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Application of quantum computation in predicting the neutron drip line in oxygen isotopic chain

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Atomic nuclei are complex many-body systems composed of nucleons interacting via strong nuclear force. Understanding nuclear properties from the nucleon-nucleon force is one of the main goals of low-energy nuclear physics. Like other quantum many-body problems, the structure of atomic nuclei can be effectively solved using configuration-interaction methods. One such method that is very successful in solving many-body problems of nuclear structure is the nuclear shell model [1, 2, 3]. But, the exponential increase in Hilbert space with increasing nucleon numbers has become a computational challenge for classical computers. Quantum computers are emerging as promising tools for solving many-body problems across the spectrum of physical sciences. These devices are natural quantum systems in which the principles of quantum mechanics, like the superposition principle and entanglement, are embedded.

In the noisy intermediate-scale quantum era [4], variational algorithms have become a standard approach to solving quantum many-body problems. Here, we present variational quantum eigensolver (VQE) [5] results of selected oxygen isotopes within the shell model description. The aim of this work was to locate the neutron drip line of the oxygen chain using unitary coupled cluster (UCC) type ansatze [6] with different microscopic interactions (DJ16 [7], JISP16 [8], and N3LO [8]), in addition to a phenomenological USDB [9] interaction. While initially infeasible to execute on contemporary quantum hardware, the size of the problem was reduced significantly using qubit tapering techniques in conjunction with custom circuit design and optimization. The optimal values of ansatz parameters from classical simulation were taken for the DJ16 interaction, and the tapered circuits were run on IonQ's Aria [10], a trapped-ion quantum computer. After applying gate error mitigation for three isotopes, we reproduced exact ground state energies within a few percent error. The post-processed results from hardware also clearly showed ^{24}O as the drip line nucleus of the oxygen chain. Future improvements in quantum hardware could make it possible to locate drip lines of heavier nuclei.

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Presentation type

Oral presentation

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