

# Singular analysis of RPA diagrams in coupled cluster theory

Heinz-Jürgen Flad

Zentrum Mathematik, Technische Universität München  
Boltzmannstr 3, D-85748 Garching

Coupled cluster theory is presently considered as the ultimate benchmark in quantum chemistry. The present work focuses on nonlinear coupled cluster models within the random phase approximation (RPA). Solutions of these models are commonly represented by series of Goldstone diagrams. We present a detailed asymptotic analysis of these so-called RPA diagrams using techniques from singular analysis and discuss their computational complexity within adaptive approximation schemes. In particular, we provide a connection between RPA diagrams and classical pseudo-differential operators which enables an efficient treatment of the linear and nonlinear interactions in these models. Finally, we discuss a best  $N$ -term approximation scheme for RPA-diagrams and provide the corresponding convergence rates.

This is joint work with Gohar Flad-Harutyunyan (TU München)