Séminaire de Chimie Théorique

Salle conférence, 3eme Est, bat. A12

Mercredi 8 Juin à 11:00

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A Sturmian Approach for ionization processes of atoms and molecules

The Sturmian approach, using Generalized Sturmian Functions (GSF), is a spectral method that has been applied successfully both for structure calculations [1] and for the study of several ionization processes [2] with atomic targets.
GSF are two-body functions that solve a Sturm-Liouville problem. They can be used as a basis set to solve correlated three-body bound or scattering problems. When compared with other basis functions, the GSF increase expansions convergence rates because they diagonalize the kinetic energy and the main (Coulomb) interactions. Moreover, the whole GSF set can be chosen to possess asymptotic conditions appropriate for the physical problem under consideration: bound-type behavior with a specific asymptotic charge are chosen for bound states, while – for example - outgoing behavior with a given adequate energy are taken for solving scattering processes.
In this presentation, I will review the GSF method and show some applications in three-body correlated (bound and continuum) atomic systems. I will also briefly describe the recent extension and implementation of the Sturmian approach for single ionization of molecules by photon and electron impact [3].

References
(1) G. Gasaneo et al., Adv. Quantum Chem. **67**, 153 (2013) ; J.M. Randazzo et al., Phys. Rev. A **81** 042520 (2010)
(2) M.J. Ambrosio et al., J Phys. B **48** 055204 (2015) ; J.M. Randazzo et al., Eur. J. Phys. D, **69**, 189 (2015) ; M.J. Ambrosio et al., Phys. Rev. A, **92**, 042704 (2015)
(3) C.M. Granados-Castro et al., Adv. Quantum Chem., **73**, 3 (2016); C.M. Granados-Castro, PhD Thesis – Université de Lorraine (2016)

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