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 $\{\xi_j, \eta_j\}$, $j=1,2,3$ [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-

lations of the continuum wave function is performed. A study of the convergence rate as a function of the number of the quasi-Sturmians used is presented. Some conclusion are given in Section V. Atomic units are used throughout.

2 Coulomb three-body system in parabolic coordinates

2.1 General considerations

We consider three particles of masses m_1, m_2, m_3, charges Z_1, Z_2, Z_3 and momenta $\mathbf{k}_1$, $\mathbf{k}_2$, $\mathbf{k}_3$. The Hamiltonian of the system in the center of mass frame of reference is given by

$$\hat{H} = -\frac{1}{2\mu_{12}}\Delta_{\mathbf{R}} - \frac{1}{2\mu_3}\Delta_{\mathbf{r}} + \frac{Z_1Z_2}{r_{12}} + \frac{Z_2Z_3}{r_{23}} + \frac{Z_1Z_3}{r_{13}}, \tag{1}$$

where $\mathbf{r}_{ls}$ denotes the relative coordinates

$$\mathbf{r}_{ls} = \mathbf{r}_l - \mathbf{r}_s, \quad r_{ls} = |\mathbf{r}_{ls}|, \tag{2}$$

$\mathbf{R}$ and $\mathbf{r}$ are the Jacobi coordinates

$$\mathbf{R} = \mathbf{r}_1 - \mathbf{r}_2, \quad \mathbf{r} = \mathbf{r}_3 - \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2}. \tag{3}$$

The reduced masses are defined as

$$\mu_{12} = \frac{m_1m_2}{m_1+m_2}, \quad \mu_3 = \frac{m_3(m_1+m_2)}{m_1+m_2+m_3}. \tag{4}$$

In the Schrödinger equation

$$\hat{H}\Phi = E\Phi \tag{5}$$

the eigenenergy $E > 0$ is given by

$$E = \frac{1}{2\mu_{12}}\mathbf{K}^2 + \frac{1}{2\mu_3}\mathbf{k}^2, \tag{6}$$

where $\mathbf{K}$ and $\mathbf{k}$ are the momenta conjugate to the variables $\mathbf{R}$ and $\mathbf{r}$. By substituting

$$\Phi = e^{i(\mathbf{K}\cdot\mathbf{R} + \mathbf{k}\cdot\mathbf{r})}\Psi \tag{7}$$

into (5), we arrive at the equation for the reduced wave function Ψ

$$\left[-\frac{1}{2\mu_{12}}\Delta_{\mathbf{R}} - \frac{1}{2\mu_3}\Delta_{\mathbf{r}} - \frac{i}{\mu_{12}}\mathbf{K}\cdot\nabla_{\mathbf{R}} - \frac{i}{\mu_3}\mathbf{k}\cdot\nabla_{\mathbf{r}} + \frac{Z_1Z_2}{r_{12}} + \frac{Z_2Z_3}{r_{23}} + \frac{Z_1Z_3}{r_{13}}\right]\Psi = 0. \tag{8}$$

The leading-order asymptotic terms of Ψ in the Ω_0 domain are expressed in terms of the generalized parabolic coordinates [13]

$$\begin{aligned}\xi_1 &= r_{23} + \hat{\mathbf{k}}_{23}\cdot\mathbf{r}_{23}, \quad \eta_1 = r_{23} - \hat{\mathbf{k}}_{23}\cdot\mathbf{r}_{23},\\ \xi_2 &= r_{13} + \hat{\mathbf{k}}_{13}\cdot\mathbf{r}_{13}, \quad \eta_2 = r_{13} - \hat{\mathbf{k}}_{13}\cdot\mathbf{r}_{13},\\ \xi_3 &= r_{12} + \hat{\mathbf{k}}_{12}\cdot\mathbf{r}_{12}, \quad \eta_3 = r_{12} - \hat{\mathbf{k}}_{12}\cdot\mathbf{r}_{12},\end{aligned} \tag{9}$$

where $\mathbf{k}_{ls} = \frac{\mathbf{k}_l m_s - \mathbf{k}_s m_l}{m_l + m_s}$ is the relative momentum, $\hat{\mathbf{k}}_{ls} = \frac{\mathbf{k}_{ls}}{k_{ls}}$ and $k_{ls} = |\mathbf{k}_{ls}|$. The operator in the square brackets, denoted by $\hat{D}$, can be decomposed into two terms [13]

$$\hat{D} = \hat{D}_0 + \hat{D}_1, \tag{10}$$

where the operator $\hat{D}_0$ contains the leading term of the kinetic energy and the total potential energy

$$\hat{D}_0 = \sum_{j=1}^{3} \frac{1}{\mu_{ls}(\xi_j + \eta_j)} \left[\hat{h}_{\xi_j} + \hat{h}_{\eta_j} + 2k_{ls}t_{ls}\right], \quad \text{for } j \neq l,s \text{ and } l < s, \tag{11}$$

$$\hat{h}_{\xi_j} = -2\left(\frac{\partial}{\partial\xi_j}\xi_j\frac{\partial}{\partial\xi_j} + ik_{ls}\xi_j\frac{\partial}{\partial\xi_j}\right), \tag{12}$$

$$\hat{h}_{\eta_j} = -2\left(\frac{\partial}{\partial\eta_j}\eta_j\frac{\partial}{\partial\eta_j} - ik_{ls}\eta_j\frac{\partial}{\partial\eta_j}\right). \tag{13}$$

