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

IJCLab

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1. Introduction



Problematics for many-body systems

• Create ansätzes 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 many-body Hamiltonians.



• Obtain the quantum state evolution.







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

2. Mapping a physical problem into a quantum computer



Many-body Hamiltonians

Nuclear Superfluidity. Pairing in Finite Systems, by D.M. Brink and R.A. Broglia, Contemporary Physics. (2010)

• Pairing model
$$(\hat{N}_p = \hat{a}_p^{\dagger} \hat{a}_p + \hat{a}_{\bar{p}}^{\dagger} \hat{a}_{\bar{p}}, \hat{P}_p^{\dagger} = \hat{a}_p^{\dagger} \hat{a}_{\bar{p}}^{\dagger})$$
:

 $\widehat{H}_P = \sum_p \varepsilon_p \,\widehat{N}_p - g \sum_{p,q} \widehat{P}_p^{\dagger} \widehat{P}_q$



• Fermi-Hubbard model ($\hat{n}_{i,\sigma} = \hat{a}_{i,\sigma}^{\dagger} \hat{a}_{i,\sigma}, \sigma = \{\uparrow, \downarrow\}$):

A. Altland and B. Simons, Interaction effects in the tight-binding system. Condensed Matter Field Theory. Cambridge University Press. pp. 58 (2006).

Jordan-Wigner transformation(JWT) and Trotter evolution

JWT Operators → Pauli matrices

 $\widehat{H}_{\varepsilon} + \widehat{H}_{a}$. As $[\widehat{H}_{\varepsilon}, \widehat{H}_{a}] \neq 0$:

Guido Fano, S. M. Blinder, Mathematical Physics in Theoretical Chemistry, 377 (2019).

Ovrum E, Hjorth-Jensen M. arXiv:0705.1928v1 (2007)

A. Khamoshi, F. A. Evangelista, and G. E. Scuseria, Quantum Sci. Technol. 6, 014004 (2021).

$$a_p^{\dagger} = \bigotimes_{k=1}^{p-1} Z_k \otimes Q_p^{\dagger} \bigotimes_{k=p+1}^N I_k \qquad \qquad \widehat{Q}_p^{\dagger} = \frac{1}{2} \left(X_p - iY_p \right) = \begin{pmatrix} 0 & 0\\ 1 & 0 \end{pmatrix}_p$$

Seniority zero scheme \rightarrow No broken pairs: $\hat{P}_p^{\dagger} = \hat{a}_p^{\dagger} \hat{a}_{\bar{p}}^{\dagger} = \hat{Q}_p^{\dagger}$. 1 pair \leftrightarrow 1 qubit.

• Trotter-Suzuki decomposition. E.g. Pairing Hamiltonian $\hat{H}_P = \underbrace{\sum_p \varepsilon_p \hat{N}_p}_{\hat{H}_s} \underbrace{-g \sum_{p,q} \hat{P}_p^{\dagger} \hat{P}_q}_{\hat{H}_q} =$

H. F. Trotter, Proc. Am. Math. Soc. 10, 545 (1959)

$$e^{-it\hat{H}_P} \approx \left(e^{-i\hat{H}_g \frac{t}{n}} e^{-i\hat{H}_\varepsilon \frac{t}{n}}\right)^n$$



Pairing problem

• Single-particle operator:



Hubbard Hamiltonian

• Single-particle operator:

$$\widehat{U}_U(t) = e^{-i\widehat{H}_U t/\hbar} = \prod_{\alpha} CR(\phi)$$

 $CR(\phi) \rightarrow$



Yamada et al. High Performance LOBPCG Method for Solving MultipHigh-Performance Hubbard Model: Efficiency of Communication Avoiding Neumann Expansion Preconditioner. 10.1007/978-3-319-69953-0_14. (2018).

• Two-particle operator:

with $\phi = -tU/\hbar$.

$$\widehat{U}_{J}(t) = e^{-i\widehat{H}_{J}t/\hbar} = \prod_{\alpha} M_{\alpha,\alpha+1}$$

$$M_{\alpha,\alpha+1} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\lambda) & i \sin(\lambda) & 0 \\ 0 & i \sin(\lambda) & \cos(\lambda) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}_{\alpha,\alpha+1} \to R_X(-2\lambda)$$

 $R(\phi)$

with $\lambda = Jt/\hbar$.

3. Quantum Ansätzes: Symmetry breaking and restoration



Variational Quantum Eigensolver (VQE)

• Hamiltonian decomposition $\rightarrow \hat{H} = \beta_1 \hat{V}_1 + \beta_2 \hat{V}_2 + \cdots$.



