Quantum computing description of atomic nuclei: challenges and opportunities

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A short highlight of today’s nuclear physics challenges

From QCD to atomic nuclei phenomena
A short highlight of today’s nuclear physics challenges

Some phenomenology

Strongly interacting fermions

Quantum self-bound Fermi droplets

to atomic nuclei phenomena
A short highlight of today’s nuclear physics challenges

Actual tendency: Towards Full Configuration-Interaction (ab-initio) description?

Strongly interacting fermions

- Start from the full Hamiltonian
- Obtain the energy spectra

Challenges

- The interaction is highly non-perturbative
- Starting from 2005: new generations of interactions were developed getting rid of the short-range part

Still the strong interaction is rather elusive: emergence of 3-body (and more generally multi-body) interaction

So far, we can assume that we have a starting Hamiltonian

\[ H = H_{1\text{-body}} + H_{2\text{-body}} + \cdots \]
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Actual tendency: Towards Full configuration-Interaction description?

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

Atomic nuclei are mesoscopic systems (particle Number ranges from 2 to 300+). When mass increases we have an exponential growth of the Hilbert space.

In \textit{pf} shell:
- $^{56}\text{Ni}$: 1,087,455,228
- $^{78}\text{Ni}$: 210,046,691,518

In \textit{pf-sdg} space:
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Actual tendency: Towards Full configuration-Interaction description?

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

Nuclei are small superfluid systems

Current status

A specificity: atomic nuclei like to break spontaneously symmetries

Symmetry Restored (SR) state (multi-reference)

Described by breaking U(1) symmetry

Symmetry Preserving HF state

Symmetry Breaking (SB) state

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

Nuclei do present rotational bands

Nuclei might be deformed

(How) Can Quantum computers help?
What we have started to do

Further Quantum or hybrid Quantum-Classical Post-processing

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, ...)

Symmetry Restored (SR) state (multi-reference)

Symmetry Breaking (SB) state
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

\[ |\Phi_0\rangle = \prod_i (u_i + v_i a_i^\dagger a_i^\dagger) |\rangle \]

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

\[ H_P = \sum_{i>0} \varepsilon_i (a_i^\dagger a_i + a_i^\dagger a_i^\dagger) - g \sum_{i,j>0} a_i^\dagger a_j^\dagger a_j a_i \]

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

State ordering is important!

Initial (symmetry breaking) state preparation

\[ |\Psi\rangle = \exp \left\{ - \sum_{i>0} \varphi_i \left( a_i^\dagger a_i^\dagger - a_i a_i^\dagger \right) \right\} |0\rangle \]

Equivalent universal gate on pairs

\[ e^{-i\theta (XY + YX)/2} = e^{-i\theta Y} \]


States labels \( i \quad \bar{i} \quad \ldots \)

Qubits labels \( 0 \quad 1 \quad 2 \quad \ldots \quad n \quad n+1 \)

\[ a_i^\dagger a_i^\dagger \rightarrow Q_n^+ Q_{n+1}^+ \]

Simplified circuit (generalized Bell state)

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

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

All calculations here are done with IBM qiskit toolkit.
Restoration of particle number symmetry

The counting statistics problem

Example of mixing for 12 qubits (with qiskit)

Direct estimate of Counting statistics

Projection on particle number

\[ |\Psi\rangle = \sum_{N} c_N |N\rangle \rightarrow |N\rangle \]

For 2 qubits

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

\[ |N = 0\rangle \quad \propto |N = 1\rangle \quad |N = 2\rangle \]

A possible way to perform the projection is to use
The Quantum-Phase-Estimation method with \(N\) itself

The quantum-Phase estimation (QPE) algorithm

For known eigenvalue problems

Assume a unitary operator \( U \)

Assume an eigenstate \( |\Psi\rangle \) Such that \( U |\Psi\rangle = e^{2\pi i \varphi} |\Psi\rangle \)

\[ \begin{align*}
|0\rangle &\quad H \quad \times e^{8\pi i \varphi} \\
|0\rangle &\quad H \quad \times e^{4\pi i \varphi} \\
|0\rangle &\quad H \quad \times e^{2\pi i \varphi} \\
|\Psi\rangle &\quad n=3 \quad U U^2 U^4 \quad |\Psi\rangle
\end{align*} \]

\[ \begin{align*}
&\frac{1}{\sqrt{2}} (|0\rangle + e^{2\pi i \varphi} |1\rangle) \\
&\frac{1}{\sqrt{2}} (|0\rangle + e^{2\pi i 2\varphi} |1\rangle) \\
&\frac{1}{\sqrt{2}} (|0\rangle + e^{2\pi i 4\varphi} |1\rangle)
\end{align*} \]