Here $t_{ls} = \frac{Z_l Z_s \mu_{ls}}{k_{ls}}$ and $\mu_{ls} = \frac{m_l m_s}{m_l + m_s}$. $\hat{D}_1$ represents the remaining part of the kinetic energy operator [13] which, in the case of the $(e^-, e^-, \mathrm{He}^{++}) = (123)$ system with $m_3 = \infty$, takes the form [21]

$$\begin{aligned}\hat{D}_1 = \sum_{j=1}^{2}(-1)^{j+1}\Big[&\mathbf{u}_j^- \cdot \mathbf{u}_3^- \frac{\partial^2}{\partial\xi_j\partial\xi_3} + \mathbf{u}_j^- \cdot \mathbf{u}_3^+ \frac{\partial^2}{\partial\xi_j\partial\eta_3}\\ &+ \mathbf{u}_j^+ \cdot \mathbf{u}_3^- \frac{\partial^2}{\partial\eta_j\partial\xi_3} + \mathbf{u}_j^+ \cdot \mathbf{u}_3^+ \frac{\partial^2}{\partial\eta_j\partial\eta_3}\Big],\end{aligned} \tag{14}$$

where

$$\mathbf{u}_j^{\pm} = \hat{\mathbf{r}}_{ls} \mp \hat{\mathbf{k}}_{ls}. \tag{15}$$

The asymptotic behavior of Ψ is determined by the operator $\hat{D}_0$. In particular, there exist solutions to the equation

$$\hat{D}_0\Psi_{C3} = 0, \tag{16}$$

which satisfy the Redmond conditions in Ω_0. These solutions are the well-known C3 wave function. Ψ_{C3} is expressed in terms of a product of three Coulomb waves. For example, Ψ_{C3} with pure outgoing behavior is written as

$$\Psi_{C3} = \prod_{j=1}^{3} {}_1F_1\left(it_{ls}, 1; -ik_{ls}\xi_j\right). \tag{17}$$

In turn, $\hat{D}_1$ is regarded as a perturbation which does not violate the asymptotic conditions [13, 14].

2.2 Formal solution of the problem

At first sight, given the Green's function operator $\hat{\mathcal{G}} = \hat{D}_0^{-1}$ (see [15]), one could take into account the non-orthogonal term $\hat{D}_1$ of the kinetic energy operator by putting it into the kernel of the Lippmann-Schwinger type equation

$$\begin{aligned} \Psi &= \Psi_{C3} - \hat{\mathcal{G}}\hat{\mathcal{V}}\Psi, \\ \hat{\mathcal{V}} &\equiv \hat{D}_1. \end{aligned} \tag{18}$$

If the kernel $\hat{\mathcal{G}}\hat{\mathcal{V}}$ is compact, then the integral equation (18) can be solved by an algebraic method based on the fact that a compact operator may be uniformly approximated by operators of finite rank. For this purpose a set of square-integrable parabolic Laguerre basis functions [22]

$$|\mathfrak{N}\rangle \equiv \mathfrak{B}_{\mathfrak{N}}(\xi,\eta) = \prod_{j=1}^{3} \phi_{n_j m_j}(\xi_j,\eta_j), \tag{19}$$

$$\phi_{n_j m_j}(\xi_j,\eta_j) = \psi_{n_j}(\xi_j)\,\psi_{m_j}(\eta_j), \tag{20}$$

$$\psi_n(x) = \sqrt{2b_j}\,e^{-b_j x} L_n(2b_j x), \tag{21}$$

could be used. The index $\mathfrak{N}$ lists all the indexes of the basis function $\mathfrak{N}=\{n_1,m_1,n_2,m_2,n_3,m_3\}$ and the argument (ξ,η) of the function $\mathfrak{B}_{\mathfrak{N}}(\xi,\eta)$ represents in compact form the dependence on all the parabolic coordinates. The basis functions (20), (21) are parametrized with different Coulomb Sturmian exponents b_j for each pair $\{\xi_j,\eta_j\}$, $j=\overline{1,3}$. Thus, the operator $\hat{\mathcal{V}}$ is represented by its projection $\hat{\mathcal{V}}^{\mathcal{N}}$ onto a subspace of basis functions,

$$\hat{\mathcal{V}}^{\mathcal{N}} = \sum_{\mathfrak{N},\mathfrak{N}'=0}^{\mathfrak{N}_0} |\mathfrak{N}\rangle \langle\mathfrak{N}|\hat{\mathcal{V}}|\mathfrak{N}'\rangle \langle\mathfrak{N}'|, \tag{22}$$

and the solution Ψ of the problem is obtained for $\hat{\mathcal{V}}^{\mathcal{N}}$. Inserting $\hat{\mathcal{V}}^{\mathcal{N}}$ into Eq. (18) then leads to a finite matrix equation for the expansion coefficients $[\underline{a}]_{\mathfrak{N}} = \langle\mathfrak{N}|\Psi\rangle$,

$$\underline{a} = \underline{a}^{(0)} - \underline{\mathcal{G}}\,\underline{\mathcal{V}}\,\underline{a}, \tag{23}$$

which has the solution

$$\underline{a} = (\underline{1} + \underline{\mathcal{G}}\,\underline{\mathcal{V}})^{-1}\,\underline{a}^{(0)}. \tag{24}$$

Here $[\underline{\mathcal{G}}]_{\mathfrak{N}\mathfrak{N}'} = \langle\mathfrak{N}|\hat{\mathcal{G}}|\mathfrak{N}'\rangle$ and $[\underline{\mathcal{V}}]_{\mathfrak{N}\mathfrak{N}'} = \langle\mathfrak{N}|\hat{\mathcal{V}}|\mathfrak{N}'\rangle$ are the Green's function operator and potential operator matrices of the size $\mathfrak{N}_0+1$, and $\underline{a}^{(0)}$ is the coefficient vector of Ψ_{C3}. The wave function Ψ is expressed in terms of the solution of Eq. (23)

$$\Psi = \Psi_{C3} - \sum_{\mathfrak{N}=0}^{\mathfrak{N}_0} [\underline{C}]_{\mathfrak{N}}\hat{\mathcal{G}}|\mathfrak{N}\rangle, \tag{25}$$

where $\underline{C} = \underline{\mathcal{V}a}$.

