IONIZATION PROCESSES OF ATOMS AND MOLECULES: A STURMIAN APPROACH

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Résumé

The ionization of atoms and molecules by photon or charged particle impact is a N-body Coulomb problem. Its quantum mechanical study requires, amongst other things, an adequate description of continuum states. In practical calculations one needs accurate wave functions, on large radial domains, corresponding to one or two active electrons escaping in the field of the ionized target.
In the last ten years a Sturmian approach, using Generalized Sturmian Functions (GSF), has been developed and applied successfully both for structure calculations [1,2,3] and for the study of several ionization processes with atomic (by impact of electrons [4], protons [5] or photons [6]) and, more recently, with molecular (by impact of photons [7] or electrons [8]) targets.

GSF are two-body functions that solve a Sturm-Liouville problem. They can be used as a numerically efficient orthogonal and complete basis set to solve correlated Coulomb three-body bound or scattering problems. 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 property makes the GSF method particularly adapted when applied to describe charged particles in their long-range Coulomb interaction.

In the presentation, I will briefly review the GSF method and show some applications in three-body correlated continuum systems.

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