# NEW SOLUTIONS FOR AN OLD PROBLEM: AN EFFICIENT AND ROBUST SOLVER FOR LINEAR RESPONSE EQUATIONS

T. Nottoli, D. Cianchino, I. Gianní, R. Alessandro, F. Pes, **F. Lipparini**
Department of Chemistry and Industrial Chemistry, University of Pisa
Via G. Moruzzi 13, I-56124 Pisa, Italy
filippo.lipparini@unipi.it

Linear response theory is one of the most powerful tools in computational quantum chemistry, as it allows to directly connect calculation with experimental spectroscopic measurements. In linear response theory, excitation energies and transition moments, that are associated with the positions and intensities of the peaks in spectra, are compute as the eigenvalues and eigenvectors of a generalized eigenvalue problem. As such a problem can be very large, the development of efficient iterative algorithms is paramount. In this contribution, we start from the state of the art algorithm, originally proposed by Olsen almost 40 years ago [1], and using a simple, but effective strategy, recast it into a new iterative procedure which is not only more efficient, but also particularly robust from a numerical point of view [2]. We compare the algorithm not only to the Olsen method, but also to a recent proposed modification of the latter [3], and to a more specialized algorithm that is commonly use in the special case of time-dependent Density Functional Theory [4].

## References

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