We performed different studies of this equation and we found that the kernel is not compact when is expressed in terms of L^2-spaces. Actually the problem is that the standard L^2 bases do not possess the appropriated asymptotic behavior of the problem. Thus, this means that the asymptotic behavior has to be constructed and then the perturbation operator $\hat{D}_1$ (14) seems to be not bounded. However, if the basis already possesses the asymptotic behavior of the problem, then, the operator turns to be of a short range and then becomes compact and manageable.

Even when what we just mentioned is possible, we will explore an alternative approach to the problem based on the study of the driven equation

$$\left[\hat{D}_0 + \hat{D}_1\right] \Psi_{sc} = -\hat{D}_1 \Psi_{C3}, \tag{26}$$

where the wave function Ψ is split into an outgoing (incoming) part Ψ_{C3} and a scattering Ψ_{sc} part

$$\Psi = \Psi_{sc} + \Psi_{C3}. \tag{27}$$

Note that the inhomogeneity in (26) is a square-integrable function. Eq. (25) in turn gives a hint as to how the solution Ψ_{sc} to (26) may be constructed with the help of the square-integrable basis (19). Namely, we suppose that the wave function Ψ can be expressed in the form (25), i. e., propose to expand Ψ_{sc} as

$$\Psi_{sc} = \sum_{\mathfrak{N}=0} [\underline{c}]_{\mathfrak{N}} |\mathcal{Q}_{\mathfrak{N}}\rangle, \tag{28}$$

where

$$|\mathcal{Q}_{\mathfrak{N}}\rangle \equiv \hat{\mathcal{G}} |\mathfrak{N}\rangle. \tag{29}$$

We will call $|\mathcal{Q}_{\mathfrak{N}}\rangle$ *quasi-Sturmian functions*. The word 'quasi' refers to the fact that in order to obtain these functions there is no need to solve a Sturm-Liouville equation.

3 Quasi Sturmian functions

According with the definition of Eq. (29) the QS functions satisfy the following driven equation

$$\hat{D}_0 \mathcal{Q}_{\mathfrak{N}}(\xi, \eta) = \mathfrak{B}_{\mathfrak{N}}(\xi, \eta) \tag{30}$$

and they possess the same asymptotic behavior as the Green's function $\hat{\mathcal{G}}$. In this case we are using on the right-hand-side the Laguerre type basis functions $\mathfrak{B}_{\mathfrak{N}}(\xi, \eta)$, but any basis set can be used. However, to preserve the asymptotic behavior of the $\mathcal{Q}_{\mathfrak{N}}$ functions, the extent of the basis functions in the configuration space has to be finite. A closed form expression for the Green's function $\hat{\mathcal{G}}$ was given in Ref. [23] and this allows one to express the QS functions in terms of special functions. The right hand side of (30) depends on the indexes $\mathfrak{N}$, thus for each set of values $\mathfrak{N}$ we have different functions $\mathcal{Q}_{\mathfrak{N}}$. All of these functions form a complete basis set even when they are not orthogonal.

When solving Eq. (26) with the proposal (28) we enforce the solution to possess the correct outgoing behavior of the scattering function. This is similar to what it is observed when generalized Sturmian functions are used [8, 9]. The completeness of the $\mathcal{Q}_{\mathfrak{N}}$, the short-range of both the right-hand-side and $\hat{D}_1\mathcal{Q}_{\mathfrak{N}}$ allow to assure that this expansion converges. To exemplify this affirmation we will solve in the following sections a two-dimensional model problem presented in [21]. We will use a product of one-dimensional QS functions obtained from one-dimensional Green's function

$$\mathcal{Q}_n(k,\xi) \equiv \int d\xi' G^{(+)}(k;\xi,\xi')\psi_n(\xi'). \tag{31}$$

This will allow us to probe the convergence of the expansion of two-dimensional scattering wave function before considering a very elaborate and cumbersome six-dimensional case as required for the full three-body problem.

3.1 Definitions and asymptotic behaviors

We start with the Green's function which satisfies the equation

$$\left[-2\frac{\partial}{\partial\xi}\xi\frac{\partial}{\partial\xi} - 2ik\xi\frac{\partial}{\partial\xi} + 2kt\right] g^{(+)}\left(k;\xi,\xi'\right) = \delta(\xi-\xi') \tag{32}$$

One of the solutions of the equation (32) can be written

$$g^{s(+)}\left(k;\xi,\xi'\right) = \frac{\Gamma(it)}{2}\,{}_1F_1\left(it,1,-ik\xi_<\right) U\left(it,1;-ik\xi_>\right) e^{ik\xi'}. \tag{33}$$

Lets us define the functions

$$\mathfrak{q}_n^s(k,\xi) \equiv \int d\xi' g^{s(+)}(k;\xi,\xi')\psi_n(\xi'), \tag{34}$$

It follows from (33) and (34) that

$$\mathfrak{q}_n^s(k,\xi) \underset{\xi\to\infty}{\sim} v_n U\left(it,1;-ik\xi\right), \tag{35}$$

where

$$\begin{aligned} v_n &\equiv \frac{\Gamma(it)}{2}\int_0^\infty d\xi\, {}_1F_1\left(it,1,-ik\xi\right) e^{ik\xi}\psi_n(\xi) \\ &= \frac{1}{\sqrt{2b}}\left(\frac{1+\omega}{2\omega}\right)^{1-it}(-\omega)^{-n}\frac{\Gamma(it)\Gamma(n+1-it)}{n!\Gamma(1-it)}\,{}_2F_1(-n,it;it-n;\omega), \\ \omega &= \frac{b-ik}{b+ik}. \end{aligned} \tag{36}$$

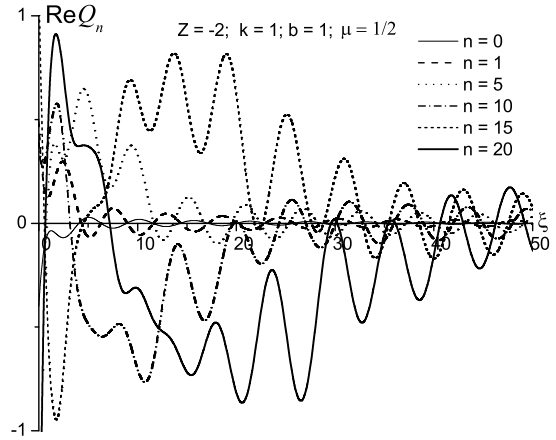

Figure 1: Real parts of QS functions $\mathcal{Q}_n$ (51), (43), (40) for $Z=-2$, $k=1$, $b=1$, $\mu=\frac{1}{2}$.

