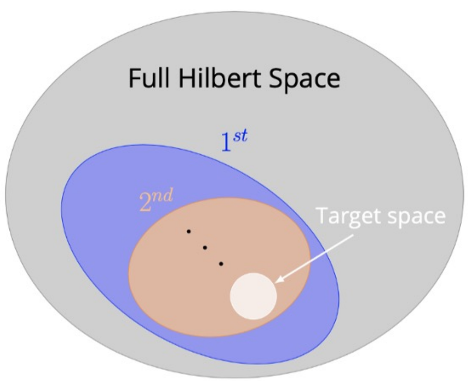
Standard Quantum Phase estimation



Iterative Quantum Phase estimation

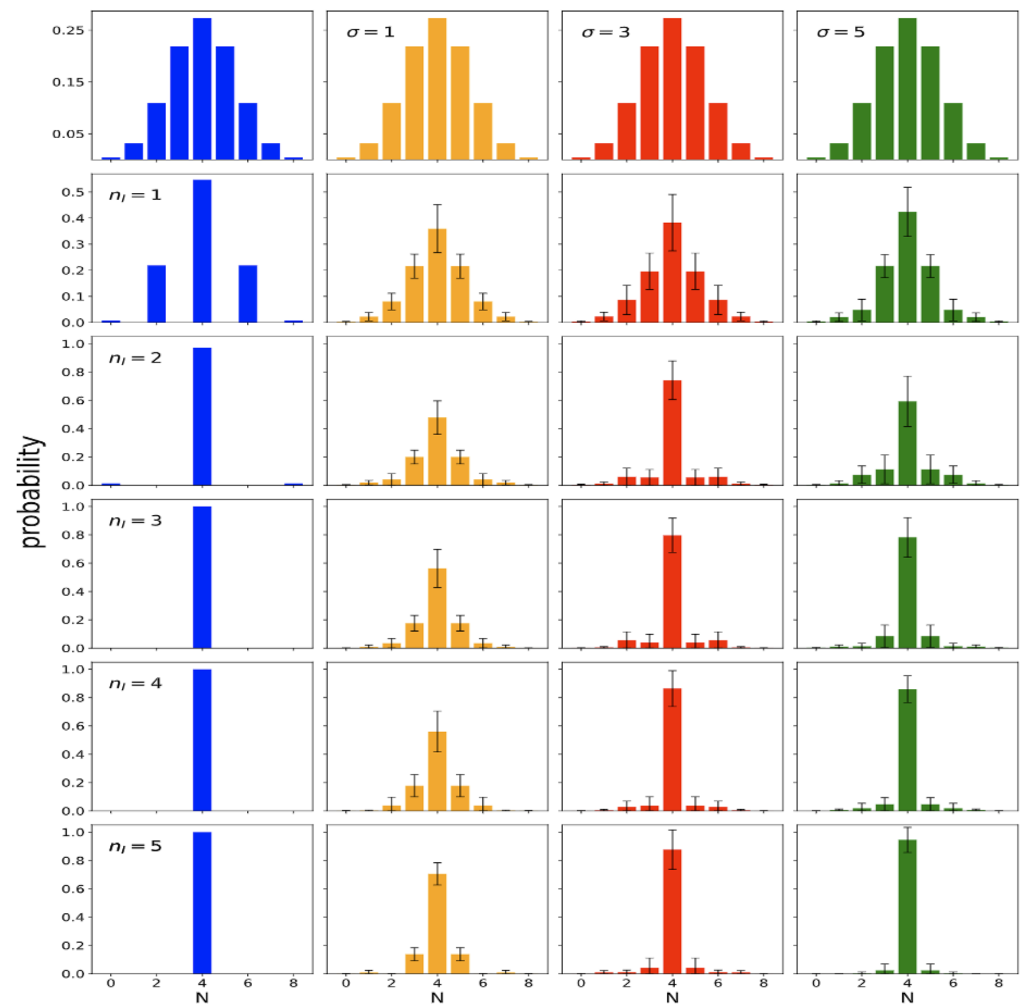


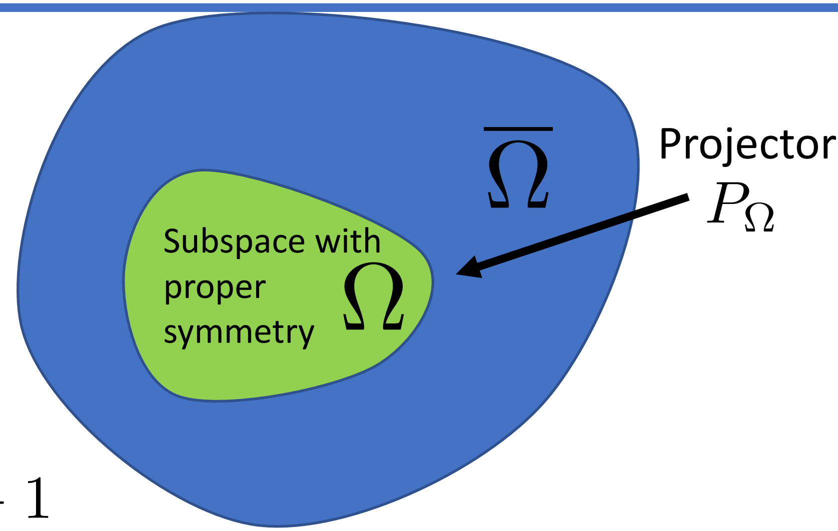
$$\hat{V}^{(k)} = e^{i\phi_k \hat{N}} \qquad \phi_k = \frac{\pi}{2^k}$$



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

Iterative QPE   Rodeo algorithm with different resolution





Grover Classification operator

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

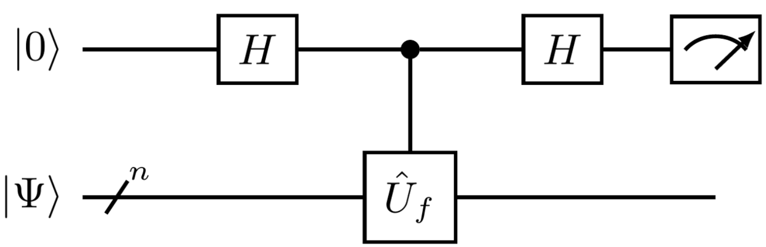
Lov K. Grover, Phys. Rev. Lett. **79**, 325 (1997)

