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A spectral approach based on generalized Sturmian functions for two- and three-body scattering problems

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Abstract

A methodology based on generalized Sturmian functions is put forward to solve two- and three-body scattering problems. It uses a spectral method which allows for the inclusion of the correct asymptotic behavior when solving the associated driven Schrödinger equation. For the two-body case, we demonstrate the equivalence between the exterior complex scaling (ECS) and the Sturmian approaches and illustrate the latter by using Hulthén Sturmian functions. Contrary to the ECS approach, no artificial cut-off of the potential is required in the Surmian approach. For the three-body scattering problem, the theoretical framework is presented in hyperspherical coordinates and a set of hyperspherical generalized Sturmian functions possessing outgoing asymptotic behavior is introduced. The Sturmian procedure is a direct generalization of the method discussed for the two-body problem; thus, the comparison with the ECS method is similar. For both the two- and three-body cases, Sturmian bases are efficient as they possess the correct outgoing behavior, diagonalize part of the potentials involved and are essentially localized in the region where the unsolved interaction is not negligible. Moreover, with the Sturmian basis, the operator $(H - E)$ is represented by a diagonal matrix whose elements are simply the Sturmian eigenvalues.

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(Some figures may appear in colour only in the online journal)

1. Introduction

Different and successful methods such as, e.g., the convergent close coupling [1, 2], the *J*-matrix [3] and the exterior complex scaling (ECS) [4–6] have been developed to deal with the description of collision processes between three particles. In general, these methods require an enormous amount of computational resources. The application of the same methods to the

study of the next step, the four-body problem, is presently prohibitive from the computational point of view (see, e.g., [7]). This is proved by the fact that none of the mentioned approaches have been applied as a pure *ab initio* treatment to the study of, e.g., double ionization of helium by electron impact; only approximated versions have been used instead.

For this reason, it is important to continue to develop techniques which improve the efficiency of existing approaches. In this paper, we present and discuss the application of generalized Sturmian functions (GSF) to solve two- and three-body scattering problems.

Recently, a method based on Sturmian functions has been proposed to deal with scattering and structure problems; its efficiency was illustrated in a number of applications (see [8–12] and references therein). It was noted that the developed method contains as a particular case the ECS. The Sturmian method allows one to set proper outgoing boundary conditions, as done by the ECS; however, contrary to the latter, it does not require the rotation of the coordinate, thus avoiding the difficulty associated with the divergence of the driven term. We shall show how to implement the method for solving the two-body driven equation and discuss the equivalence between the Sturmian and the ECS [13] approaches.

The implementation of the ECS method to scattering problems was first proposed by Rescigno and co-workers [13]. Since then, the method has proved to be one of the most successful to deal with a large variety of processes [4, 14–19]. The ECS procedure (see, e.g., [5, 6]) is based on the separation of the total wavefunction as the sum of an asymptotic (or approximated) solution of the problem and a scattering function [20, 21] with, respectively, standing- and outgoing-wave behavior at large distances. This separation leads straightforwardly to a driven Schrödinger equation for the scattering part. Within the ECS approach, two methods have been proposed to solve it: (i) the use of a complex rotation of the radial coordinate is performed on the driven equation and (ii) the use of complex basis sets. In [13], the authors showed that the rotation of the coordinate is equivalent to considering the rotation on the coordinate of the basis functions. In this paper, we follow that idea and implement it in a particular form using a GSF basis. As already demonstrated in [12], these can be built possessing adequate incoming or outgoing behavior, so that all basis functions possess the same behavior at large distances. We will show that the use of Sturmian functions within the context of ECS presents at least two advantages. First, GSF allow us to naturally impose the correct scattering behavior on the solutions of the driven equation, thus avoiding some problems appearing upon rotation of the coordinate in the driven equation [22]. Second, the efficiency of the method can be increased because the basis makes diagonal the operator $(H - E)$ and is localized in the region where the interaction takes place.

