Coupled cluster theory: towards an algebraic geometry approach [1]

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Coupled cluster theory produced arguably the most widely used high-accuracy computational quantum chemistry methods. Despite the approach's overall great computational success, its mathematical understanding is so far limited to results within the realm of functional analysis. The coupled cluster amplitudes, which are the targeted objects in coupled cluster theory, correspond to solutions to the coupled cluster equations, which is a system of polynomial equations of at most fourth order. The high-dimensionality of the electronic Schrödinger equation and the non-linearity of the coupled cluster ansatz have so far stalled a formal analysis of this polynomial system. We present the first algebraic investigations that shed light on the coupled cluster equations and the root structure of this ansatz. This is of paramount impor- tance for the *a posteriori* evaluation of coupled cluster calculations, where alternative benchmark procedures cannot be employed. To that end, we investigate the root structure by means of Newton polytopes. We derive a general v-description, which is subsequently turned into an h-description for explicit examples. This perspective re- veals an apparent connection between *Pauli's exclusion principle* and the geometrical structure of the Newton polytopes. Moreover, we provide numerical simulations of two computationally tractable systems, namely, the two electrons in four spin orbitals system and the three electrons in six spin orbitals system. These simulations provide novel insight into the physicality of the coupled cluster solutions when the coupled cluster ansatz is truncated.

REFERENCES

[1] F. M. Faulstich and M. Oster, *Coupled cluster theory: Towards an algebraic geometry for- mulation*, arXiv:2211.10389.