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Bardeen–Cooper–Schrieffer(BCS) ansatz

• BCS theory \rightarrow first microscopic theory of superconductivity.

$$|\Phi_{BCS}\rangle = \prod_{p} (u_p + v_p \hat{P}_p^{\dagger}) |0\rangle_p$$
1 qubit

With $\hat{P}_p^{\dagger} = \hat{a}_p^{\dagger} \hat{a}_{\bar{p}}^{\dagger}$. 1 pair \leftrightarrow 1 qubit.

• Equation:



Chernodub, Maxim. Can nothing be a superconductor and a superfluid?. Proceedings of Science. (2011).

$$\left|\Phi_{BCS}\left(\{\theta_{p}\}\right)\right\rangle = \bigotimes_{p=0}^{N-1} \left[\sin(\theta_{p})|0\rangle_{p} + \cos(\theta_{p})|1\rangle_{p}\right] = \prod_{p=0}^{N-1} R_{Y}(\pi - 2\theta_{p})|0\rangle_{p}$$

Symmetry breaking:

Superposition of states with different number of pairs.

$$q_{0}:|0\rangle - \left[\operatorname{R}_{Y}\left(\theta\left[0\right]\right)\right] - \left[\operatorname{R}_{Y}\left(\theta\left[1\right]\right)\right] - \left[\operatorname{R}_$$



Quantum BCS minimization

Define: 1.

2.

- $\varepsilon_p = p\Delta e, g \rightarrow \text{Pairing Hamiltonian}.$
- Number of pairs n_p . Tolerance ϵ_{tol} for $|\langle \Phi_{BCS} \{\theta_p\} | \hat{N} | \Phi_{BCS} \{\theta_p\} \rangle n_p|$. Guess:
- $\{\theta_p\}$ and the Fermi energy λ .





While
$$|\langle \hat{N} \rangle - n_p| \ge \epsilon_{tol}$$
:
1. Minimize $C(\{\theta_p\}) = \langle \Phi_{BCS}\{\theta_p\} | \hat{H}_P | \Phi_{BCS}\{\theta_p\} \rangle - \langle \Phi_{BCS}\{\theta_p\} | \lambda(\hat{N} - n_p) | \Phi_{BCS}\{\theta_p\} \rangle$:
1. $\langle \Phi_{BCS}\{\theta_p\} | \hat{H}_P | \Phi_{BCS}\{\theta_p\} \rangle \rightarrow \text{Quantum Computer.}$

2.
$$\langle \Phi_{BCS} \{ \theta_p \} | \widehat{N} | \Phi_{BCS} \{ \theta_p \} \rangle \rightarrow \text{Classical computer:}$$

$$\langle \Phi_{BCS} \{ \theta_p \} | \hat{N} | \Phi_{BCS} \{ \theta_p \} \rangle = \sum_p \cos^2(\theta_p)$$

$$\Rightarrow \{\theta'_p\}.$$
2. $\lambda' = \lambda + \Delta e(n_p - \langle \Phi_{BCS}\{\theta'_p\} | \widehat{N} | \Phi_{BCS}\{\theta'_p\} \rangle).$
3. $\lambda' \to \lambda \text{ and } \{\theta'_p\} \to \{\theta_p\}.$



Symmetry restoration on a given number of particles with QPE

• Quantum Phase Estimation (QPE) \rightarrow eigenvalues { θ_k } and eigenstates { ϕ_k }:



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



Denis Lacroix, Phys. Rev. Lett. 125, 230502 (2020)

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

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

• Q-PAV:

• Q-VAP:

$$|\Psi(n_1, n_2, ...)\{\theta\}\rangle \xrightarrow{VQE} min(\langle \Psi|H|\Psi\rangle) \xrightarrow{\widehat{\mathcal{P}}_{n_k}^{QPE}} n_k, |\Psi(n_k)\rangle$$

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

8 sites, 4 pairs. $\Delta E/E(\%) \rightarrow$ Percentage of error on the ground state energy.