Although more elaborate, a strategy similar to that presented for the two-body case is also implemented for the three-body problem. It is done in hyperspherical coordinates because the three-body wavefunction asymptotically behaves as a spherical wave in only one coordinate, the hyper-radial coordinate [23]. For electron impact ionization problems, for example, if one uses the spherical coordinates $(\mathbf{r}_1, \mathbf{r}_2)$ for two electrons, the solution is usually expanded in partial waves and outgoing behavior is imposed on each radial coordinate (r_1, r_2) for the two-continuum wavefunction. Within the ECS approach [6], for example, an external rotation of each spherical coordinate is performed; even though a numerical approximation to the exact solution of the problem is found, difficulties in representing its asymptotic behavior are encountered (the same happens when using the standard Sturmian approach [8]). Indeed, a larger than necessary numerical domain is required to extract the scattering information, since a good representation of the hyperspherical wave has to be found on a squared contour, rather than on a natural hyperspherical one. Moreover, slow convergency rates are to be expected; for the Coulomb problem, the inter-electronic correlation is not included in the basis and generally implies a slow partial wave expansion of the wavefunction. Thus, to treat three-body

ionization or fragmentation problems, it is natural and convenient to use hyperspherical, rather than spherical, coordinates. In this paper, GSF in hyperspherical coordinates (HGSF) are introduced. We do that following the ideas of Macek and Ovchinnikov [24] but we generalize their proposal by using also Sturmian functions in the hyper-radius possessing outgoing (or incoming) behavior. Within this approach, an exterior complex rotation of the hyper-radial coordinate can be performed on the Sturmian equation. This leads to a basis-based ECS for the three-body problem. This approach is a variant of the proposal of McCurdy and co-workers [6], with the important advantage that the asymptotic condition is imposed on a natural hyperspherical contour. Within the present approach, the divergences associated with the driven term of the scattering equation disappear, avoiding the necessity of introducing an artificial cut-off on the interaction potential. Because of the similarities with the two-body problem approach, the properties and conclusions can be extended straightforwardly.

The rest of the paper is arranged as follows. In section 2, we present the two-body scattering formulation and propose using Sturmian basis to solve the standard driven equation. The efficiency of the method is illustrated through Hulthén Sturmian functions. The three-body scattering problem (for two electrons in interaction with a heavy nucleus) is presented in section 3.1. In section 3.2, a set of completely correlated basis hyperspherical GSF is defined in terms of intermediate Sturmian functions. The solution of the driven Schödinger equation is discussed in section 3.3. Finally, a summary is presented in section 4.

Atomic units ($\hbar = e = 1$) are used throughout.

2. Two-body scattering problem

2.1. Formulation of the problem

The two-body scattering problem is described by the Schrödinger equation $[H - E]\Phi(r) = 0$ with a positive energy $E = k^2/(2\mu)$ (μ is the reduced mass). For two particles interacting via a spherically symmetric potential $V(r)$, the radial equation, with the convenient transformation $\Phi(r) = \Psi(r)/r$, reads

$$(h_l - E)\Psi(r) = 0, \tag{1}$$

with the Hamiltonian $h_l = \mathcal{T}_l + V(r)$, where $\mathcal{T}_l = -\frac{1}{2\mu}\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2}\right)$ represents the reduced kinetic energy operator and l is the angular momentum eigenvalue. The free-particle solution $\Psi_0(r)$ of the simplified problem (without potential)

$$(\mathcal{T}_l - E)\Psi_0(r) = 0 \tag{2}$$

is known

$$\Psi_0(r) = kr j_l(kr), \tag{3}$$

where $j_l(z)$ represents the spherical Bessel function of order l [25]; $\Psi_0(r)$ behaves at large distances as $\sin\left(kr - \frac{\pi}{2}l\right)$ and corresponds to a unitary flux.

It is quite common in scattering theory (e.g, [20, 21]) to separate the solution of the scattering problem into two terms,

$$\Psi(r) = \Psi_0(r) + \Psi_{\mathrm{sc}}(r), \tag{4}$$

where $\Psi_0(r)$ is taken as initial—asymptotic—state (corresponding to no scattering) and $\Psi_{\mathrm{sc}}(r)$ is the scattering term describing the dynamics of the collision process. In principle, $\Psi_{\mathrm{sc}}(r)$ should have pure outgoing behavior, denoted $\Psi^+_{\mathrm{sc}}(r)$; the corresponding wavefunction (4) is denoted $\Psi^+(r)$. Replacing decomposition (4) into equation (1), we obtain the following driven Schrödinger equation for $\Psi_{\mathrm{sc}}(r)$:

