Exploring the electronic structures of small molecules with qiskit nature v0.7
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Introduction
Quantum computing brings a promising alternative to the current ab-initio methods in molecular modeling. Qiskit Nature offers a tool-set to perform different basic quantum algorithm based calculations. However, the transition from “classical” codes into quantum algorithm based methods involves a given learning curve, a different way of defining calculation workflows and rethinking computational costs. This poster is an attempt to go an step beyond the basic examples provided in the documentation and tutorials.

A collection of electronic structure calculations for a set of small molecules using Qiskit Nature (version 0.7) is presented, together with some common approaches to reduce the size of the problem. The reference electronic structure was produced with the PySCF driver with a minimal STO-3G basis set. The parametrized circuit was produced with the standard Transformer

The calculations were performed locally (on a PC) and in the QASM simulator on the IBM Cloud.

Mappers and options
Further reduction can be achieved through the different mapping and options for the qubit operators. While Jordan-Wigner and Parity mappers with default options map the spin operators 1 to 1, fixing the amount of particles and especially using the tapered reduction can provide a meaningful size reduction.

In order to start reducing the size of the problem, the active space was easily reduced by applying the FreezeCoreTransformer with default options.

Influence of number of shots and resilience (QASM simulator)
A calculation for the H$_2$ molecule with different number of shots and resilience (error mitigation) method are compared the exact value (red line) in the following chart. As it could be expected, the amount of shots increase the accuracy of the calculation. The resilience has a limited impact, because of the size of the system and the simulated backend. The red line indicates the exact ground state (NP) energy, numeric values below the bars the difference of the averaged energy (4 calculations) with the exact energy, and inside the bars (red numbers) the standard deviation of the 3 values.

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We can observer that the results have an acceptable reproducibility.

Results on quantum hardware (ibmq_ehningen)
The results of a single calculation set are displayed below. As it could be expected, the estimated energy values on the left are further away from the exact value (red line) compared to the graph above, and the resilience method doesn't seem to have a big effect on the result.

Computation cost (QASM simulator)
The computing costs for the calculations on the QASM simulator (graph on the left side) were measured as the total value for solving the GroundStateSolver, including the (almost neglectable) queuing time and averaged over the 4 calculations. As it could be expected, the resilience level 0 (no error mitigation) represented by the red line, the resilience level 1 (TREX), represented by orange bars, and a much clearer overhead for the case of resilience level 2 (ZNE), represented as green bars.

Conclusions
I still have a lot to test in my journey towards optimal calculations with qiskit nature. Next steps will involve running equivalent calculations on further systems and trying to make a picture of computing costs for each accuracy expectation. Corrections and further steps will be published soon.

And, I am definitely open to discuss possible collaborations with anyone interested.

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