Some aspects of simulation of complex many-body systems on quantum computers

Nuclear Physics Team - Theory Pole

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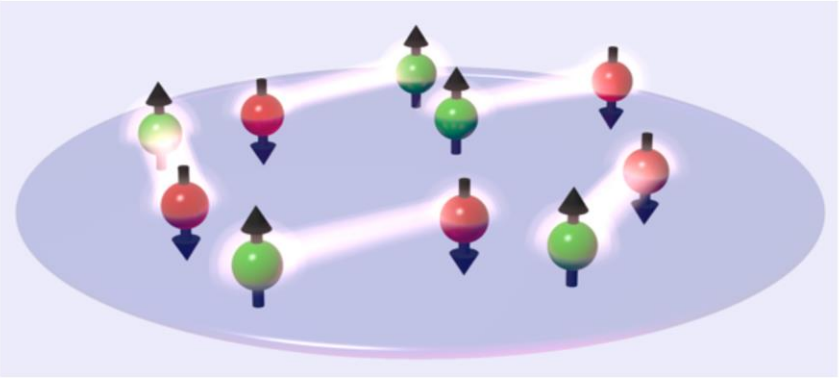
1. Introduction

What does a many-body problem look like?

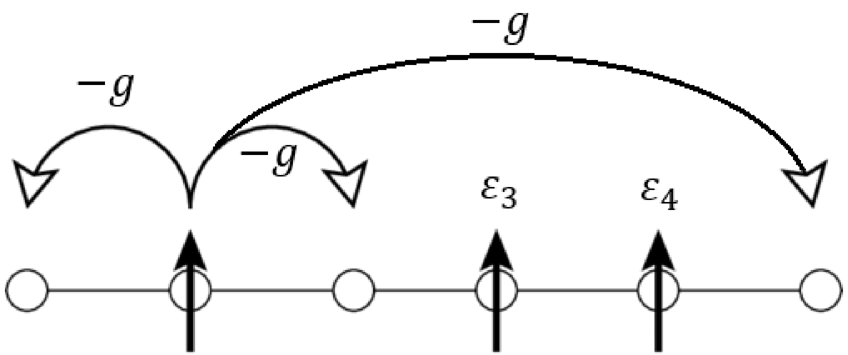
- Many-body problem → Many quantum particles in interaction.



https://www.uni-heidelberg.de/presse/news2016/pm20160128_what-are-the-special-properties-of-an-atomic-gas.html

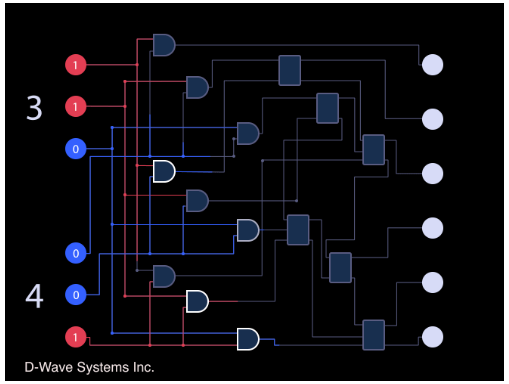
- Pairing model:

$$\hat{H}_p = \sum_i \varepsilon_i \hat{a}_i^\dagger \hat{a}_i - g \sum_{i,j} \hat{a}_i^\dagger \hat{a}_j$$



Why solve many-body problems with quantum computers?

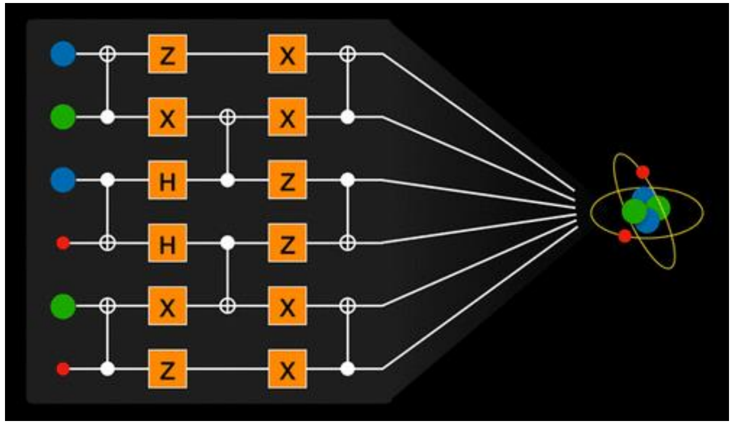
- Resources for the description of the configuration space ($2^{n_{qubits}}$) :



https://www.engadget.com/2018-10-04-d-wave-takes-quantum-computers-mainstream-with-leap.html

Classical computer $\rightarrow$ exponential scaling.