$$(h_l - E)\,\Psi_{\mathrm{sc}}(r) = -V(r)\Psi_0(r). \tag{5}$$

Solutions of this equation possessing pure outgoing behavior can be obtained only if the driven term falls off to zero sufficiently fast. This is a requirement of the standard theory of scattering. Long-range potentials are acceptable as long as one modifies the way of extracting the scattering information [22]; this happens, for example, when dealing with potentials possessing a Coulomb tail. If the potential $V(r)$ is of short range, a possible representation for the asymptotic form of $\Psi_{\rm sc}^{+}(r)$ is given by the Riccati–Hankel functions [25], denoted $H_l^{\pm}(0,r)$, which are irregular at the origin and behave asymptotically as $\mathrm{e}^{\pm \mathrm{i}\left(kr-\frac{\pi}{2}l\right)}$. For long-range potentials, however, the treatment should be developed within the framework of a distorted wave approach. For Coulomb plus short-range potentials, the proper recipe is given in section 4.2 of [6]. Recently [22], a reformulation has been proposed which allows us to formulate the scattering problem for both short- and long-range potentials, including the pure Coulomb case. For Coulombic asymptotic behavior $z_1 z_2/r$ (let $\alpha = z_1 z_2 \mu/k$ define the Sommerfeld parameter), the scattering wavefunction $\Psi_{\rm sc}(r)$ has incoming ($H_l^{-}(\alpha,r)$) or outgoing ($H_l^{+}(\alpha,r)$) behavior which, at large distances, behave as

$$H_l^{\pm}(\alpha,r) \longrightarrow \mathrm{e}^{\pm \mathrm{i}\left(kr-\alpha\ln(2kr)-\frac{\pi}{2}l\right)}; \tag{6}$$

the functions $H_l^{\pm}(\alpha,r)$, which are linear combinations of the regular and irregular Coulomb functions, are irregular close to the origin. The asymptotic behavior of $\Psi_{\rm sc}(r)$ provides the transition matrix $A_l = \mathrm{e}^{\mathrm{i}\delta_l}\sin(\delta_l)$ (or the scattering matrix $S_l = \mathrm{e}^{2\mathrm{i}\delta_l}$) in terms of the scattering phase-shift δ_l.

2.2. Use of generalized Sturmian basis to solve the driven equation

Sturmian functions may be used as an appropriate basis to deal with scattering problems (see [8, 9, 12] and references therein). These functions satisfy the equation

$$[\mathcal{T}_l + \mathcal{U}(r) - E]\, S_{n,l}(r) = -\beta_n \mathcal{V}(r) S_{n,l}(r), \tag{7}$$

where $\mathcal{U}(r)$ and $\mathcal{V}(r)$ are, respectively, the *auxiliary* and *generating* potentials and β_n are the eigenvalues; the energy E is taken as an externally fixed value ($E \geqslant 0$ for scattering problems). Assuming that $r = x$ is a point located in a region where the generating potential is negligible, equation (7) comes with the two-point boundary conditions

$$S_{n,l}^{\pm}(r=0) = 0, \tag{8a}$$

$$S_{n,l}^{\pm}(r=x) \to H_l^{\pm}(\alpha,x); \tag{8b}$$

$\alpha = 0$ when $\mathcal{U}(r)$ is short range. As in all two-point boundary value problems, the Sturmian functions $S_{n,l}^{\pm}(r)$ (assumed normalized) form a complete

$$\sum_n S_{n,l}^{\pm}\left(r'\right)\mathcal{V}(r) S_{n,l}^{\pm}(r) = \delta(r-r') \tag{9}$$

and orthogonal set

$$\left\langle S_{n',l}^{\pm}\right|\mathcal{V}(r)\left|S_{n,l}^{\pm}\right\rangle = \int_0^{\infty} \mathrm{d}r\, S_{n',l}^{\pm}(r)\mathcal{V}(r) S_{n,l}^{\pm}(r) = \delta_{n',n}. \tag{10}$$

Note that the functions are orthogonal with respect to the generating potential $\mathcal{V}(r)$ and that no conjugation symbol appears in equation (10).