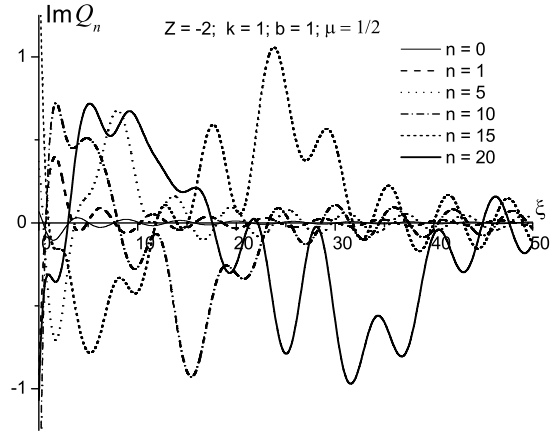

Figure 2: The same as in Fig. 1 but for the imaginary parts.

Using the integral representation for the Whittaker functions [24] we can write

$$g^{s(+)}(k;\xi,\xi') = \frac{1}{2} e^{i\frac{k}{2}(\xi'-\xi)} \int_0^\infty dz \exp\left\{ i\frac{k}{2}(\xi+\xi')\cosh(z) \right\} \times \left[\coth(\frac{z}{2})\right]^{-2it} I_0\left(-ik\sqrt{\xi\xi'}\sinh(z)\right), \tag{37}$$

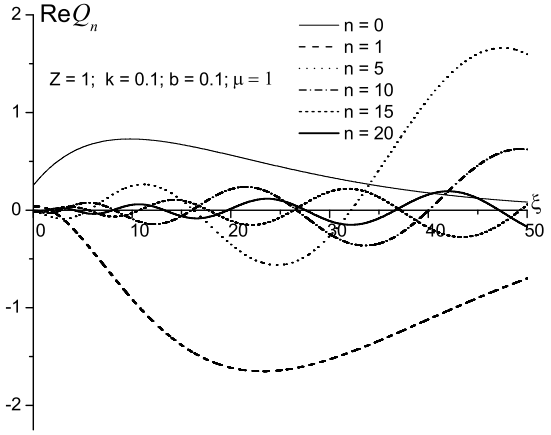

Figure 3: The same as in Fig. 1 but for $Z=1$, $k=0.1$, $b=0.1$, $\mu=1$.

where I_ν is the modified Bessel function [24]. Inserting (37) into the integral (34), we get

$$\mathfrak{q}_n^s(k,\xi)=\frac{(-1)^n}{\sqrt{2b}}\int_0^1 \frac{dx\,x^{it-1}}{(1-\frac{ik}{b}-x)}\left(\frac{1+\frac{ik}{b}-x}{1-\frac{ik}{b}-x}\right)^n \exp\left(\frac{ik\xi x}{1-\frac{ik}{b}-x}\right) \times L_n\left[\frac{\frac{2k}{b}k\xi x}{(1-\frac{ik}{b}-x)(1+\frac{ik}{b}-x)}\right]. \tag{38}$$

Expanding the exponential factor in (38) $\mathfrak{q}_n^s$ can be expressed in the form

$$\mathfrak{q}_n^s(k,\xi)=\frac{e^{-b\xi}}{\sqrt{2b}}\frac{1+\omega}{2\omega}\sum_{m=0}^{\infty}\frac{(b\xi)^m}{m!}\left[\sum_{\ell=0}^{n}(-1)^\ell\binom{n}{\ell}\frac{(2b\xi)^\ell}{\ell!}\left\{\sum_{j=0}^{n-\ell}(-1)^j\binom{n-\ell}{j}\left(\frac{1+\omega}{\omega}\right)^j \times\frac{\Gamma(m+j+1)\Gamma(it+\ell)}{\Gamma(it+\ell+m+j+1)}{}_2F_1\left(it-\ell,m+j+1;it+\ell+m+j+1;\frac{1+\omega}{2\omega}\right)\right\}\right]. \tag{39}$$

Assuming that there exist a factor x^ϵ, $\epsilon=+0$ in the integrand, we can perform the integral (38) by parts

$$\mathfrak{q}_n^s(k,\xi)=\frac{1}{2kt}\psi_n(\xi)-\frac{(-1)^n}{it\sqrt{2b}}\int_0^1 dx\,x^{it} \times\frac{d}{dx}\left\{\frac{\left(1+\frac{ik}{b}-x\right)^n}{\left(1-\frac{ik}{b}-x\right)^{n+1}}\exp\left(\frac{ik\xi x}{1-\frac{ik}{b}-x}\right)L_n\left[\frac{\frac{2k}{b}k\xi x}{(1-\frac{ik}{b}-x)(1+\frac{ik}{b}-x)}\right]\right\}. \tag{40}$$

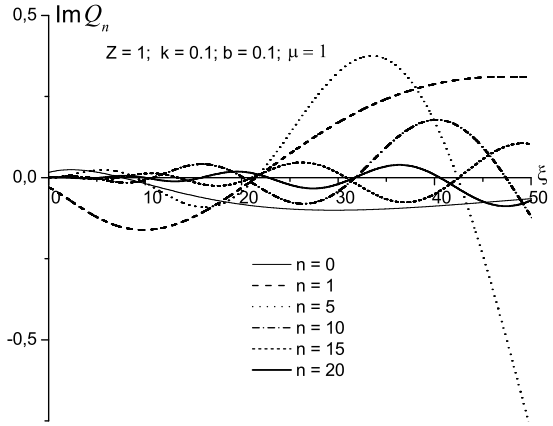

Figure 4: The same as in Fig. 3 but for the imaginary parts.

