



Linear Response on a Quantum Computer

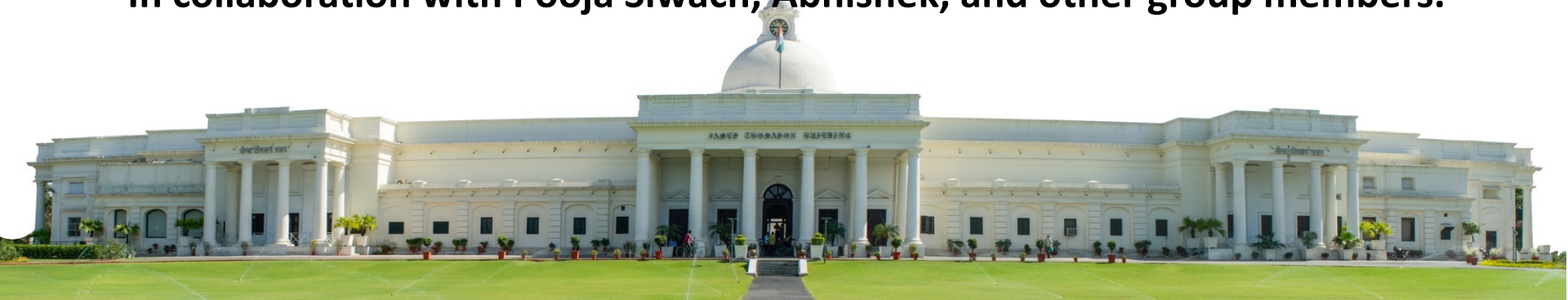
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A Quantum Algorithm for the Linear Response of Nuclei

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Abstract

We present a quantum algorithm to obtain the response of the atomic nucleus to a small external electromagnetic perturbation. The Hamiltonian of the system is presented by a harmonic oscillator, and the linear combination of unitaries (LCU) based method is utilized to simulate the Hamiltonian on the quantum computer. The output of the Hamiltonian simulation is utilized in calculating the dipole response with the SWAP test algorithm. The results of the response function computed using the quantum algorithm are compared with the experimental data and provide a good agreement. We show the results for ^{120}Sn and ^{208}Pb to corroborate with the experimental data in Sn and Pb region and also compare the results with those obtained using the conventional linear response theory.

arXiv:2210.08757v1 [quant-ph] 17 Oct 2022

Introduction

- Remapped a nuclear physics problem into a quantum computing problem by Jordan-Wigner and Gray code encoding.
- Prepared excited states on a quantum computer, a critical initial step to studying nuclear dynamics within linear-response theory.
- Calculated energies using a Linear Combination of Unitaries(LCU).
- Developed algorithm for the calculation of linear response on a quantum computer.
- Compared the results obtained using QASM simulator with the experimental and classical computation results.

Nuclear Physics to QC Problem

We start with a second quantization representation of Hamiltonian

$$H = \sum_{ij} h_{ij} a_i^\dagger a_j \quad \text{where} \quad h_{ij} = \langle i | \hat{T} + \hat{V} | j \rangle$$

is computed classically. We used JWT and GC transformations to encode $a_i^\dagger a_j$ operator into qubit operators.

- JWT

Occupation \longrightarrow Qubit orientation

Ex.: $|1100\rangle \longrightarrow |\uparrow\uparrow\downarrow\downarrow\rangle$

$$\hat{a}_j \longrightarrow \sigma_j^{(-)}$$

$$\hat{a}_j^\dagger \longrightarrow \sigma_j^{(+)},$$

$$\sigma^{(+)} = \frac{1}{2}(X - iY) = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$$

$$\sigma^{(-)} = \frac{1}{2}(X + iY) = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix},$$

Siwach Pooja, & Arumugam, P. (2021) *Phys. Rev. C*, 104, 034301.

- GC

$$a_i^\dagger a_j + a_j^\dagger a_i = \prod_{\alpha \in T(i,j)} P_\alpha^{(i,\alpha)} \left(\prod_{\beta \in S(i,j)} Q_\beta^{(i,\beta)} + \prod_{\beta \in S(i,j)} Q_\beta^{(j,\beta)} \right) \times [1 + \delta_{i,j}],$$

where,

$$P_\alpha^{(0)} = \frac{1}{2}(1 + Z_\alpha), P_\alpha^{(1)} = \frac{1}{2}(1 - Z_\alpha),$$

$$Q_\beta^{(0)} = \frac{1}{2}(X_\beta + iY_\beta), Q_\beta^{(1)} = \frac{1}{2}(X_\beta - iY_\beta),$$