The generating potential $\mathcal{V}(r)$ is arbitrary but defined to be of short range (say R_0) and shorter than that of $\mathcal{U}(r)$. In that way, for values of r such that $\mathcal{V}(r)$ is negligible, all the Sturmian functions $S_{n,l}^{\pm}(r)$ satisfy

$$[\mathcal{T}_l + \mathcal{U}(r) - E]\, S_{n,l}^{\pm}(r) = 0, \tag{11}$$

and thus possess the same energy and the same (e.g., outgoing) asymptotic behavior ruled by $\mathcal{U}(r)$. These properties allow us to define an appropriate basis set to deal with scattering problems, and we can use it to solve the driven equation (5). Indeed, expanding $\Psi_{\rm sc}(r)$ and $V(r)\Psi_0(r)$ in Sturmian functions

$$\Psi^{\pm}_{\rm sc}(r) = \sum_n a_n S^{\pm}_{n,l}(r), \tag{12}$$

$$-V(r)\Psi_0(r) = \sum_n b_n \mathcal{V}(r) S^{\pm}_{n,l}(r), \tag{13}$$

and replacing into (5), we obtain

$$\sum_n a_n \left[V(r) - \mathcal{U}(r) + \beta_n \mathcal{V}(r)\right] S^{\pm}_{n,l}(r) = \sum_n b_n \mathcal{V}(r) S^{\pm}_{n,l}(r). \tag{14}$$

Choosing the auxiliary potential $\mathcal{U}(r)$ to be the interaction $V(r)$, only the generating potential remains on the lhs. Projecting on the left by $S^{\pm}_{n',l}(r)$, integrating on the coordinate and using the orthogonality property (10), we end up with

$$\sum_n \beta_n \delta_{n',n} a_n = b_{n'}. \tag{15}$$

Thus, a matrix equation $\bar{\mathbf{s}}\,\mathbf{a} = \mathbf{b}$ is obtained and can be solved by standard matrix methods.

Taking the asymptotic limit of (12) yields

$$\Psi^{\pm}_{\rm sc}(r) \to \sum_n a_n \, \mathrm{e}^{\pm \mathrm{i}\left[kr - \alpha \ln(2kr) - \frac{\pi}{2} l\right]} = A_l \, \mathrm{e}^{\pm \mathrm{i}\left[kr - \alpha \ln(2kr) - \frac{\pi}{2} l\right]}, \tag{16}$$

which leaves us with the simple definition $A_l = \sum_n a_n$ for the transition amplitude.

The Sturmian basis functions transformed the operator $(h_l - E)$ into a diagonal matrix $\bar{\mathbf{s}}$ whose elements are simply the Sturmian eigenvalues. This can be seen in an alternative form. Equation (5) can be rewritten as

$$\Psi^{\pm}_{\rm sc}(r) = G^{\pm} V(r) \Psi_0(r) \tag{17}$$

in terms of Green's function $G^{\pm}$ which is responsible for providing the correct asymptotic behavior to $\Psi^{\pm}_{\rm sc}(r)$. Now, Green's function satisfies the equation

$$(h_l - E) G^{\pm}(E, r, r') = \delta(r - r'), \tag{18}$$

and can be expanded in terms of Sturmians functions as follows:

$$G^{\pm}(E, r, r') = \sum_n g_n S^{\pm}_{n,l}(r') S^{\pm}_{n,l}(r). \tag{19}$$

Replacing this expansion into (18), using equation (7) and taking $\mathcal{U}(r) = V(r)$, we find

$$-\sum_n g_n \beta_n S^{\pm}_{n,l}(r') S^{\pm}_{n,l}(r) \mathcal{V}(r) = \delta(r - r'). \tag{20}$$

By comparison with the closure relation (9), we deduce that $g_n = -1/\beta_n$. This means that Green's function is diagonal in the generalized Sturmian representation. Besides, the representation is optimized since the asymptotic region is associated with the range of the generating potential $\mathcal{V}(r)$; the asymptotic form of $G^{\pm}$ is directly given by the correct asymptotic behavior of the Sturmian functions. This is clear since equation (7) can be written as

$$\frac{1}{\beta_n} S^{\pm}_{n,l}(r) = -G^{\pm} \mathcal{V}(r) S^{\pm}_{n,l}(r), \tag{21}$$

and thus the Sturmian functions are eigenfunctions of the operator $G^{\pm}\mathcal{V}(r)$ with the eigenvalue $-1/\beta_n$ [26–28].

At this point, a comparison with the ECS can be performed. Similar to what we have just described, the ECS approach also uses spectral methods to represent the operator $(h_l - E)$; the main difference with our proposal, however, is that we are using basis functions that diagonalize the interaction and the kinetic energy, and the Green's function itself. Besides, the generating potential $\mathcal{V}(r)$ can be defined as having the range of the driven term, implying that all the basis functions are concentrated in the region where the driven term $V(r)\Psi_0(r)$ is not negligible.

