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An analytically solvable three-body break-up model problem in hyperspherical coordinates

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Abstract. An analytically solvable S-wave model for three particles break-up processes is presented. The scattering process is represented by a non-homogeneous Coulombic Schrödinger equation where the driven term is given by a Coulomb-like interaction multiplied by the product of a continuum wave function and a bound state in the particles coordinates. The closed form solution is derived in hyperspherical coordinates leading to an analytic expression for the associated scattering transition amplitude. The proposed scattering model contains most of the difficulties encountered in real three-body scattering problem, e.g., non-separability in the electrons' spherical coordinates and Coulombic asymptotic behavior. Since the coordinates' coupling is completely different, the model provides an alternative test to that given by the Temkin-Poet model. The knowledge of the analytic solution provides an interesting benchmark to test numerical methods dealing with the double continuum, in particular in the asymptotic regions. An hyperspherical Sturmian approach recently developed for three-body collisional problems is used to reproduce to high accuracy the analytical results. In addition to this, we generalized the model generating an approximate wave function possessing the correct radial asymptotic behavior corresponding to an S-wave three-body Coulomb problem. The model allows us to explore the typical structure of the solution of a three-body driven equation, to identify three regions (the driven, the Coulombic and the asymptotic), and to analyze how far one has to go to extract the transition amplitude.

1 Introduction

The efficient treatment of collision problems is of fundamental importance in atomic and molecular physics. One key feature to treat ionization processes is the ability to describe three-body collision processes. For single ionization processes huge progress has been made in the last few years. Methods such as the convergent close coupling [1], the J-matrix [2] and the exterior complex scaling [3] have yielded many successful results. They managed to describe accurately a double continuum, i.e. two electrons escaping from a nucleus. This is the case of single ionization of hydrogen ($(e, 2e)$ process) and the double photoionization of helium ($(\gamma, 2e)$ process). This very satisfactory picture suggests that all the methods provide an appropriate description of the the double continuum of a three-body Coulomb system (or at least they numerically manage to find convergence towards the exact solution of the problem). This idyllic situation, however, is not encountered when applying the same double continuum wave function to describe, for example, the double ionization of helium ($(e, 3e)$ process) by high energy electron impact (within the first Born approximation, the four-body problem can be treated as a three-body one). Several ab initio methods (including time-dependent ones [4]) do not reproduce absolute experimental $(e, 3e)$ data, and do not agree with each other (see a review of the situation in Ref. [5], and the recent J-matrix contribution [6]). This is difficult to understand (and accept) because they should all provide the exact (numerical) solutions of the three-body problem. Of course, though using the same tools, the application of rather well established methods to certain collision processes or specific kinematic domains may be problematic due to convergence issues.

Since the situation is still unclarified for the $(e, 3e)$ case, and with the aim to search for explanations, it may be useful to further test the existing methods on a simplified three-body problem. This is what historically has been done before the electron-hydrogen problem was numerically solved [7]. Indeed, the S-wave model [8,9] – often referred to as Temkin-Poet model – calculations have played a very important role in the developments of theoretical and numerical methods. Higly accurate calculations used as benchmark were presented in, e.g., references [10,11].

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This model is the lowest order of the real physical problem but contains most of its technical difficulties. Model calculations for $(e, 3e)$ can be found throughout the collision literature. Single- and double-ionization processes in electron scattering from a model helium atom have been calculated by Pindzola et al. using a time-dependent close-coupling approach [12]. Plottke and co–workers made a systematic study of single ionization [13] of an S-wave model helium using the convergent close-coupling method. A similar model was considered by Horner et al. [14] who studied excitation and single ionization with low projectile energies. Bartlett and Stelbovics considered the same model for the study of various two electron processes, and particularly $(e, 3e)$, using the propagating exterior complex scaling method [15,16]. More recently, J-matrix calculations of electron-helium S-wave scattering have been presented by Konovalov et al. [17]. All these benchmark studies are useful, in general, as they allow to put on a strong footing different numerical methods which do not necessarily yield converging results when applied to complicated scattering processes which involve several ingredients. When the model is close enough to the description of a given process it serves also to provide physical insight. However, there are also studies based on models who do not involve physical interactions (see, e.g. [18,19]), and do not necessarily produce measurable quantities, but serve to illustrate the efficiency of a novel numerical method or to intervalidate two different methods.

Since most of the ab initio methods available for describing the double continuum seem to agree with each other for the electron hydrogen ionization (and the Temkin-Poet subcase), and to some extent for double photoionization of helium, it may be useful to test the three-body problem in a different way. This is what is proposed in the present paper. We introduce a three-body scattering model problem which (i) contains similar difficulties to the real problem (Coulomb potential and non-separability); (ii) tests the double continuum in a different manner; and (iii) has an analytical solution, thus providing an unquestionable solid test for any numerical method.

A three-body scattering problem is described by the Schrödinger equation $[H - E]\,\Psi^+ = 0$ where Ψ^+ has outgoing behavior. One way to describe break-up processes consists in splitting the total wave function as $\Psi^+ = \Psi_0 + \Psi^+_{sc}$ [20,21]. Here Ψ_0 is a known asymptotically prepared initial state (corresponding to no scattering) which solves an approximate (asymptotic) Hamiltonian H_0, i.e., $[H_0 - E]\,\Psi_0 = 0$; Ψ^+_{sc} is the scattering wave function, defined with outgoing wave asymptotic behavior, which possesses all the dynamics information. If W is the neglected interaction, i.e. $H = H_0 + W$, then Ψ^+_{sc} solves the driven Schrödinger equation $[H - E]\,\Psi^+_{sc} = -W\Psi_0$ which comes generally with two conditions: regularity at the origin and pure outgoing behavior at large distances.

The S-wave break-up model proposed in this paper applies to any three charged particles, and is presented in hyperspherical rather than spherical coordinates, thus testing the coupling between the interparticle distances in a different way than, say, the Temkin-Poet approach. When solving three-body break-up processes, hyperspherical coordinates are known to be better suited to deal with proper asymptotic boundary conditions. Indeed, when the three particles are far from each other, the three-body wave function asymptotically behaves as a distorted spherical wave which depends on all the coordinates (Peterkop's asymptotics) [22–24]. In our model, the interaction W neglected in the initial channel is given by a Coulomb-like potential in the hyperradius ρ. A bound-free initial state Ψ_0 is considered and built as the symmetrized product of a standing spherical wave and a bound state. The scattering wave function of our model is expanded in terms of Jacobi polynomials for the hyperangular part. The coupled hyperradial solutions, regular at the origin and with outgoing asymptotic behavior, are found analytically. This is the essential feature of our model. As far as we know, no other meaningful example of three-body scattering model, analytically solvable, as the one presented here has been provided in the literature.

The analytical results are validated through the application of an hyperspherical Sturmian approach recently formulated to treat three-body break-up problems [25,26]. In the numerical study presented in this paper, the scattered wave function is evaluated through an expansion in terms of hyperspherical Sturmian functions (HSF). These are constructed here with a complete set of coupled hyperangular Jacobi polynomials and hyperradial Sturmian functions, the latter already accounting for the appropriate boundary conditions. As the basis elements possess the correct asymptotic behavior, the hyperspherical Sturmian approach is expected to be very efficient.