We have found in our numerical calculations that it is preferable to use this representation rather than the series (39).

Note that the Green's function

$$g^{(+)}(k;\xi,\xi') = \frac{\Gamma(it)}{2}{}_1F_1(it,1,-ik\xi_<)\,[U(it,1;-ik\xi_>) - \alpha\,{}_1F_1(it,1,-ik\xi_>)]\,e^{ik\xi'}, \tag{41}$$

also meets the equation (32). In particular, with

$$\alpha = e^{-\pi t}\Gamma(1-it) \tag{42}$$

the asymptotic behavior of the function

$$\mathfrak{q}_n(k,\xi) \equiv \int d\xi' g^{(+)}(k;\xi,\xi')\psi_n(\xi') = \mathfrak{q}_n^s(k,\xi) - \alpha\,{}_1F_1(it,1,-ik\xi)\,v_n, \tag{43}$$

in view of the asymptotic formulae

$${}_1F_1(it,1,-ik\xi) \underset{\xi\to\infty}{\sim} \frac{e^{\pi t}}{\Gamma(1-it)}(-ik\xi)^{-it}\left(1-\frac{t^2}{ik\xi}\right) + \frac{e^{-ik\xi}}{\Gamma(it)}(-ik\xi)^{it-1}, \tag{44}$$

$$U(it,1,-ik\xi) \underset{\xi\to\infty}{\sim} (-ik\xi)^{-it}\left(1-\frac{t^2}{ik\xi}\right), \tag{45}$$

becomes

$$\mathfrak{q}_n(k,\xi) \underset{\xi\to\infty}{\sim} v_n \frac{e^{-\frac{\pi t}{2}}}{ik}\frac{\Gamma(1-it)}{\Gamma(it)}\frac{e^{-ik\xi+it\ln k\xi}}{\xi}. \tag{46}$$

These (decaying) functions (43) serve as a basis for the quasi-Sturmian construction. We note only that the Green's function $G^{(+)}$ which satisfies the equation

$$\hat{\mathfrak{h}}(k)G^{(+)}(k;\xi,\xi') = \delta(\xi-\xi'), \tag{47}$$

$$\hat{\mathfrak{h}}(k) = \frac{1}{\mu\xi}\left[-2\frac{\partial}{\partial\xi}\xi\frac{\partial}{\partial\xi} - 2ik\xi\frac{\partial}{\partial\xi} + 2kt\right], \tag{48}$$

is related to (41) by

$$G^{(+)}(k;\xi,\xi') = \mu g^{(+)}(k;\xi,\xi')\xi'. \tag{49}$$

Thus, it follows from the recurrence relation

$$\xi\psi_n = \frac{1}{2b}[-(n+1)\psi_{n+1} + (2n+1)\psi_n - n\psi_{n-1}] \tag{50}$$

that the one-dimensional quasi-Sturmian of Eq. (31) are expressed in terms of $\mathfrak{q}_n$ (43)

$$\mathcal{Q}_n = \frac{\mu}{2b}[-(n+1)\,\mathfrak{q}_{n+1} + (2n+1)\,\mathfrak{q}_n - n\,\mathfrak{q}_{n-1}]. \tag{51}$$

In Figs. 1-4 we present the plots of various QS functions for different parameters and energies used in our calculations below.

3.2 Laguerre representation of the Quasi Sturmian functions

3.2.1 Expressions for the $\mathfrak{q}_n$ and $\mathcal{Q}_n$ functions

The coefficients in the basis set (21) expansion of the Green's function (33)

$$g^{s(+)}(k;\xi,\xi') = \sum_{m,n=0}^{\infty} \psi_m(\xi) g^{s(+)}_{mn}(k)\psi_n(\xi) \tag{52}$$

are expressed in terms of well-known special functions

$$\begin{gathered} g^{s(+)}_{mn}(k) = \tfrac{i}{2k}\tfrac{\omega-1}{\omega^{n+1}}\, p_\nu(t;\omega)\, q^{(+)}_\mu(t;\omega), \\ \nu = \min(n,m), \mu = \max(n,m), \end{gathered} \tag{53}$$

where

$$p_n(t;\omega) = \frac{(-1)^n}{n!}\frac{\Gamma(n+1-it)}{\Gamma(1-it)}\,{}_2F_1(-n,it;it-n;\omega), \tag{54}$$

$$q^{(+)}_n(t;\omega) = (-1)^n\frac{n!\Gamma(it)}{\Gamma(n+1+it)}\,{}_2F_1\left(it,n+1;n+1+it;\omega^{-1}\right). \tag{55}$$

Then, it follows from (41), (36), (57), (56) and the expression

$$a_n = \sqrt{\frac{2}{b}}\left(\frac{1+\omega}{2}\right)^{it}(-1)^n\frac{\Gamma(n+1-it)}{n!\Gamma(1-it)}\,{}_2F_1(-n,it;it-n;\omega). \tag{56}$$

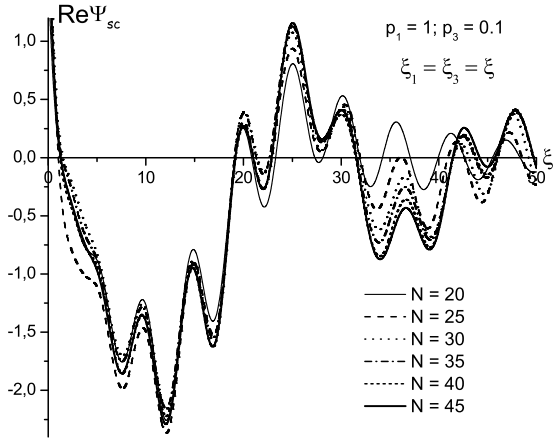

Figure 5: Convergence of the equation (70) solution real part vs the number N of the basis quasi-Sturmians used in the calculation (for each of the coordinates ξ_1 and ξ_3) on the diagonal $\xi_1 = \xi_3$.