QFT\(^{-1} \quad 2^{n_r} \varphi \quad \bigotimes \quad |\Psi\rangle

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
QPE applied to the number of persons

Practical details

\[ U_N = \prod_j U_j \]
\[ U_i = |0_i\rangle\langle 0_i| + \exp(i\pi/2^{n_0-1})|1_i\rangle\langle 1_i| \]
\[ U_i = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/2^{n_0-1}} \end{bmatrix} \]

Example: Qubit counting statistics

Initial state

\[ |0_j\rangle \otimes n_q \rightarrow R_Y(\varphi) \otimes [\cos(\varphi/2)|0_j\rangle + \sin(\varphi/2)|1_j\rangle] \]

\[ P(A) = C_{n_q}^A p^A (1 - p)^{n_q-A} \]

\[ p = \sin^2(\varphi/2) \]

\[ \varphi = \frac{\pi}{4} \]
\[ \varphi = \frac{\pi}{2} \]
\[ \varphi = \frac{3\pi}{4} \]

\[ 6/2^4 = 1/2 + 1/4 + 0/8 \equiv [110] \]
Eigenvalues-Ground state and excited states

\[ \bigotimes_{n_r} |0\rangle \xrightarrow{H \otimes n_r} \sum_{n_q} \alpha_k |\phi_k\rangle \xrightarrow{QPE[U_S]} \xrightarrow{QFT^{-1}} \lambda_k |\phi_k\rangle \]

Initial configuration with symmetry breaking state
Symmetry operator eigenvalues encoding
In the register qubits
Symmetry restoration through measurement

**Measurement**

**Example of an event:**

\[ |011 \cdots 010\rangle^{(\lambda)} \otimes |\phi_A^{(\lambda)}\rangle = A^{(\lambda)} \]

**Degenerate case**

For the degenerate case, this should give the exact solution

\[ H = -g \sum_{i,j>0} a_i^\dagger a_i^\dagger a_j a_j \]

\[ \langle \phi_A^{(\lambda)} \big| H \big| \phi_A^{(\lambda)} \rangle \]

**BCS/HFB state**

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

**Projected BCS or with varying number Of particles**

**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 $n_q$ qubits
- Assume that $S$ has discrete eigenvalues $\{\lambda_0 \leq \cdots \leq \lambda_M\}$ with $\lambda_k = am_k$
- Define the operator
  \[
  U_S = \exp \left\{ 2\pi i \left[ \frac{S - \gamma_0}{a2^{n_0}} \right] \right\}
  \]
- Eigenvalues of $U_S$ are given by $e^{2\pi i \theta_k}$ with $\theta_k = (m_k - m_0) / 2^{n_0}$

If $(m_k - m_0) < 2^{n_0}$ then $\theta_k < 1$ and $\theta_k$ 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
- $J_z = \hbar m$
- $J^2 = \hbar^2 j(j + 1)$

Projection on total spin

Projection on $S^2$ and $S_z$ components

$$|\Psi\rangle = \sum_{s_i \in \{0,1\}} \Psi_{s_1, \ldots, s_N} |s_1, \ldots, s_n\rangle.$$  

Illustration

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

The full basis can eventually be constructed

P. Siwach and DL, arXiv:2106.10867
Coming back to our superconducting problem

Combining projection with variational method

### Possible optimization schemes

**Variational**

Symmetry-Breaking ansatz

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

**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

**Pair occupation are now encoded**

\[ E_{\text{SB+projection}} \]

\[ E_{\text{SB state}} \]

\[ E_{\text{GS}} \]

8 particles on 8 equidistant levels

**Percentage of error**

- Exact
- BCS
- Q-PAV
- Q-VAP
Post-processing of projected states

Complete strategy

- Initial state preparation (HF, BCS, P-VAP, Q-VAP)
- Purely quantum method: Quantum Phase Estimation
- Hybrid Quantum-Classical Quantum Krylov method

Diagram:

1. Symmetry Breaking (SB) state
2. Symmetry Restored (SR) state (multi-reference)
3. Symmetry operator eigenvalues encoding in the register qubits