In this report we thus present a three-body fragmentation model which can be used to test different numerical approaches. It is solved analytically and verified numerically, and can thus serve as a benchmark and a strong challenge for other ab initio methods. As the analytical solution is known, the model is also used to explore how the three-body asymptotic regimes are reached in different spatial domains and different kinematics; the proposed analysis may help in identifying possible convergence difficulties of existing methods in particular at low energies. This is the aim of this paper.

The rest of this paper is arranged as follows. In Section 2, we present the model scattering problem. Section 3 provides analytical expressions for the scattering wave function, as well as for the transition amplitude. In Section 4, hyperspherical Sturmian functions with outgoing wave asymptotic behavior are defined, and the numerical implementation to solve the scattering problem is presented. Numerical and analytical results are then compared. Section 5 is dedicated to asymptotic considerations of the Temkin-Poet problem. A brief summary is given in Section 6.

Atomic units are used throughout.

2 Model potential and scattering problem

Consider three particles of masses m_1, m_2 and m_3, and charges Z_1, Z_2 and Z_3; for illustration, and for the present

discussion, we may take for simplicity a nucleus of charge $Z_3 = Z > 0$, and two electrons with $Z_1 = Z_2 = -1$. The Hamiltonian of the system can be written in terms of any of three pairs of Jacobi or mass-scaled Jacobi coordinates [25,27]. The hyperspherical coordinates are one hyperradius ρ and five hyperangular coordinates (denoted collectively by ω_5). Leaving aside the four polar angles, and for presentation purposes, in what follows we shall simply use

$$\rho = \sqrt{r_1^2 + r_2^2}, \quad \alpha = \arctan(r_2/r_1), \tag{1}$$

i.e. $r_1 = \rho\cos\alpha$ and $r_2 = \rho\sin\alpha$, where r_1 and r_2 are the usual spherical coordinates of two particles (electrons) with respect to the third one (nucleus).

2.1 Model potential

For three-body scattering problems, the full Coulomb interaction potential

$$V(\rho,\omega_5) = \frac{Z_1Z_3}{r_1} + \frac{Z_2Z_3}{r_2} + \frac{Z_1Z_2}{r_{12}}, \tag{2}$$

(r_{12} is the inter-electronic distance) may be written in hyperspherical coordinates as

$$\begin{aligned} V(\rho,\omega_5) &= \frac{Z_1Z_3}{\rho\cos\alpha} + \frac{Z_2Z_3}{\rho\sin\alpha} + \frac{Z_1Z_2}{\rho\sqrt{1-\sin(2\alpha)\cos\theta_{12}}} \\ &= \frac{C(\omega_5)}{\rho}, \end{aligned} \tag{3}$$

where $\cos\theta_{12} = \hat{\mathbf{r}}_1 \cdot \hat{\mathbf{r}}_2$ defines the angle between particles 1 and 2. $C(\omega_5)$ may be viewed as an angular dependent charge and the corresponding three-body problem is notoriously difficult. In principle, the scattering solution $\Psi_{\rm sc}(\rho,\omega_5)$ should have, in the region where all the particles are far from each other, the following outgoing Peterkop-type asymptotic behavior [22,23]

$$\Psi^+_{\rm sc}(\rho,\omega_5) \propto A(\omega_5)\rho^{-5/2} e^{i\left(K\rho - \frac{C(\omega_5)}{K}\log[2K\rho]\right)}, \tag{4}$$

where $A(\omega_5)$ is the scattering amplitude, and K is the hyperspherical momentum related to the energy $E = \frac{K^2}{2\mu}$ of the system.

In the S-wave Temkin-Poet model, the interelectronic potential $1/r_{12}$ is spherically averaged and replaced by $1/r_>$ where $r_> = \max(r_1, r_2)$. The resulting potential, and thus the three-body Schrödinger equation, is quasi separable in spherical coordinates r_1 and r_2. A coupling exists through the domain, i.e., whether r_1 is larger/smaller than r_2. In terms of hyperspherical coordinates, the "charge" $C(\omega_5)$ is replaced by $\tilde{C}(\alpha)$ with

$$\tilde{C}(\alpha) = -\frac{Z}{\cos\alpha} - \frac{Z}{\sin\alpha} + \begin{cases} \frac{1}{\cos\alpha} & 0 \le \alpha \le \frac{1}{4}\pi \\ \frac{1}{\sin\alpha} & \frac{1}{4}\pi \le \alpha \le \frac{1}{2}\pi. \end{cases} \tag{5}$$

Thus only an α dependence is retained. In these coordinates, the Schrödinger equation corresponding to the Temkin-Poet model provides a simplified version of the physical problem which tests the angular separation at $\alpha = \pi/4$. Note that, in the case of hydrogen ($Z = 1$), in each domain the potential reduces simply to $-1/r_2$ or $-1/r_1$. Though rather simple, the model contains the essential difficulties of the real problem (Coulomb potentials and non-separability) thus providing a very interesting benchmark which served to validate many numerical methods.

In the model we present and study in this paper, we suggest something different. We replace $C(\omega_5)$ by a constant charge $\mathcal{C}$, i.e. the following Coulomb potential

$$V(\rho) = \frac{\mathcal{C}}{\rho}; \tag{6}$$

the model interaction can be considered as either attractive ($\mathcal{C} > 0$) or repulsive ($\mathcal{C} < 0$). Note that the potential is not one of the three Coulomb interactions that appear in the physical case (3). Although seemingly simple in hyperspherical coordinates, it is not separable in spherical coordinates r_1 and r_2; assuming for example that $r_2 < r_1$, their coupling is very particular

$$\begin{aligned} \frac{\mathcal{C}}{\sqrt{r_1^2 + r_2^2}} &= \frac{\mathcal{C}}{r_1}\left[1 - \frac{1}{2}\left(\frac{r_2}{r_1}\right)^2 + \ldots\right] \\ &= \frac{\mathcal{C}}{\rho\cos\alpha}\left[1 - \frac{1}{2}\tan^2\alpha + \ldots\right], \end{aligned} \tag{7}$$

where the second equality illustrates the expansion in terms of the hyperangle α. The lowest order (first term) of expansion (7) corresponds to retaining the first term of the real potential (3). The model potential (6) therefore tests the r_1 and r_2 dependence in a way which differs substantially from the Temkin-Poet model. On top of that, it offers the possibility to make a detailed and interesting asymptotic investigation of the scattering wave function. Indeed, for a given "angular" set (fixed ω_5), the angular dependent charge $C(\omega_5)$ takes a constant value and thus the physical three-body potential reduces to our model. The knowledge of the analytic solution will allow us to investigate for what hyperradius the corresponding asymptotic regime is actually reached. By varying the angles, one may explore different asymptotic domains, and related convergence issues.

