Variational quantum eigensolver boosted by adiabatic connection

Katarzyna Pernal[1], Fabijan Pavosevic[2], Libor Veis[3]

[1] *Institute of Physics, Lodz University of Technology, 90-924, Lodz, Poland*
[2] *Algorithmiq Ltd., Kanavakatu 3C, FI-00160 Helsinki, Finland*
[3] *J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, v.v.i., Dolejškova 3, 18223 Prague 8, Czech Republic*

In this work we integrate the variational quantum eigensolver (VQE) [1, 2] with the adiabatic connection (AC) method [3, 4] for efficient simulations of chemical problems on near-term quantum computers. The orbital optimized VQE methods [5] are employed to capture the strong correlation within an active space, while the classical AC corrections recover the dynamical correlation effects comprising electrons outside of the active space. On two challenging strongly correlated problems, namely the dissociation of N_2 and the electronic structure of the tetramethyleneethane biradical, we show that the combined VQE-AC approach enhances the performance of VQE dramatically. Moreover, since the AC corrections do not bring any additional requirements on quantum resources or measurements, they can literally boost the VQE algorithms. Our work paves the way towards quantum simulations of real-life problems on near-term quantum computers.

References

[1] A. Peruzzo, J. McClean, P. Shadbolt, M.-H. Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik, and J. L. O'Brien, *Nat. Commun.* **5** (2014).

[2] Y. Cao, J. Romero, J. P. Olson, M. Degroote, P. D. Johnson, M. Kieferová, I. D. Kivlichan, T. Menke, B. Peropadre, N. P. D. Sawaya, S. Sim, L. Veis, and A. Aspuru-Guzik, *Chem. Rev.* **119**, 10856 (2019).

[3] K. Pernal, *Phys. Rev. Lett.* **120** (2018).

[4] E. Pastorczak, K. Pernal, *J. Chem. Theory Comput.* **14**, 3493 (2018).

[5] W. Mizukami, K. Mitarai, Y. O. Nakagawa, T. Yamamoto, T. Yan, and Y. Ohnishi, *Phys. Rev. Res.* **2**, 033421 (2020).