Quantum simulation of lepton-nuclei scattering

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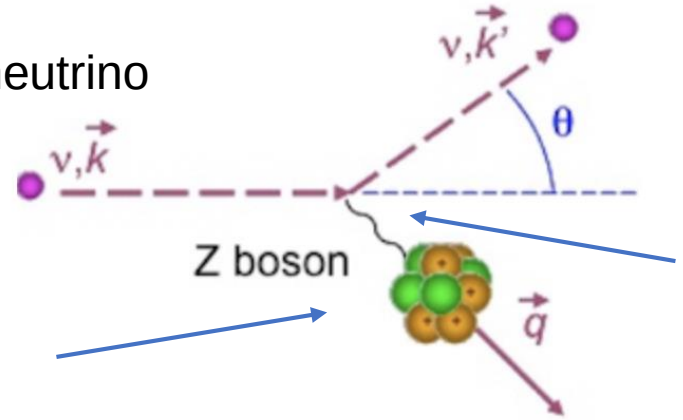
Oriel Kiss, Michele Grossi, Sofia Vallecorsa,
Federico Sanchez and Thomas Papenbrock

Motivation and Overview:

- Quantum many-body systems are challenging for classical computers due to the exponential scaling of the Hilbert space.
- We propose to use quantum devices to simulate scattering experiments by computing two points response functions.

Incoming neutrino



momentum transfer described by H_I (external probing).

Nuclei described by H_0.
Starts in its ground state.

Ground state preparation
with the Variational Quantum Eigensolver (VQE)

Variational principle:

$$E_0 \leq \frac{\langle \psi(\theta)| H |\psi(\theta)\rangle}{\langle \psi(\theta)|\psi(\theta)\rangle}.$$

We are looking for a state which minimize the expectation value of H_0.

6Li nuclei with an 4He inert core (12 orbitals in the shell model):

$$H = \sum_i \epsilon_i \hat{a}_i^\dagger \hat{a}_i + \frac{1}{2} \sum_{ijkl} V_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l,$$

Unitary Coupled Clusters (UCC) ansatz

$$|\psi(\boldsymbol{\theta})\rangle = e^{i(\hat{T}(\boldsymbol{\theta}) - \hat{T}^\dagger(\boldsymbol{\theta}))} |\psi_0\rangle.$$

Hartree Fock solution

$$\hat{T} = \hat{T}_1 + \hat{T}_2 + \dots$$

Cluster operators

$$\hat{T}_1 = \sum_{i \in \text{virt}; \alpha \in \text{occ}} \theta_i^\alpha \hat{a}_i^\dagger \hat{a}_\alpha$$

Single fermionic excitation terms

$$\hat{T}_2 = \sum_{i,j \in \text{virt}; \alpha,\beta \in \text{occ}} \theta_{ij}^{\alpha\beta} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_\alpha \hat{a}_\beta.$$