2.2 Scattering model problem

As briefly described in the introduction, the wave function $\Psi(\rho,\omega_5)$ for a collision process may be separated in two parts $\Psi(\rho,\omega_5) = \Psi_0(\rho,\omega_5) + \Psi_{sc}(\rho,\omega_5)$ where $\Psi_0(\rho,\omega_5)$ is a known initial state, eigensolution of an approximate Hamiltonian $H_0 = H - W$ (H is the full Hamiltonian and W is the neglected, unsolved, interaction); $\Psi_{sc}(\rho,\omega_5)$, on the other hand, is a wave function solving all the interactions $V(\rho,\omega_5)$. According to this separation, the function $\Psi_{sc}(\rho,\omega_5)$ satisfies a driven Schrödinger equation

$$\begin{aligned} (T + V(\rho,\omega_5) - E)\,\Psi_{sc}(\rho,\omega_5) &= -W(\rho,\omega_5)\Psi_0(\rho,\omega_5) \\ &= \varphi(\rho,\omega_5), \end{aligned} \tag{8}$$

where $\varphi(\rho,\omega_5)$ denotes the driving term. Equation (8) must be solved imposing outgoing behavior to $\Psi_{sc}(\rho,\omega_5)$ for large values of ρ ($\rho \to \infty$). With our model potential (6) the Schrödinger equation to be solved reads

$$\left[-\frac{1}{2\mu}\frac{1}{\rho^5}\frac{\partial}{\partial\rho}\left(\rho^5\frac{\partial}{\partial\rho}\right)+\frac{\Lambda^2}{2\mu\rho^2}+\frac{\mathcal{C}}{\rho}-E\right] \times \Psi(\rho,\alpha)=\varphi(\rho,\alpha), \quad (9)$$

where the dependence is limited to ρ and α as no polar angles are considered here.

Above, the kinetic energy operator takes the form

$$T=-\frac{1}{2\mu}\left[\frac{1}{\rho^5}\frac{\partial}{\partial\rho}\left(\rho^5\frac{\partial}{\partial\rho}\right)-\frac{\Lambda^2}{\rho^2}\right],$$

where Λ^2 is the grand orbital angular momentum operator

$$\Lambda^2=-\frac{1}{\sin^2\alpha\cos^2\alpha}\frac{d}{d\alpha}\left(\sin^2\alpha\cos^2\alpha\frac{d}{d\alpha}\right) +\frac{\mathbf{j}^2}{\cos^2\alpha}+\frac{\mathbf{l}^2}{\sin^2\alpha}, \quad (10)$$

where $\mu=\sqrt{m_1m_2m_3/(m_1+m_2+m_3)}$ is the three-body reduced mass of the system, and $\mathbf{j}$ and $\mathbf{l}$ denote the rotational and centrifugal angular momentum operators. The eigenfunctions of Λ^2 are known for any quantum numbers j and l. However, as we consider a S-wave model, we can set $j=l=0$. In this case, the functions

$$\Omega_n(\alpha)=\mathcal{N}_n\ {}_2F_1\left(-n,n+2,\frac{3}{2};\sin^2\alpha\right), \quad (11)$$

with $\mathcal{N}_n=4(n+1)/\sqrt{\pi}$, satisfy the eigenvalue equation

$$\Lambda^2\Omega_n(\alpha)=\lambda_n(\lambda_n+4)\Omega_n(\alpha), \quad (12)$$

with $\lambda_n=2n$ ($n=0,1,\ldots$); ${}_2F_1$ represents Gauss hypergeometric function [28]. The eigenfunctions $\Omega_n(\alpha)$ are Jacobi polynomials: they form a complete set and satisfy the orthonormality relation

$$\int_0^{\pi/2}\Omega_n(\alpha)\Omega_m(\alpha)\sin^2\alpha\cos^2\alpha\ d\alpha=\delta_{nm}. \quad (13)$$

In our model the initial state is taken to be a symmetrized bound-free product of a standing spherical wave in the relative coordinate r_1 between the incoming particle and the center of the target and a bound-like state in the target coordinate r_2; the interaction neglected in the initial channel is given, for example by a Yukawa potential $e^{-a\rho}/\rho$. More specifically, we take the following source (driving term)

$$\varphi(\rho,\alpha)=\rho^t e^{-a\rho}\frac{1}{2}\left[\frac{\sin r_1}{r_1}\frac{\sinh r_2}{r_2}+\frac{\sin r_2}{r_2}\frac{\sinh r_1}{r_1}\right], \quad (14)$$

with a parameter a such that $\Re(a)>1$. At large distances, the decreasing exponential $e^{-a\rho}$ gives an overall asymptotically vanishing source (the hyperradial width of the source depends on $\Re(a)$). The bound-like state comes from the combination of $e^{-a\rho}$ with $\sinh r_j/r_j$ ($j=1,2$): it is well-behaved close to $r_j=0$, and for large values of r_j, the dominant asymptotic behavior reads $e^{-a\rho}\sinh r_j \propto e^{-a\rho+r_j}$ thus simulating an angularly screened hydrogenic s state in coordinate r_j. The sinus term in r_i ($i\neq j$) is the Bessel function of order zero, and represents a free standing wave. In (14), the real power $t\geq -1$ is arbitrary; when $t=0$, $\rho^t e^{-a\rho}\sinh r_j/r_j$ ($j\neq i$) represents the product of a Coulomb-like potential multiplied by a bound-like s state. Hence, the driven term (14) can be associated to a physical bound-free picture as would appear in a scattering problem (see Eq. (8)); moreover, as we shall see in the next sections, it allows for an analytical solution of the driven Schrödinger equation (9).

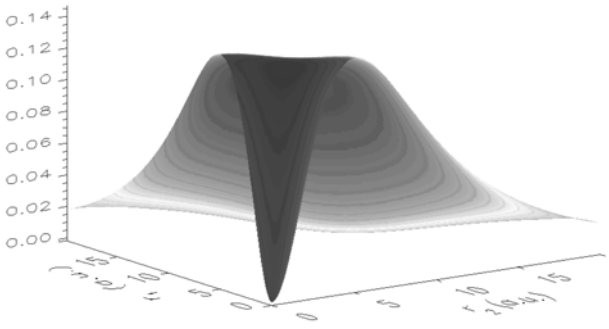

Fig. 1. The source $\varphi(\rho,\alpha)\rho^{5/2}$, as it appears on the right-hand-side of equation (20), is plotted as a function of the spherical coordinates r_1 and r_2. $\varphi(\rho,\alpha)$ is defined by equation (14), and here $t=0$ and $a=2$.

The source (14) may be expanded in a series of Jacobi polynomials $\Omega_n(\alpha)$ as (see details in the Appendix)

$$\varphi(\rho,\alpha)=\sum_{n=0}^{\infty}b_n f_n(\rho)\Omega_n(\alpha), \quad (15)$$

where

$$f_n(\rho)=e^{-a\rho}\rho^{2n+t} \quad (16)$$

$$b_n=\frac{1}{\mathcal{N}_n}\frac{1}{2^{2n}\left(\frac{3}{2}\right)_n n!}\frac{[(-1)^n+1]}{2}. \quad (17)$$

Notice that due to the symmetry of the source, the summation in expansion (15) is limited to even numbers n only.

In Figure 1, we plot $\varphi(\rho,\alpha)\rho^{5/2}$ as a function of the more familiar spherical variable r_1 and r_2, for $a=2$ and $t=0$. The factor $\rho^{5/2}$, that appears in the reduced form (20) of equation (9), is added for illustration purposes. At large r_1 and r_2, the source behaves as the product of a Coulombic potential, multiplied by a decreasing exponential (representing a hydrogenic bound state) and a Bessel function (continuum state). Note that for r_i larger than say 5 a.u. the source is already vanishing. The source function $\varphi(\rho,\alpha)$ is reproduced to an accuracy of 10^{-3} up to the hyperradius $\rho=60$ through the expansion (15) with 45 terms. For larger hyperradius ρ, the number of terms needed in the expansion increases proportionally to ρ.