We used Harmonic Oscillator Potential:

$$h_{N'N} = \langle N' | (\hat{T} + \hat{V}) | N \rangle = \hbar\omega \left[\left(N + \frac{3}{2} \right) \delta_N^{N'} \right]$$

For 120 Sn:

$$H_{JW} = 12I - 2.25Z_0 - 2.75Z_1 - 3.25Z_2 - 3.75Z_3$$

$$H_{GC} = 3I - 0.5Z_0 - 1.125Z_1 - 1.875Z_2 - 1.375Z_0Z_1 - 1.625Z_0Z_2 - 0.25Z_0Z_1Z_2$$

Preparation of Excited States

For the state preparation algorithm, the main idea is to exploit the time-evolution operator:

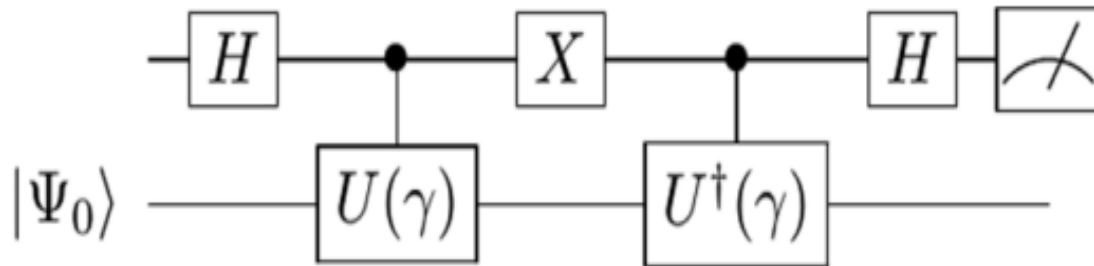
$$U(\gamma) = \exp(-i\gamma O) = \cos(\gamma O) - i \sin(\gamma O)$$

associated with the excitation operator O to produce the approximate state

$$|\Psi_A(\gamma)\rangle \propto \sin(\gamma O)|\Psi_0\rangle = |\Phi_E\rangle + \mathcal{O}(\gamma^2)$$

A. Roggero et al., (2020) *Phys. Rev. C*, 102, 064624.

State preparation circuit:



The state obtained after the measurement is :

$$|\Omega(\gamma)\rangle = |0\rangle \otimes \cos(\gamma O)|\Psi_0\rangle - i |1\rangle \otimes \sin(\gamma O)|\Psi_0\rangle$$