Mathematical expression:

\[ \sum \alpha_k |\phi_k\rangle \]

with prob. \( |\alpha_k|^2 \)
Illustration of the QPE method with projected state

Initial state preparation

$|0\rangle \rightarrow H^{\otimes n_r}QPE[U_S] \rightarrow |\phi_k\rangle$

Some technical details

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

For the propagator, we used the Trotter-Suzuki method

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

$U(\tau) = \prod U(\Delta\tau) \rightarrow \prod U_{\varepsilon}(\Delta\tau)U_g(\Delta\tau)$

$H_P = \sum_{i>0} \varepsilon_i (a_i^\dagger a_i + a_i^{\dagger\dagger} a_i) - g \sum_{i,j>0} a_i^\dagger a_i^{\dagger\dagger} a_j a_j$

$\prod_p \begin{pmatrix} 1 & 0 \\ 0 & \exp(-2i\varepsilon_p \Delta t) \end{pmatrix}$

$\prod_{p>q} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\lambda_{pq}) & i \sin(\lambda_{pq}) & 0 \\ 0 & i \sin(\lambda_{pq}) & \cos(\lambda_{pq}) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$

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

$R_X(-2\lambda)$

$R(\varphi_p)$
Illustration of the QPE method with projected state
Krylov Based methods

Hilbert space

Important 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

\[ O_{ij} = \langle \Phi_i | \Phi_j \rangle \quad H_{ij} = \langle \Phi_i | H | \Phi_j \rangle \]

Generalized eigenvalue problem

\[ |\xi_\alpha\rangle = \sum_n c_n(\alpha) |\Psi_n\rangle \quad \sum_n c_n(\alpha) H_{in} = E_\alpha \sum_n c_n(\alpha) O_{in} \]

Our first attempt: use the generating function of H

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

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

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

Quantum Krylov method

Highly Truncated Hilbert space

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

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

\[
O_{ij} = \langle \Phi_i | \Phi_j \rangle = \langle \Psi | e^{-i(\tau_j - \tau_i) H} | \Psi \rangle \quad H_{ij} = \langle \Psi | H e^{-i(\tau_j - \tau_i) H} | \Psi \rangle
\]

Initial state preparation

\[
\sum \alpha_k |\phi_k\rangle
\]

Hadamard test for the real part of \(O\) and \(H\)

\[
|0\rangle \rightarrow H \rightarrow \lambda_k \rightarrow 0/1
\]

Modified Hadamard test for the imaginary part

\[
|0\rangle \rightarrow H \rightarrow R(\pi/2) \rightarrow \lambda_k \rightarrow 0/1
\]

Diagonalization on a classical computer
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

\[ \tau_{\text{QPE}} + 2\tau_{\text{QPE}} + \cdots + 2^{n_q-1}\tau_{\text{QPE}} \]

\[ \tau_{\text{tot}}(n_q) = (2^{n_q} - 1) \tau_{\text{QPE}} \]
Some summary and prospects

We are starting to explore many-body techniques for quantum computing

We made a focus on symmetry-breaking and symmetry restoration

Interesting results on Q-VAP + CI techniques

E. A. Ruiz Guzman and DL, in preparation

Ongoing/starting projects

More Systematic exploration of quantum ansatz

Atomic nuclei on lattices

Quantum Machine Learning

J. Zhang thesis

Y. Beaujeault-Taudiere (postdoc)
Few initiated applications in the world in the two infinities field

**Lattice gauge theories**

Zohar, Kolck, Savage, ...

**N-body problem**

**N-body nuclear systems**

Dumitrescu, Hagen, Carlson, Papenbrock...

**Dynamics: e, ν scattering**

Roggero, Carlson, ...

**Applications to data mining (event classification)**

**Dark matter**

Mocz, Szasz

**CMS-detector (with LLR)**

QC2I is a computing project supported by IN2P3, the French national nuclear and particle physics institute. Its goal is to explore the possible applications of the emerging quantum computing technologies to particles and nuclear physics problems as well as astrophysics. The main tasks are:

- to identify, within IN2P3, scientists/engineers/technicians who are interested in using quantum technologies,
- to facilitate the access and training on quantum computers,
- to identify milestones applications for nuclear/particle physics and astrophysics,
- to design dedicated algorithms and proof of principle applications.

The project action has three main directions: Prepare the Quantum Computing Revolution (PQCR), Quantum Machine Learning (QML), Complex Quantum Systems Simulation (CQSS)
Thank You