Assume we are able to encode the projector

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

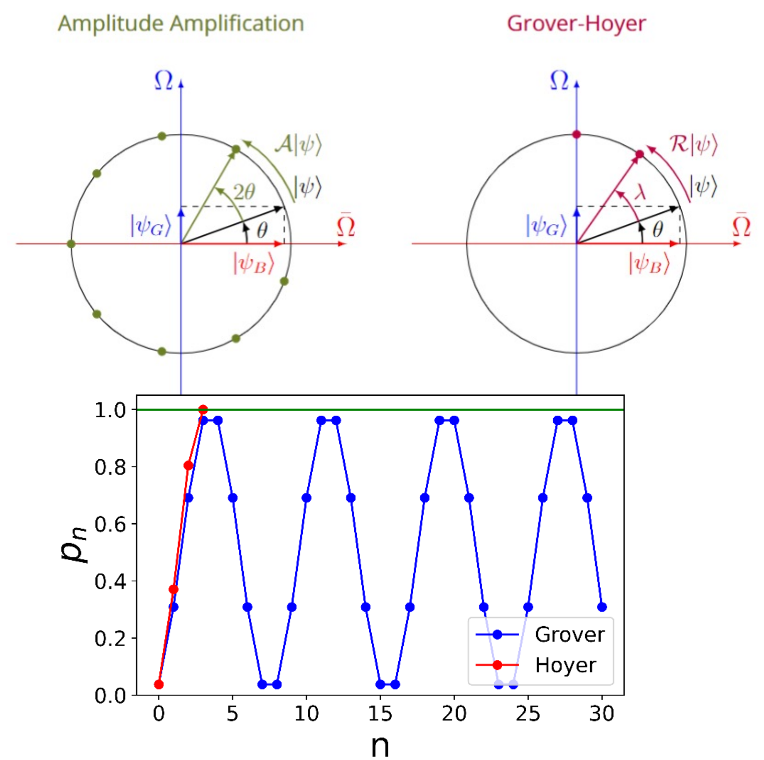
Methods based on projectors

Oracle + Hadamard test



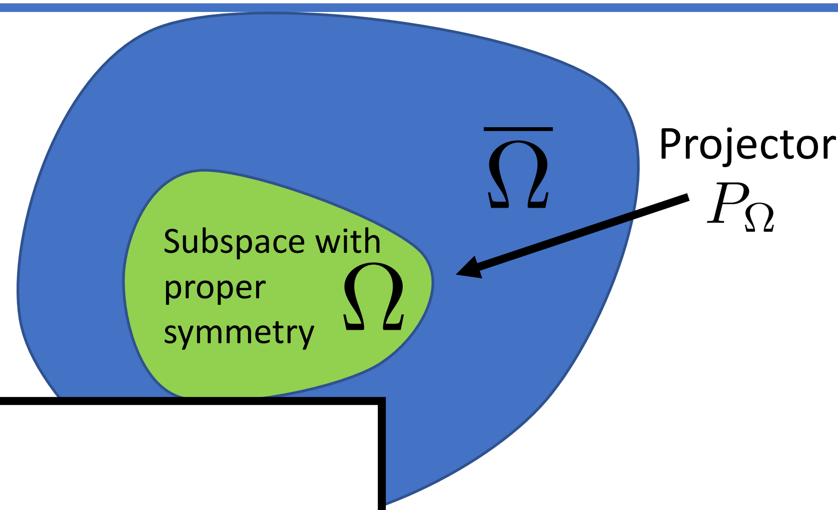
$$\frac{1}{2}\{|0\rangle \otimes [I + \hat{U}_f]|\Psi\rangle + |1\rangle \otimes [I - \hat{U}_f]|\Psi\rangle\} = |0\rangle|\Psi_B\rangle + |1\rangle|\Psi_G\rangle$$

Grover technique



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

Symmetry restoration using Projection operators and Oracles



Grover Classification operator

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

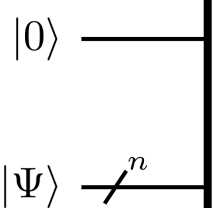
Lov K. Grover, Phys. Rev. Lett. **79**, 325 (1997)