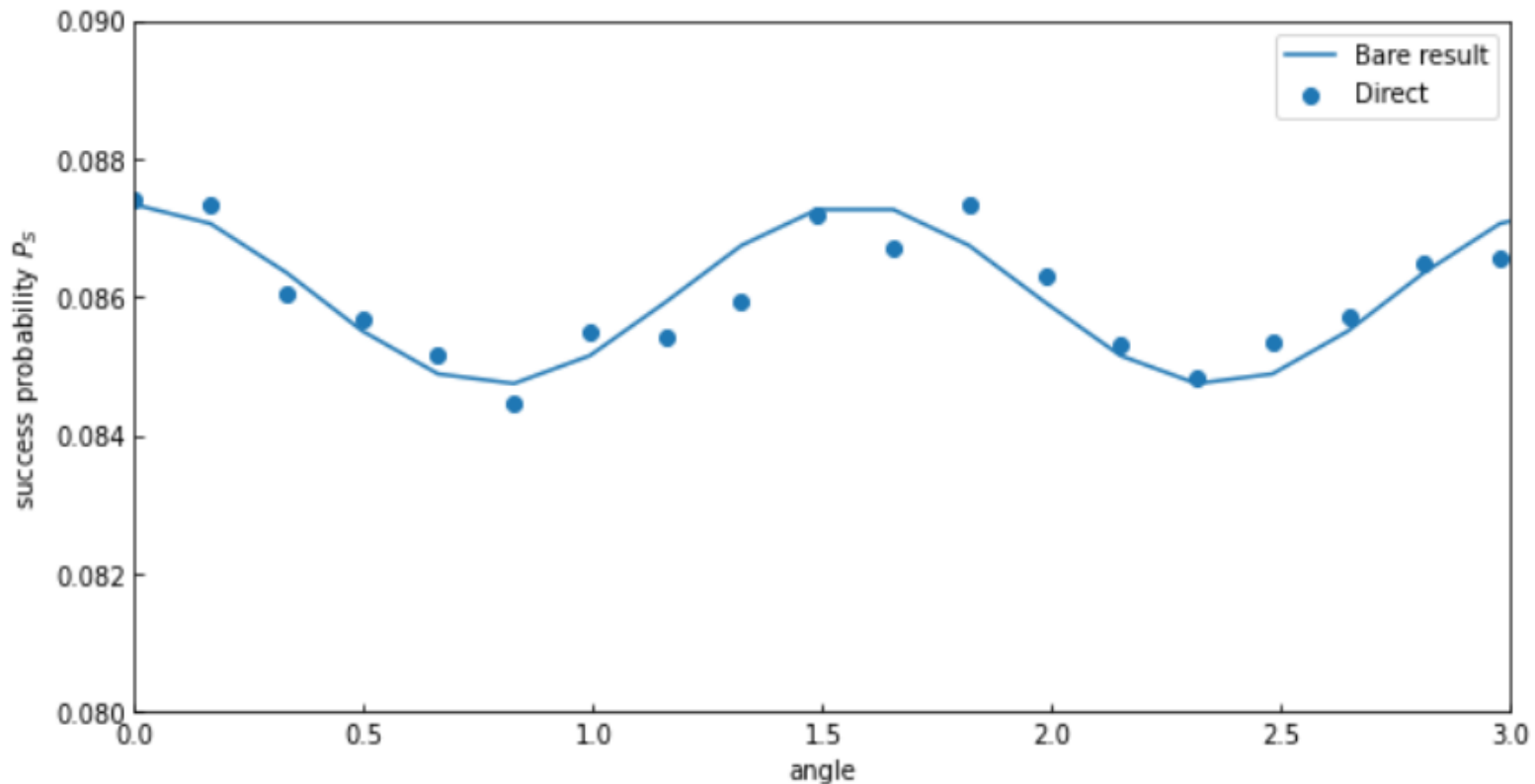
$$|\Psi_A(\gamma)\rangle = \frac{-i}{\sqrt{\langle\Psi_0|\sin^2(\gamma O)|\Psi_0\rangle}} \sin(\gamma O)|\Psi_0\rangle$$

A. Roggero et al., (2020) *Phys. Rev. C*, 102, 064624.

State preparation Results

We use $\theta \in [0, \pi]$ for the simple excitation operator

$$O(\theta) = \cos(\theta)X + \sin(\theta)1$$



Nuclear Response Function

We use separable interaction of the form:

$$\hat{H}' = \hat{H} + \frac{1}{2} \sum_{\alpha=1}^3 \kappa_{\alpha} \hat{D}_{\alpha}^{\dagger} \hat{D}_{\alpha}$$

The response function matrix is calculated as:

$$R_{\alpha\beta}^0 = \sum_{\nu} \frac{\langle 0 | \hat{D}_{\alpha} | \Psi_{\nu} \rangle \langle \Psi_{\nu} | \hat{D}_{\beta}^{\dagger} | 0 \rangle}{E - (e_{\nu} - e_0) + i\Gamma}$$

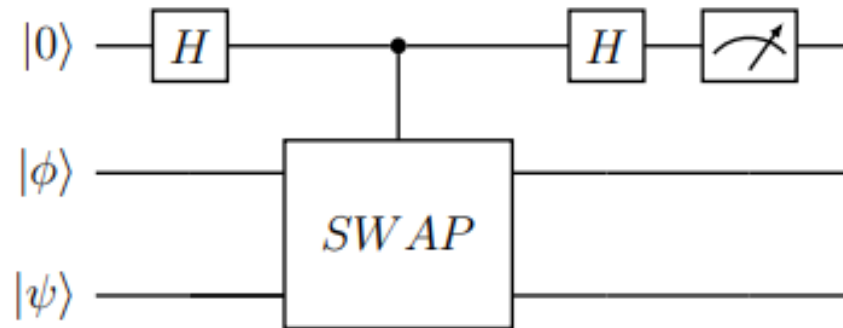
And the cross-section is related to the response function as:

$$\sigma(E) = \frac{-4\pi e^2 E}{\hbar c} \sum_{\alpha=1}^3 \text{Imag}(R_{\alpha\alpha})$$

