Quantum computational simulation to calculate the deuteron binding energy

Abhisek Roy Ranchi
Central University of Jharkhand, Ranchi 835 205, India

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This paper in a nutshell, introduces quantum computational techniques used in nuclear physics to provide us with a new path forward in the exploration of many-body systems that are of central importance to nuclear physics, such as the deuteron (the simplest case of a many body system). The purpose of this paper is to bind QC algorithms with calculations based on complex nuclei, which unravel important details about the properties of matter, and formation of heavy elements. This research approaches towards low-energy nuclear many-body problems by simulating the lightest of complex nuclei, the deuteron, and by applying the VQE algorithm (quantum algorithm to find ground state energy) we generate binding energies of the deuteron accurate to a reasonable error. This research direction leads us to a better understanding of how quantum computation and information could be applied to a range of light nuclei, using QC hardware that is expected to be available during the immediate next few years. Another feature of this research is that it also explores the presently available quantum computers at IBM called the IBM Q-Experience (Q-X), which can be accessed remotely via the web and can serve to facilitate many quantum computational experiments. This research proves how useful a tool the IBM Q-X is to devise new quantum algorithms and test them for nuclear physics as well as other diverse fields of physics.

Keywords: Quantum algorithm, VQE algorithm, Simulation, Deuteron binding energy, QC hardware

1 Introduction

Calculations of nuclear bonding energy are resource demanding in particular, computational time scales exponentially with the nucleon number $A^{1,2}$. In contrast to that, usage of quantum computers would allow an efficient (in polynomial time)$^3$ calculation and speed-up for other beyond-mean-field (correlation energy including) methods. With a quantum simulation of the deuteron binding energy on quantum processors, it is possible to compute the B.E. of the deuteron to within a few percent of error. This would be a bold move towards scalable nuclear structure computations on a quantum processor.$^3$

Solving many-body problems over a quantum simulation reveals several challenges such as wave function-based methods in nuclear physics face the exponential growth of Hilbert space with increasing number of nucleons. Also, the quantum Monte Carlo methods are confronted with the fermion sign problem$^6$.

Quantum computers promise to reduce the computational complexity of simulating quantum many-body systems from exponential to polynomial$^3$ and thus, make calculations more accessible. This paper aims to present a quantum computation of the deuteron, a bound state of the proton and neutron, and use publicly available quantum computer from IBM Q-Experience$^3$.

2 Problem Formulation

General nuclear structure Hamiltonian in second quantization (considering no-pair approximation and nucleonic structure with at most $k$-body interactions) has a form$^{3,5}$.

$$H = \sum_{n=1}^{N} \sum_i \sum_j V^{(n)}(i_n, j_n) \hat{a}^+(i_n) \hat{a}(j_n), \quad \ldots (1)$$

Where,

$$\hat{a}(j_n) = \hat{a}(j_1) \hat{a}(j_2) \ldots \hat{a}(j_n), \quad \ldots (2)$$

$$\hat{a}(i_n) = \hat{a}^+(i_n) \hat{a}^+(i_{n-1}) \ldots \hat{a}^+(i_1), \quad \ldots (3)$$

$$V^{(n)}(i_n, j_n) = \langle i_1, i_2, \ldots i_n | V^{(n)} | j_1, j_2, \ldots j_n \rangle, \quad \ldots (4)$$

In the standard formulation, number of creation and annihilation operators for the given type of nucleon must be same in each term in Eq. (1). Creation and annihilation operators, as connected to two distinct types of fermions have to obey anticommutation relations and commute with operators for the other nucleonic type$^6$.

But the problem of quantum computing the deuteron B.E. is that we have to adjust the employed

*Corresponding author (E-mail: abhisekroy95quanta@gmail.com)
Hamiltonian, the wave function preparation, and the computational approach. We will use a discrete variable representation in the harmonic oscillator basis for the Hamiltonian\textsuperscript{7,8}. Then, the deuteron Hamiltonian will have the form\textsuperscript{7},

\[ H_N = \sum_{n=0}^{N-1} \langle n | (T + V) | n \rangle a_n^+ a_n \ldots \ldots \quad (5) \]

2.1 Mapping the deuteron into qubits

Quantum computers manipulate qubits by operations based on Pauli matrices (denoted by \(X_q\), \(Y_q\), and \(Z_q\) on qubit \(q\))\textsuperscript{1}. The deuteron creation and annihilation operators can be mapped onto Pauli matrices as:

\[ a_n^+ \rightarrow \frac{1}{2} \prod_{j=0}^{n-1} (-Z_j) (X_n - iY_n), \]

\[ a_n \rightarrow \frac{1}{2} \prod_{j=0}^{n-1} (-Z_j) (X + iY_n). \]

To compute the ground state energy of deuteron we employ the following strategy. We determine the ground-state energy of the Hamiltonian (5) for \(N = 1, 2, 3\) and use those values to extrapolate the energy to the infinite-dimensional space\textsuperscript{7}.

All sources of quantum computer power—superposition (Hadamard gate application), parallelism, entanglement and destructive interference (the inverse QFT)\textsuperscript{9,10} are exploited in the formulation of the gates and this would lead to an exponential speed up for energy calculation when compared to classical computer-based procedure under an important preposition that both initial eigenvector guess and evolution operator application (in general it is a 1-qubit gate and should be decomposed into elementary one and two-qubit gates from universal quantum logic gate set\textsuperscript{4}).

The comparison of the ground state energy values of \(H_2\) obtained through simulation is compared with the values of ground state of the exact values of the \(H_2\) ground state energies, shown in Table 1.

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<th>(O(KLe^{-4kl}))</th>
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E from exact diagonalization.

<table>
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</table>

E from quantum computing.

Fig. 1 – Experimentally determined energies for \(H_2\) (top) and expectation values of the Pauli terms that enter the two-qubit Hamiltonian of \(H_2\) as determined on the QX (center) and 19Q (bottom) chips.

Experimental results are denoted by symbols. Theoretical results are denoted by lines.

Pauli term appearing in the Hamiltonian is measured on the quantum chip. The results of the simulation from the QX-10 and 19Q chips, and its experimentally determined energies of \(H_2\) are shown in Fig. 1. We recall that quantum-mechanical measurements are stochastic even for an isolated system, and the noise enters through undesired couplings with the environment.

4 Conclusions

This paper presents a quantum algorithm feasible for \(H_2\) ground state energy calculations, with the initial eigenvector guess (identical to Hartree-Fock solution). For excited states, linear combination of a smaller set of configurations should be used as an initial eigenvector guess. The studies should carry on
for $^4$He and later to be extended to larger nuclei. Different quantum algorithms should be investigated as well.

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References