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Quasi-Sturmian basis functions for two- and three-body scattering problems. JESSICA A. DEL PUNTA, LORENZO UGO ANCARANI, Universite de Lorraine, Metz, France, GUSTAVO GASANEO, Universidad Nacional del Sur, Bahia Blanca, Argentina — For quantum three-body scattering processes, one important theoretical issue is how to impose to the wave function the correct asymptotic behavior. In many methods the problem is solved using basis functions that generally do not possess the correct behavior at large distances. One exception is given by the Generalized Sturmian Functions (GSF) [1] which are defined taking into account the interactions of the problem under consideration, thus making them an efficient basis set. We present in this work an alternative set of basis functions, named Quasi Sturmian Functions (QSF). Starting with the two-body case [2], QSF satisfy a non-homogeneous differential equation, and may be constructed with a selected asymptotic behavior (e.g. outgoing). Contrary to GSF, these basis functions have analytical closed form for the case of a Coulomb potential. Moreover, we showed that the QSF provide a superior convergency rate when solving a two-body scattering problem. For the three-body case, we propose a representation using hyperspherical coordinates. While the angular variables are treated in a parametric way, the hyperradial part of these new QSF basis functions are obtained by a generalization of the method used for the two-body problem. As a consequence, analytical expressions can be given for these new QSF and the desired Coulomb asymptotic behavior in the hyperradial coordinate can be imposed.

[1] G. Gasaneo et al, Adv. Quantum Chem., 67, 153 (2013) [2] J. A. Del Punta el al, J. Math. Phys., 55, 052101 (2014).

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