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Quantum computing of the 6Li nucleus via ordered unitary coupled cluster

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The variational quantum eigensolver (VQE) is an algorithm to compute ground and excited state energy of quantum many-body systems. A key component of the algorithm and an active research area is the construction of a parametrized trial wavefunction –a so called variational ansatz. The wavefunction parametrization should be expressive enough, i.e. represent the true eigenstate of a quantum system for some choice of parameter values. On the other hand, it should be trainable, i.e. the number of parameters should not grow exponentially with the size of the system. Here, we apply VQE to the problem of finding ground and excited state energies of the odd-odd nucleus 6Li. We study the effects of ordering fermionic excitation operators in the unitary coupled clusters
ansatz on the VQE algorithm convergence by using only operators preserving the Jz quantum number. The accuracy is improved by two order of magnitude in the case of descending order. We first compute optimal ansatz parameter values using a classical state-vector simulator with arbitrary measurement accuracy and then use those values to evaluate energy eigenstates of 6Li on a superconducting quantum chip from IBM. We post-process the results by using error mitigation techniques and are able to reproduce the exact energy with an error of 3.8% and 0.1% for the ground state and for the first excited state of 6Li, respectively.

Significance

We compute the ground and first excited state energy of the 6Li nuclei in the shell model using a quantum processor, which has not been done before.

References

https://arxiv.org/abs/2205.00864

Experiment context, if any

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