E. A. Ruiz Guzman and D. Lacroix, Phys. Rev. C **105**, 024324 (2022)



4. Ground and excited energies of many-body Hamiltonians

4.1 Quantum Phase Estimation (QPE)

4.2 Generating function technique

4.3 Quantum Krylov



Quantum Phase Estimation(QPE) for Energy Spectrum Hamiltonian Phase Estimation



 $U^m = e^{-i\hat{H}\frac{l}{2^m}}$ with $m = 1, 2, ..., r \cdot r \rightarrow \text{Number of ancilla qubits.}$



Quantum Phase Estimation(QPE) for Energy Spectrum Hamiltonian Phase Estimation

E. A. Ruiz Guzman and D. Lacroix, Phys. Rev. C **105**, 024324 (2022)

• E.g. Pairing, 8 levels, 4 pairs:





Generating function

• Generating function of a Hamiltonian \hat{H} is:

$$F(t) = \langle \psi | e^{-i\hat{H}t} | \psi \rangle$$

• Moments of the Hamiltonian:

$$\left\langle H^k \right\rangle = \left\langle \psi \middle| H^k \middle| \psi \right\rangle$$

• Relation between them:

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

Plots generating function

- Pairing. 8 sites \rightarrow 8 qubits. $|\psi_0\rangle = |00001111\rangle$. g = 1. $\varepsilon_{p=1,\dots} = 2p$
- Hubbard. 4 sites \rightarrow 8 qubits. $|\psi_0\rangle = \frac{1}{\sqrt{6}}(|00110011\rangle + \cdots)$. U = J = 1.



- Points \rightarrow Average of 10⁴ measurements on a perfect quantum computer.
- Lines \rightarrow Exact results.

Quantum Krylov Moments $\langle H^k \rangle$

Cristian L. Cortes et al. Phys. Rev. A **105**, 022417 (2022)

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• Change of basis \rightarrow Krylov basis of size M:

 $\left\{\chi_j\right\} = \left\{|\Psi\rangle, H|\Psi\rangle, H^2|\Psi\rangle, \dots, H^{M-1}|\Psi\rangle\right\}$

- $\langle \chi_m | H | \chi_n \rangle = \langle \Psi | H^{m+n+1} | \Psi \rangle = i^{m+n+1} \frac{d^{m+n+1}F(t)}{dt^{m+n+1}} \Big|_{t=0}$
- Diagonalization of $\langle \chi_m | H | \chi_n \rangle$ in reduced space \rightarrow Approximated E_k
- E.g. 8 levels, 4 particles.





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Quantum Krylov Evolutions $\langle He^{\tau} \rangle$

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Cristian L. Cortes et al. Phys. Rev. A **105**, 022417 (2022)

• Change of basis \rightarrow Krylov basis of size M:

$$\left\{\Phi_{j}\right\} = \left\{|\Psi\rangle, e^{-i\tau_{1}H}|\Psi\rangle, \dots, e^{-i\tau_{M-1}H}|\Psi\rangle\right\}$$

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



• Hadamard Test $\rightarrow \langle \Phi_m | H | \Phi_n \rangle = \langle \Psi | H e^{-i(\tau_m - \tau_n)H} | \Psi \rangle$

Diagonalization of $\langle \Phi_i | H | \Phi_j \rangle$ in reduced space \rightarrow Approximated E_k

E. A. Ruiz Guzman and D. Lacroix, Phys. Rev. C **105**, 024324 (2022)





Evolution of the survival probability

• $P_M(|\psi_0\rangle) = |\langle \psi_0 | \psi(t) \rangle|^2$



E. A. Ruiz Guzman and D. Lacroix, arXiv:2104.08181. (2021)



Imaginary time evolution

D. Horn and M. Weinstein, Phys. Rev. D 30, 1256 (1984)

Kazuhiro Seki, Seiji Yunoki, Phys. Rev. X Quantum 2, 010333 (2021)

• Ground state energy:

$$E_{GS} = \lim_{\tau \to \infty} \langle \psi(\tau) | \hat{H} | \psi(\tau) \rangle = \lim_{\tau \to \infty} E(\tau)$$

with
$$|\psi(\tau)\rangle = \frac{e^{-\tau/2\hat{H}}}{\sqrt{\langle\psi_0|e^{-\tau\hat{H}}|\psi_0\rangle}}|\psi_0\rangle.$$

• Taylor approximation of $\dot{E}(\tau)$:

$$\frac{dE(\tau)}{d\tau} \approx -\sum_{n=0}^{L} \frac{(-\tau)^n}{n!} \kappa_{n+2}$$

 $\{\langle H^n \rangle\}_{L+2} \rightarrow \{\kappa_n\}_{L+2} \text{ and } \{\kappa_n\} \text{ cumulants.}$

• Padé approximation [m,n]:

$$P_{mn}(\tau) = \frac{\sum_{j=0}^{m} a_j \tau^j}{\sum_{j=0}^{n} b_j \tau^j}$$



Imaginary time evolution-Results E. A. Ruiz Guzman and D. Lacroix, arXiv:2104.08181. (2021)

