EXCITED STATES FROM LOCAL METHODS

Danylo Kats, Martin Schütz

Theoretische Chemie, Universität Regensburg
Universitätsstraße 31, D-93040 Regensburg, Germany

The calculation of excitation energies and first-order properties of excited states with *a-priori* restricted local methods is a challenging task, since one needs information about the state-character *before* the calculation. One possibility is to take it from an initial lower level method calculation like CCS [1, 2, 3]. Yet such an approach is too strongly dependent on the quality of this initial calculation.
With the Laplace-transform formalism [4, 5] we are able to solve this problem by adapting the local approximations on-the-fly during the calculation [6]. As a further advantage, the Laplace-transform technique considerably speeds up the convergence, reduces the I/O rate and memory usage. Furthermore, it permits multi state calculations and a new type of local approximations from Laplace transformed quantities.
Test calculations on various molecules demonstrate robustness and accuracy of the new method.

Literature:

[1] T.Korona, H.J.Werner, *J. Chem. Phys.* 118 (2003) 3006
[2] D.Kats, T.Korona, and M.Schütz, *J. Chem. Phys.* 125 (2006) 104106
[3] D.Kats, T.Korona, and M.Schütz, *J. Chem. Phys.* 127 (2007) 064107
[4] J. Almlöf, *Chem. Phys. Letters* 181 (1991) 319
[5] D.Kats, D.Usvyat, and M.Schütz, *Phys. Chem. Chem. Phys.* 10 (2008) 3430
[6] D.Kats, M.Schütz, *J. Chem. Phys.* 131 (2009) 124117