for the coefficients of the Kummer function expansion

$$ {}_1F_1(it,1,-ik\xi) = \sum_{n=0}^{\infty} a_n \psi_n(\xi), \tag{57}$$

that

$$ g^{(+)}_{mn}(k) = g^{s(+)}_{mn}(k) - \alpha a_m v_n. \tag{58}$$

Finally, from (31) it follows that

$$ \mathcal{Q}_n(k,\xi) = \sum_{m=0}^{\infty} G^{(+)}_{mn}(k)\psi_m(\xi), \tag{59}$$

where

$$ G^{(+)}_{mn} = \frac{\mu}{2b}\left[-(n+1)g^{(+)}_{mn+1} + (2n+1)g^{(+)}_{mn} - n g^{(+)}_{mn-1}\right]. \tag{60}$$

3.2.2 Expansion for the derivatives of $\mathcal{Q}_n$

To obtain the coefficients for the expansion

$$ \frac{d}{d\xi}\mathcal{Q}_n(k,\xi) = \sum_{m=0} C_{mn}(k)\psi_m(\xi) \tag{61}$$

let us calculate the integral

$$ C_{mn}(k) = \int_0^{\infty} \psi_m(\xi)\frac{d}{d\xi}\mathcal{Q}_n(k,\xi) \tag{62}$$

by parts

$$\begin{aligned}\int_0^\infty \psi_m(\xi)\tfrac{d}{d\xi}\mathcal{Q}_n(k,\xi) &= -\psi_m(0)\mathcal{Q}_n(k,0)-\int_0^\infty\left[\tfrac{d}{d\xi}\psi_m(\xi)\right]\mathcal{Q}_n(k,\xi)\\ &= -\sqrt{2b}\mathcal{Q}_n(k,0)+b\left[\int_0^\infty \psi_m(\xi)\,\mathcal{Q}_n(k,\xi)+2\sum_{\ell=0}^{m-1}\int_0^\infty \psi_\ell(\xi)\,\mathcal{Q}_n(k,\xi)\right].\end{aligned} \tag{63}$$

From (59) it follows that

$$C_{mn}(k) = -\sqrt{2b}\,\mathcal{Q}_n(k,0)+b\left[G^{(+)}_{mn}(k)+2\sum_{\ell=0}^{m-1}G^{(+)}_{\ell n}(k)\right]. \tag{64}$$

Similarly, we obtain that the coefficients d_n of the derivative of (57) expansion

$$\frac{d}{d\xi}{}_1F_1(it,1,-ik\xi) = \sum_{n=0}^{\infty} d_n\psi_n(\xi), \tag{65}$$

are

$$d_n = -\sqrt{2b}+b\left[a_n+2\sum_{m=0}^{n-1}a_m\right]. \tag{66}$$

4 A model problem

4.1 Statement of the problem

As mentioned above, the full three-body problem is very complicated. So we decided, first, to test the methodology by solving a simpler problem. We found one model problem which contains many characteristics of the full one. This was introduced in 1997 in the treatment of a double continuum wave function for two electrons interacting with a heavy ion [21]. This is actually an extension of the Φ_2 model designed to deal with two heave ions and one electron [25]. In Ref. [21] the authors introduced an approximation to the full two-electron Schrödinger equation. This equation was obtained by demanding very particular kinematical conditions on the system. The equation to be solved is

$$\left[\hat{\mathfrak{h}}_1(k_1)+\hat{\mathfrak{h}}_3(k_3)-8\frac{k_3}{k_1}\frac{\partial^2}{\partial\xi_1\partial\xi_3}\right]\Psi(\xi_1,\xi_3)=0. \tag{67}$$

In this contribution we solve this equation using our QS functions.

To start with the study, we divide the wave function Ψ into two parts

$$\Psi(\xi_1,\xi_3) = \Psi_{C2}(\xi_1,\xi_3)+\Psi_{sc}(\xi_1,\xi_3), \tag{68}$$

where

$$\Psi_{C2}(\xi_1,\xi_3) = {}_1F_1\left(i\frac{\mu_1 Z_1}{k_1},1,-ik_1\xi_1\right){}_1F_1\left(i\frac{\mu_3 Z_3}{k_3},1,-ik_3\xi_3\right). \tag{69}$$

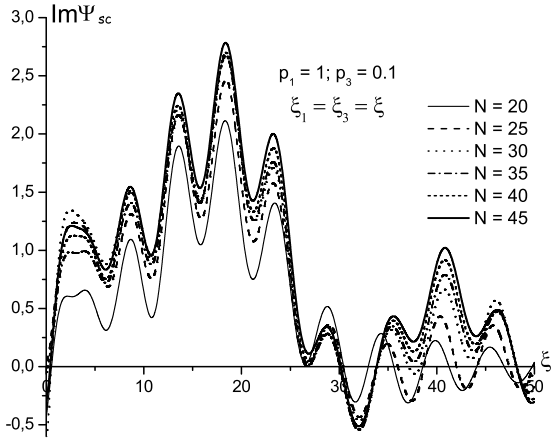

Figure 6: The same as in Fig. 5 but for the solution imaginary part.