One further remark. If spherical, rather than hyperspherical, coordinates are used, the model driven equation reads

$$\left[-\frac{1}{2r_1^2}\frac{\partial}{\partial r_1}\left(r_1^2\frac{\partial}{\partial r_1}\right)-\frac{1}{2r_2^2}\frac{\partial}{\partial r_2}\left(r_2^2\frac{\partial}{\partial r_2}\right)+\frac{\mathcal{C}}{\sqrt{r_1^2+r_2^2}}-E\right]\Psi(r_1,r_2)=\left[\sqrt{r_1^2+r_2^2}\right]^t\times e^{-a\sqrt{r_1^2+r_2^2}}\frac{1}{2}\left[\frac{\sin r_1}{r_1}\frac{\sinh r_2}{r_2}+\frac{\sin r_2}{r_2}\frac{\sinh r_1}{r_1}\right]. \quad (18)$$

The Coulomb potential is simple in hyperspherical, but not in spherical, coordinates. The driven term is not separable in either set of coordinates, not even asymptotically. Thus, the model equation (9) together with the source (14) provides a physically meaningful Coulomb scattering problem which presents typical three-body problem difficulties including non-separability.

3 Analytical solution

To solve the driven equation (9) with the source (14), we shall first provide the general solution Ψ_H^G of the corresponding homogenous equation (Sect. 3.1), and then the particular solution Ψ_{NH}^P (Sect. 3.2). The general solution Ψ_{NH}^G of the problem, its asymptotic limit and the transition amplitude, will be given in Section 3.3. All this can be provided in analytic form.

It is convenient first to make the change of function

$$\Psi(\rho,\alpha)=\frac{\bar{\Psi}(\rho,\alpha)}{\rho^{\frac{5}{2}}}, \quad (19)$$

so that the non-homogeneous differential equation to solve reads

$$\left[-\frac{1}{2\mu}\frac{\partial^2}{\partial\rho^2}+\frac{\Lambda^2+15/4}{2\mu\rho^2}+\frac{\mathcal{C}}{\rho}-E\right]\bar{\Psi}(\rho,\alpha)=\rho^{5/2}\varphi(\rho,\alpha). \quad (20)$$

(We take this opportunity to signal a typographical mistake in Eq. (15) of Ref. [25], where $-15/4$ appears instead of $15/4$.)

3.1 General solution of the homogeneous differential equation

The homogeneous equation corresponding to equation (20) can be readily solved by variable separation. The angular part is given by $\Omega_n(\alpha)$, and property (12) yields a centrifugal barrier $[\lambda_n(\lambda_n+4)+15/4]/(2\mu\rho^2)=\nu_n(\nu_n+1)/(2\mu\rho^2)$ where $\nu_n+1=\frac{5}{2}+\lambda_n=\frac{5}{2}+2n$. The general solution (regular at the origin) of the hyperradial Coulomb equation reads

$$\Psi_H^G(\rho,\alpha)=\frac{1}{\rho^{\frac{5}{2}}}\sum_n\chi_n(\rho)\Omega_n(\alpha) \quad (21)$$

where

$$\chi_n(\rho)=N_C(\nu_n)e^{iK\rho}\rho^{\nu_n+1}\,{}_1F_1(a_n,c_n;-2iK\rho), \quad (22)$$

with

$$a_n=i\eta+\nu_n+1 \quad (23a)$$

$$c_n=2\nu_n+2, \quad (23b)$$

and where $\eta=\mathcal{C}\mu/K$ defines the Sommerfeld parameter. The normalization constant

$$N_C(\nu_n)=\frac{(2K)^{\nu_n+1}}{2}\frac{|\Gamma(a_n)|}{\Gamma(c_n)}e^{-\frac{\pi}{2}\eta}, \quad (24)$$

is chosen in order to provide the following asymptotic behavior

$$\chi_n(\rho)\to\sin\left(K\rho-\eta\ln(2K\rho)-\frac{\pi}{2}\nu_n+\sigma_c(\nu_n)\right), \quad (25)$$

where the Coulomb phase-shift is given by $\sigma_C(\nu_n)=\mathrm{Arg}[\Gamma(a_n)]$.

3.2 Particular solution of the non-homogeneous differential equation

As the potential appearing on the left-hand-side of equation (20) does not depend on the angular variables, it may be convenient to express the solution as a combination of radial and angular functions:

$$\Psi_{NH}^P(\rho,\alpha)=\frac{1}{\rho^{\frac{5}{2}}}\sum_n b_nR_n(\rho)\Omega_n(\alpha). \quad (26)$$

Replacing into (20) and using again property (12), we obtain

$$\sum_n\Omega_n(\alpha)\left[-\frac{1}{2\mu}\frac{\partial^2}{\partial\rho^2}+\frac{\nu_n(\nu_n+1)}{2\mu\rho^2}+\frac{\mathcal{C}}{\rho}-E\right](b_nR_n(\rho))=\rho^{\frac{5}{2}}\varphi(\rho,\alpha), \quad (27)$$

where the source $\varphi(\rho,\alpha)$ is given by equation (15). By projecting on the angular functions $\Omega_n(\alpha)$, and using the orthonormality property (13), we get the following hyperradial equation

$$\left[-\frac{1}{2\mu}\frac{d^2}{d\rho^2}+\frac{\nu_n(\nu_n+1)}{2\mu\rho^2}+\frac{\mathcal{C}}{\rho}-E\right]R_n(\rho)=\rho^{\frac{5}{2}}f_n(\rho). \quad (28)$$

Introducing the change of function

$$R_n(\rho)=(-2\mu)(-2iK)^{-2-t}e^{iK\rho}\rho^{2n+5/2}v_n(\rho) \quad (29)$$

the equation for $v_n(\rho)$ results

$$\left[\rho\frac{d^2}{d\rho^2}+(2iK\rho+c_n)\frac{d}{d\rho}+2iKa_n\right]v_n(\rho)=(-2iK)^{2+t}e^{-iK\rho}\rho^{-2n+1}f_n(\rho).$$

