Compressing VQE circuit with applications in the study of small molecule

A.V Tomut*, M Vasilescu*
* Faculty of Physics, Babeş-Bolyai University, Kogalniceanu 1, Cluj-Napoca, Romania.

PRESENTER: **Andrei Voicu Tomut**
tomutvoicuandrei@gmail.com

ABSTRACT: Quantum computers allow us efficiently solve problems that would generally be intractable for classical hardware. An example of such a problem would be determining the minimum eigenvalue of an operator. Although technology is in a state of continuous development, right now, the dimensions of real QPUs are small, and quantum computing simulators are limited. We tested various methods of optimizing the dimensions of such a circuit in order to reduce the number of qubits as well as the number of gates. The results show dependence between optimization time and circuit dimensions. So we can say now in which situations the optimization step is helpful or redundant.

METHOD

This research's novelty element consists of applying the matchgate compression rule presented by Richard Jozsa and Akimasa Miyake on a variational circuit[1].

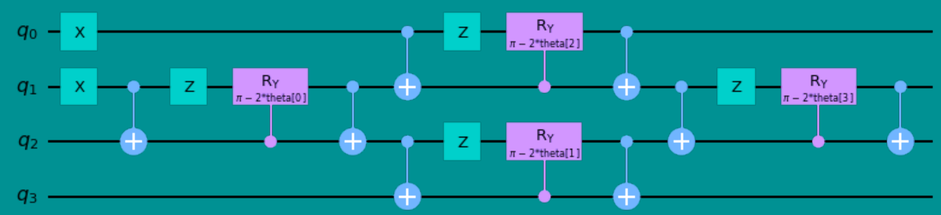
First, the electronic hamiltonian of the target molecule (ex.: H2) was mapped to qubits using Jordan Weegner transformation.
The ansatz was build from gates that conserve the number of electrons, so the circuit needs to be initialized with the first n_e qubits in state |1> where n_e is the number of electrons in the system. Then we run the VQE with the uncompressed ansatz to check the convergence (fig2).

$$G(t) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & cos(t) & sin(t) & 0 \\ 0 & sin(t) & -cos(t) & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

Before starting the compression, we selected a piece of the hamiltonian formed only by the observable that need only one Z measurement because their compression is easier (fig 3). However, even this small improvement can generate saving by reducing the computing power.
The general form of compression by Walter León Boyajian in " Matchgate circuits and compressed quantum computation."[2] (Table).

Can we use matchgate compression to reduce the number of qubits needed to study the Molecular Hamiltonian?

fig.1 :Matchgate ansatz for H2 molecule simulation



	Initial circuit	Compressed circuit
Initial state	ρ_{in}	$\rho_{in}^{=} = \frac{1}{2n}[I + iS(\rho_{in})]$
Observable	$H = \frac{i}{2}\sum_{j\neq k=0}^{2n-1} a_{jk}c_j c_k$	$H^{=} = \frac{i}{2}\sum_{j\neq k=0}^{2n-1} a_{jk}\lvert j><k\rvert$
Operator	$U_l = e^{iH_l}$	$R = e^{4h_l}$

Table: compression rules

Take a picture to get acces to a code sample

RESULTS

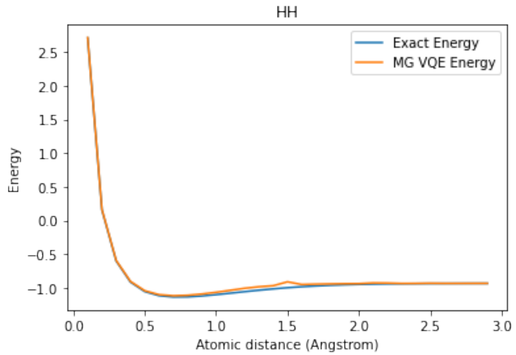


fig.2: VQE energy versus exact energy for hydrogen molecule and the ansatz from fig.1.

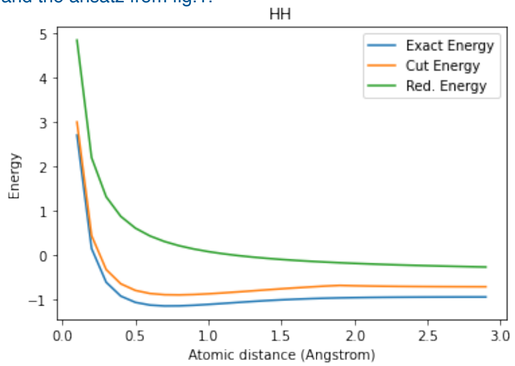


fig.3: A comparison between the best results that we can get using the compressed circuit and the target values, for hydrogen molecule.

CONCLUSIONS

Naw, we can say that applying the matchgate technique requires to manny approximation, so we can't guaranty a practical result even for the easy to compress part of the hamiltonian.

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References:

[1] Matchgates and classical simulation of quantum circuits arXiv:0804.4050
[2] " Matchgate circuits and compressed quantum computation." https://inis.iaea.org/collection/NCLCollectionStore/_Public/48/059/48059246.pdf?r=1&r=1