Quasi-Sturmian Approach to the Three-Body Continuum Coulomb Problem

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Abstract

The three-body continuum Coulomb problem is treated in terms of generalized parabolic coordinates. Specifically, the original problem is reduced to a driven equation where the 'perturbation' operator contains the non-orthogonal part of the kinetic energy operator. As a test of this approach, a simple two-dimensional model problem is solved numerically by using so-called parabolic quasi-Sturmian basis representation. Convergence of the solution is achieved as the basis set is enlarged.

Keywords: *Three-body Coulomb system; parabolic coordinates; driven equation; quasi-Sturmians; convergence*

1 Introduction

The three-body continuum Coulomb problem is one of 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 calculations of such processes have been developed recently including a convergent close coupling (CCC) approach [1, 2], a Coulomb–Sturmian separable expansion method [3, 4] and a J-matrix method [5, 6, 7]. In all these approaches (see also [8, 9]), the continuous Hamiltonian spectrum is represented in the context of complete square integrable bases. Despite an enormous progress made so far in discretization and subsequent numerical solutions of three-body differential and integral equations of Coulomb scattering theory, a number of related mathematical problems remain open. Actually, the use of a product of two fixed charge Coulomb waves for two outgoing electrons as an approximation to the three-body continuum state, is typical for 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 in the two-body problem this type of definition of the "free particle solution" is not leading to divergent solutions [10]. In addition, in the three-body case, approaches like the exterior complex scaling [11] and generalized Sturmian approaches [8] 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 of these differences between the solutions corresponding to the LS type and driven equations.

On the other hand, it is well known [12, 13] that the Schrödinger equation for a three-body Coulomb system at large particle separations, i. e., in the so-called region Ω_0, is separable in terms of 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 Ref. [15]. Thus, at first glance, one can get an impression that the three-body Coulomb problem can be recast as a Lippmann–Schwinger type equation, where the potential energy operator coinciding with the non-orthogonal part of

the kinetic energy operator, is expressed in terms of second partial mixed derivatives with respect to the parabolic coordinates. No complete studies of the compactness of the kernel of this integral equation can be found in the literature (see discussion in Ref. [16]). Actually, a differential operator of this type seems to be unbounded in the Hilbert space, and therefore finding formal solutions of the corresponding Lippmann–Schwinger equation could be difficult. To avoid these problems, an alternative approach can be used by considering an inhomogeneous Schrödinger equation with a square integrable driven term. 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., Refs. [17, 18] and references therein) which are eigensolutions of a Sturm–Liouville differential or integral equation and form a complete set of basis functions, the QS functions 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 of driven type instead of Lippmann–Schwinger 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-dimensional Coulomb wave operators $\hat{\mathfrak{h}}_1$ and $\hat{\mathfrak{h}}_3$, contains a 'perturbation' term $\frac{\partial^2}{\partial\xi_1\,\partial\xi_3}$.

This paper is organized as follows. We introduce notations, recall the generalized parabolic coordinate definition and convert the three-body Coulomb problem into a driven equation in Sec. 2. We present in Sec. 3 a simple two-dimensional model and briefly outline the parabolic QS approach. Calculations of model continuum wave function are also described in Sec. 3. Our aim is to study the rate of convergence as the basis set used to describe the 'perturbation' operator is enlarged. The calculations show that the convergence can be achieved on the basis of a reasonable size with appropriately chosen basis parameters. Sec. 4 contains a brief discussion of the overall results. 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 after separating out the center-of-mass motion 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 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 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 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 Eq. (5), we obtain an equation for the reduced wave function Ψ:

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

Leading-order asymptotic terms of Ψ in the Ω_0 domain are expressed in terms of 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 square brackets in Eq. (8) 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 kinetic energy and the total potential energy:

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

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

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

Here $t_{ls} = \frac{Z_l Z_s \mu_{ls}}{k_{ls}}$ and $\mu_{ls} = \frac{m_l m_s}{m_l + m_s}$. The operator $\hat{D}_1$ represents the remaining part of kinetic energy [13] which, in the case of the (e^-, e^-, He^{++}) = (123) system with $m_3 = \infty$, takes the form [19]:

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

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 of the equation

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

such that the total wave functions (7) satisfy Redmond conditions [20] in Ω_0. These solutions are well-known $C3$ wave functions. Ψ_{C3} are expressed in terms of products of three Coulomb waves. For example, Ψ_{C3} with pure outgoing behavior is written as