Quantum computer $\rightarrow$ polynomial scaling.



https://pubs.acs.org/doi/10.1021/acs.chemrev.8b00803

- Various quantum algorithms that have up to an exponential speed-up over their classical counterparts.

- Dynamical quantum computing ecosystem with real devices available for the public (e.g., IBM experience).

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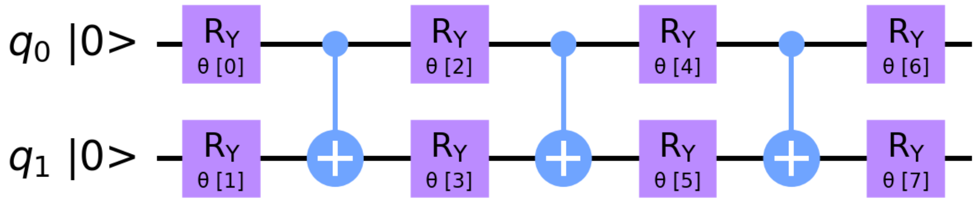
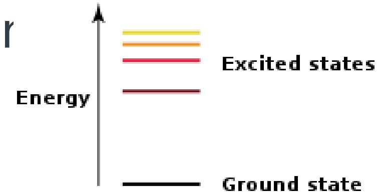
Problematics

- Create ansatzes that can reproduce the eigenstates of a Hamiltonian.



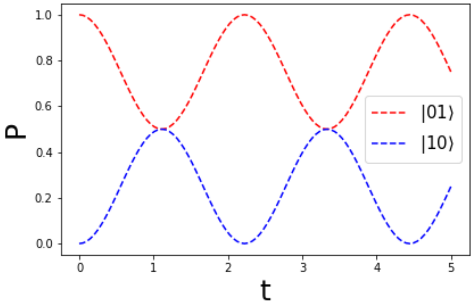
Ansatz: Circuit that creates a variational quantum state $|\Psi(\{\theta\})\rangle$ in a quantum register.

- Find the spectrum of a many-body Hamiltonian



- Obtain the quantum state evolution/dynamics.

$$e^{-itH}|\psi_0\rangle \rightarrow$$



Notes:

- Applications made on schematic Pairing or Hubbard Hamiltonian.
- Hamiltonians encoded on qubits using the Jordan-Wigner transformation.

2. Ansatzes

Bardeen–Cooper–Schrieffer(BCS) ansatz

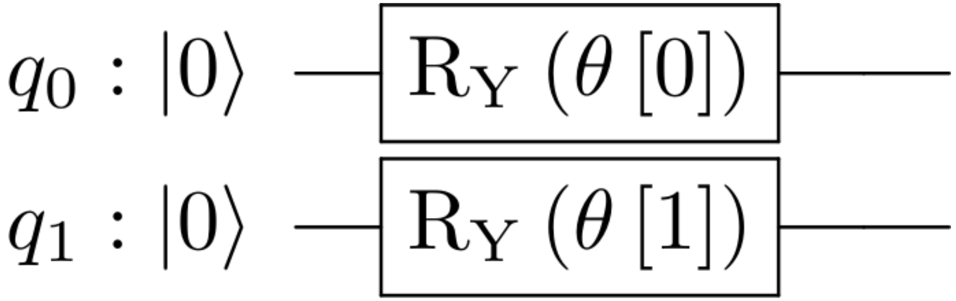
- BCS theory →first microscopic theory of superconductivity.

- Equation:

$$|\mathrm{BCS}(\{\theta_p\})\rangle = \bigotimes_{p=0}^{N-1}\left[\sin(\theta_p)|0\rangle_p + \cos(\theta_p)|1\rangle_p\right] = \prod_{p=0}^{N-1} R_Y(\pi - 2\theta_p)|0\rangle_p$$

Superposition of states with different number of pairs.

