Coupled cluster theory: Towards an algebraic geometry formulation

Fabian M. Faulstich,[1] Mathias Oster[2]

[1]*Department of Mathematics,RensselaerPolytechnicInstitute,Troy,NY*
[2]*IGPM,RWTHAachen,Germany*

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 degree four. 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. In this article, we present algebraic investigations that shed light on the coupled cluster equations and the root structure of this ansatz. This is of importance for the *a posteriori* evaluation of coupled cluster calculations. 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 reveals an apparent connection between *Pauli's exclusion principle* and the geometrical structure of the Newton polytopes. We also propose an alternative characterization of the coupled cluster equations projected onto singles and doubles as cubic polynomials on an algebraic variety with certain sparsity patterns. 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 root structure of the coupled cluster solutions when the coupled cluster ansatz is truncated.