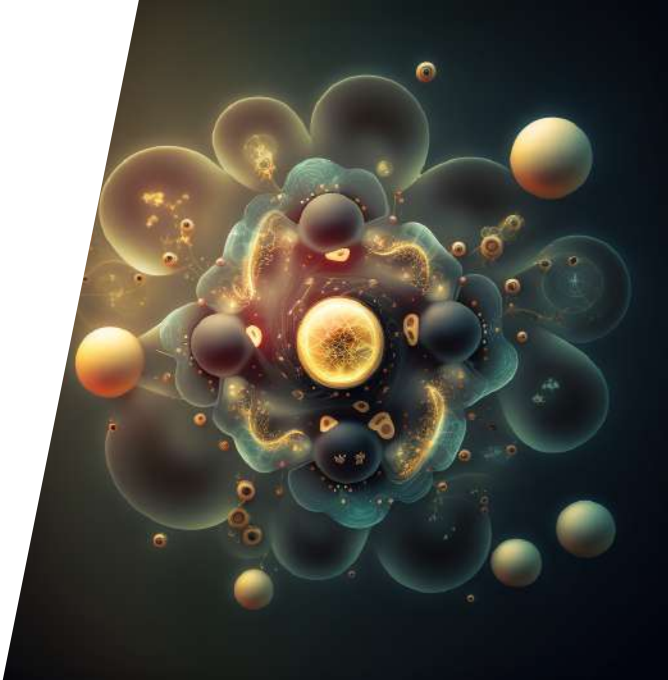
APPLICATION OF HYBRID QUANTUM-CLASSICAL COMPUTING ALGORITHMS FOR QUANTUM SIMULATION OF NUCLEAR PHYSICS PROCESSES

Luca Nigro (Università degli Studi di Milano)

Enrico Prati (Università degli Studi di Milano)



the Quantum Intelligence Lab - Milan

Università Statale Milano

Istituto di Fotonica e Nanotecnnologie

Politecnico Milano

CNR-IFN Milano

Quantum Team

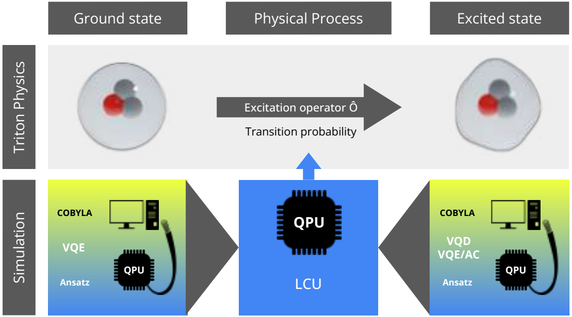
- Enrico Prati (Head, UNIMI)
- Paolo Zentilini (UNIMI)
- Luca Nigro (UNIMI)
- Francesco Monzani (UNIMI)
- Lorenzo Moro (POLIMI)
- Gabriele Agliardi (IBM POLIMI)
- Sebastiano Corli (POLIMI)
- Marco Maronese (UNIBO IIT)
- Lorenzo Rocutto (UNIBO)
- Andrea Zanetti (POLIMI)
- Davide Noè (Tohoku University)
- Matteo Di Giancamillo (POLIMI)
- Manuel Peracci (POLIMI)
- Rebecca Casati (UNIMI)
- Stefano Bruni (POLIMI)

The problem

There are problems that are too harsh to tackle with an analytical approach. An example would be determining the quantum state of a composite physical system.

No one has presented a pipeline that exploits a quantum computer in order to simulate a transition between quantum states.

The solution: a hybrid quantum-classical pipeline



- **VQE:** Variational Quantum Eigensolver
- **VQD:** Variational Quantum Deflation
- **VQE/AC:** Variational Quantum Eigensolver with Automatically-adjusted Constraints
- **LCU:** Linear Combination of Unitaries

Index

- Previous work
- My work
- Results
- Conclusion

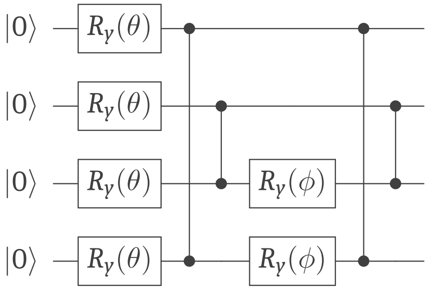
Quantum computing for neutrino-nucleus scattering