- Circuit:



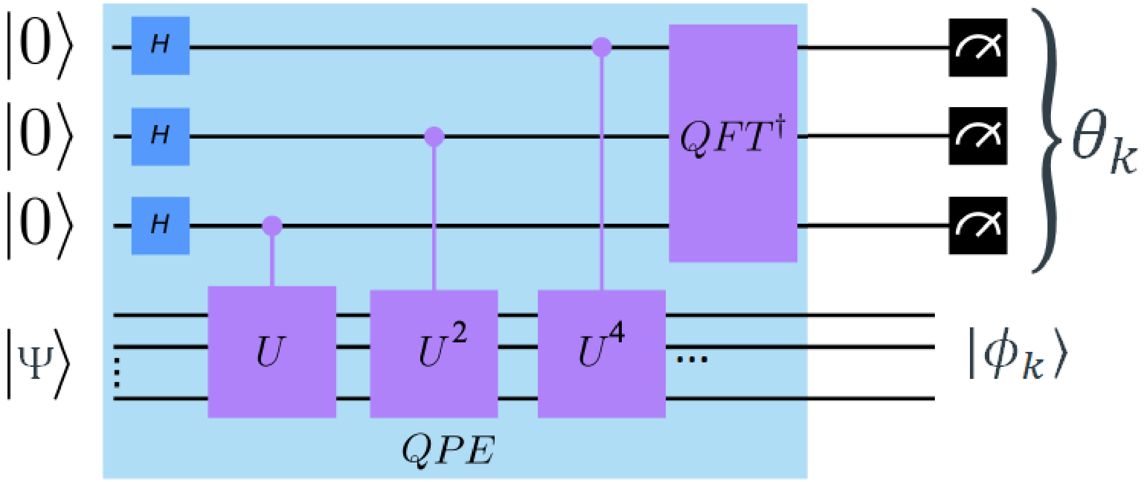
Projection on a fixed number of particles

- Quantum Phase Estimation (QPE) $\longrightarrow$ eigenvalues $\{\theta_k\}$ and eigenstates $\{\phi_k\}$:

$$\boldsymbol{M}\vec{x} = \lambda\vec{x}$$

$$\boldsymbol{M} \to U,\ \lambda \to e^{2\pi i\theta_k},\ \vec{x} \to |\phi_k\rangle$$

$$U|\phi_k\rangle = e^{2\pi i\theta_k}|\phi_k\rangle$$



https://www.swissquantumhub.com/quantum-supremacy-quantum-hybrid-hhl-algorithm-for-solving-a-system-of-linear-equation/

- Projection:

$$|\Psi(n_1, n_2, \dots)\rangle \to QPE(\hat{N}) \to n_k, |\Psi(n_k)\rangle$$

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Variational Quantum Eigensolver (VQE)

- Hamiltonian decomposition → $H = H_1 + H_2 + \cdots$.

- VQE:

https://www.theverge.com/circuitbreaker/2018/6/12/17453918/ibm-summit-worlds-fastest-supercomputer-america-department-of-energy

$$\{\theta\}$$

↑

$$\{\nabla\theta\}$$

↑

$$\langle H\rangle = \langle H_1\rangle + \langle H_2\rangle + \cdots$$

→

$$|\Psi(\{\theta\})\rangle$$

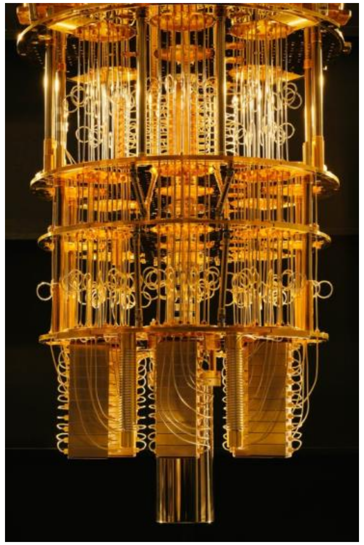
↓

$$\langle\Psi|H_1|\Psi\rangle$$

$$\langle\Psi|H_2|\Psi\rangle$$

…

←



https://pulsenews.co.kr/view.php?year=2019&no=321975

Quantum-Projection After Variation (Q-PAV) and Quantum-Variation After Projection (Q-VAP)

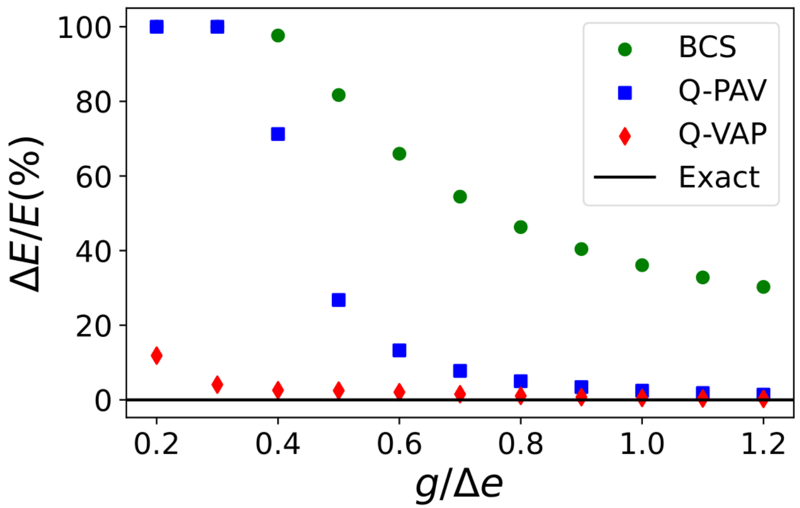
- Q-PAV:

