Computing molecular properties in multireference coupled-cluster theory

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In single-reference coupled-cluster theory the computation of molecular properties builds on two intimately related and now well-established formalisms: Gradient theory [1] and response theory [2]. Here, I want to report on our progress in using these approaches within the framework of internally contracted multireference coupled-cluster (icMRCC) theory [3] with the aim of applying the theory to questions beyond molecular energies.
In one line of our work, we apply the quasi-energy response formalism to icMRCC theory. The approach gives access to excitation energies [4], expectation values [5], and static and dynamic response functions [6]. We will in particular discuss the application to hyperfine coupling tensors [5] and outline some of the subtle problems that occur in the computation of icMRCC response functions [6].
A second thread starts from the multistate generalization of icMRCC theory [7] and focusses on the computation of properties for (quasi-)degenerate states. In particular we will discuss some initial results for the computation of spin-orbit coupling matrix elements of $^2\Pi$ radicals [8].

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