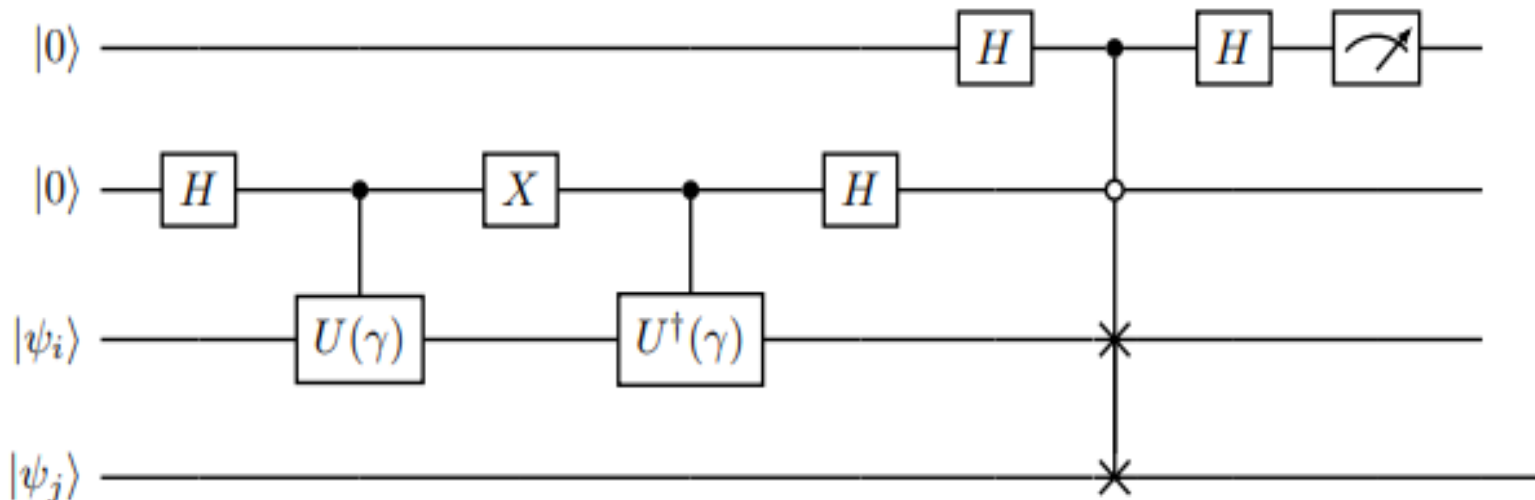
K. Huang et al., The Journal of Physical Chemistry Letters 13, 9114 (2022).

B. L. Berman and S. C. Fultz, Rev. Mod. Phys. 47, 713 (1975).

Quantum circuit that performs the SWAP test to calculate overlap:

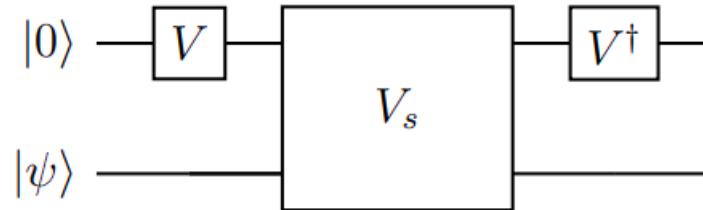


Overall quantum circuit:



Energy Calculation

Quantum circuit to calculate energy using the Linear Combination of Unitaries (LCU)



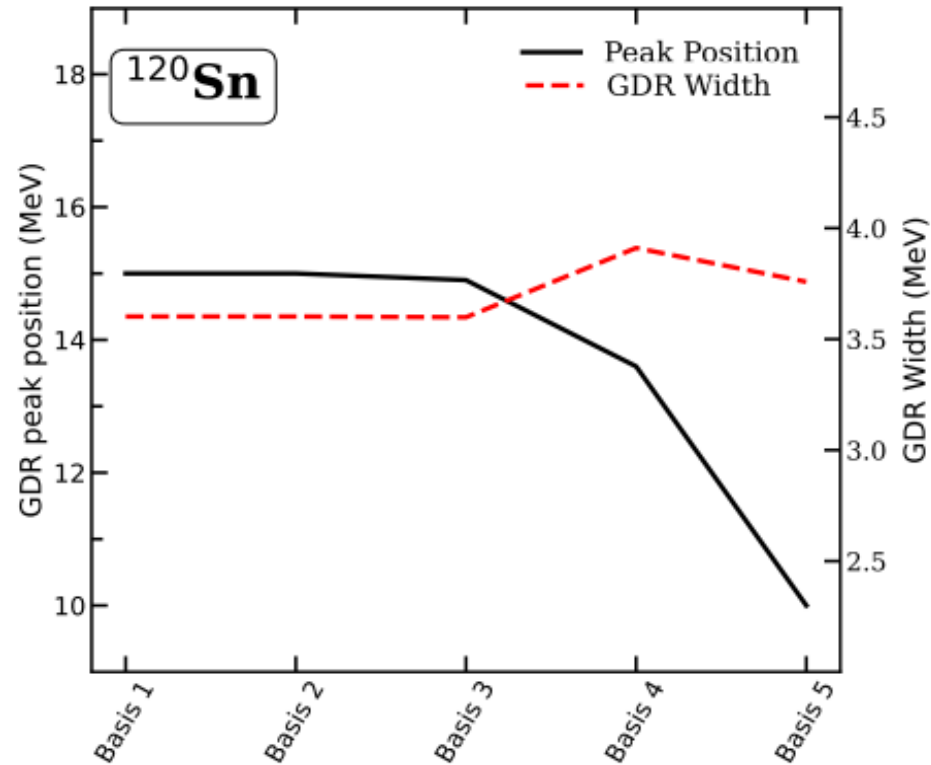
$$H = \sum_{i=0}^{k-1} a_i U_i \text{ with } a_i > 0 \forall i \in [0, k-1].$$