$$|\Psi(n_1, n_2, \dots)\{\theta\}\rangle \xrightarrow{VQE} min(\langle\Psi|H|\Psi\rangle) \xrightarrow{QPE(\hat{N})} n_k, |\Psi(n_k)\rangle$$

- Q-VAP:

$$|\Psi(n_1, n_2, \dots)\{\theta\}\rangle \xrightarrow{QPE(\hat{N})} n_k, |\Psi(n_k)\rangle \xrightarrow{VQE} min(\langle\Psi(n_k)|H|\Psi(n_k)\rangle)$$

8 levels, 4 particles.
$\Delta E/E(\%)$ → Percentage distance to the ground state.

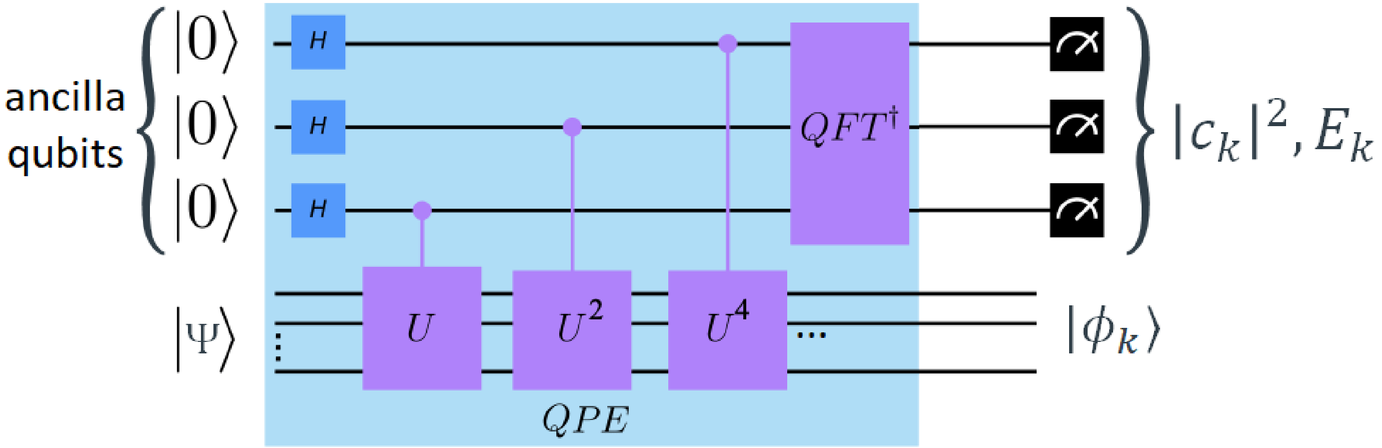


3. Post-processing

Quantum Phase Estimation(QPE) for Hamiltonians

Hamiltonian Phase Estimation

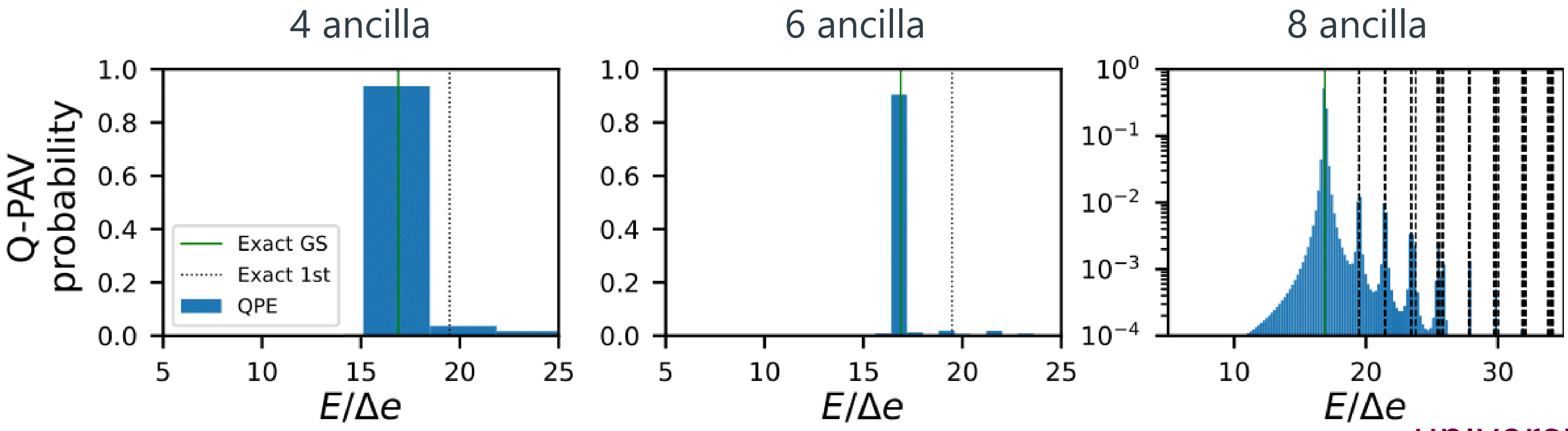