Our description of the Sturmian method implemented to deal with scattering problems shows that it is equivalent to the ECS in the sense that a matrix representation of $(h_l - E)$ and $(h_l - E)^{-1}$ is used to solve the problem, and a similar type of linear system of equations appears. In the Sturmian case, the basis is optimized to have not only the energy of the problem but also the appropriate asymptotic behavior (8*b*). The difference from the ECS approach is, up to this point, that we are not performing a rotation of the coordinate. However, this can be performed. Within the Sturmian method, it is more convenient to define Sturmian functions with the rotated coordinate rather than using the rotation of the driven equation (5). Consider a smooth exterior complex rotation of the coordinate, denoted $\tau(r, \eta)$, which at the origin and until a point close to R_0 behaves as r and for large $r > R_0$ behaves as $r\,\mathrm{e}^{\mathrm{i}\eta}$. For rotation $r > R_0$, will transform all the basis functions with, e.g., outgoing behavior into

$$S^{+}_{n,l}(\tau(r, \eta)) \to H^{+}_{l}(\alpha, r\,\mathrm{e}^{\mathrm{i}\eta}); \tag{22}$$

thus, for large values of r, $H^{+}_{l}(\alpha, r\,\mathrm{e}^{\mathrm{i}\eta}) \to \mathrm{e}^{\mathrm{i}\left[kr\,\mathrm{e}^{\mathrm{i}\eta} - \alpha \ln\left(2kr\,\mathrm{e}^{\mathrm{i}\eta}\right) - \frac{\pi}{2}l\right]} \to 0$ as desired. All the basis functions possess the same outgoing behavior; thus, all of them will decrease asymptotically in the same form.

Within the ECS method [6], a divergence of the driven term of equation (5) appears when performing an exterior complex rotation; as a consequence, the method requires an artificial cut-off of the potential on the right-hand side of the driven equation. It is clear that this artifice is completely avoided when using Sturmian functions, as no incoming wave behavior is allowed. Besides, the use of this basis for solving the driven Schrödinger equation can considerably increase the efficiency of the standard ECS as proposed in, e.g., [13]. For illustration, we consider here Sturmian functions corresponding to the Hulthén potential $\mathcal{V}(r) = -\mathrm{e}^{-r/R_0}/(1 - \mathrm{e}^{-r/R_0})$. In figure 1, we plot the real and imaginary parts of the Sturmian functions versus r; here $R_0 = 10$ and $\mathcal{U}(r) = 0$ [12]. One can easily observe that all the basis functions possess the same asymptotic behavior for values of $r > R_0$; all of them have the same energy, here $E = 0.6$. If we assume that the range of the driven term is that of the generating potential, let us say R_0, then we clearly see how the efficiency of the basis is increased because all the nodes are located in that region. In this way, the convergence rate of expansion (12) of the scattering wavefunction is accelerated, the convergence itself being guaranteed by the fact that $V(r)\Psi_0(r)$ is short range.

In figure 2, we plot (with dots) as a function of the real part of the radial coordinate the real (top panel) and imaginary (bottom panel) parts of two of the Sturmian functions plotted in figure 1; for the same values of E and R_0, the eigenvalues are $\beta = -0.08 + \mathrm{i}0.438\,178$ and $\beta = -2.88 + \mathrm{i}2.629\,07$. For comparison, the real and imaginary parts of the Sturmian functions, $n = 1$ (long dashed line) and $n = 6$ (dashed line), with the real coordinate are included. We use here a smooth complex rotation of the coordinate such as the one proposed by Karlsson [29], i.e. $\tau(r, \eta) = r + \mathrm{i}\tan\eta g(r)$ with $g(r) = 0$ if $r < \bar{R}_0$ and $g(r) = (r - \bar{R}_0)^2$ if $r > \bar{R}_0$. All the basis functions have the same behavior as the one observed in figure 1 for the real values of r. For values of r larger than $\bar{R}_0$ (here $\bar{R}_0 = 15$), those with the rotation in the

