J. At. Mol. Sci.
doi: 10.4208/jams.121312.012013a

Vol. 4, No. 4 , pp. 302-320
November 2013

Solving a three-body continuum Coulomb problem with quasi-Sturmian functions

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Received 13 December 2012; Accepted (in revised version) 20 January 2013
Published Online 30 August 2013

Abstract. The scattering problem of three particles interacting via Coulomb potentials is studied using generalized parabolic coordinates. The scattering solutions are obtained by solving a driven equation. The 'perturbation' operator appearing in the driven term is the non-orthogonal part of the kinetic energy operator. The approximated solution appearing in the driven term is the product of two two-body Coulomb wave functions. As a test for our proposal, a simple two-dimensional model problem has been solved numerically by using so called parabolic quasi-Sturmian basis representation. Convergence of the solution has been obtained as the basis set is enlarged.

PACS: 34.50.Fa, 34.10.+x, 03.65.Nk

Key words: three-body coulomb system, parabolic coordinates, driven equation, quasi-Sturmians, convergence

1 Introduction

The three-body continuum Coulomb problem is one of the fundamental unresolved problems of theoretical physics. In atomic physics, a prototype example is a two-electron continuum which arises as a final state in electron-impact ionization and double photoionization of atomic systems. Several discrete-basis-set methods for the calculation of such processes have recently been developed including convergent close coupling (CCC) [1,2], the Coulomb-Sturmian separable expansion method [3,4], the J-matrix method [5–7], the Generalized Sturmian approach [8, 9]. In all these approaches the continuous Hamiltonian spectrum is represented in the context of complete square integrable bases. Despite the enormous progress made so far in discretization and subsequent numerical solutions

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of three-body differential and integral equations of the Coulomb scattering theory, a number of related mathematical problems remain open. Actually, the use of a product of two fixed charge Coulomb waves for the two outgoing electrons as an approximation to the three-body continuum state is typical of these approaches. As a consequence, a long-range potential appears in the kernel of the corresponding Lippmann-Schwinger (LS) equation. Since this integral equation is, in principle, non-compact, its formal solution therefore should be divergent. Note, however that for the two-body problem this type of definition for the 'free particle solution' is not leading to a divergent solution [10]. In addition, for the three-body case approaches such as the exterior complex scaling [11] and the generalized Sturmian approaches [8, 9] lead to correct solutions for the driven equation from which the LS equations are derived. One of the aims of this paper is to understand the reason for that differences between the solution corresponding to LS type and driven equations.

On the other hand, it is well known [12, 13] that for large particle separations (in the Ω_0 region) the Schrödinger equation for a three-body Coulomb system is separable in terms of so called generalized parabolic coordinates $\left\{\xi_j,\eta_j\right\}$, $j=1,2,3$ [13, 14]. Moreover, a representation of the corresponding Green's function operator has been derived in [15]. Thus, at first glance it would seem that a formal solution for the three-body Coulomb problem can be expressed in the form of a Lippmann-Schwinger-type equation, where the potential operator, which coincides with the non-orthogonal part of the kinetic energy operator, is expressed in terms of second partial mixed derivatives whit respect to the parabolic coordinates. No complete studies of the compactness of the kernel of this integral equation can be found in the literature [16]. Actually, a differential operator of this type seems to be unbounded in a Hilbert space and therefore the corresponding LS equation could presents difficulties in its formal solution. To avoid these problems, an alternative approach can be performed by considering an inhomogeneous Schrödinger equation whose driven term is square integrable. In this paper we formulate a procedure for solving the driven equation using so called quasi-Sturmian (QS) functions. Unlike Sturmian functions (see, e. g., [17–20] and references therein), which are eigensolutions of a Sturm-Liouville differential or integral equation, and form a complete set of basis functions, the QS are constructed from square-integrable basis functions with the help of an appropriate Coulomb Green's function operator. In order to test practically the QS approach and the solution to an equation of a driven type instead of LS equations we consider a simple two-dimensional model problem on the plane (ξ_1,ξ_3). Here the total wave operator, aside from the one-dimension Coulomb wave operators $\hat{\mathfrak{h}}_1$ and $\hat{\mathfrak{h}}_3$, contains the 'perturbation' term $\frac{\partial^2}{\partial\xi_1\partial\xi_3}$.

This paper is organized as follows. In Section II we introduce the notations, recall the generalized parabolic coordinates definition and express a formal solution for the three-body Coulomb problem in the form of a driven equation. In Section III we present the quasi-Sturmian functions and its properties. We also present its representation in terms of Laguerre basis functions and some of its properties. In Section IV a simple two-dimensional model is presented and used to test the parabolic QS approach. The calcu-