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A Sturmian approach for ionization processes of atoms and molecules[1]

LORENZO UGO ANCARANI, Universite de Lorraine, Metz, France

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 deal with two- or three-body bound or scattering problems. By construction, 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. This important intrinsic property makes GSF basis sets - and thus the whole approach - computationally efficient. In the case of ionization, a specific feature of our methodology is that the scattering amplitude and the corresponding cross section are extracted directly from the asymptotic part of the scattering function without requiring the evaluation of a matrix element. Compared to the case of many-electron atoms several extra challenges occur for molecules: the scattering problem is generally multicenter and highly non-central, and the molecular orientation must also be taken into account. These features make the computational task much more cumbersome and expensive than for atomic targets. The Sturmian approach with GSF has been recently extended and implemented to study single ionization of small polyatomic molecules by photon and electron impact [3]. Results for a variety of single and double ionization processes will be presented. [1] G. Gasaneo et al., Adv. Quantum Chem. **67,** 153 (2013). [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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