

Quantum computing description of strongly interacting atomic nuclei: challenges and opportunities

D Lacroix

► To cite this version:

D Lacroix. Quantum computing description of strongly interacting atomic nuclei: challenges and opportunities. Quantum computing for quantum chemistry, Nov 2024, Montpellier, France. hal-04799783

HAL Id: hal-04799783 https://hal.science/hal-04799783v1

Submitted on 23 Nov 2024

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers. L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



Distributed under a Creative Commons Attribution - NonCommercial 4.0 International License



Quantum computing description of strongly interacting atomic nuclei *and neutrinos*: challenges and opportunities

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)





Initial motivations



IN2P3 communication newsletter



Courtesy M. Savage

d



Bau

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

A focus on neutrino oscillation physics simulated on quantum computers







A focus on neutrino oscillation physics simulated



on quantum computers

Illustration of the Hamiltonian (2 flavor approx)

N-1

$$H_{\nu} = \frac{1}{N} \sum_{\substack{i=0\\N-1}} \sin(2\theta_{\nu}) X_{i} - \cos(2\theta_{\nu}) Z_{i}$$
$$H_{\nu\nu} = \sum_{\substack{i$$

- 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





A focus on neutrino oscillation physics simulated

on quantum computers



Illustration of the Hamiltonian (2 flavor approx)

Oscillation H_{ν} =

Coupling

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







or with optimization





A focus on neutrino oscillation physics

Is also pushing the limit of classical simulation













Illustration with small superconductors

Illustration with the Richardson Hamiltonian

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

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

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

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

$$H_{\rm P} = \sum_{i>0} \varepsilon_i (a_i^{\dagger} a_i + a_{\overline{i}}^{\dagger} a_{\overline{i}}) - g \sum_{i,j>0} a_i^{\dagger} a_{\overline{i}}^{\dagger} a_{\overline{j}} a_j$$
Jordan-Wigner transfo: $\frac{1}{2}(I_i - Z_i)$ State ordering is important !

 φ_i

Initial (symmetry breaking) state preparation

$$|\Psi
angle = \exp\left\{-\sum_{i>0} \varphi_i \left(a_i^{\dagger} a_{\overline{i}}^{\dagger} - a_{\overline{i}} a_i\right)\right\} |0
angle$$

Equivalent universal gate on pairs

Pairing Hamiltonian



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



$$a_i^{\dagger} a_{\overline{i}}^{\dagger} \longrightarrow Q_n^+ Q_{n+1}^+$$

$$= \varphi$$

$$|\Psi\rangle = \prod_{n>0} e^{i\varphi(X_n Y_{n+1} + Y_n X_{n+1})/2} |-\rangle$$

Simplified circuit (generalized Bell state)

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

$$R_Y(\varphi)$$



Quantum computing for atomic nuclei

Superfluidity can be described by breaking particle number

BCS circuit

 $e^{-i\theta Y}$

Illustration for small superfluids

Example of mixing for 12 qubits (with qiskit)



Projection on particle number

$$\Psi\rangle = \sum_{N} c_{N} |N\rangle \Rightarrow |N\rangle$$

0/1

n

For 2 qubits

 $\bigotimes_n |0\rangle$

$$\begin{split} |\Psi\rangle &= \alpha |00\rangle + \beta |01\rangle + \gamma |10\rangle + \delta |11\rangle \\ |N &= 0\rangle \qquad \propto |N &= 1\rangle \qquad |N &= 2\rangle \end{split}$$

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



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

The quantum-Phase estimation (QPE) algorithm



qubit. After measurement, I have the projection on the associated particle number component

Eigenvalues-Ground state and excited states

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



H was encoded on the full Fock space with $A < n_q$ For the degenerate case, this should give the exact solution

More on symmetry restoration techniques on quantum computer



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

Exploration of different methods for the symmetry restoration



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



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)



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



Symmetry restoration using Projection operators and Oracles



Methods based on projectors

Oracle + Hadamard test

 $|0\rangle$

 $|\Psi\rangle$

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

H

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

Assume we are able to encode the projector

 \hat{U}_f

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

$$P_{\Omega} \implies U_f = +1P_{\Omega} - 1(1 - P_{\Omega}) = 2P_{\Omega} -$$

Grover technique



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

Symmetry restoration using Projection operators and Oracles



Symmetry restoration by quantum tomography

Classical shadow technique





E.A. Ruiz Guzman and D. Lacroix, EPJA 60 (2024)

Coming back to our superconducting problem



Is the breaking of symmetries always a good idea?