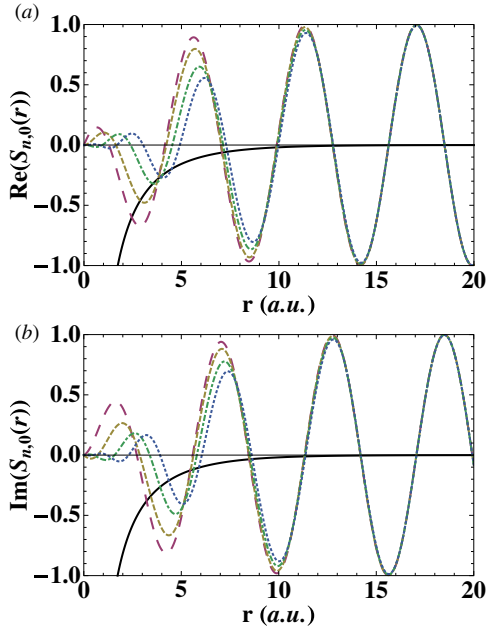

Figure 1. Real and imaginary parts of four Hulthén Sturmian functions $S_{n,0}(r)$ ($n = 1$–4) for the angular momentum $l = 0$, range $R_0 = 10$ and energy $E = 0.6$. The Hulthén potential (solid line) is also shown.

coordinate decrease exponentially to zero. We can fix $\bar{R}_0$ as being equal to, greater or smaller than R_0 depending on the convenience in the calculations to be performed and depending on the size (extension) of the driven term.

A complete connection between the ECS and the Sturmian approach discussed above can be established if the set of Sturmian functions is derived from the equation

$$[\mathcal{T}_l(\tau(r,\eta)) + \mathcal{U}(\tau(r,\eta)) - E]\,\bar{S}_{n,l}(\tau(r,\eta)) = -\beta_n \mathcal{V}(\tau(r,\eta))\bar{S}_{n,l}(\tau(r,\eta)), \tag{23}$$

with the two-point boundary conditions

$$\bar{S}_{n,l}(r=0) = 0, \tag{24a}$$

$$\bar{S}_{n,l}\,[\tau(r,\eta) = \tau(x,\eta)] \to H_l^{\pm}(\alpha, x). \tag{24b}$$

The boundary condition at large values of the coordinate is imposed for a real value x of the radial coordinate and the parameter η enters parametrically through the relation $\tau(r,\eta) = \tau(x,\eta)$. Here, we are giving not only the optimal basis functions to be used on scattering problems but also the way of obtaining them. All the methods discussed in [8, 9, 12] (and references therein) can be applied to solve the complex rotated Sturmian equation. The limit $\eta \to 0$ can be easily taken and will lead to Sturmian functions obtained over the real axis of the coordinate. The use of a smooth exterior complex rotation of the coordinate avoids the occurrence of a discontinuity of the derivative of the basis functions contrary to the ECS proposal [6].

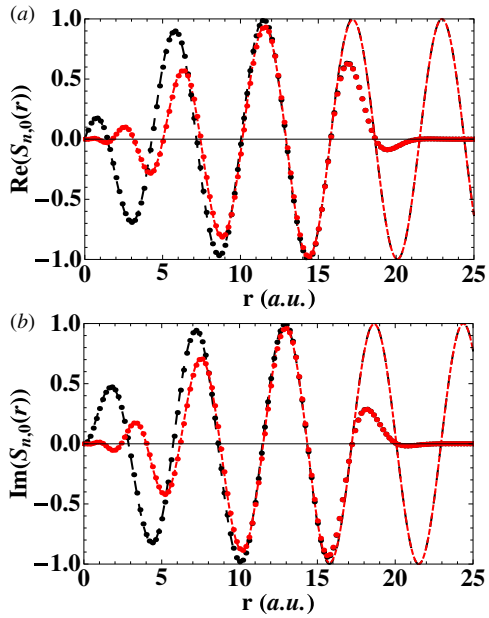

Figure 2. Real and imaginary parts (plotted with dots) of two of the Hulthén Sturmian functions $S_{n,0}(r)$ ($n = 1$ and $n = 6$) obtained after a smooth complex rotation (see the text) as a function of the real part of the radial coordinate ($l = 0$, $R_0 = 10$ and $E = 0.6$). For comparison, the real and imaginary parts of the Sturmian functions, $n = 1$ (long dashed line) and $n = 6$ (dashed line), with the real coordinate are included.

