Compression of sets of products of atomic orbitals, with applications to TDDFT and GW

D. Foerster CPMOH/LOMA, University of Bordeaux I, France
d.foerster@cpmoh.u-bordeaux1.fr

Molecular orbitals in clusters or molecules can be conveniently expressed as linear combinations of localized atomic orbitals. Products of overlapping orbitals occur in electronic densities and these, by contrast, are linearly dependent. An improved solution of this well known technical problem leads to

(i) a new solution of the Petersilka-Gossmann-Gross equation of TDDFT -
(ii) a new $O(N^3)$ implementation, without plasmon parametrization, of Hedin's GW scheme.

Here we describe aspects of the compression algorithms we developed and their effect on the accuracy of spectra and electronic spectral functions in TDDFT and GW, respectively.

References

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See also the contribution by P. Koval on "$O(N^3)$ GW" at the session on HPC.