

Title: Electron-Molecule Collision Calculations Based On The First Born Approximation and EOM-CCSD

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Abstract: There is a long history of important developments in quantum theory supported exclusively on scattering experiments. Concerning particularly the subfield of electron collision, there are still important topics such as atmospheric chemistry and the growing relevance of electron energy loss spectroscopy to name just a few[1].

The Born approximation is as old as quantum mechanics itself, and it is still the fundamental tool for collisions within fast electrons. While keeping the energy of the bound states as a lower limit, the Born approximation is the prevalent theoretical treatment for electron-molecule collisions [2]. Therefore, the main issue to be attacked is the dependence on the molecular wave functions. The method is very sensitive to the quality of the wave functions and the theoretical apparatus of highly correlated methods are of fundamental importance.

The problem of electron scattering by molecule has not profited decades of developments of quantum chemistry methods, which is evidenced by the absence of calculations of properties related to scattering problems in modern quantum chemistry computational packages. This led us to work on methods for practical computation of scattering amplitudes based on high quality wave functions. Very successful applications were found by using density matrices obtained from equation of motion – coupled cluster singles and doubles(EOM-CCSD)[3] and configuration interaction(CI). The convenience of using an Octave [4] scripts has an immediate trade off on computer time, although for an average ten minute computation we were able to obtain good accuracy. These results are presented here for a series of small molecules used as benchmark. Results include some scattering experiments never simulated before with quantitative accuracy.

Key-words: Scattering, Collision, EOM-CCSD, Born Approximation

Support: CNPq

References:

- [1] Brydson, R. "Electron Energy Loss Spectroscopy" (2001) A. Köhler (editor) , Royal Microscopical Society MICROSCOPIC HANDBOOKS Volume 48, BIOS Scientific Publishers Ltd, Oxford, UK
- [2] M. Inokuti, Rev. Mod. Phys. 43, 3 (1971). 297-347.
- [3] J. F. Stanton and R. J. Bartlett, J. Chem. Phys., 98 (1993) 7029-39.