$$V |0\rangle^{\otimes n_a} = \frac{1}{\sqrt{\Lambda}} \sum_i \sqrt{a_i} |i\rangle \quad \text{where } \Lambda = \sum_i a_i$$

$$V_s = \sum_{i=0}^L |i\rangle \langle i| \otimes U_i$$

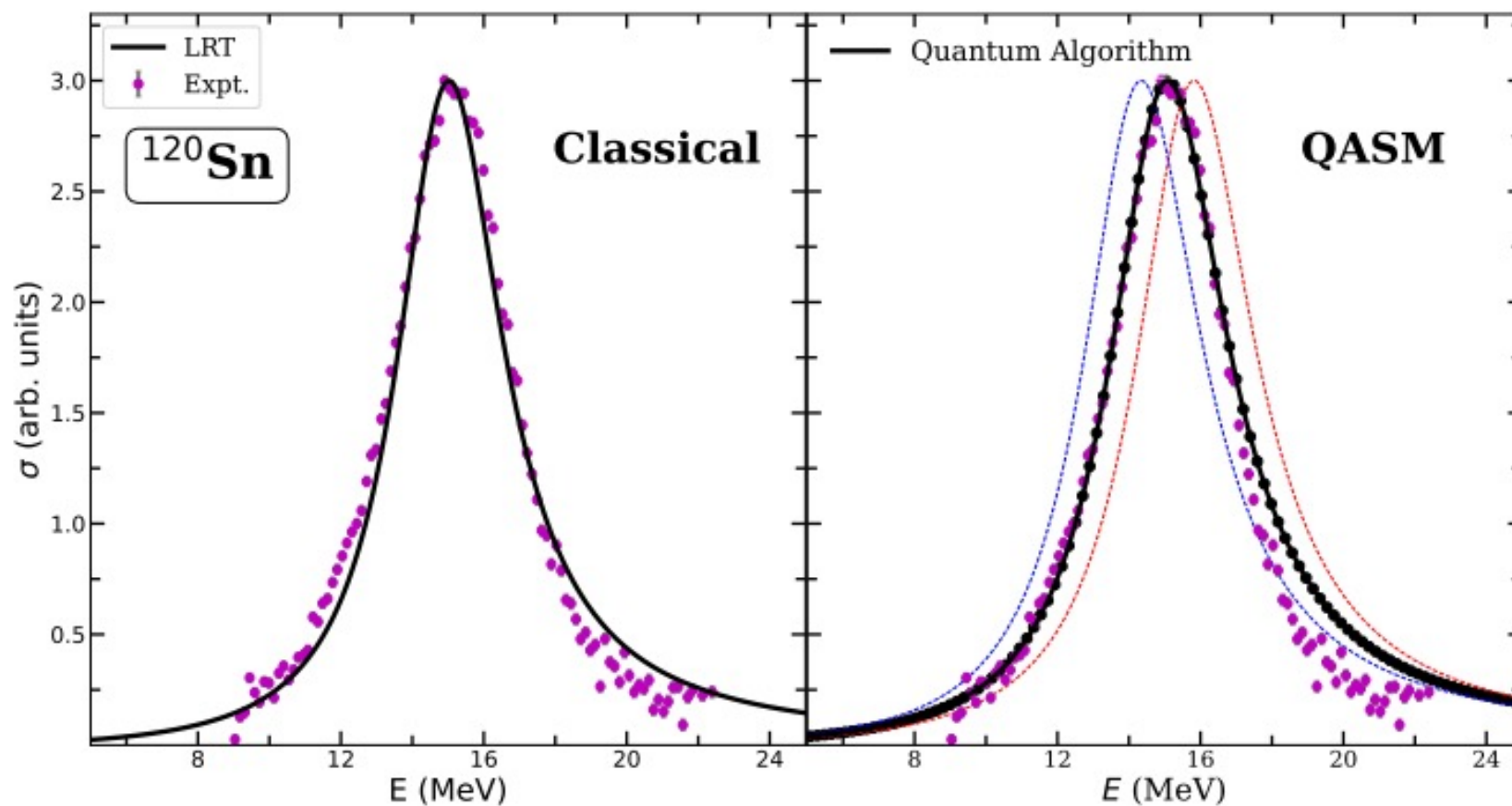
Siwach Pooja, & Arumugam, P. (2022) *Phys. Rev. C*, 105, 064318.
A. M. Childs and N. Wiebe, *Quantum Inf. Comput.* 12, 901 (2012).