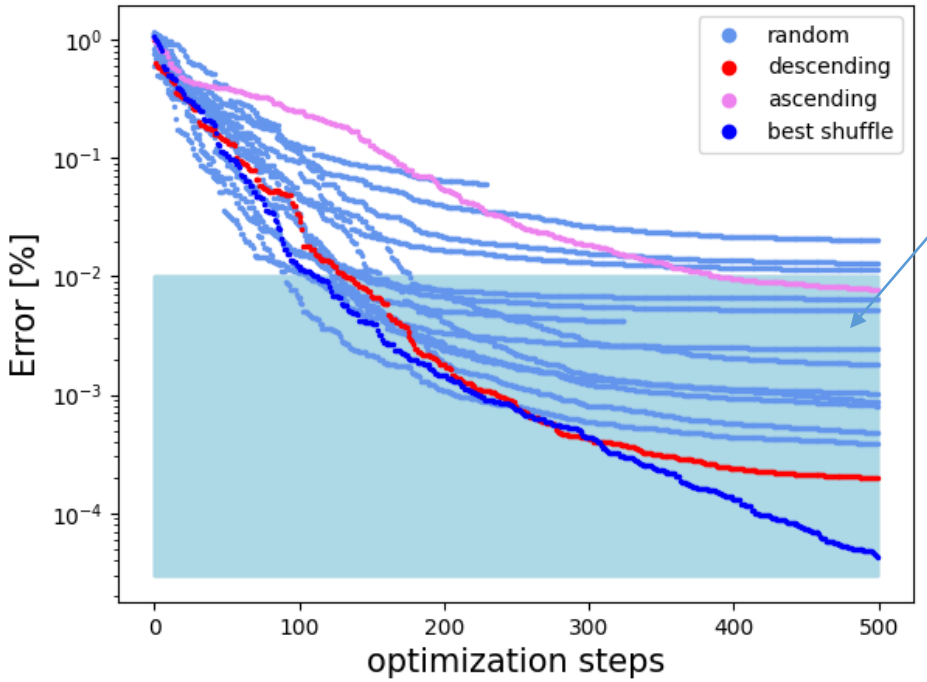
Double fermionic excitation terms

Comparison of different ansatz

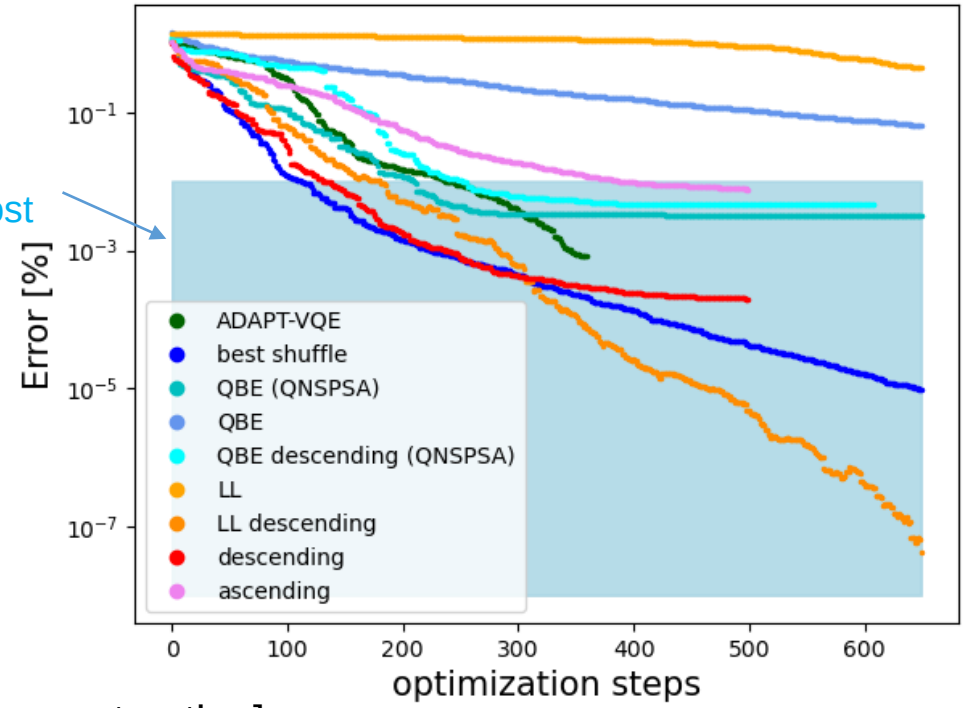
The effect of shuffling the fermionic excitations operators. We should order them in descending order of magnitude (of the corresponding term in the hamiltoninan).

The quantum circuits are simulated on the QTI nodes.

Best approach: train the ansatz recursvily in descending order. Qubit Based Excitation UCC: adapted to NISQ devices



1% barrier needed for most applications



[Paper currently under construction]

Theoretical Framework

Scalable model for a nuclei

Pionless EFT on a lattice with M sites and A nucleons from N_f different species (spin = +/- 1, isospin = +/- 1).

$$H = -t \sum_{f=1}^{N_f} \sum_{\langle i,j \rangle} c_{i,f}^{\dagger} c_{j,f} + 2dtA$$

Kinetic energy (hopping)

$$+ U \sum_{i=1} \sum_{f<f'}^{N_f} n_{i,f} n_{i,f'} + V \sum_{f<f'<f''}^{N_f} \sum_{i=1} n_{i,f} n_{i,f'} n_{i,f''}$$

Two and three body on-site interaction

$$+ U \sum_{f=1}^{N_f} n_{1,f} + V \sum_{f<f'}^{N_f} n_{1,f} n_{1,f'}$$

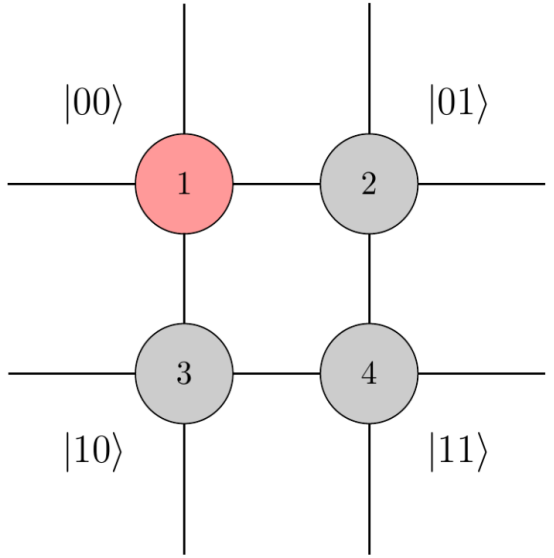
Potential of a frozen nucleon

External linear probing

$$H_I(\mathbf{q}_k) = \sum_{f=1}^{N_f} \rho_f(\mathbf{q}_i) = \sum_{f=1}^{N_f} e_f \sum_i e^{i\mathbf{q}_k \cdot \mathbf{r}_i} n_{i,f} \,,$$

Mapping to qubits

First quantisation needs $\log_2(M)N_f$ qubits.