•
$$L = 10 \rightarrow \{\langle H^k \rangle\}_{12}$$

• $\frac{dE(\tau)}{d\tau} = \dot{E}(\tau)$



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5. Alternative methods for symmetry restoration



Symmetry restoration on a given number of particles with the IQPE-like method

• Iterative-QPE(IQPE)-like:





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At most $n_{IOPE} = \lfloor \log_2(n) \rfloor + 1$

Symmetry restoration on a given number of particles by Amplitude Amplification

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

Peter Hoyer, Phys. Rev. A 62, 052304 (2000)

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• Grover operator:

$$\widehat{G} = \widehat{R}_{\Psi} \widehat{U}_{f}$$

$$\widehat{U}_{f}|k\rangle = (-1)^{x} \text{ with } x \left\{ \begin{array}{l} 0 & if \ |k\rangle \in |\Psi_{B}\rangle \\ 1 & if \ |k\rangle \in |\Psi_{G}\rangle \\ |\Psi_{G/B}\rangle = \{|k\rangle \text{ such that: } \widehat{N}|k\rangle = /\neq A|k\rangle \} \right\}$$

$$\bullet \text{ E.g. } p_{n} = \left| \left\langle \Psi_{G} \left| \widehat{G}^{n} \right| \Psi \right\rangle \right|^{2}, 8 \text{ qubits, } A = 4 \text{ and } \theta = \angle |\Psi\rangle |\Psi_{B}\rangle = \frac{\pi}{4}, \quad \bigotimes_{\substack{0.6 \\ 0.4 \\ 0.2 \\ 0.0 \\$$

 $|\Psi_G\rangle$

Symmetry restoration on a given number of particles by Oracle+Hadamard Test

• Oracle+Hadamard projection:



$$\frac{1}{2}\left\{|0\rangle \otimes \left[I + \widehat{U}_{f}\right]|\Psi\rangle + |1\rangle \otimes \left[I - \widehat{U}_{f}\right]|\Psi\rangle\right\} = |0\rangle|\Psi_{B}\rangle + |1\rangle|\Psi_{G}\rangle$$



Symmetry restoration on a given number of particles Generic Projector as Linear Combination of Unitaries(LCU)

• Symmetry operator \hat{S} with eigenvalues $\lambda_1, \lambda_2, ..., \lambda_{\Omega}$. Generic projector:

$$\hat{\mathcal{P}}_{\alpha} = \sum_{k=0}^{M} \beta_k e^{i\phi_k \hat{S}} \qquad \beta_k = \frac{1}{M+1} e^{-i\phi_k (\xi_{\alpha} + \lambda_1)} \qquad \phi_k = \frac{2\pi k}{a(M+1)}$$

with $\xi_{\alpha} = \lambda_{\alpha} - \lambda_1 = am_{\alpha}$, $m_{\alpha} \in [0, m_{\Omega}]$ and $M = m_{\Omega}$.

• If $\hat{S} = \widehat{N}$:

$$\widehat{\mathcal{P}}_N = \frac{1}{n_q+1} \sum_{k=0}^{n_q} e^{i\phi_k \widehat{N}} \qquad \phi_k = \frac{2\pi k}{n_q+1}$$



Symmetry restoration on a given number of particles Generic Projector as Linear Combination of Unitaries(LCU)

$$\hat{\mathcal{P}}_{n_{k}} |\Psi(n_{0}, n_{1}, \dots, n_{q})\rangle = |\Psi(n_{k})\rangle$$

$$\hat{B}|0\rangle^{\bigotimes n_{LCU}} = \frac{1}{\mathcal{N}} \sum_{k=0}^{2^{n_{LCU}-1}} \beta_{k} |k\rangle$$

$$\hat{G}_{k} = e^{i\phi_{k}\hat{S}}$$

$$\text{with } \mathcal{N} = \sqrt{\sum_{k} |\beta_{k}|^{2}}, \beta_{k>M} = 0 \text{ and } \hat{G}_{k>M} = I.$$

$$\hat{G}_{k} = e^{i\phi_{k}} \beta_{k>M} = 0 \text{ and } \hat{G}_{k>M} = I.$$

$$\hat{G}_{k} = e^{i\phi_{k}\beta}$$

$$\hat{G}_{k>M} = I.$$

$$\hat{G}_{k} = e^{i\phi_{k}\beta}$$

$$\hat{G}_{k} = e^{i\phi_{k}\beta}$$

$$\hat{G}_{k>M} = I.$$

$$\hat{G}_{k} = e^{i\phi_{k}\beta}$$

• Projected expected value of $\hat{H} = \sum_{j=0} \gamma_j \hat{V}_j$:

$$\left\langle \Psi \middle| \widehat{H} \widehat{\mathcal{P}}_{n_k} \middle| \Psi \right\rangle = \sum_{k,j} \gamma_j \beta_k \left\langle \Psi \middle| \widehat{V}_j \widehat{G}_k \middle| \Psi \right\rangle$$