Assume w

P_Ω

Methods

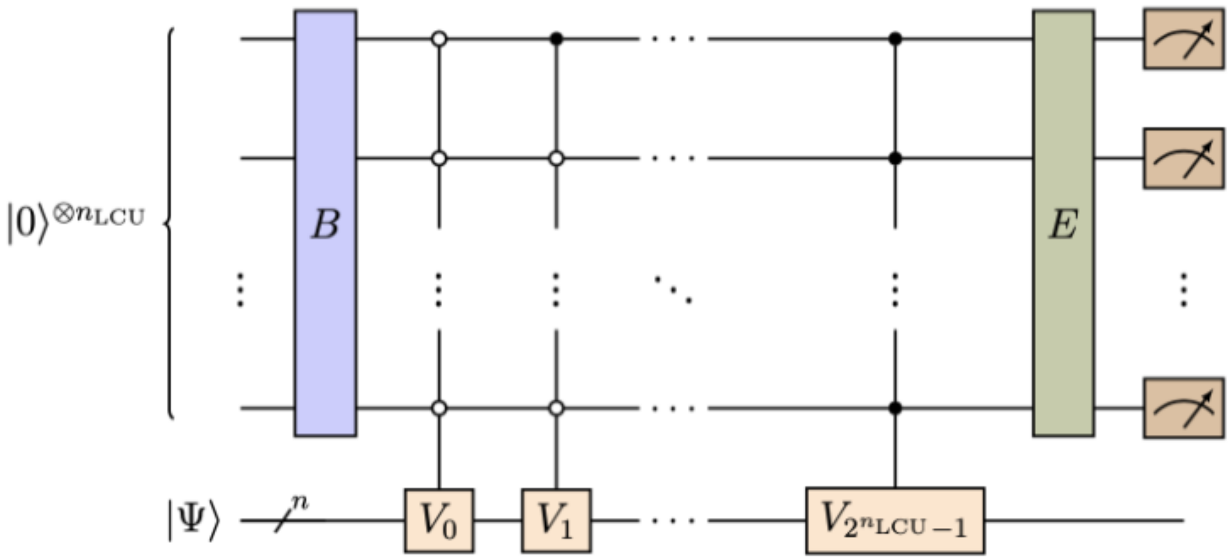
Oracle + H

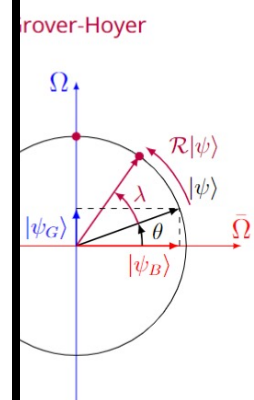


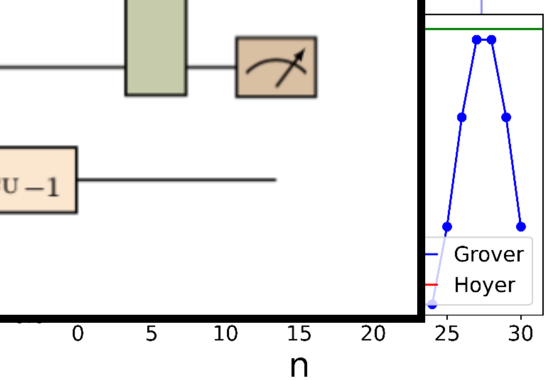
$\frac{1}{2}\{|0\rangle \otimes [I + \hat{U}$

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







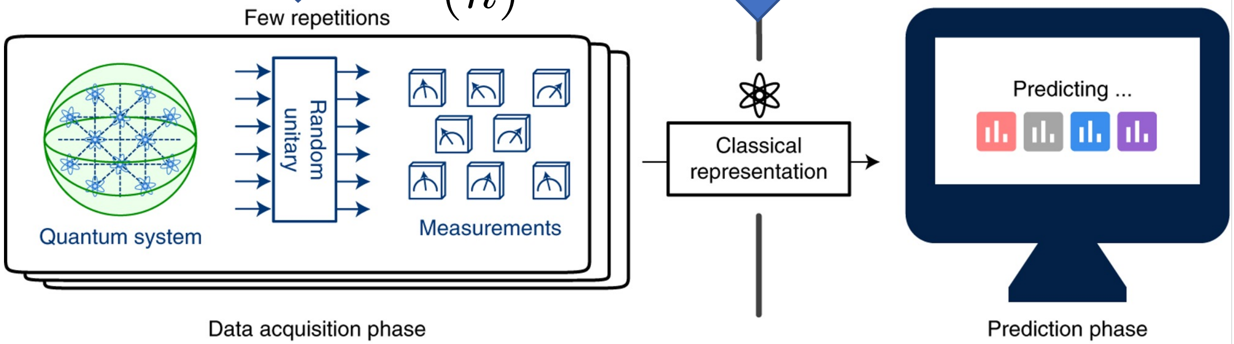
E. A. Ruiz Guzman and D. Lacroix, Phys. Rev. **C 107**, 034310 (2023)