Next we introduce the following change of variable $r = -2iK\rho$, and use the definition (16) of the source to get

$$\left[r\frac{d^2}{dr^2} + (c_n - r)\frac{d}{dr} - a_n\right] v_n(r) = e^{\gamma r} r^{1+t}, \tag{30}$$

where $\gamma = \frac{1}{2}\left(1 + \frac{a}{iK}\right)$. This latter form of the non-homogeneous differential equation is exactly the one studied quite in details in [29] (see Eq. (18)). The particular solution, regular at the origin, is given analytically by equation (23) of [29] with the labelling replacement $[k, l, \sigma, \lambda] \rightarrow [K, \nu_n, 1+t, a]$. Writing the final result for $R_n(\rho)$ we have:

$$R_n(\rho) = (-2\mu)e^{iK\rho}\rho^{\nu_n+3+t}\frac{1}{(2+t)(c_n+1+t)} \times \Theta^{(1)}\left(\begin{array}{c} 2{+}t, 1 \,|\, c_n+1+t, a_n{+}2{+}t \\ a_n{+}\,2{+}t \,|\, 3{+}t, c_n+2{+}t \end{array}\middle| \, ;{-}2iK\gamma\rho, {-}2iK\rho\right), \tag{31}$$

where $\Theta^{(1)}$ is a two variables hypergeometric function introduced and discussed in reference [30] in a different context, and whose series representation is given by

$$\Theta^{(1)}\left(\begin{array}{c} \mathfrak{a}_1, \mathfrak{a}_2 \,|\, \mathfrak{b}_1, \mathfrak{b}_2 \\ \mathfrak{c}_1 \,|\, \mathfrak{d}_1, \mathfrak{d}_2 \end{array}\middle| \, ; x_1, x_2\right) = \sum_{m_1=0}^{\infty}\sum_{m_2=0}^{\infty} \frac{(\mathfrak{a}_1)_{m_1}(\mathfrak{a}_2)_{m_2}(\mathfrak{b}_1)_{m_1}(\mathfrak{b}_2)_{m_1+m_2}}{(\mathfrak{c}_1)_{m_1}(\mathfrak{d}_1)_{m_1+m_2}(\mathfrak{d}_2)_{m_1+m_2}} \frac{x_1^{m_1}x_2^{m_2}}{m_1!m_2!}. \tag{32}$$

It is interesting to note that, when a is real, the particular solution $R_n(\rho)$ is a real function [29].

From the asymptotic study [31] of the $\Theta^{(1)}$ function, if $\Re(a) > 0$ the large ρ behavior $R_n(\rho)$ of reads

$$R_n(\rho) \rightarrow b_n N_{source} \cos\Big[K\rho - \eta\ln(2K\rho) - \frac{\pi}{2}(\nu_n + t + 3) + \delta(\nu_n, 1+t, a)\Big] \tag{33}$$

where

$$N_{source} = (-2\mu)\frac{(1)_{1+t}(2\nu_n+2)_{1+t}}{(2\nu_n+2)_{2t+4}}\frac{|\,{}_2F_1|}{N_C(\nu_n+t+2)} \tag{34}$$

is a constant fixed by the source; above

$$\delta(\nu_n, 1+t, a) = \sigma_C(\nu_n + t + 2) - \Delta, \tag{35}$$

and

$${}_2F_1\left(t+2, 2\nu_n+t+3, i\eta+\nu_n+t+3; \gamma\right) = |\,{}_2F_1|e^{i\Delta}. \tag{36}$$

As can be seen from equation (33), the solution $R_n(\rho)$ possesses both incoming and outgoing behaviors.

3.3 General solution of the non-homogeneous differential equation

To build the general solution of the non-homogeneous differential equation, we have to combine the results (22) and (31) of the previous two subsections. In order to find a pure outgoing behavior, we propose the following solution for the scattering problem

$$H_n^+(\rho) = \mathcal{A}_n\chi_n(\rho) + R_n(\rho), \tag{37}$$

where the constant $\mathcal{A}_n$ will be chosen appropriately below. According to (25) and (33), the function $H_n^+(\rho)$ behaves for large values of ρ as

$$H_n^+(\rho) \rightarrow \mathcal{A}_n \sin\Big(K\rho - \eta ln\,(2K\rho) - \frac{\pi}{2}\nu_n + \sigma_c(\nu_n)\Big) + N_{source}\cos\Big[K\rho - \eta\ln(2K\rho) - \frac{\pi}{2}(\nu_n + t + 3) + \delta(\nu_n, 1+t, \delta)\Big]. \tag{38}$$

We can choose $\mathcal{A}_n$ in such a way to eliminate the incoming wave [32]. This is achieved by setting

$$\mathcal{A}_n = iN_{source}e^{i\phi(\nu_n)} \tag{39}$$

with $\phi(\nu_n) = \sigma_c(\nu_n) + \frac{\pi}{2}(t+3) - \delta(\nu_n, 1+t, a)$. With this choice we find the required $H_n^+(\rho)$ outgoing behavior

$$H_n^+(\rho) \rightarrow N_{source}\ \cos(\phi(\nu_n))\ e^{i(K\rho - \eta\ln(2K\rho) - \frac{\pi}{2}\nu_n + \sigma_c(\nu_n))}. \tag{40}$$

The complete solution of the problem is then

$$\Psi_{NH}^G(\rho, \alpha) = \frac{1}{\rho^{\frac{5}{2}}}\sum_n b_n\left(\mathcal{A}_n\chi_n(\rho) + R_n(\rho)\right)\Omega_n(\alpha). \tag{41}$$

Asymptotically it behaves, in accordance with reference [22], as

$$\Psi_{NH}^{G+}(\rho, \alpha) \rightarrow f(\alpha)\frac{e^{i(K\rho - \eta\ln(2K\rho))}}{\rho^{\frac{5}{2}}}, \tag{42}$$

providing the following analytical expression for the transition amplitude

$$f(\alpha) = \sum_n b_n\left(N_{source}\cos(\phi(\nu_n))\ e^{i(-\frac{\pi}{2}\nu_n + \sigma_c(\nu_n))}\Omega_n(\alpha)\right). \tag{43}$$

4 Numerical verification and results

The basic idea in using Sturmian functions to solve scattering problems is to increase the convergence rate when calculating both the scattering wave function as well as transition amplitudes (see [25,26,33–38] and references therein). This can be achieved by providing the basis functions with the appropriated information (physics) of the problem, in particular the correct asymptotic behavior

that the scattering function has. In this way the expansion on the basis is restricted to the region where the "interaction" between the particles takes place. Besides, the basis functions may diagonalize some of the interaction appearing on the Hamiltonian of the full scattering problem, so that some of the relevant physical information will be already built in the basis functions themselves.

To solve general three-body systems we recently developed a method based on the use of hyperspherical Sturmian functions (HSF) [25,26]. Here we propose to use a product of coupled functions, and expand the numerical solution of the scattering problem (9) as

$$\Psi^{NUM}(\rho,\alpha) = \frac{1}{\rho^{\frac{5}{2}}} \sum_m \sum_n a_{n,m} S^+_{n,m}(\rho)\, \Omega_n(\alpha), \quad (44)$$

where, for the angular part, and for this particular problem, we have taken the Jacobi polynomials $\Omega_n(\alpha)$ presented in Section 2.2. Coupled to these, for a given n, we take a HSF set of hyperradial functions $S_{n,m}(\rho)$ satisfying the equation

$$\left[-\frac{1}{2\mu}\frac{1}{\rho^5}\frac{\partial}{\partial\rho}\left(\rho^5\frac{\partial}{\partial\rho}\right) + \frac{\lambda_n(\lambda_n+4)}{2\mu\rho^2} + U(\rho) - E\right] \times \frac{S_{n,m}(\rho)}{\rho^{5/2}} = \beta_{n,m} V_g(\rho) \frac{S_{n,m}(\rho)}{\rho^{5/2}}, \quad (45)$$

where $U(\rho)$ and $V_g(\rho)$ are, respectively, the auxiliary and the generating potentials; here E is externally fixed (as the energy of the system) while $\beta_{n,m}$ are the eigenvalues. For Sturmian functions, generally [33–37], the range of the generating potential $V_g(\rho)$ – assumed of short range – is taken similar to that of the left-out interaction, i.e., in relation with the driving term in equation (9). The auxiliary potential $U(\rho)$ is taken here equal to the interaction potential, i.e., in our model problem $U(\rho) = \mathcal{C}/\rho$. With this choice, asymptotically equation (45) reduces to a Coulomb homogeneous equation providing all basis HSF, a unique – and appropriate – asymptotic behavior, i.e., the one of the full solution sought after; for our problem we choose outgoing behavior