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

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

2.2 Formal solution of the problem

At first glance, given the Green's function operator $\hat{\mathcal{G}} = \hat{D}_0^{-1}$ (see Ref. [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, 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, e. g., a set of square-integrable parabolic Laguerre basis functions [21]

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

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

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

could be used. The index $\mathfrak{N}$ represents all 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 parabolic coordinates. The basis functions (20), (21) are parametrized by different Coulomb–Sturmian parameters b_j for each pair of $\{\xi_j,\eta_j\}$, $j = \overline{1,3}$. 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 $\hat{\mathcal{V}}^{\mathcal{N}}$. Substituting $\hat{\mathcal{V}}$ by $\hat{\mathcal{V}}^{\mathcal{N}}$ in Eq. (18) we obtain 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 a 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 rank of $\mathfrak{N}_0+1$, and $\underline{a}^{(0)}$ is the coefficient vector of Ψ_{C3}, i. e., $\left[\underline{a}^{(0)}\right]_{\mathfrak{N}} = \langle\mathfrak{N}|\,\Psi_{C3}\,\rangle$. The wave function Ψ is expressed in terms of the solution (24):

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

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

We performed various studies of Eq. (18) and found out that its kernel is not compact when expressed in terms of L^2 spaces. Actually, the problem is that any L^2 basis does not possess the appropriate asymptotic behavior. Thus the correct asymptotic behavior is to be implemented and then the perturbation operator $\hat{D}_1$ [see Eq. (14)] seems to be not bounded. However, if the basis possess already the asymptotic behavior of the problem, $\hat{D}_1$ turns out to be a short range operator and becomes compact and manageable.

We explore an alternative approach to the problem based on a 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 splitted into outgoing (ingoing) Ψ_{C3} and scattered Ψ_{sc} parts,

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

Note, the inhomogeneity in Eq. (26) is a square-integrable function. Equation (25) gives a hint on how to construct a solution Ψ_{sc} of Eq. (26) 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., we 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 call the function $|\mathcal{Q}_{\mathfrak{N}}\rangle$ a *quasi-Sturmian function*. The word 'quasi' refers to that there is no need to solve a Sturm–Liouville equation to obtain these functions.

According to the definition (29), the QS functions satisfy a driven equation

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

and possess the same asymptotic behavior as the kernel $G(E;\xi,\eta,\xi',\eta')$ at large values of ξ, η and finite ξ', η'. We are using here the Laguerre basis functions $\mathfrak{B}_{\mathfrak{N}}(\xi,\eta)$, though any basis sets can be used. However, to preserve the asymptotic behavior of $\mathcal{Q}$ functions, the extension on the configuration state of basis functions has to be finite. A representation of the kernel $G(E;\xi,\eta,\xi',\eta')$ in the basis (19) was given in Ref. [22] and this allows for a closed form expression for QS functions. The right-hand-side of Eq. (30) depends on indexes $\mathfrak{N}$, thus for each set of values $\mathfrak{N}$ we have a particular function $\mathcal{Q}_{\mathfrak{N}}$. These functions form a complete basis even though they are not orthogonal.

By solving Eq. (26) with the proposition (28) we enforce the solution (27) to possess the correct outgoing asymptotic behavior of scattering function. This is similar to what is observed when generalized Sturmian functions are used [8, 9]. The completeness of the $\mathcal{Q}_{\mathfrak{N}}$ basis, the short range of both the right-hand-side of Eq. (26) and $D_1\mathcal{Q}_{\mathfrak{N}}$ assure convergence of the expansion. To exemplify this affirmation, we solve in the next section a two-dimensional model problem presented in Ref. [19]. We use a product of 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 allows us to probe the convergence of 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 A model problem

3.1 Statement of the problem

A model double continuum electron wave function was presented in 1997 in Ref. [19]. The model used a two-variable hypergeometric function Φ_2 to represent two electrons interacting with a heavy charged nucleus and with each other. An approximate two-electron Schrödinger equation was also numerically solved in Ref. [19]. This equation was associated with very particular kinematic conditions. The model equation is

$$\left[\hat{\mathfrak{h}}_1(k_1) + \hat{\mathfrak{h}}_3(k_3) - 8\frac{k_3}{k_1}\frac{\partial^2}{\partial\xi_1\partial\xi_3}\right]\Psi(\xi_1,\xi_3) = 0, \tag{32}$$

where a one-dimensional Coulomb wave operator $\hat{\mathfrak{h}}$ is defined as

$$\hat{\mathfrak{h}}(k) = \frac{1}{\mu\xi}\left[-2\frac{\partial}{\partial\xi}\xi\frac{\partial}{\partial\xi} - 2ik\xi\frac{\partial}{\partial\xi} + 2kt\right], \quad kt = \mu Z. \tag{33}$$

We use this model as a starting point of our QS test in this work. This allows us to deal with an equation which contains most of the difficulties of the full three-body problem like a non-separability and scattering type asymptotics of solutions.