$$\left.\begin{aligned} H|\phi_k\rangle &= E_k|\phi_k\rangle \\ |\Psi\rangle &= \sum_k c_k\,|\phi_k\rangle \end{aligned}\right\} \rightarrow\ QPE(H,|\Psi\rangle) \rightarrow \{|c_k|^2, E_k\}$$



https://www.swissquantumhub.com/quantum-supremacy-quantum-hybrid-hhl-algorithm-for-solving-a-system-of-linear-equation/

E.g. 8 levels,

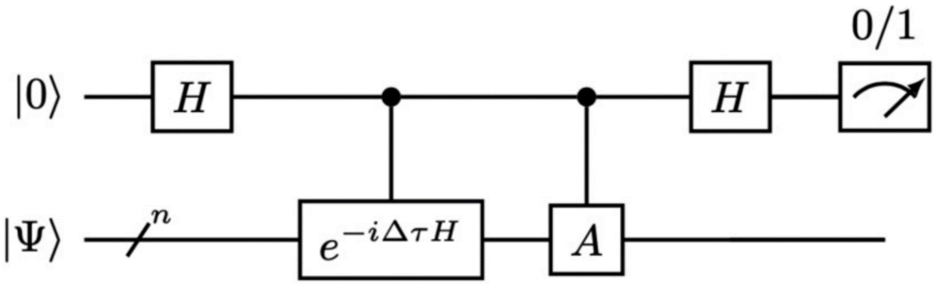
4 particles



Quantum Krylov

- Change of basis → Krylov basis of size M:

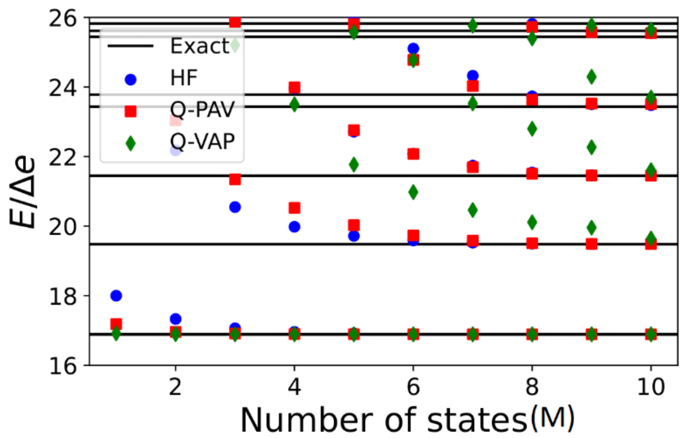
$$\{\Phi_j\} = \{|\Psi\rangle, e^{-i\tau_1 H}|\Psi\rangle, \dots, e^{-i\tau_{M-1} H}|\Psi\rangle\}$$



- Hadamard Test → $\langle\Phi_i|H|\Phi_j\rangle = \langle\Psi|He^{-i(\tau_j-\tau_i)H}|\Psi\rangle$