$$S^+_{n,m}(\rho) \to e^{i(K\rho - \eta\ln(2K\rho))}. \quad (46)$$

From this behavior, the transition amplitude can be easily extracted from $\Psi^{NUM}(\rho,\alpha)$, since

$$\Psi^{NUM}(\rho,\alpha) \to \frac{e^{i(K\rho-\eta\ln(2K\rho))}}{\rho^{\frac{5}{2}}} \sum_n \left(\sum_m a_{n,m}\right) \Omega_n(\alpha), \quad (47)$$

yielding, by comparison with (42),

$$f(\alpha) = \sum_n \left(\sum_m a_{n,m}\right) \Omega_n(\alpha). \quad (48)$$

Note that all the basis functions $S_{n,m}(\rho)$ are regular on the whole domain, and satisfy, for any n, closure and orthogonality relations with respect to the generating potential. Different techniques can be implemented to numerically generate the Sturmians functions as explained with details in references [25,37]. The Schrödinger equation, in our case the driven equation (9), is transformed into an algebraic problem which can be easily solved using standard matrix techniques [25,26,37]. Actually, for the source (14) considered in our model, the problem reduces even further: the expansion coefficients $a_{q,p}$ are directly obtained, and are proportional to simple one dimensional integrals.

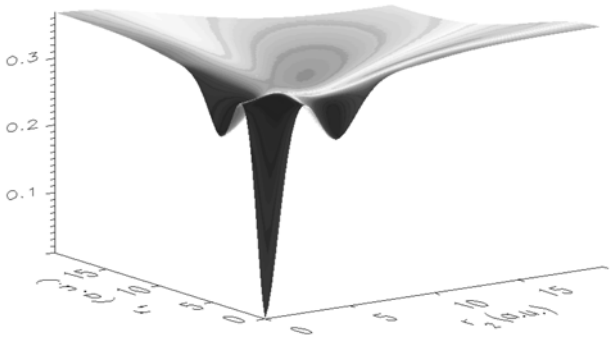

Fig. 2. The modulus of the reduced numerical scattering solution $\Psi^{NUM}(\rho,\alpha)\rho^{\frac{5}{2}}$ as given by equation (44), is plotted as a function of r_1 and r_2. The hyperspherical momentum $K = 1$ a.u., i.e., the energy $E = 0.5$ a.u.

From equation (45) we see that the HSF basis functions diagonalize not only the kinetic energy but also the Coulomb interaction $\mathcal{C}/\rho$ of the scattering equation (9). This choice, and the adequate asymptotic behavior, makes the HSF basis particularly efficient. To illustrate this, let us look at the scattering solution and the transition amplitudes, comparing the analytical results (Sect. 3) with the numerical HSF expansion (44). We take hereafter a reduced mass $\mu = 1$, the momentum of the system $K = 1$ (i.e., the energy $E = 0.5$ a.u.), the parameter of the exponential in the source is taken to be $a = 2$, and the interaction product charges as $\mathcal{C} = -1$ ($\mathcal{C} = 1$ has also been tested, and provides a similar analysis).

The HSF used in our calculation were defined in such a way that all of them have the correct asymptotic behavior of the problem fixed by $\mathcal{C}$ and K. Thus most of the Hamiltonian is diagonalized by the basis functions, and only the coupling produced by the driven term has to be dealt with. In that sense, the generating potential $V_g(\rho)$ has to be defined according to the source term. As can be seen in Figure 1, the source is of short range, and for values of ρ larger than 30, it can be considered as zero: in that region the scattering asymptotic regime should be already reached. We therefore defined the generating potential as having that range so that the constructed basis functions need to expand only the inner region. More specifically, we have taken $V_g(\rho)$ as being a Yukawa potential in ρ with a parameter similar to the one appearing in the right-hand-side of equation (9).

In Figure 2, we plot the modulus of the numerical scattering solution $\Psi^{NUM}(\rho,\alpha)\rho^{5/2}$ given by equation (44) (the modulus is shown as to avoid the oscillations which would crowd the figure). While hyperspherical coordinates are used to calculate it, the solution is presented as a function of the more familiar spherical variable r_1 and r_2

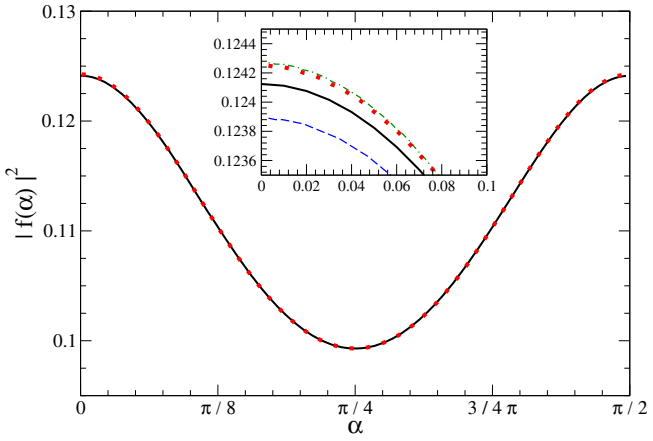

Fig. 3. (Color online) The analytical (full line) and numerical (dotted line) transition amplitude for $K = 1$ a.u., are shown as a function of α. Inset: partial summations (different hyperangular quantum numbers n in equation (48) for the numerical transition amplitudes, with 2 terms (dashed line), 3 terms (dot-dashed line), and 8 terms (dotted line).

allowing one to appreciate the symmetry related to that of the source. Overall excellent agreement (not shown as practically indistinguishable) is found with the analytical solution (41). For the numerical results, we used 8 hyperangular and 15 hyperradial terms; we observed, however, that an indistinguishable curve can be obtained by using as few as a total of 16 terms in expansion (44). It is remarkable that although the source expansion (15) needs a large number of terms (specially for large ρ values), the expansion (44) needs only a very few terms. This is related to the intrinsic adequate property set into the basis itself.

In Figure 3, we compare the exact transition amplitude (43) obtained with only $n = 8$ terms (full line) with the one calculated numerically through expression (48). It is shown here in squared modulus, and presents a U-shaped form typical of double photoionization or electron impact ionization single differential cross sections. The symmetry with respect to $\alpha = \pi/4$ (i.e. $r_1 = r_2$) is clearly observed. Coming back to Figure 2, one can observe how, as r_1 and r_2 both increase (and thus ρ also) the value of the reduced function tends (see Eqs. (47) and (48)) to the shape of the transition amplitude presented in Figure 3. Finally, the very fast convergence of the numerical expansion (48) can be easily appreciated through the partial n summations (dashed lines); the exact result is reached to an accuracy of 10^{-4} with only 3 terms (summing the correspondent terms for $n = 0, 2$ and 4).