We start with splitting the wave function Ψ into two parts,

$$\Psi = \Psi_{sc} + \Psi_{C2}, \tag{34}$$

where

$$\Psi_{C2}(\xi_1,\xi_3) = {}_1F_1\left(i\frac{\mu_1 Z_1}{k_1},\, 1,\, -ik_1\xi_1\right){}_1F_1\left(i\frac{\mu_3 Z_3}{k_3},\, 1,\, -ik_3\xi_3\right). \tag{35}$$

This transforms Eq. (32) into a driven equation

$$\left[\hat{\mathfrak{h}}_1(k_1) + \hat{\mathfrak{h}}_3(k_3) - 8\frac{k_3}{k_1}\frac{\partial^2}{\partial\xi_1\partial\xi_3}\right]\Psi_{sc}(\xi_1,\xi_3) = 8\frac{k_3}{k_1}\frac{\partial^2}{\partial\xi_1\partial\xi_3}\,\Psi_{C2}(\xi_1,\xi_3). \tag{36}$$

The scattering function Ψ_{sc} is assumed to have a purely outgoing behavior and can be expressed as a finite series in terms of products of QS functions (31):

$$\Psi_{sc}(\xi_1,\xi_3) = \sum_{n_1,n_3=0}^{N-1} c_{n_1n_3}\,\mathcal{Q}_{n_1}(p_1,\xi_1)\,\mathcal{Q}_{n_3}(p_3,\xi_3). \tag{37}$$

Note, p_j is not necessary equal k_j. The one-dimensional Green's function $G^{(+)}$ satisfies the equation

$$\hat{\mathfrak{h}}(k)\,G^{(+)}(k;\,\xi,\xi') = \delta(\xi-\xi'). \tag{38}$$

A detailed description of QS functions (31) will be presented soon elsewhere.

Due to an obvious relation

$$\hat{\mathfrak{h}}(k) = \hat{\mathfrak{h}}(p) - \frac{2i}{\mu}(k-p)\frac{\partial}{\partial\xi}, \tag{39}$$

we obtain the following system of linear equations for the unknown coefficients $c_{n_1n_3}$ after substituting $\Psi_{sc}(\xi_1,\xi_3)$ in Eq. (36) by its expansion (37) and projecting onto $\psi_{m_1}(\xi_1)\,\psi_{m_3}(\xi_3)$:

$$\sum_{n_1,n_3=0}^{N-1}\left\{\delta_{m_1n_1}\,G^{(3)(+)}_{m_3n_3}(p_3) + G^{(1)(+)}_{m_1n_1}(p_1)\,\delta_{m_3n_3} - \left[\frac{2i}{\mu_1}(k_1-p_1)\,C^{(1)}_{m_1n_1}(p_1)\,G^{(3)(+)}_{m_3n_3}(p_3)\right.\right.$$
$$\left.\left. + G^{(1)(+)}_{m_1n_1}(p_1)\,\frac{2i}{\mu_3}(k_3-p_3)\,C^{(3)}_{m_3n_3}(p_3) + 8\frac{k_3}{k_1}\,C^{(1)}_{m_1n_1}(p_1)\,C^{(3)}_{m_3n_3}(p_3)\right]\right\}c_{n_1n_3}$$
$$= 8\frac{k_3}{k_1}\,d^{(1)}_{m_1}\,d^{(3)}_{m_3}, \tag{40}$$

where $0 \leq m_1, m_3 \leq N-1$, and $C^{(j)}_{m,n}$ and $d^{(j)}_m$ are respectively the coefficients of expansion in basis functions ψ_m of derivatives of QS functions (31) and of derivatives of confluent hypergeometric functions which arise in Eq. (36) due to Eqs. (37) and (35).