A. Roggero, Phys. Rev. D (2020).

Second Quantization Hamiltonian

$$H = 8t + \frac{U}{2} - 2t\sum_{k=1}^{4} X_k - \frac{U}{4}\left[Z_1 Z_4 + Z_2 Z_3\right] - \frac{U}{4}\sum_{j<k<l} Z_j Z_k Z_l$$

Ansatz



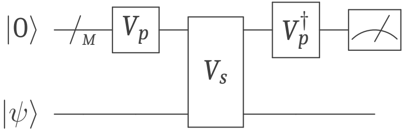
Demonstration that a quantum computer can determine the ground state of the triton. Require starting from a **spin-isospin Hamiltonian** mapped into a quantum circuit, and then minimized with Variational Quantum Eigensolver (VQE).

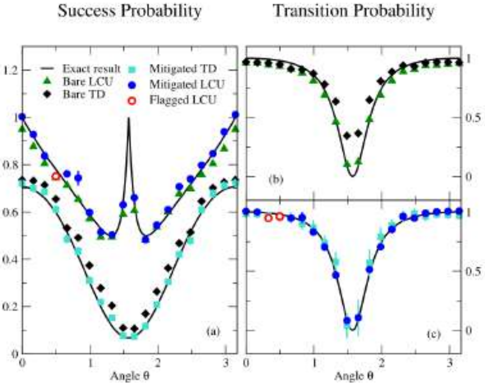
Preparation of excited states for nuclear dynamics

A. Roggero, Phys. Rev. C (2020).

LCU (Linear Combination of Unitaries) method allows embedding a weighted sum of unitary operators in a unitary gate.

$$\widehat{O}(\vartheta) = \alpha(\vartheta)\mathbb{I} + \beta(\vartheta)X + \gamma(\vartheta)Z$$

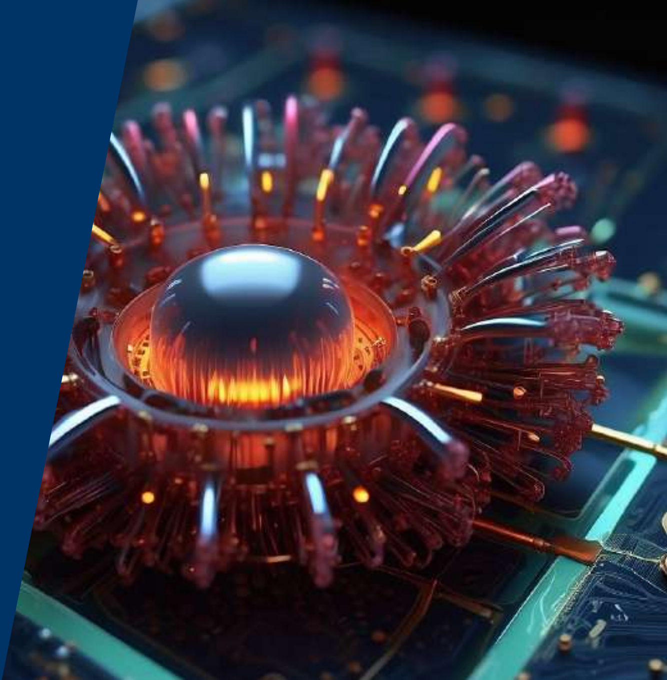




Evaluation of magnetic dipole transition probability for $p(n,\gamma)d$ reaction by using LCU method.

Index

- Previous work
- My work
- Results
- Conclusion



Mapping to qubit

Under S-wave approximation, each nucleon has a spin-isospin state $|t\ s\rangle$ that has to be mapped into qubits state.

$$|n\downarrow\rangle = |00\rangle \qquad |p\downarrow\rangle = |10\rangle$$

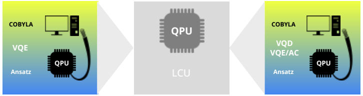
$$|n\uparrow\rangle = |01\rangle \qquad |p\uparrow\rangle = |11\rangle$$

One nucleon is set to be static in the state $|n\downarrow\rangle$, so we need 4 qubits.