Second quantisation (via Jordan-Wigner):
More natural but needs MN_f qubits.

Transition probability

Fermi Golden rule

$$S(\omega, \mathbf{q}_k) = \sum_n |\langle \Psi_0 | H_I(\mathbf{q}_k) | n \rangle|^2 \, \delta(E_n + \omega - E_0) \,,$$

From frequency to time domain…

$$\begin{aligned} S(\omega, \mathbf{q}_k) &= \int_{-\infty}^{\infty} \frac{d\tau}{2\pi} e^{i\omega\tau} \langle \Psi_0 | H_I(\tau, \mathbf{q}_k) H_I(\mathbf{q}_k) | \Psi_0 \rangle \\ &= \int_{-\infty}^{\infty} \frac{d\tau}{2\pi} e^{i\omega\tau} C(\tau, \mathbf{q}_k) \,, \end{aligned}$$

The two point correlation function

$$\begin{aligned} C(\tau, \mathbf{q}_k) &= \langle \Psi_0 | U^\dagger(\tau) H_I(\mathbf{q}_k) U(\tau) H_I(\mathbf{q}_k) | \Psi_0 \rangle \\ &= \langle U^\dagger(\tau) H_I(\mathbf{q}_k) U(\tau) H_I(\mathbf{q}_k) \rangle \,, \end{aligned}$$

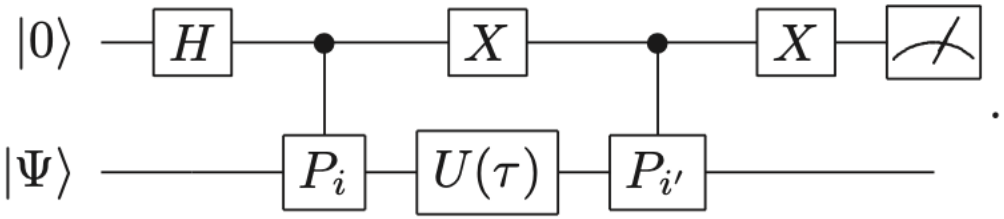
will be estimated on a quantum computer.

Write H_I in the Pauli basis: $H_I(\mathbf{q}_k) = \sum_{i=1}^{L} \alpha_i(\mathbf{q}_k) P_i \,,$

The two point correlation function can be expended as

$$C(\tau, \mathbf{q}_k) = \sum_{i,i'=1}^{L} \alpha_{i'}(\mathbf{q}_k) \alpha_i(\mathbf{q}_k) s_{i',i}(\tau) \,,$$