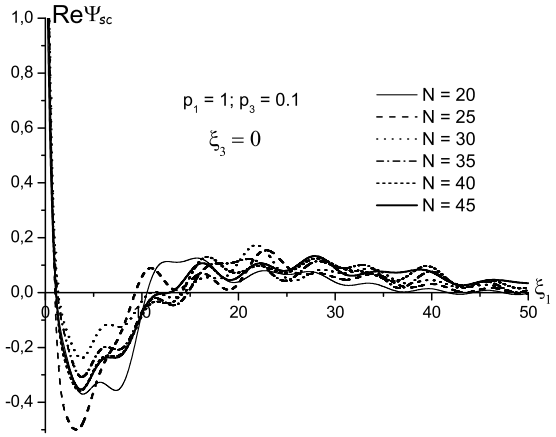

Figure 7: The same as in Fig. 5 but on the axis ξ_1.

This transforms Eq. (67) into the driven equation

$$\left[\hat{\mathfrak{h}}_1(k_1)+\hat{\mathfrak{h}}_3(k_3)-8\frac{k_3}{k_1}\frac{\partial^2}{\partial\xi_1\partial\xi_3}\right]\Psi_{sc}(\xi_1,\xi_3)=8\frac{k_3}{k_1}\frac{\partial^2}{\partial\xi_1\partial\xi_3}\Psi_{C2}(\xi_1,\xi_3). \tag{70}$$

The scattering function $\Psi_{sc}(\xi_1,\xi_3)$ is assumed to have purely outgoing behavior and can be expressed as a finite series of the QS functions (31) products

$$\Psi_{sc}(\xi_1,\xi_3)=\sum_{n_1,n_3=0}^{N-1} c_{n_1n_3}\,\mathcal{Q}_{n_1}(p_1,\xi_1)\,\mathcal{Q}_{n_3}(p_3,\xi_3). \tag{71}$$

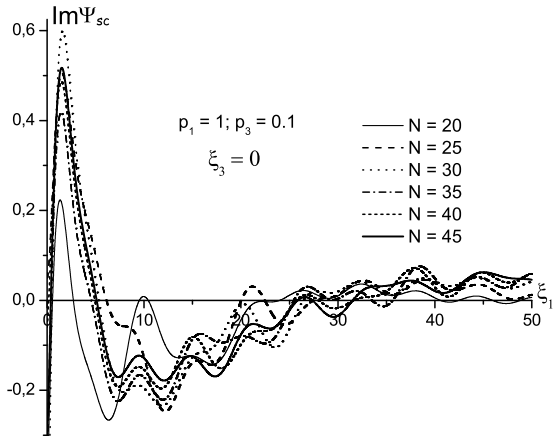

Figure 8: The same as in Fig. 6 but on the axis ξ_1.

Note that in (71) it is not necessary that the parameters p_j be equal to the momenta k_j. Rather than use two-dimensional functions obtained from the action of the separable part of Eq. (67), we propose here an expansion in products of one-dimensional functions. This is one of the aims of the paper, to see whether this expansion works and whether it is efficient.

Inserting the expansion (71) into (70) and projecting onto $\psi_{m_1}(\xi_1)\psi_{m_3}(\xi_3)$ gives, in

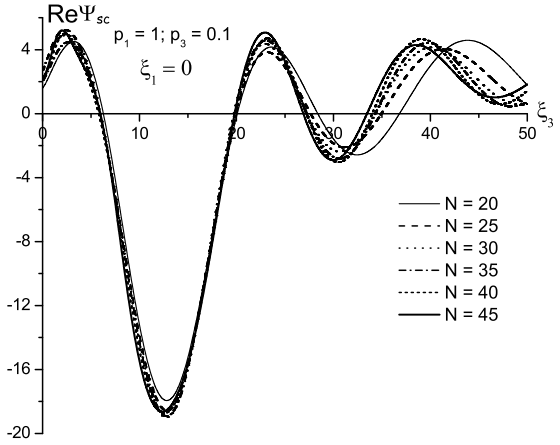

Figure 9: The same as in Fig. 5 but on the axis ξ_3.

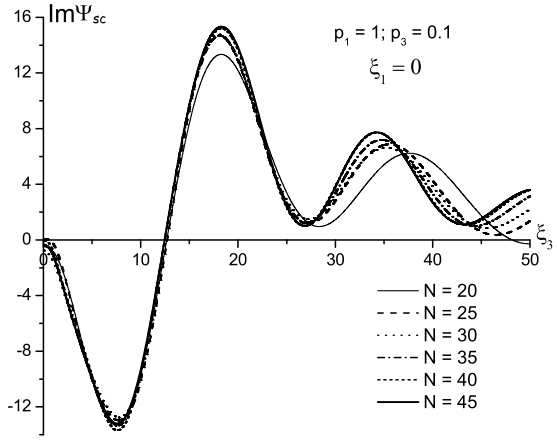

Figure 10: The same as in Fig. 6 but on the axis ξ_3.

view of the evident relation

$$\hat{\mathfrak{h}}(k) = \hat{\mathfrak{h}}(p) - \frac{2i}{\mu}(k-p)\frac{\partial}{\partial\xi}, \tag{72}$$

the following system of linear equations for the unknown coefficients $c_{n_1 n_3}$

$$\begin{aligned}
&\sum_{n_1,n_3=0}^{N-1}\Bigg\{\delta_{m_1 n_1} G^{(3)(+)}_{m_3 n_3}(p_3) + G^{(1)(+)}_{m_1 n_1}(p_1)\delta_{m_3 n_3} - \Bigg[\frac{2i}{\mu_1}(k_1-p_1)C^{(1)}_{m_1 n_1}(p_1) \\
&\qquad \times G^{(3)(+)}_{m_3 n_3}(p_3) + G^{(1)(+)}_{m_1 n_1}(p_1)\frac{2i}{\mu_3}(k_3-p_3)C^{(3)}_{m_3 n_3}(p_3) \\
&\qquad + 8\frac{k_3}{k_1}C^{(1)}_{m_1 n_1}(p_1)C^{(3)}_{m_3 n_3}(p_3)\Bigg]\Bigg\} c_{n_1 n_3} \\
&= 8\frac{k_3}{k_1} d^{(1)}_{m_1} d^{(3)}_{m_3}, \qquad 0 \le m_1, m_3 \le N-1,
\end{aligned} \tag{73}$$

where $C^{(j)}_{m,n}$ and $d^{(j)}_m$ are defined by (64) and (66), respectively.