But nuclei have both spin (s) and isospin (t) (neutron/proton)



This increases the number of qubits $S_z,\ S^2,\ \pi$

$$S_z, S^2, T_z, T^2, \pi$$

Symmetry-breaking states become extremely hard to control Symmetry restoration becomes very demanding

J. Zhang, PhD thesis (2025).

Use of adaptative methods

And try to control symmetry breaking

Iterative construction of the ansatz

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

$$\Rightarrow$$
 Start from a state $|\Psi_0
angle=|n=0
angle$

Built iteratively the ansatz such as:

$$|n
angle = e^{i heta_n A_n} |n-1
angle = \prod_{k=1}^n e^{i heta_k A_k} |0
angle$$

Such that $A_n \in \{O_1, \cdots, O_\Omega\}$

S



ADAPT-VQE applied to the Superfluid problems: only spins





Extension to spin and isospin



Is breaking symmetries always a good idea?

Extension to the proton-neutron pairing Hamiltonian problem

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

Different Hamiltonian limit

S_z/T_z	Isoscalar			Isovector		
Case	-1	0	1	-1	0	1
1				\checkmark		\checkmark
2		\checkmark			\checkmark	
3				\checkmark	\checkmark	\checkmark
4	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark

Different operator pool in ADAPT-VQE breaking or not symmetries

	Particle number	Seniority	Parity
H-pool	\checkmark	\checkmark	\checkmark
QEB-pool	\checkmark	×	\checkmark
Qubit-pool	×	×	\checkmark



J. Zhang, DL, and Y. Beaujeault-Taudière, arXiv:2408.17294

Is breaking symmetries always a good idea?

Extension to the proton-neutron pairing Hamiltonian problem

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

Different Hamiltonian limit

S_z/T_z	Isoscalar			Isovector		
Case	-1	0	1	-1	0	1
1				\checkmark		\checkmark
2		\checkmark			\checkmark	
3				\checkmark	\checkmark	\checkmark
4	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark

Different operator pool in ADAPT-VQE breaking or not symmetries

	Particle number	Seniority	Parity
H-pool	\checkmark	\checkmark	\checkmark
QEB-pool	\checkmark	×	\checkmark
$\operatorname{Qubit-pool}$	×	×	\checkmark



J. Zhang, DL, and Y. Beaujeault-Taudière, arXiv:2408.17294

What about excited states?



(SR) state (multi-reference)

١	$ \bullet E $			Spectral methods
1	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		Today's challenges: -Identify pilot applications, -Reduce the Quantum resou- -Develop novel quantum algorithm -1 1	Getting excited states urces gorithms $\sigma = +1$ $\sigma = -1$
	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	J,M angle o [M] angle
	q = 2N		q = N	Use first quantization
		ſ	$X_{\alpha} = 1_{\alpha}\rangle \langle 0_{\alpha} + 0_{\alpha}\rangle \langle 1_{\alpha} ,$ $Y_{\alpha} = i 1_{\alpha}\rangle \langle 0_{\alpha} - i 0_{\alpha}\rangle \langle 1_{\alpha} ,$	$q = \lceil \log_2 N \rceil$
		Ì	$egin{aligned} &I_{lpha} = \imath_{ 1_{lpha}\rangle\langle 0_{lpha} } - \imath_{ 0_{lpha}\rangle\langle 1_{lpha} }, \ &Z_{lpha} = 0_{lpha} angle\langle 0_{lpha} - 1_{lpha} angle\langle 1_{lpha} \end{aligned}$	
	Н	$\overline{\varepsilon} = \frac{\varepsilon}{2} \sum_{\alpha}^{2}$	$\sum_{m=1}^{N} Z_{lpha} + rac{V}{4} \sum_{lpha eq eta}^{N} (X_{lpha} X_{eta} - Y_{lpha} Y_{eta}),$	



J. Romero et al, PRC 105 (2022)

Solving the Lipkin model with using 2 qubits only with hybrid quantum-classical method



Y. Beaujeault-Taudière and DL, PRC 109, 024327 (2024)



The main goal was to find pilot applications for Quantum Computing where Qc can be disruptive compared to CC

We first focused on the problem of Many-body / symmetries (that could be useful beyond many-body problems) - and developed various Techniques (QPE, Oracle, Shadow, Hilbert Space expansion, ... mostly post NISQ techniques)



We are now gaining expertise on algorithmic, noise, ...



Our current interest are: variational ansatz and expressivity, equilibrium and non-equilibrium properties, entanglement growth, ...