Choice of basis size



Basis Label	Basis Size
Basis 1	$N = 0$ to 10
Basis 2	$N = 2$ to 8
Basis 3	$N = 3$ to 6
Basis 4	$N = 4$ to 6
Basis 5	$N = 4$ to 5

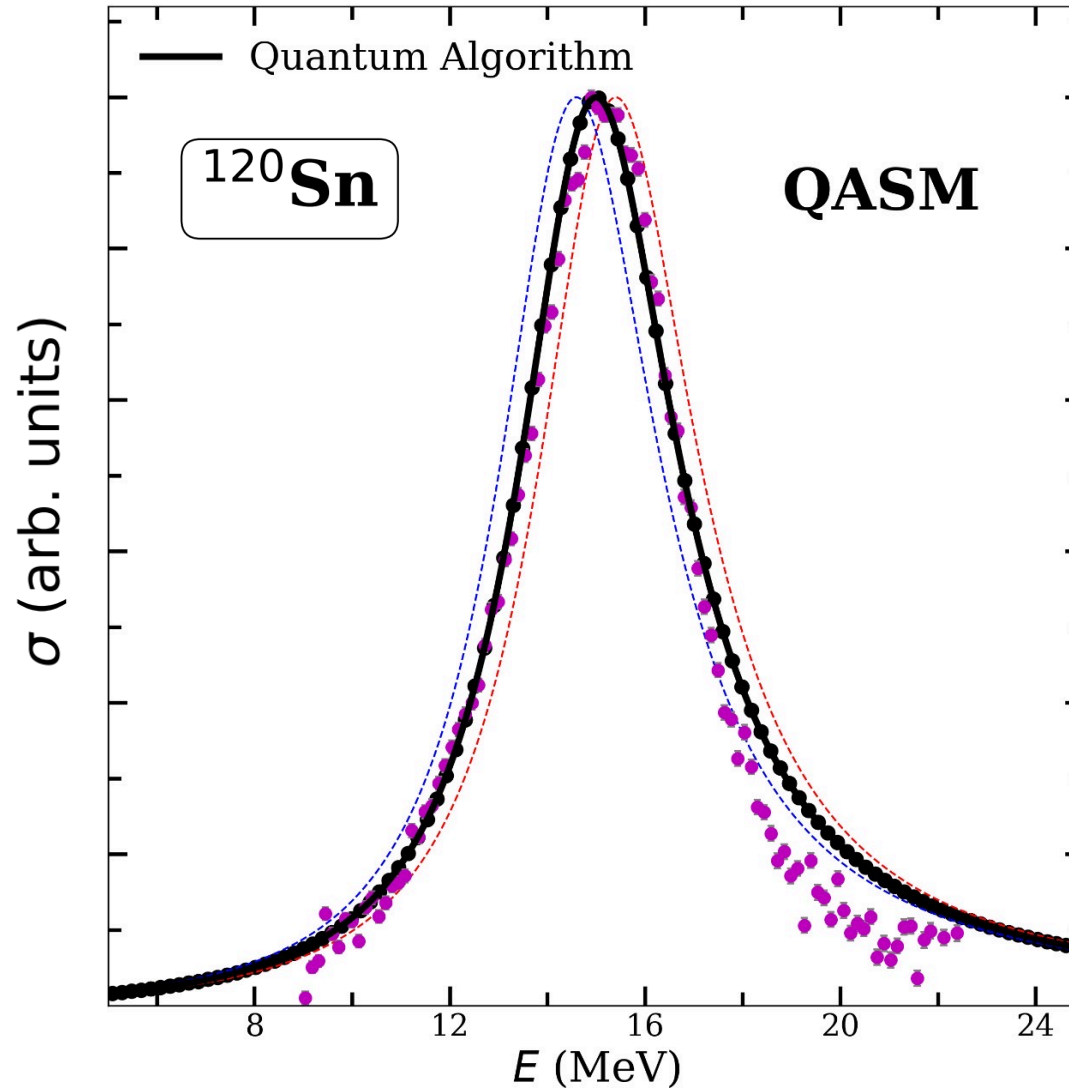
Results

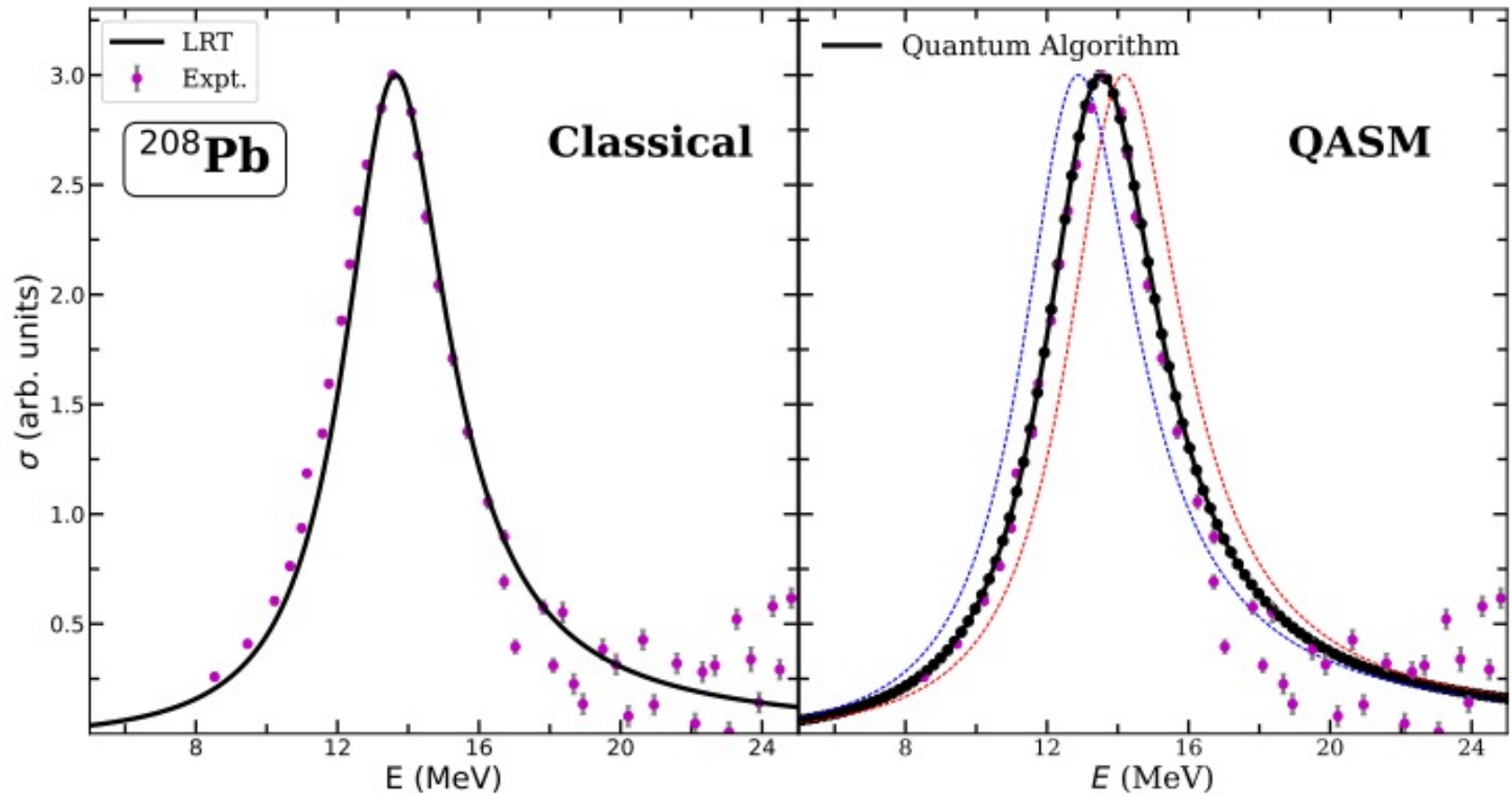


(a) Classical computation.

(b) Quantum simulation.