3. Three-body scattering problems: a hyperspherical approach

When applied to two-body scattering problems, the ECS method and the Sturmian proposal presented in section 2 are based on the same principle: solving a driven equation to find a function which possesses pure, e.g., outgoing behavior at large distances. As explained in the introduction, to treat three-body ionization or fragmentation problems it is more natural and convenient to use hyperspherical, rather than spherical, coordinates. In order to maintain a Sturmian approach like in section 2, we need to use Sturmian functions in hyperspherical coordinates and impose proper outgoing behavior. One possible way of introducing such functions has been presented in [30]. Here, we will introduce a different set similar to the one used by Macek and Ovchinnikov [24].

3.1. Formulation in hyperspherical coordinates

The Hamiltonian for a system of three particles of masses m_1, m_2 and m_3 can be written in terms of any of three pairs of Jacobi coordinates $\mathbf{r}_{ij}$, $\mathbf{R}_{k,ij}$ or mass-scaled Jacobi coordinates $\mathbf{x}_k$ and $\mathbf{X}_k$ [30],

$$\mathbf{x}_k = \left(\frac{\mu_{ij}}{\mu}\right)^{1/2} \mathbf{r}_{ij}, \qquad \mathbf{X}_k = \left(\frac{\mu}{\mu_{ij}}\right)^{1/2} \mathbf{R}_{k,ij},$$

for $k = 1, 2, 3$ and $i \neq j \neq k$. The two-body reduced mass for the ij pair of particles is $\mu_{ij} = m_i m_j/(m_i + m_j)$, while the three-body one is $\mu = \sqrt{m_i m_j m_k/(m_i + m_j + m_k)}$. The

hyper-radius ρ, defined as $\rho^2 = x_k^2 + X_k^2$, is independent of the particular choice of k. The remaining five hyperangular coordinates (denoted collectively by ω_5) include the hyperangle

$$\tan\alpha_k = \frac{X_k}{x_k}$$

and the polar angles θ_{x_k}, ϕ_{x_k} and θ_{X_k}, ϕ_{X_k} defining the orientations $\widehat{\mathbf{x}}_k$ and $\widehat{\mathbf{X}}_k$ of the Jacobi vectors in the center-of-mass reference frame. We will drop the subindex k in the following, so the previous definitions allow one to write $x = \rho\cos\alpha$ and $X = \rho\sin\alpha$.

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

$$\Lambda^2 = -\frac{1}{\sin^2\alpha\cos^2\alpha}\frac{\mathrm{d}}{\mathrm{d}\alpha}\left(\sin^2\alpha\cos^2\alpha\frac{\mathrm{d}}{\mathrm{d}\alpha}\right) + \frac{\mathbf{j}^2}{\cos^2\alpha} + \frac{\mathbf{l}^2}{\sin^2\alpha}, \tag{25}$$

where $\mathbf{j}$ and $\mathbf{l}$ denote the rotational and centrifugal angular momentum operators, respectively. The Schrödinger equation to be considered is

$$[T + V(\rho,\omega_5) - E]\,\Psi(\rho,\omega_5) = 0, \tag{26}$$

where $V(\rho,\omega_5)$ describes the interaction potentials between the particles. When dealing with two-electron systems (and a nucleus of charge Z), the interaction potential reads [24]

$$\begin{aligned} V(\rho,\omega_5) =& -\frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} \\ =& -\frac{Z}{\rho\cos\alpha} - \frac{Z}{\rho\sin\alpha} + \frac{1}{\rho\sqrt{1-\sin(2\alpha)\cos\theta_{12}}} = \frac{C(\omega_5)}{\rho}, \end{aligned} \tag{27}$$

where $\cos\theta_{12} = \hat{\mathbf{r}}_1\cdot\hat{\mathbf{r}}_2$ defines the inter-electron angle. We can use the well-known partial wave expansion [31]

$$\frac{1}{r_{12}} = \frac{1}{\rho}\sum_{l=0}^{\infty} P_l(\cos\theta_{12}) \begin{cases} \sec\alpha\tan^l\alpha & 0 \leqslant \alpha \leqslant \frac{1}{4}\pi \\ \csc\alpha\cot^l\alpha & \frac{1}{4}\pi \leqslant \alpha \leqslant \frac{1}{2}\pi, \end{cases} \tag{28}$$

to separate the angle α from the other variables. Besides, expanding the Legendre polynomials in the spherical angles $\{\theta_1,\phi_1,\theta_1,\phi_1\}$