Symmetry restoration by quantum tomography

Classical shadow technique

Random rotations of the computational basis $U_{(n)}$

Storing of pseudo classical bits $\mathbf{b}^{(n)} = b_{q-1}^{(n)} \cdots b_0$



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

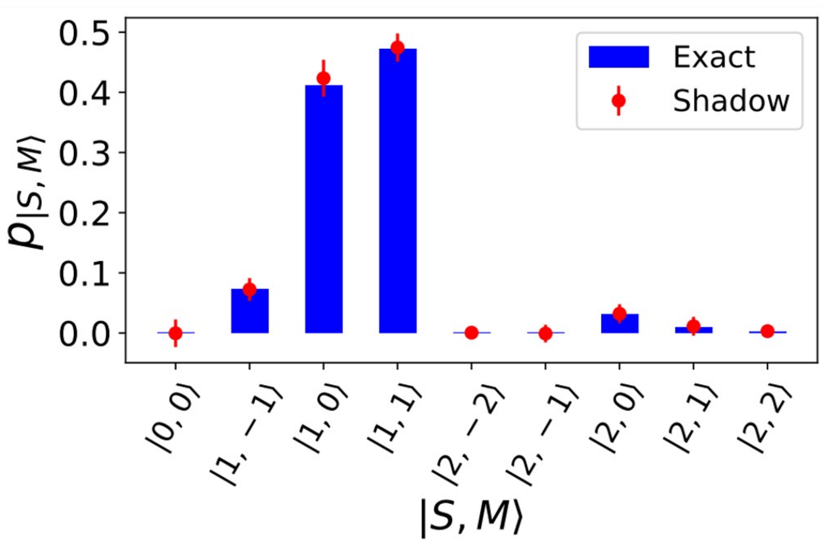
Snapshot

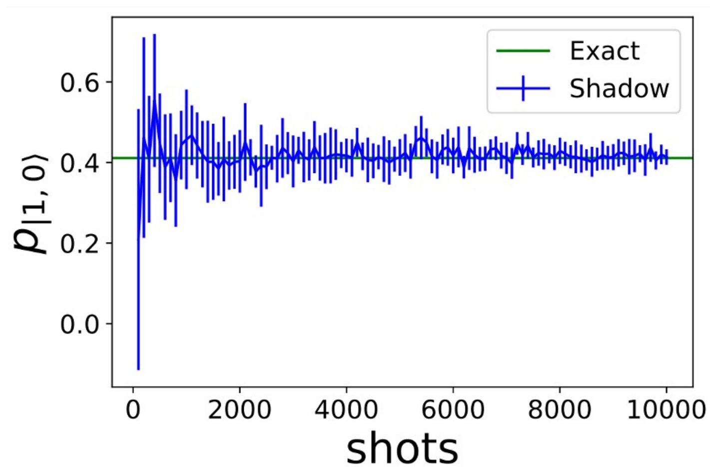
$$\rho^{(n)} = |\mathbf{b}^{(n)}\rangle\langle\mathbf{b}^{(n)}|$$

Inverse transformation average

$$\langle O\rangle = \frac{1}{N_{\text{evt}}}\sum_n \text{Tr}\left(O U_{(n)}^{\dagger}\rho^{(n)}U_{(n)}\right)$$

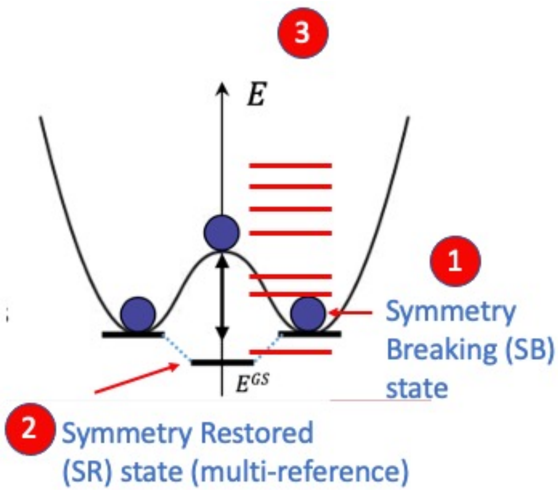
+ optimization on the convergence





E.A. Ruiz Guzman, PhD thesis, in preparation

Some summary and prospective

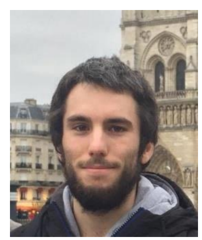


- We made a quite extensive focus on the symmetry problem (symmetry breaking/symmetry restoration
- Several techniques have been used to perform symmetry restoration (QPE, Grover, Shadow)
- We also explored a bit of postprocessing to get the ground state and excited states

Collaborators

IJCLab
Irène Joliot-Curie
Laboratoire de Physique des 2 Infinis

Department of Physics
Research, teaching and outreach in Physics at UW–Madison



E. A. Ruiz Guzman (PhD) J. Zhang (PhD) Y. Beaujeault-Taudiere (postdoc) P. Siwach (postdoc)