Where the matrix elements can be estimated via a Hilbert test,

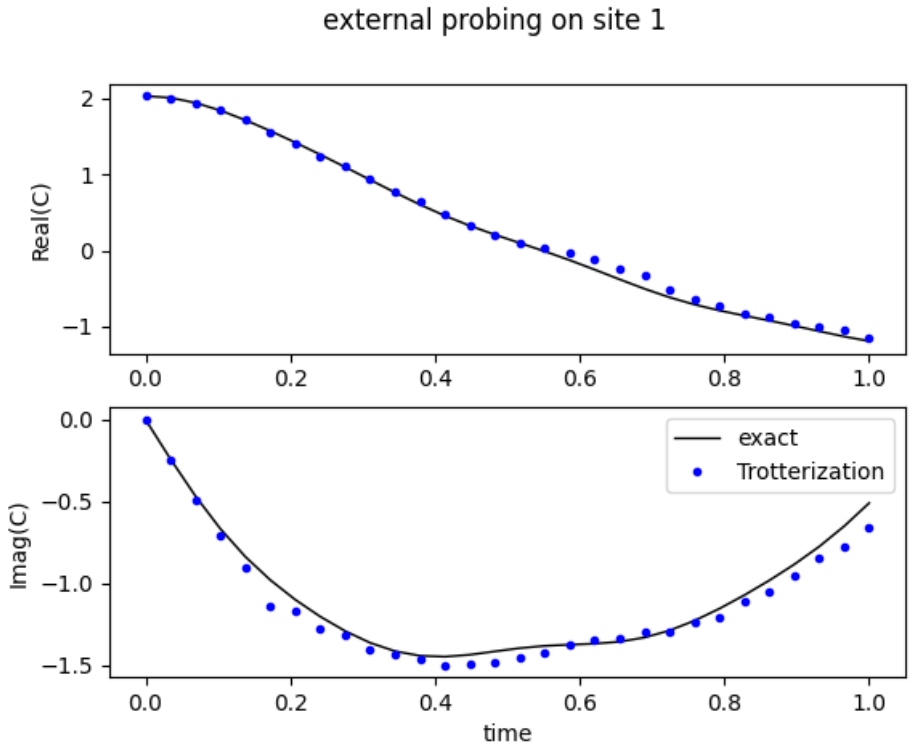


with

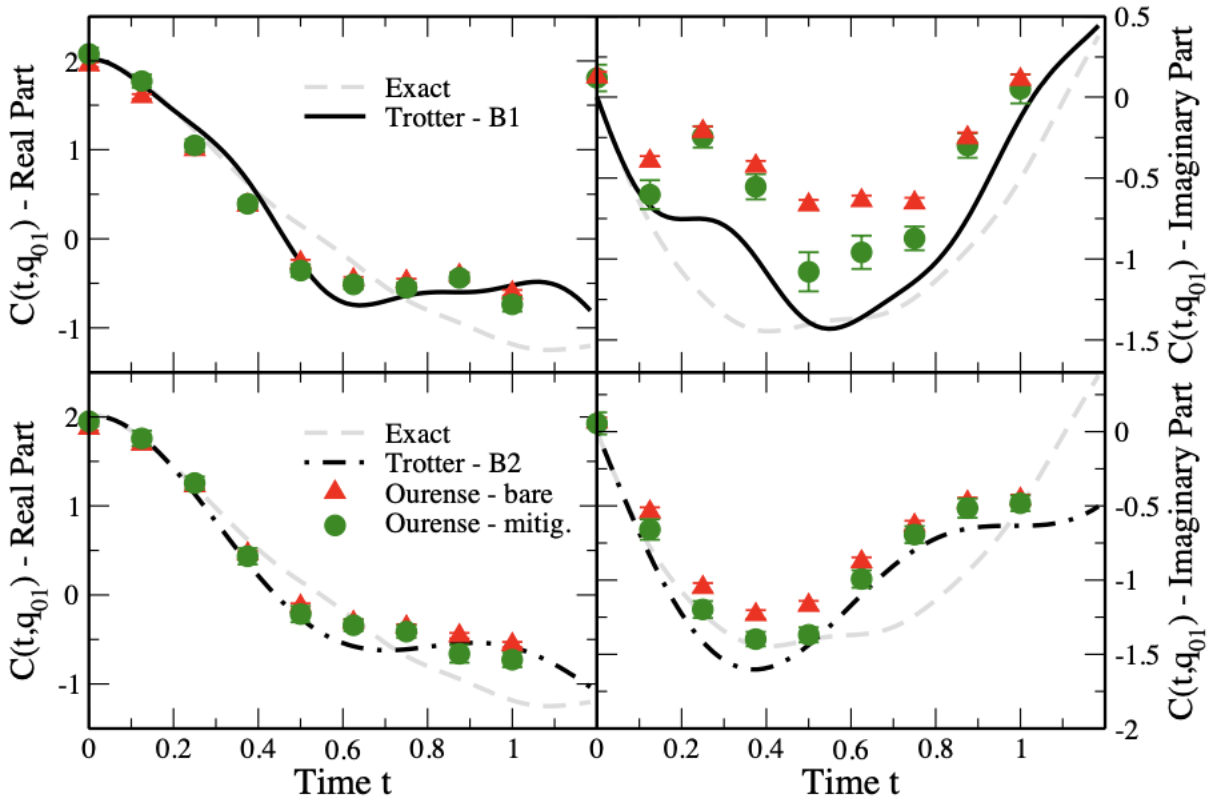
$$\langle X \rangle = \mathcal{R}e\left(s_{i'i}(\tau)\right) \,, \quad \langle Y \rangle = -\mathcal{I}m\left(s_{i'i}(\tau)\right) \,,$$

Results on a (2x2) lattice

with $\left\lfloor \frac{t}{10} \right\rfloor$ Trotter steps on qasm simulator



With 1 Trotter step on quantum hardware (ibmq_ourense), from *Nuclear two point correlation functions on a quantum computer,* Roggero et al.



Conclusions and Future Work

1. We have a framework to extract physical insights about scattering experiments using time evolution on quantum devices.
2. Replace Trotterization with variational and stochastic techniques.
3. Use quantum machine learning (on quantum data) to discriminate between different phases.

Thanks for your attention!
Questions?

oriel.kiss@cern.ch
sofia.vallecorsa@cern.ch

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