4.2 Results

We follow Ref. [21] and put $Z_1 = -2$, $\mu_1 = 1$, $k_1 = 1$, and $Z_3 = 1$, $\mu_3 = \frac{1}{2}$, $k_3 = 0.4$. Intuitively one expects that convergence can be achieved provided that the sum of the first two ('unperturbed') terms in the figure brackets on the left-hand-side of Eq. (73) appears to be much larger than the ('perturbation') term in the square brackets. We believe that it should be possible to affect the ratio between these two parts of the matrix element by varying the basis parameters p_j.

Our calculations show that the convergence rate and numerical stability may be significantly improved by taking appropriate values of p_1 and p_2. The results obtained with parameters $p_1=1$ and $p_3=0.1$ (the Laguerre scale factors b_j are equal to the p_j) are shown in Figs. 5-10 where we plot the real and imaginary parts of the scattering wave function Ψ_{sc} on the diagonal $\xi_1=\xi_3$ and the axes ξ_1 and ξ_3. We can see in all the figures that the convergence is achieved showing that the method works. Results for $N=45$ are shown in Figs. 11, 12.

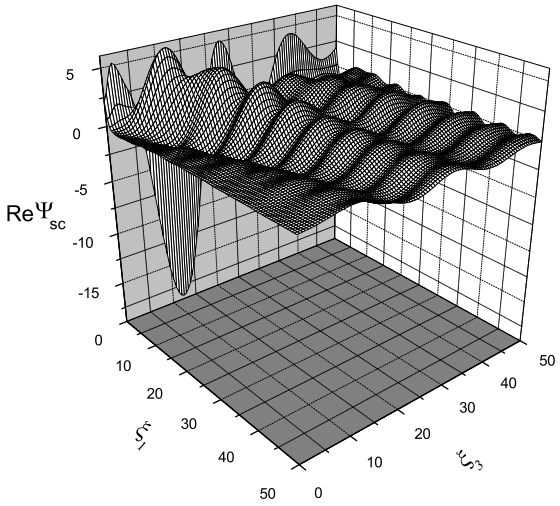

Figure 11: The solution Ψ_{sc} to Eq. (70) (obtained with $N=45$) real part.

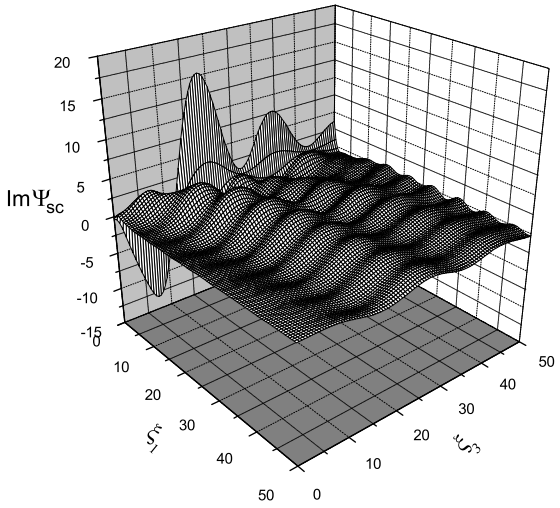

Figure 12: The same as in Fig. 11 but for the imaginary part.

5 Conclusions

In this contribution we presented a study of the three-body scattering problem written in parabolic coordinates. It is well known that the C3 wave function [14] possesses the correct asymptotic behavior in the Ω_0 region where all the particles are far from each other. Thus, this is a good starting point to formulate a Lipmann-Schwinger type equation or a driven equation. This means, if we consider the C3 function as the asymptotic solution, the scattering part (the remaining part of the solution) will satisfy an equation having a compact kernel or a short range driven term. Due to the character of the perturbation corresponding to the C3 function [26], the use of standard L^2 basis is not appropriated. Instead, it turns to be necessary to use basis functions possessing the asymptotic behavior corresponding to the problem being considered. Generalized Sturmian [18] can be used. The numerical implementation of the calculation of this type of functions in parabolic coordinates is part of our actual investigations. In this contribution we introduced a set of basis functions that we named quasi-Sturmian functions. They are defined differently from the generalized Sturmian as they are solutions of a driven differential equation. We proposed here the use of QS functions which are the solutions of a driven equation which includes the separable part of the full three-body kinetic energy in the Klar's parabolic coordinates and also all the Coulomb interactions. In the right-hand-side of (30) any basis set can be used. Depending on the type of the driven term appearing in the full three body equation, the use of one or other of the bases can be more efficient. The basis on the right-hand-side should be chosen to obtain the fastest convergence of the driven term. The QS functions form a complete basis set and this allows to expand the scattering wave function we are looking for. All the QS basis elements possess the correct asymptotic behavior of the full three-body problem in the Ω_0 region. This means that, in principle, only the inner region where the interaction between all the particles takes place must be expanded.

In this contribution we tested the efficiency of the proposed method by applying it to a two-dimensional problem which possesses most of the properties of the full problem: the non-separability and the scattering type boundary conditions. Instead of using non-separable two-dimensional QS functions, products of one-dimensional ones in terms of the parabolic coordinates appearing in the model problem were utilized. We showed that convergence is reached for the scattering wave function with a reasonable number of basis functions. A more extensive study of the properties of the QS functions for bases of different types in the driven terms will be presented soon elsewhere.

Acknowledgments. One of the authors (GG) thanks the support by PGI (24/F049) of the Universidad Nacional del Sur. GG acknowledge also the support of ANPCyT (PICT08/0934) (Argentina) and PIP 200901/552 CONICET (Argentina).

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