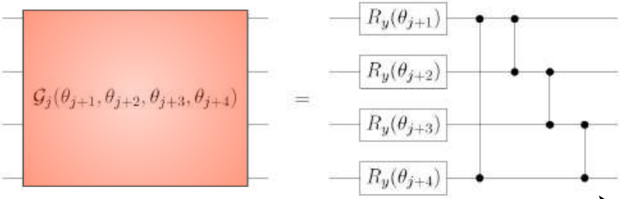
The ground state $|g\rangle$ and the excited state $|e\rangle$ in second quantization are mapped into

$$|g\rangle = |01\rangle \qquad |e\rangle = |10\rangle$$

Ansatz parametrization

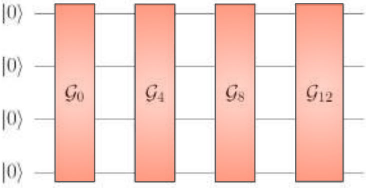


Single block



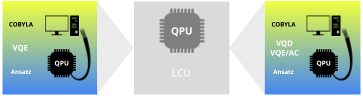
Circular scheme of entanglement

Full ansatz



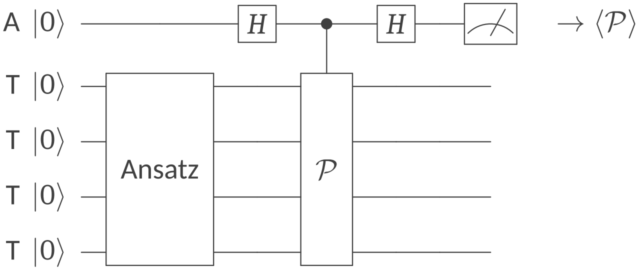
16 parameters in total

VQE circuit to perform minimization of a multi-qubit Pauli operator $\mathcal{P}$

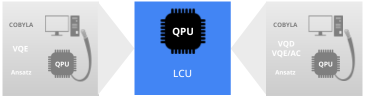


$$H = \sum_i \mathcal{P}_i \quad \Rightarrow \quad \langle H \rangle = \sum_i \langle \mathcal{P}_i \rangle$$

- Minimum energy
  $\rightarrow$ ground state
  $\Rightarrow \quad \theta_g^{\text{opt}}$
- Minimum energy + constraints
  $\rightarrow$ 1^{st} excited
  $\Rightarrow \quad \theta_e^{\text{opt}}$



LCU circuit

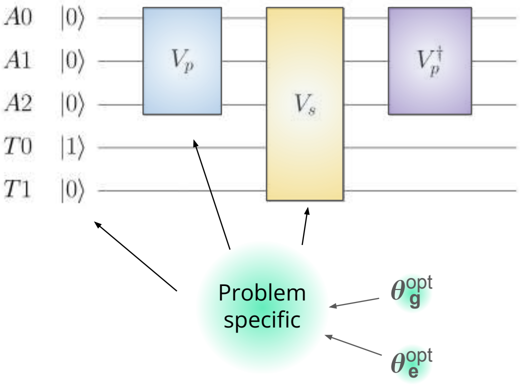


$$O = \alpha + \frac{\gamma}{2}(Z_0 - Z_1) + \frac{\beta}{2}(X_0X_1 + Y_0Y_1)$$

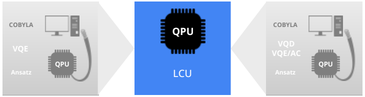
$$= \begin{pmatrix} \alpha & 0 & 0 & 0 \\ 0 & \alpha+\gamma & \beta & 0 \\ 0 & \beta & \alpha-\gamma & 0 \\ 0 & 0 & 0 & \alpha \end{pmatrix}$$

α, β and γ are determined by θ_g^{opt} and θ_e^{opt}. They are also functions of the dipole polarization angle ϑ.

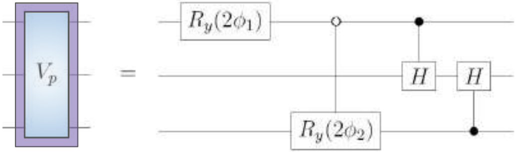
Linear combination of unitaries



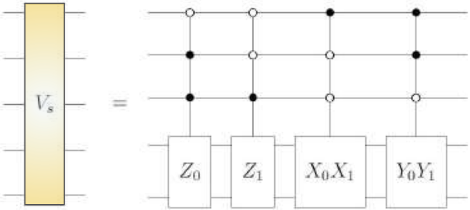
LCU unitaries



Prepare unitary



Select unitary

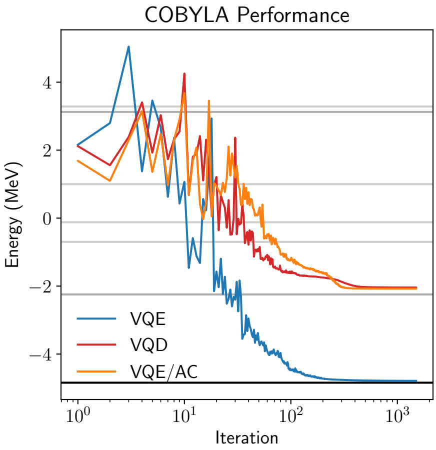


The angles ϕ_1 and ϕ_2 are determined by θ_g^{opt} and θ_e^{opt}.

