Topological Index and Homotopy in Coupled-Cluster theory

Mihály A. Csirik and Andre Laestadius

Hylleraas Centre, Department of Chemistry, University of Oslo, Norway

Contact email: m.a.csirik@kjemi.uio.no

We propose a comprehensive mathematical framework for Coupled-Cluster-type methods based on topological degree theory [1]. This allows us to establish more general existence results than [10] and deduce local information about the solutions of the CC equations. The idea of constructing a homotopy for CC theory is not new, and has been extensively studied in the past [11, 12, 8, 5, 7, 4, 2, 3, 6]. We consider the more recent Kowalski–Piecuch (KP) homotopy [9] from a mathematical point of view and use it as a theoretical tool to prove the existence of a truncated CC solution. This follows from a more general result guaranteeing the existence of a whole solution curve of the KP homotopy.

References

- [1] Mihály A. Csirik and Andre Laestadius. Coupled-cluster theory revisited. arXiv preprint arXiv:2105.13134, 2021.
- [2] K. Jankowski and K. Kowalski. Physical and mathematical content of coupled-cluster equations. II. on the origin of irregular solutions and their elimination via symmetry adaptation. *The Journal of chemical physics*, 110(19):9345–9352, 1999.
- [3] K. Jankowski and K. Kowalski. Physical and mathematical content of coupled-cluster equations. IV. impact of approximations to the cluster operator on the structure of solutions. *The Journal of chemical physics*, 111(7):2952–2959, 1999.
- [4] K. Jankowski, K. Kowalski, I. Grabowski, and H.J. Monkhorst. Correspondence between physical states and solutions to the coupled-cluster equations. *International journal of quantum chemistry*, 75(4-5):483–496, 1999.
- K. Jankowski, K. Kowalski, and P. Jankowski. Multiple solutions of the single-reference coupled-cluster equations.
 I. H4 model revisited. International Journal of Quantum Chemistry, 50(5):353–367, 1994.
- [6] Fábris Kossoski, Antoine Marie, Anthony Scemama, Michel Caffarel, and Pierre-Francois Loos. Excited states from state specific orbital optimized pair coupled cluster. arXiv preprint arXiv:2104.03746, 2021.
- [7] K. Kowalski and K. Jankowski. Full solution to the coupled-cluster equations: the H4 model. *Chemical physics letters*, 290(1-3):180–188, 1998.
- [8] J. Paldus, M. Takahashi, and B.W.H. Cho. Degeneracy and coupled-cluster approaches. International Journal of Quantum Chemistry, 26(S18):237–244, 1984.
- [9] Piotr Piecuch and Karol Kowalski. In search of the relationship between multiple solutions characterizing coupled-cluster theories. In *Computational chemistry: reviews of current trends*, pages 1–104. World Scientific, 2000.
- [10] Reinhold Schneider. Analysis of the projected coupled cluster method in electronic structure calculation. Numerische Mathematik, 113(3):433–471, 2009.
- [11] Tomislav P. Živković. Existence and reality of solutions of the coupled-cluster equations. International Journal of Quantum Chemistry, 12(S11):413-420, 1977.
- [12] Tomislav P. Živković and Hendrik J. Monkhorst. Analytic connection between configuration-interaction and coupled-cluster solutions. *Journal of Mathematical Physics*, 19(5):1007–1022, 1978.