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Extracting Information from Partial Hamiltonian of Simple Molecules for Designing Efficient Variational Quantum Eigensolvers

This work aims to study the qubit Hamiltonian of a molecule term-by-term to understand their contributions, and if any information can be extracted by just considering a few selected terms of the Hamiltonian, a technique called partial Hamiltonian analysis (PHA). The transformation of a molecular Hamiltonian from the fermionic space to the qubit space[1] provides us with a series of qubit operators in sum-of-product format, with each component being a qubit operator. The important question to answer would be if we can extract any useful information by considering the partial Hamiltonian, and if we can diagonalize the whole Hamiltonian by analyzing just some of its terms, hence making the overall computation smaller.
The PHA method can be summarized as follows: Consider a qubit Hamiltonian, consisting of n terms,
\begin{equation}
H_{full} = H_1 + H_2 + \cdots + H_n
\end{equation}

The variational quantum eigensolver finds a wavefunction that minimizes the energy,
\begin{equation}
H_{full}\mid \Psi_{full}\rangle =E_{full}\mid \Psi_{full}\rangle
\end{equation}

Now, with PHA, we try to consider only certain terms of the Hamiltonian, assuming that since the Hamiltonian is in sum-of-products format, the wavefunction that minimizes the partial Hamiltonian might minimize the overall Hamiltonian.
\begin{equation}
H_{partial} = H_1 + H_2 + \cdots + H_m (m<n)
\end{equation}

and,
\begin{equation}
H_{partial} \mid \Psi_{partial}\rangle =E' \mid \Psi_{partial}\rangle
\end{equation}

\begin{equation}
\langle \Psi_{full} \mid H_{full} \mid \Psi_{full} \rangle \stackrel{?}{=} \langle \Psi_{partial} \mid H_{partial} \mid \Psi_{partial} \rangle
\end{equation}
The criteria for constructing the partial hamiltonian of a molecule, based on the data obtained in Figure 1 can be explained as: (i) The term in the full hamiltonian with the largest co-efficient (usually the identity term) must be considered; (ii) All the terms having only 'I', 'Z', or both gates must be considered; and (iii) In case convergence is not achieved, additional terms can be added based on the value of the coefficient. Terms with larger coefficients must be considered first.

Once the criteria for constructing the partial hamiltonian is finalized, the technique can be tested on some other molecule and results can be further verified. The other molecule chosen was Lithium hydride and the results are presented in Figure 2. For the generalized method, the number of shots for a certain accuracy ϵ, scale as $O(\frac{N^4}{\epsilon^2})$[2] with the number of qubits N. For partial hamiltonian analysis, if only the 'Z'and 'I'terms are considered, the number of shots for a certain accuracy ϵ, scale as $O(\frac{1}{\epsilon^2})$ with every system requiring a single circuit execution.

[1] C. D. Batista and G. Ortiz, Generalized jordan-wigner transformations, Physical Review Letters 86, 1082 (2001)
[2] Tilly, Jules, et al. "The Variational Quantum Eigensolver: A Review of Methods and Best Practices."Physics Reports, vol. 986, 5 Nov. 2022, pp. 1–128, www.sciencedirect.com/science/article/pii/S0370157322003118, https://doi.org/10.1016/j.physrep.2022.08.003.

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