3.2 Results

We follow Ref. [19] and set $Z_1 = -2$, $\mu_1 = 1$, $k_1 = 1$, and $Z_3 = 1$, $\mu_3 = \frac{1}{2}$, $k_3 = 0.4$. The convergence is intuitively expected if the sum of the first two ('unperturbed') terms in figure brackets in l.h.s. of Eq. (40) is much larger than the ('perturbation') term in square brackets. We hope to affect the ratio of these two contributions to the matrix elements by varying the values of basis parameters p_j.

Our calculations demonstrate 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 $b_j = p_j$) are shown in Figs. 1–6 where we plot real and imaginary parts of the scattering wave function Ψ_{sc} on the diagonal $\xi_1 = \xi_3$ and on the axes ξ_1 and ξ_3. The convergence is seen from the figures to be achieved; i. e., the proposed approach is reliable.

4 Conclusions

We presented in this contribution a study of three-body scattering problem expressed in parabolic coordinates. As is well-known, the C3 wave function [14] possesses a correct asymptotic behavior in the Ω_0 region where all particles are far from each other. This is a good starting point for formulating a Lippmann–Schwinger equation or driven type equations. This means that if we consider the C3 function as an asymptotic solution, the scattering part (the remaining part of the solution) should satisfy an equation having a compact kernel or a short range driven term. Due to properties of perturbation corresponding to the C3 function [23], the use of standard L^2 bases is not appropriated. Instead it is necessary to use basis functions possessing the

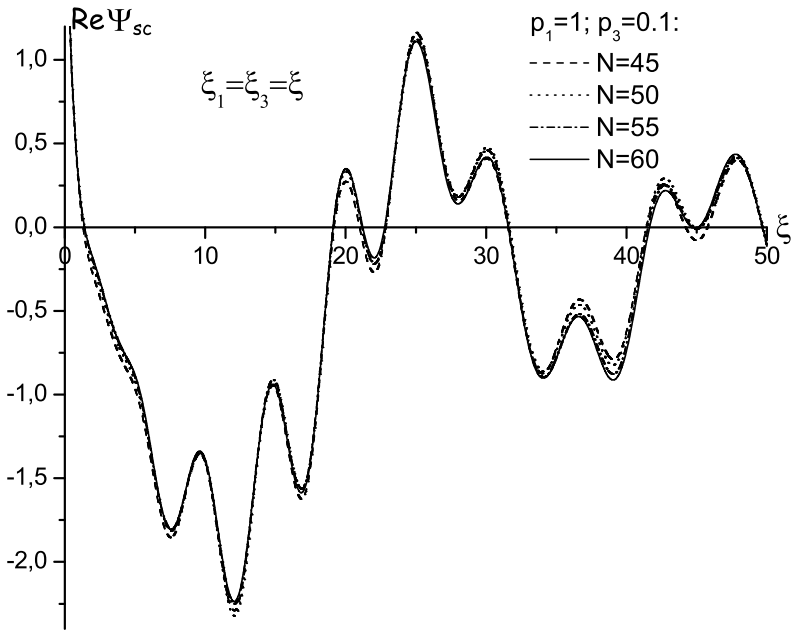

Figure 1: Convergence of the real part of solution vs the number N of basis quasi-Sturmians used in calculation on the diagonal $\xi_1 = \xi_3$.

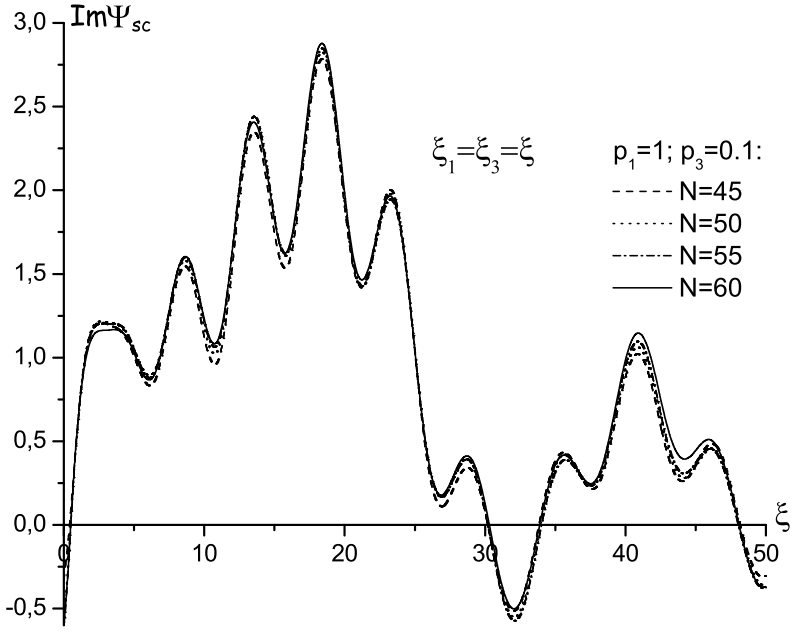

Figure 2: Same as Fig. 1 but for the imaginary part of solution.

