# Formulation of an Internally Contracted Multi-Reference Coupled-Cluster Based Linear Response Theory to Study Excited States

Pradipta Kumar Samanta[1], Matthias Hanauer,[2]
Andreas Köhn[2] and Debashis Mukherjee,[1]

[1] Raman Center for Atomic, Molecular and Optical Sciences, Indian Association for the Cultivation of Science, Kolkata, India
[2] Institut für Physikalische Chemie, Universität Mainz, Mainz, Germany

Linear Reponse (LR) theory is an effective tool to calculate the excitation energies of chemical systems which have a proper ground state description. For systems having prominent Multi-Reference (MR) characters in their electronic ground state, a number of different MR theories have been developed in the past years which can be divided into two broad categories: (a) Theories where the different model functions are used as the reference states. (b) Theories which use a contracted description, i.e., a linear combination of the model functions are exploited. The second class of theories are known as 'Internally Contracted MR' (IC-MR) theories.

In our present formulation, we have developed and implemented a linear response theory based on internally contracted multireference coupled-cluster theory (ic-MRCC-LRT, [1]). Excitation energies can be obtained, using LRT framework, as the poles of the response function when an external field acts on its ground state. The formulation of the ic-MRCC-LRT can be approached differently by treating the external field in a time-dependent [2] or time-independent manner [3]. These two approaches lead to different final expressions as here the cluster operators are non-commuting and have been truncated after doubles excitations.

We will present some pilot numerical applications of the above mentioned ic-MRCC-LRT. Our results indicate that the ic-MRCC response functions are well-behaved and the resulting excitation energies turn out to be very accurate. The method is particularly promising for the description of doubly excited states and photochemical pathways.

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