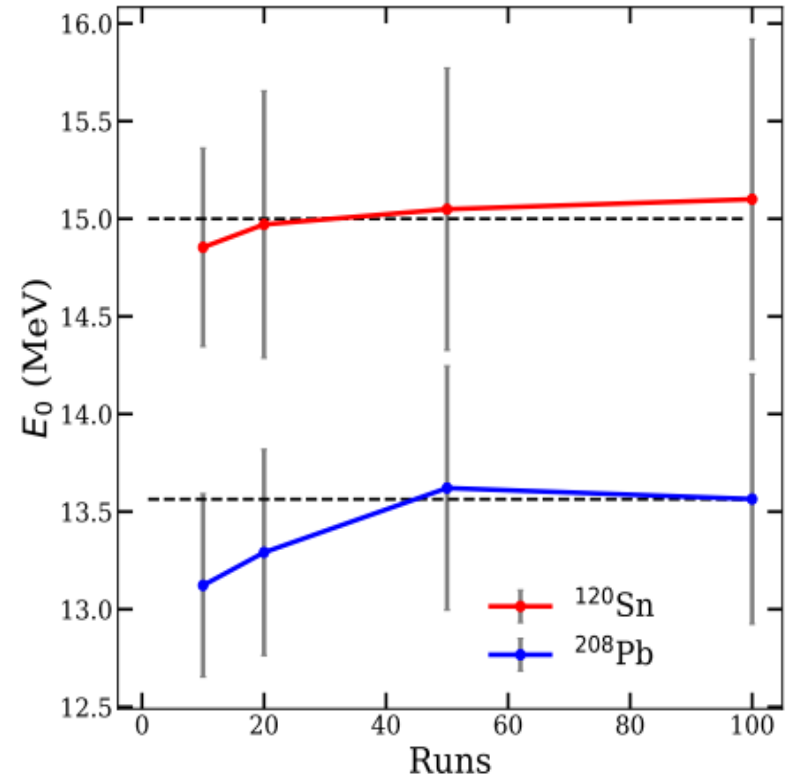
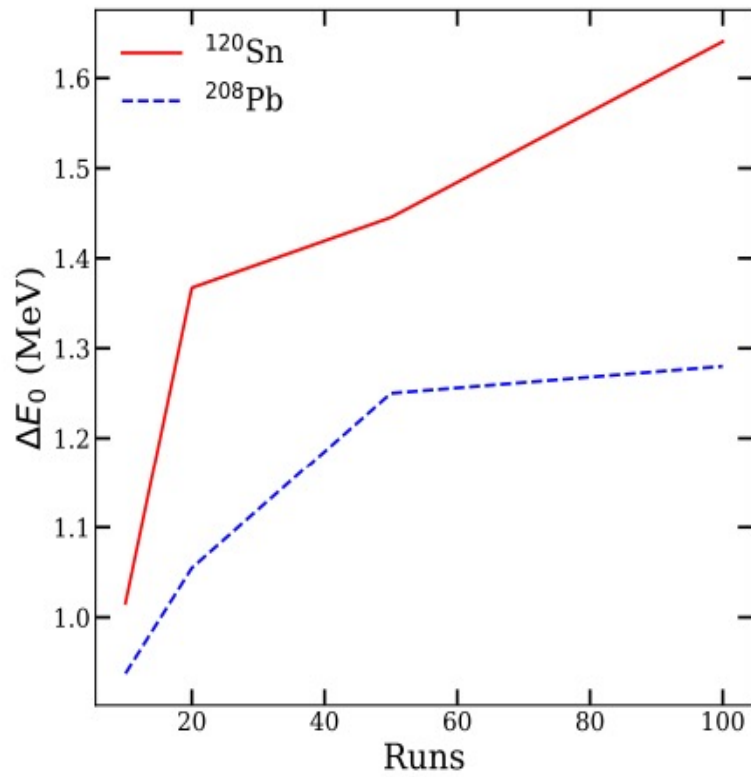
Using GC encoding





(a) Classical computation.

(b) Quantum simulation.



Conclusion

- To simulate the Hamiltonian, we used an approach based on the linear combination of unitaries (LCU), and we used the SWAP test to get the expected value of the dipole operator (overlap), which is needed to calculate the nuclear response.
- With the use of the QASM simulator, we were able to simulate a real quantum computer and compare the outcomes to both the experimental data and the results of the linear response theory's classical calculation of the response based on random phase approximation. Our results agree with the experimental data in both the Sn and Pb regions.
- We have demonstrated that only states close to the Fermi level contribute the most to the nuclear reaction; hence we have chosen a smaller basis size centered around the Fermi level in both nuclei.

Thank you.