The above illustration was given for an energy $E = 0.5$ a.u. (hyperspherical momentum $K = 1$). It is well known that the convergence of numerical methods is strongly energy dependent and becomes more difficult as the energy approaches the ionization threshold. For a much smaller hyperspherical momentum $K = 0.1$ (energy of $E = 0.005$ a.u.), we were able to reproduce the analytical transition amplitude with great accuracy (error of less than 1%) with about 20 m-terms per hyperangular quantum number n, giving a total of about 60–80 terms. This required also adapting the exponent parameter of the Yukawa generating potential (0.005 a.u.). Thus, the convergence can be reached even at very small energy values (the case $K = 0.05$ was also tested successfully).

5 Asymptotic considerations related to the Temkin-Poet problem

It is well known from scattering theory that the transition amplitude corresponding to different collision processes occurring in a given system can be extracted from the asymptotic limit of the wave function. This was shown explicitly in the previous section for the model problem proposed here. How and where to extract this information depends strongly on the problem under consideration, but some general trends can be identified. There are basically three regions to be considered when studying the solution of a driven scattering Schrödinger equation. The first one, $\mathcal{R}_1$, is the region where the driven term is different from zero. The second, $\mathcal{R}_2$, is the region starting where the driven term becomes negligible and up to the domain where the solution's asymptotic behavior begins. The third region, $\mathcal{R}_3$, is the true asymptotic region. The transition amplitude should be extracted in $\mathcal{R}_3$; to the best of our knowledge, however, no studies have been done to clarify how far from the origin this region is located when dealing with the three-body Coulomb problem. This is of importance for its numerical treatment because the problem is difficult and computationally expensive.

With a modification of our model problem we can contribute in understanding the asymptotic domains' issue. Consider the following approximate wave function

$$\Psi^{+}_{app}(\rho,\alpha) = \frac{\bar{\Psi}^{+}_{app}(\rho,\alpha)}{\rho^{\frac{5}{2}}} = \frac{1}{\rho^{\frac{5}{2}}}\sum_n d_n \bar{H}^{+}_n(\rho,\alpha)\Omega_n(\alpha) \tag{49}$$

where d_n are some coefficients, and $\bar{H}^{+}_n(\rho,\alpha)$ are defined by equation (37) but with the Temkin-Poet charge $\tilde{C}(\alpha)$ (see Eq. (5)) replacing $\mathcal{C}$. According to the study presented in Section 3.3, instead of equation (42), the asymptotic behavior of $\Psi^{+}_{app}(\rho,\alpha)$ is

$$\Psi^{+}_{app}(\rho,\alpha) \to f_{app}(\alpha)\frac{e^{i\left(K\rho - \frac{\tilde{C}(\alpha)}{K}\ln(2K\rho)\right)}}{\rho^{\frac{5}{2}}}, \tag{50}$$

that is to say it possesses Peterkop's asymptotic behavior for the Temkin-Poet model. The transition amplitude has the following analytical expression

$$f_{app}(\alpha) = \sum_n d_n \Big(N_{source}(\alpha)\cos\left[\phi(\alpha,\nu_n)\right] \times e^{i\left[-\frac{\pi}{2}\nu_n + \sigma_c(\alpha,\nu_n)\right]}\Omega_n(\alpha)\Big), \tag{51}$$

where the α dependence has been explicitly added everywhere. The approximate wave function $\Psi^{+}_{app}(\rho,\alpha)$ is interesting as it allows us to make a detailed investigation of

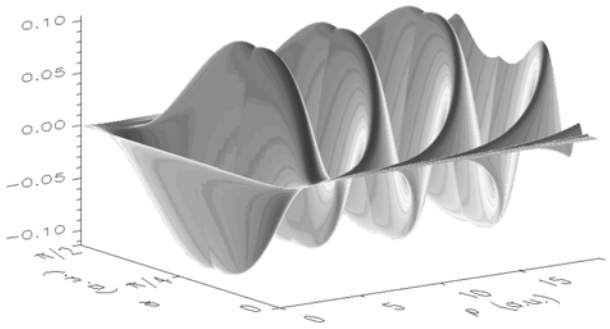

Fig. 4. The function $\bar{R}_n(\rho,\alpha)$ for $n=0$ is plotted as a function of ρ and α.

where the three regions $\mathcal{R}_i$ are located, the analysis being greatly facilitated by the knowledge of the analytic expression. The functions $\bar{H}_n^+(\rho,\alpha)$ satisfy the following non-homogeneous differential equation

$$\left[-\frac{1}{2\mu}\frac{\partial^2}{\partial\rho^2}+\frac{\nu_n(\nu_n+1)}{2\mu\rho^2}+\frac{\tilde{C}(\alpha)}{\rho}-E\right] \times \bar{H}_n^+(\rho,\alpha)=\rho^{5/2}f_n(\rho)\,, \quad (52)$$

and involve again a – α dependent – Coulomb solution of the corresponding homogeneous equation and a particular solution, noted herefater $\bar{R}_n(\rho,\alpha)$. The latter are real functions, and have been evaluated analytically for many values of α. The results for $n=0$, $Z=1$ and $K=1$ are shown in Figure 4 as a function of α and ρ. The α dependence clearly affects the radial behavior. In the region $\mathcal{R}_1$, the function depends strongly on the driven term. As already discussed through Figure 1, the driven term is not negligible for hyperradii smaller than about 5 a.u. Therefore, for $\rho>10$ a.u., the right-hand-side can be numerically considered as zero, meaning that the solution of the driven equation is already located in $\mathcal{R}_2$ where the interaction appearing on the Hamiltonian dictates the dynamics.

It remains to be seen where the function $\Psi^+_{app}(\rho,\alpha)$ reaches the asymptotic regime. The region $\mathcal{R}_3$ is attained when the functions $\bar{H}_n^+(\rho,\alpha)$ will reach their asymptotic behavior, and this for all the necessary n values to get convergence for the total wave function and the transition amplitude. For this purpose, we should compare $\bar{H}_n^+(\rho,\alpha)$ with the asymptotic expression $e^{i\left(K\rho-\frac{\tilde{C}(\alpha)}{K}\ln(2K\rho)\right)}$ for different values of n; it is simpler, however, to compare only the real function $\bar{R}_n(\rho,\alpha)$ and its asymptotic expression (33). This comparison is illustrated in Figure 5 where the functions, normalized asymptotically to one, have been plotted as a function of ρ, shown up to 150 a.u., for $\alpha=\frac{\pi}{3}$ (similar results are obtained for other values of α), and for $n=0,4$ and 8. First of all, we observe a phase shift, which is larger for larger values of n. Secondly, good agreement between the full function and the asymptotic expression is achieved for values of the hyperradial coordinate of about 100 a.u., for $n=0$. However, for higher n values, the asymptotic behavior is reached at much larger values of ρ, for example, at distances larger