They are also functions of the dipole polarization angle ϑ.

Index

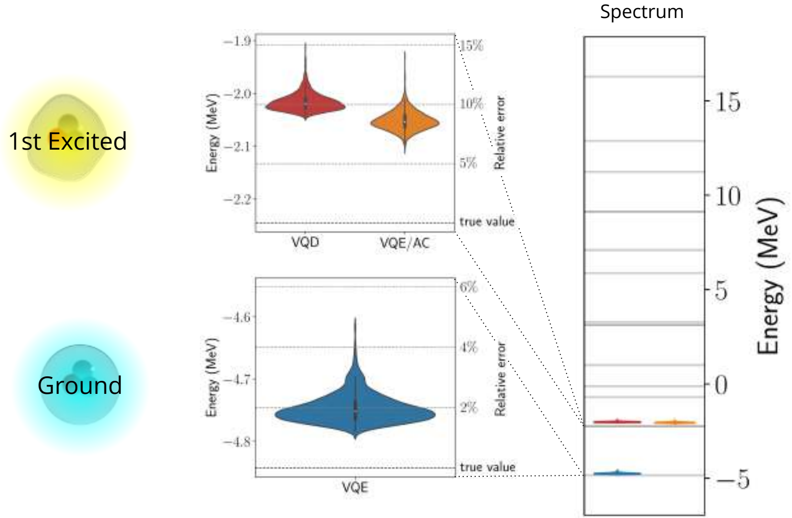
Both VQD and VQE/AC algorithms perform similarly



COBYLA: Constrained Optimization BY Linear Approximation

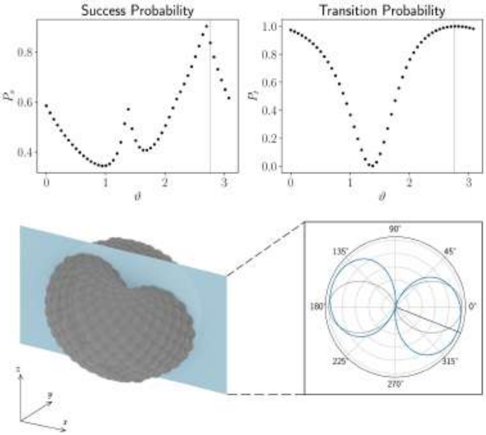
- constrained problems
- no derivative
- linear programming approximation

Low relative error for the energy expectation value



Success and transition probability

The algorithm is successful if and only if the ancilla register is measured in the state $|000\rangle$.



- Previous work
- My work
- Results
- **Conclusion**

Conclusions & Outlook

- Relative error below 2% for the ground state energy, and below 10% for the first excited state energy;
- the LCU method for triton excitation has a success probability in the range $[0.3, 0.9]$;
- this pipeline is valid for any similar transition (molecules, nucleons, quarks...);
- other reactions simulated: $d(p,\gamma)^3$He and $d(n,\gamma)t$;
- limitations due to current quantum hardware;
- next step: add orbital angular momentum.

Thank you for listening!

Magnetic dipole moment

$$\mathbf{m} = \mu_N \left[g_p (\mathbf{S}_p^1 + \mathbf{S}_p^2) + g_n (\mathbf{S}_n^1 + \mathbf{S}_n^2) \right] + \mu_N g_n \frac{1}{2} \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix}$$

$$\mathbf{m} \cdot \xi = m_x \cos\vartheta + m_z \sin\vartheta$$ ξ polarization vector

$$O = \begin{pmatrix} \langle g| \mathbf{m} \cdot \xi |g\rangle & \langle g| \mathbf{m} \cdot \xi |e\rangle \\ \langle e| \mathbf{m} \cdot \xi |g\rangle & \langle e| \mathbf{m} \cdot \xi |e\rangle \end{pmatrix} = \begin{pmatrix} \alpha + \gamma & \beta \\ \beta & \alpha - \gamma \end{pmatrix}$$

NOTE: $\mathbf{m} \cdot \xi(\vartheta)$ and the states $|g\rangle$, $|e\rangle$ are obtained with θ^{opt}.