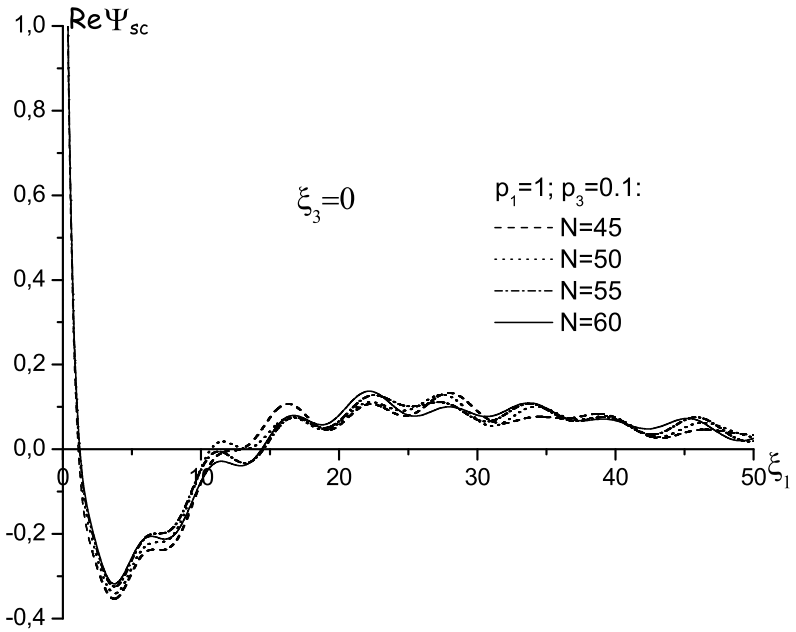

Figure 3: Same as Fig. 1 but on the axis ξ_1.

asymptotic behavior corresponding to the problem under consideration. Therefore we introduce a set of basis functions that we name quasi-Sturmian functions. They are defined as solutions of a driven differential equation which includes the separable part of the full three-body kinetic energy in generalized parabolic coordinates and also all Coulomb interactions. Any basis set can be used in the right-hand-side of Eq. (30). The choice of a convenient basis depends on the type of the driven term appearing in the full three-body driven equation. The basis in the right-hand-side of Eq. (30) should provide a fast convergence of the driven term. On the other hand, the QS

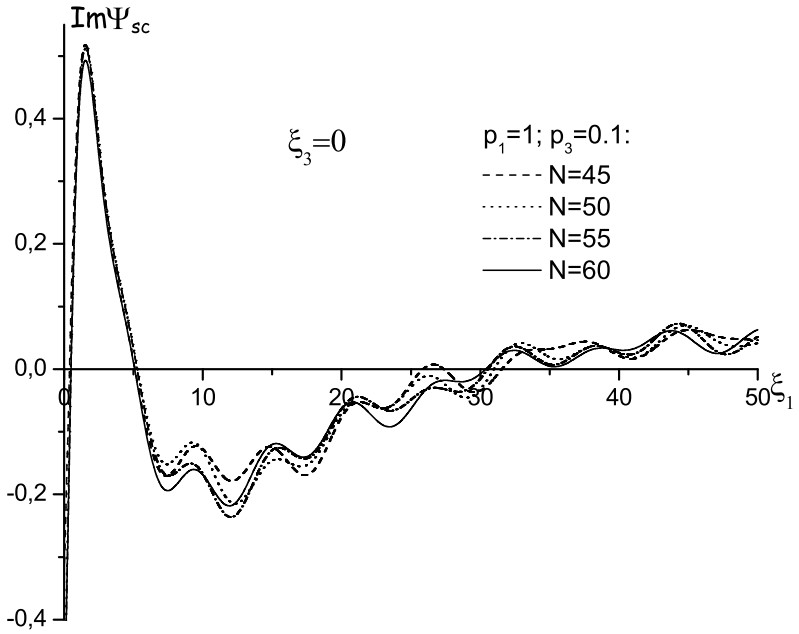

Figure 4: Same as Fig. 2 but on the axis ξ_1.