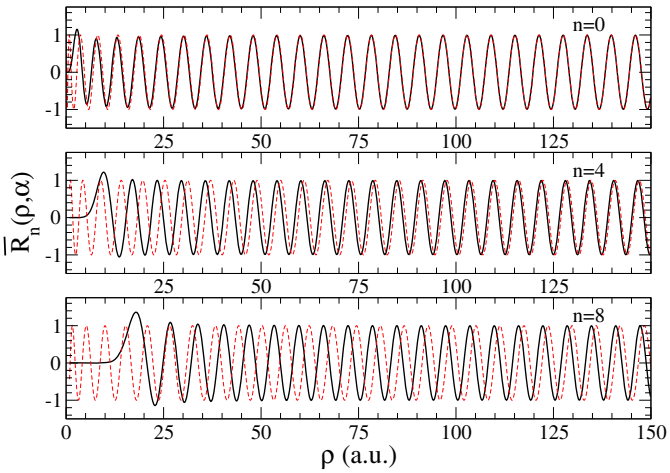

Fig. 5. (Color online) The functions $\bar{R}_n(\rho,\alpha)$ (full line) are plotted as a function of ρ, for $\alpha=\frac{\pi}{3}$, and for $n=0$ (top), $n=4$ (middle) and $n=8$ (bottom). The asymptotic expression (33) is also shown (dashed line) for comparison. Both quantities are shown with unit modulus asymptotically.

than 250 for $n=4$, and even larger than 2500 a.u., for $n=8$. This means that to accurately calculate a converged transition amplitude (say including up to $n=8$ terms), one should evaluate the wave function up to an hyperradius of about 2500–3000 a.u. When restricting the calculation to, say, 100 a.u. one observes an error of about 3%, and even a non negligible difference in shape, for the cross sections. Of course, these values correspond to the chosen physical parameters, and in particular to the system's energy. For smaller energies one should go up to much larger hyperradius values: for example, up to 30 000 a.u. for $E=0.005$ a.u. and even 60 000 a.u. for $E=0.00125$ a.u. (as a rule of thumb, for an hyperspherical momentum K, one should go to distances beyond $3000/K$). Thus, from this analysis, it seems that it is not sufficient to limit the scattering wave function calculation to a domain of about 100 or even 300 a.u.: this is directly related to the long range nature of the Coulomb interaction.

As a consequence of the above analysis, the following question arises: how methods such as the Exterior Complex Scaling [3] or our Generalized Sturmians approach [33] manage to generate the full three-body solution in a square region (r_1 and r_2) of less than 300 atomic units? Extrapolation methods have been implemented to extract the transition amplitude from a wave function defined in a region of less than 200 or 300 a.u. It is, however, fair to ask whether such extrapolations are really yielding the exact result? In order to explore and answer these questions, we are currently using our Generalized Sturmian method for different collision problems, imposing different types of asymptotic behaviors to the basis functions, and comparing the convergency obtained with spherical and hyperspherical coordinates. As illustrated in the present manuscript, hyperspherical Sturmian functions allowed to treat efficiently the model problem and to extract the transition amplitude very accurately. Only very few angular and radial basis functions were

required, but the extraction of the transition amplitude was performed, for $E = 0.5$ a.u., at hyperradius values of about 2500–3000 a.u. The model presented here has the advantage of possessing an analytic solution; this allowed us to compare the numerical to the exact solution, and finally to illustrate the efficiency of our generalized hyperspherical Sturmian approach.

6 Summary

In this report we introduced a model for three-body fragmentation/ionization which applies both for attractive or repulsive cases. The full wave function is split into a chosen bound-free initial state and a scattering wave function which satisfies a driven Schrödinger equation. We were able to find an analytical solution with outgoing wave behavior at large distances, as well as a closed form expression for the transition amplitude. As our model differs substantially from the Temkin-Poet model, it provides an alternative benchmark to test numerical three-body methods. Moreover, contrary to the Temkin-Poet model, in our case the solution is analytical. We thus invite those developing three-body codes to test them by solving the driven Schrödinger equation (18) in spherical coordinates or equation (9) in hyperspherical coordinates (results for different energies E and charge values $\mathcal{C}$ may be obtained from the authors, upon request).

The analytical results of the model scattering problem were verified numerically through an expansion on a complete basis set of the hyperspherical Sturmian functions. All hyperradial basis elements not only diagonalize the kinetic energy and the interaction, but also possess the same appropriate asymptotic behavior; thus, they only need to expand the solution in the interaction region. These properties strongly accelerate the expansion convergence rate for the scattering wave function, and allow for a straightforward extraction of the transition amplitude. Excellent agreement with the analytical results is found with only very few expansion terms.

We also extended the scattering model to allow for an hyperangular charge dependence. In that way, we were able to define an approximate S-wave three-body wave function possessing the correct Peterkop behavior at large distances. This extension allowed us to explore how the wave function takes different behaviors in different hyperradial domains. The configuration space can be subdivided in three regions. In the first one, the source term governs the wave function. In the second region, where the driven term is negligible, the dynamics are ruled purely by the (Coulomb) interactions appearing in the hamiltonian. Finally, for sufficiently large distances, the asymptotic region is reached. The proposed model allowed us to quantitatively identify at which hyperradial distances the asymptotic region is really reached, and thus how far one should go to extract the transition amplitude from the wave function itself. Similar deductions apply for other three-body problems involving Coulomb interactions, and we found that the required distances are larger than 2500 a.u. (this value, of course, depends on the energy of the system). In this respect, it has to be underlined that no full numerical calculations, with numerical grids of such size, have been performed for either $(e, 2e)$ or $(e, 3e)$ processes.

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Appendix

In this Appendix we provide the demonstration of expansion (15) for the proposed source given by equation (14). We start from the mathematical formula (8.442)(2) of reference [39], specified for $\nu = \mu = 1/2$ and taking b as purely imaginary (i.e., ib),

$$\frac{J_{1/2}(az)J_{1/2}(ibz)}{[(az/2)^{1/2}(ibz/2)^{1/2}]} = \sum_{n=0}^{\infty} \frac{(-1)^n (az/2)^{2n}\ {}_2F_1(-n, -n-1/2, 3/2; -b^2/a^2)}{n!\Gamma(3/2)\Gamma(3/2+n)}. \tag{A.1}$$

Let us set $az = \rho\cos\alpha = r_1$ and $bz = \rho\sin\alpha = r_2$. The left-hand-side is then simply $\frac{4}{\pi} j_0(r_1) j_0(ir_2) = \frac{4}{\pi}\frac{\sin r_1}{r_1}\frac{\sinh r_2}{r_2}$. On the right-hand-side, transforming the hypergeometric function ${}_2F_1$ according to formula (15.3.4) of [28], the Jacobi polynomials $\Omega_n(\alpha)/\mathcal{N}_n$ defined through equation (11) appear. After trivial simplifications, we get

$$\frac{\sin r_1}{r_1}\frac{\sinh r_2}{r_2} = \sum_{n=0}^{\infty} \frac{(-1)^n}{2^{2n}(\frac{3}{2})_n n!}\frac{\Omega_n(\alpha)}{\mathcal{N}_n}. \tag{A.2}$$

By reversing the roles of a and b, i.e., r_1 with r_2, $\sin^2\alpha$ becomes $\cos^2\alpha$; this is also equivalent to replacing α by $\pi/2 - \alpha$. Using relation (15.3.6) of [28], it is easy to show that $\Omega_n(\pi/2-\alpha) = (-1)^n\Omega_n(\alpha)$, and hence

$$\frac{\sin r_2}{r_2}\frac{\sinh r_1}{r_1} = \sum_{n=0}^{\infty} \frac{1}{2^{2n}(\frac{3}{2})_n n!}\frac{\Omega_n(\alpha)}{\mathcal{N}_n}. \tag{A.3}$$

Putting together results (A.2) and (A.3) in the source (14), we finally obtain expansion (15).

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