Symmetry restoration on a given number of particles Generic Oracle as Linear Combination of Unitaries(LCU)

• $\hat{O}_{\alpha}(\varphi,\mu) = e^{i\mu} (\hat{I} - \hat{\mathcal{P}}_{\alpha}) + e^{i\varphi} \hat{\mathcal{P}}_{\alpha}$

$$\hat{O}_{\alpha}(\varphi,\mu)|\Phi_{k}\rangle = \begin{cases} e^{i\varphi} & if \quad \hat{S}|\Phi_{k}\rangle = \lambda_{\alpha}|\Phi_{k}\rangle \\ e^{i\mu} & if \quad \hat{S}|\Phi_{k}\rangle \neq \lambda_{\alpha}|\Phi_{k}\rangle \end{cases}$$

• Projected expected value of $\hat{H} = \sum_{j=0} \gamma_j \hat{V}_j$. If \hat{H} Hermitian and $\hat{U} = \hat{V}_j$:

$$\left| 0 \right\rangle \underbrace{H}_{\hat{H}\hat{O}_{\alpha}} \left(\varphi = 0, \mu = \frac{\pi}{2} \right) \left| \Psi \right\rangle = \left\langle \Psi \right| \hat{H}\hat{\mathcal{P}}_{\alpha} \left| \Psi \right\rangle = p_0 - p_1$$

$$\left| \Psi \right\rangle \underbrace{n}_{\hat{U}} \underbrace{\hat{U}}_{\hat{U}} \underbrace{\hat{U}} \underbrace{\hat{U}}_{\hat{U}} \underbrace{\hat{U}} \underbrace{\hat{$$



Comparison of symmetry restoration methods

	# Ancilla	# Measurements	Gate resources	Ranking
QPE	$n_{QPE} = \left\lfloor \log_2 n_q \right\rfloor$	$\sim p_G = \langle \Psi_G \Psi_G \rangle$	M, controlled $e^{i\phi_k \widehat{N}}$ QFT^{\dagger}	2
LCU	$n_{LCU} = \lfloor \log_2(M+1) \rfloor$	$\sim p_G$	M, n_{LCU} -controlled $e^{i\phi_k \widehat{N}}$	4
Grover/Hoyer	0	-	2 general oracles n_G general \hat{G} , each: - 1 general oracle - 2 QSP over n_q qubits.	5
IQPE-like	1	$\sim p_G$	At most n_{IQPE} IQPE-like circuits	1
Oracle+Hadamard	1	$\sim p_G$	1 controlled Oracle \widehat{U}_f	3



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. An approximation of the evolution of $|\psi\rangle$ can be obtained with the Quantum Krylov method.
- Many approaches to performing projection have been presented. The IQPE-like approach presents itself as the best compromise in terms of resources.



Questions ?



Why solve many-body problems using quantum **computers?**

• Resources for the description of the configuration space :

Classical computer \rightarrow exponential scaling. Quantum computer \rightarrow polynomial scaling.

Smith, A., Kim, M.S., Pollmann, F. et al. npj Quantum Inf 5, 106 (2019).

Sam McArdle et al. Rev. Mod. Phys. 92, 015003 (2020).



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

- Various quantum algorithms that have up to an exponential speed-up over their classical counterparts. Montanaro, A. npj Quantum Inf 2, 15023 (2016).
- Dynamical quantum computing ecosystem with real devices available for the public and constantly improving.



Application on real platforms



IBM experience

- Public access to quantum computers
- Superconducting transmon qubits











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

Transpiling

- Basic gates (IBMQ Santiago CX, RZ, SX, X)
- Topology (IBMQ Santiago ••••••)



Written





Generating function on a Quantum Computer

• FakeSantiago.

E. A. Ruiz Guzman and D. Lacroix, arXiv:2104.08181. (2021)

- F(t) without (Blue) and with (Red) error correction.
- Classical (Black). Quantum (Green).



