Linear response on a quantum computer

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Introduction

Recent advancements in quantum computing enable us to simulate the dynamics of a quantum many-body system such as the atomic nucleus. One among the simpler problems in nuclear dynamics could be the linear response of a quantum system to a small external perturbation [1]. We offer an all-encompassing method for universal quantum computers that compute the linear response function and yield details about particular final states that may be directly used to find other nuclear observable.

We utilize the Linear Combination of Unitaries (LCU) [2] based algorithm to simulate the Hamiltonian of the system. The response is calculated by obtaining the transition probabilities from the ground state to the excited states using the SWAP test. We have chosen the deuteron to demonstrate our method, where we use the Hamiltonian derived from pionless effective field theory (EFT) [3].

Hamiltonian for the deuteron

The Hamiltonian in the second quantization notation is given by [3]

$$H = \sum_{ij} h_{ij} a_i^\dagger a_j, \tag{1}$$

$$\begin{aligned}\langle n'l'|\hat{T}|nl\rangle =& \frac{\hbar\omega}{2}\Big[\Big(2n+l+\frac{3}{2}\Big)\delta_n^{n'} \\ &- \sqrt{n\Big(n+l+\frac{1}{2}\Big)}\delta_n^{n'+1} \\ &- \sqrt{(n+1)\Big(n+l+\frac{3}{2}\Big)}\delta_n^{n'-1}\Big]\delta_l^{l'}.\end{aligned} \tag{2}$$

For the case of the deuteron with $l = 0$ ($^3S_1$ state) and the matrix element for EFT potential is given by $\langle n'|V|n\rangle = V_0\delta_n^{n'}\delta_n^0$, where the coefficient $V_0 = -5.68658111$ MeV. For basis size ($N = 4$), the Hamiltonian using Gray code (GC) encoding is [4]

$$\begin{aligned}H_4 =& 14.328I - 7.814X_0 - 3.913X_1 - 1.422Z_0 \\ &- 8.422Z_1 + 3.527X_0Z_1 + 3.913Z_0X_1 \\ &- 4.922Z_0Z_1.\end{aligned} \tag{3}$$

Preparation of excited States

The excited state is created by evolving the ground state with the time-evolution operator

$$U(\gamma) = \exp(-i\gamma O) = \cos\gamma O - i\sin\gamma O, \tag{4}$$

where the excitation operator $O(\theta) = \cos(\theta)X + \sin(\theta)I$ [5] which produces a rotation around the X direction. In Fig. 1, we give the

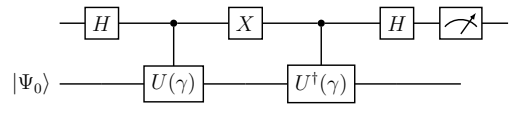

FIG. 1: The circuit for preparation of excited states.

quantum circuit to prepare the excited state.

$$|\Psi_A(\gamma)\rangle \propto \sin(\gamma O) = |\phi_O\rangle + \mathcal{O}(\gamma^2), \tag{5}$$

We prepare the auxiliary qubit in the state $|0\rangle$ and, using the given circuit evolve it to obtain the excited state. In accordance with the degree of precision we require and the possibility of success, we must select a short time period for the time parameter γ [5].

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Linear response

The dynamical response function [1],

$$S_O(\omega) = \sum_\nu |\langle\psi_\nu| O |\psi_0\rangle|^2 \delta(E_\nu - E_O - \omega), \tag{6}$$

used to completely characterize the response of a system of interacting particles owing to a perturbative probe defined by the excitation operator O. Here $|\psi_0\rangle$ is the ground state of the system with energy E_0, $|\psi_\nu\rangle$ are the final states of the reaction with energies E_ν, and ω is the energy transfer.
The probability distribution $P(y)$ is a decent approximation of $S_O(\omega)$

$$P(y) = \frac{1}{2^{2W}} \sum_\nu |\langle\psi_\nu| O |\psi_0\rangle|^2 \times \frac{\sin^2[2^W \pi(\lambda_\nu - \frac{y}{2^W})]}{\sin^2[\pi(\lambda_\nu - \frac{y}{2^W})]}, \tag{7}$$

where W is the number of ancilla qubits and $\lambda_\nu \in [0, 1]$ is the energy of ν^{th} state. We calculate the matrix element $(|\langle\psi_\nu| O |\psi_0\rangle|^2)$ of $\hat{O}$ between the ground state and excited state on the quantum computer using the SWAP test as shown in Fig. 2. The energies are calculated using the LCU [2] algorithm.

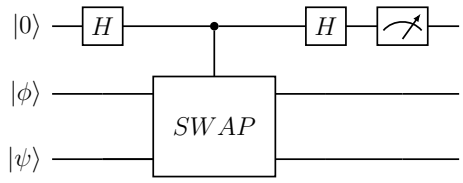

FIG. 2: SWAP test

Result and Discussion

In Fig. 3, we show our result for the response function calculated on the QASM simulator and compare it with the results obtained on the actual quantum devices (IBMQ nairobi). The exact response calculated classically using Eq. (4) is also displayed with a black dot. The error in the results because of the noise present in the actual quantum computer is shown with the shaded region. The results obtained with QASM match with the classical calculation but due to the presence of noise, the IBMQ underestimates the response. However, the position of the peaks agrees with the classical results. Our approach provides direct access to the final state resulting from an external perturbation and allows us to obtain the response which is comparable to the exact classical calculations. Our method can potentially be used as a valuable tool for corroborating with the nuclear response data.

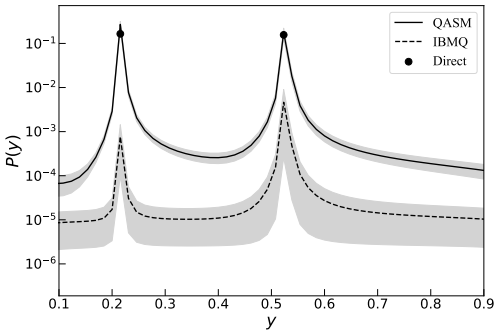

FIG. 3: Response function as a function re-scaled energies (y) for $W = 6$ ancilla qubits using the actual quantum computer (IBMQ) and QASM simulator. The shaded grey area shows the error in the result because of the noise present in the IBMQ. The exact response is also shown with black dots.

References

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