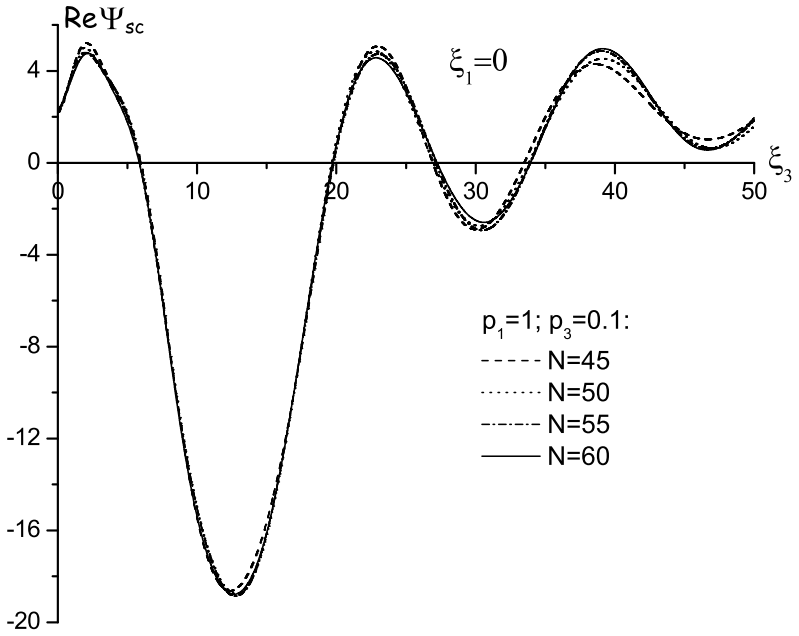

Figure 5: Same as Fig. 1 but on the axis ξ_3.

functions also form a basis set thus allowing to expand the scattering wave function we are looking for. All QS functions possess the correct asymptotic behavior of the full three-body problem. This means, in principle, that only the inner region where the interaction between all particles takes place, should be expanded.

We demonstrate an efficiency of the proposed method in this contribution by applying it to a two-dimensional problem which possesses most of the full problem difficulties: the non-separability and the scattering type boundary conditions. We probe whether we are able to achieve the convergence of the scattering wave function

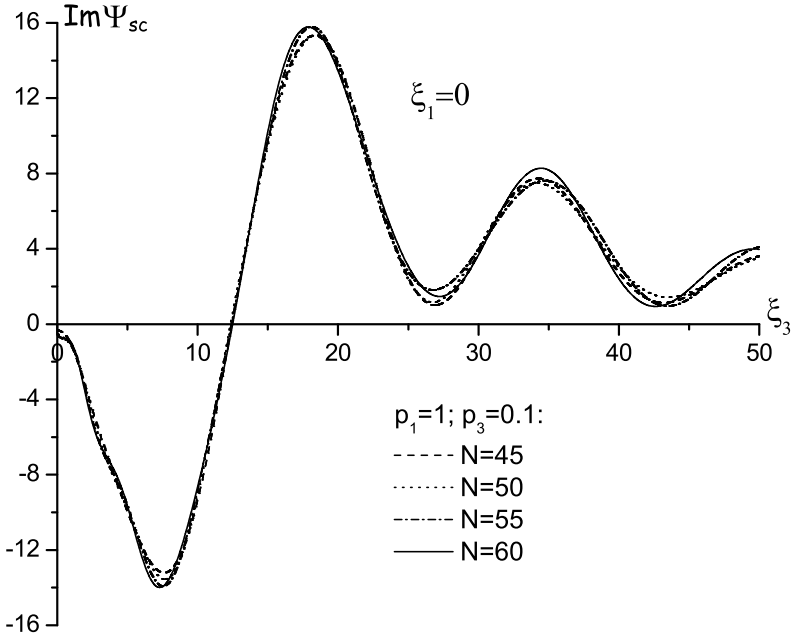

Figure 6: Same as Fig. 2 but on the axis ξ_3.

by the use of QS functions. A more extensive study of properties of QS functions associated with a different type of basis used to expand the driven term, will be presented soon elsewhere. In this study we shall present a six-dimensional function possessing both incoming and outgoing type boundary conditions.

Acknowledgements

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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