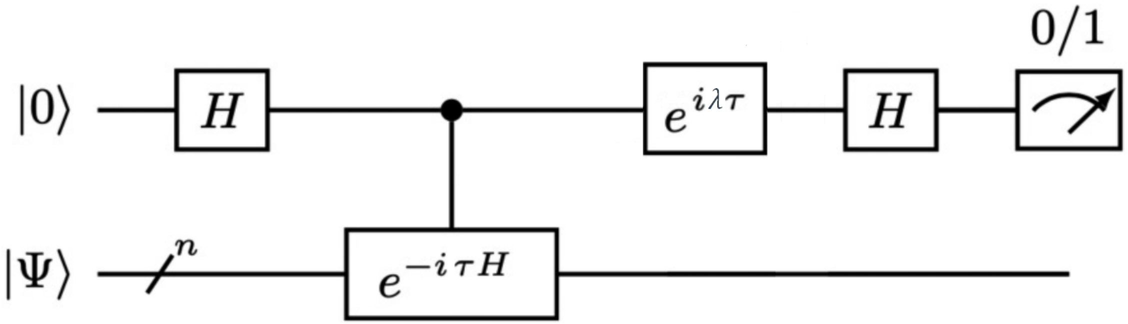
- Diagonalization of $\langle\Phi_i|H|\Phi_j\rangle$ → Approximated E_k

- E.g. 8 levels, 4 particles. $\tau_p = p * 0.3$



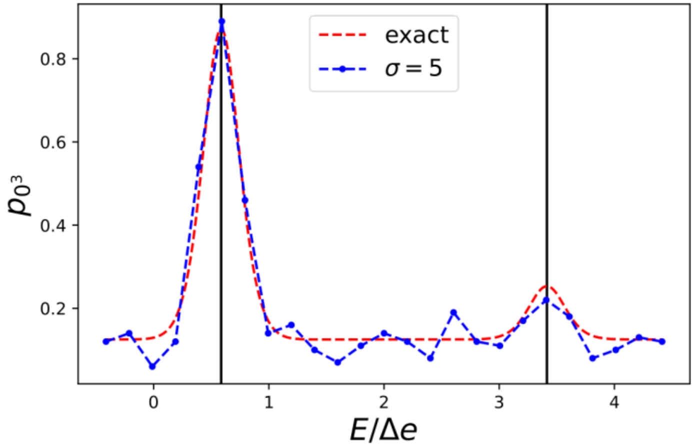
Rodeo algorithm

- $\tau \longrightarrow$ Random Gaussian distribution with standard deviation σ.



- p_{0^N} has Gaussian distributions around eigenvalues E_k

$$p_{0^N}(\lambda) = \sum_k |c_k|^2 \left[\frac{1 + e^{-(E_k-\lambda)^2\sigma^2/2}}{2}\right]^N$$



Conclusions

- We have implemented the Quantum Projection After Variation (Q-PAV) method and the Quantum Variation After Projection (Q-VAP) method. Both processes can be applied to any ansatz.

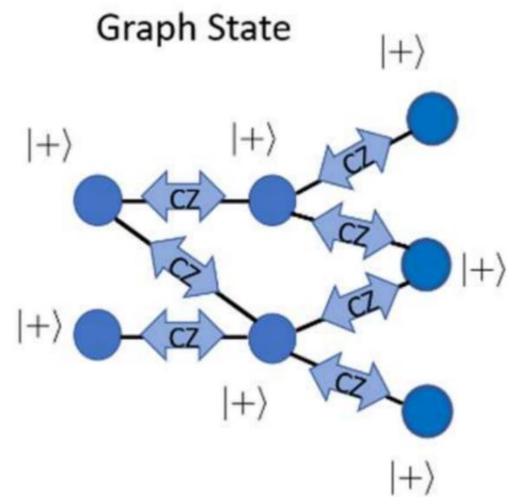
- Several post-processing methods have been explored to recover approximations of the ground and excited states energies of a Hamiltonian.

- Information about the initial state $|\psi\rangle$ can be retrieved in some of the post-processing methods (QPE, Rodeo). An approximation of its evolution can also be obtained (Quantum Krylov).

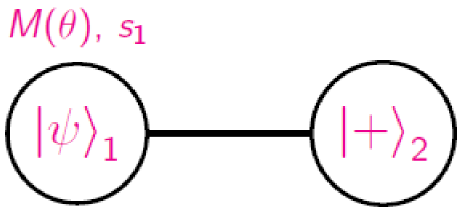
Questions ?

Measurement-Based Quantum Computing(MBQC)

- Graph states -> Entangled qubits in the state $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$:



- Gates -> Measurement over qubits on a rotated basis $\{|+_\theta\rangle, |-_\theta\rangle\}$:



$$(X_2)^{s_1} HP(-\theta)|\psi\rangle_2$$