$$P_l(\cos\theta_{12}) = \frac{4\pi}{2l+1}\sum_{m=-l}^{l}(-1)^m Y_l^{-m}\left(\hat{\mathbf{r}}_2\right) Y_l^m(\hat{\mathbf{r}}_1), \tag{29}$$

we have complete angular separation, and $C(\omega_5)$ reads explicitly

$$C(\omega_5) = -\frac{Z}{\cos\alpha} - \frac{Z}{\sin\alpha} + \sum_{l=0}^{\infty}\frac{4\pi}{2l+1}\sum_{m=-l}^{l}(-1)^m Y_{-m}^l\left(\hat{\mathbf{r}}_2\right) Y_m^l(\hat{\mathbf{r}}_1) \begin{Bmatrix} \sec\alpha\tan^l\alpha \\ \csc\alpha\cot^l\alpha \end{Bmatrix}, \tag{30}$$

where the restrictions given in (28) must be taken into account.

For collision problems, we need to solve the Schrödinger equation (26). As in section 2.1, the wavefunction $\Psi(\rho,\omega_5)$ is separated into two terms, $\Psi(\rho,\omega_5) = \Psi_0(\rho,\omega_5) + \Psi_{\mathrm{sc}}(\rho,\omega_5)$, leading to the following driven equation:

$$[T + V(\rho,\omega_5) - E]\,\Psi_{\mathrm{sc}}(\rho,\omega_5) = -W(\rho,\omega_5)\Psi_0(\rho,\omega_5), \tag{31}$$

where $W(\rho,\omega_5)$ is the interaction not solved by a given initial state $\Psi_0(\rho,\omega_5)$. Two important issues while solving this collision problem are (i) the range of the interaction $W(\rho,\omega_5)$ and (ii) the use of an appropriate matrix definition for the operator $(H-E)$ or for Green's function $(H-E)^{-1}$; here $H = T + V(\rho,\omega_5)$.

The basis set to be used has to take into account both issues: it has to be complete in the region where the interaction $W(\rho,\omega_5)$ is not negligible and outside that region has to possess the correct asymptotic behavior corresponding to all three Coulomb interactions.

3.2. Hyperspherical Sturmian functions

Sturmian functions in hyperspherical coordinates were introduced and applied by Macek and Ovchinnikov [24]. In this very interesting paper, these authors extended the Sturmian concept to various dimensions and defined the solution of the three-body Coulomb problem in a very particular way. Briefly, the solution was expressed as a contour integral with an integrand given by the product of Bessel functions depending on the hyper-radius, angular Sturmian functions depending on all the angular coordinates and a coefficient depending on the integration variable. The integration is performed over the index of the Bessel function defining what is known as a Kontorovich–Lebedev transform [32–35], which is a kind of generalized Fourier transform. The Bessel functions form a complete set but do not possess the appropriate boundary conditions; for this reason, the integral has to build the correct Coulomb logarithmic-type solution.

Here we will follow these ideas, but instead of using a Kontorovich–Lebedev representation, we will use Sturmian functions also for the hyper-radial coordinate. These functions possess the appropriate boundary conditions and depend on a discrete index rather than a continuous one as in the Kontorovich–Lebedev transform. This allows the use of matrix techniques to solve scattering problems.

To achieve this, we first define intermediate Sturmian functions both for the angular and the radial coordinate, and then use them to define full non-separable Sturmian functions.

3.2.1. Intermediate Sturmian functions. For the hyper-radial coordinate, we can introduce a set of radial functions $\bar{S}_m(\rho)$ satisfying

$$\left[-\frac{1}{2\mu}\frac{1}{\rho^5}\frac{\partial}{\partial\rho}\left(\rho^5\frac{\partial}{\partial\rho}\right)+\frac{\lambda(\lambda+4)}{2\mu\rho^2}+\mathcal{U}_{\rm int}(\rho)-E\right]\bar{S}_{m,\lambda}(\rho)=-\beta_m\mathcal{V}_{\rm int}(\rho)\bar{S}_{m,\lambda}(\rho), \tag{32}$$

which we consider as an intermediate Sturmian equation. The potential $\mathcal{U}_{\rm int}(\rho)$ can be of short or long range; $\mathcal{V}_{\rm int}(\rho)$ is a generating potential. Introducing the reduced function

$$\bar{S}_{m,\lambda}(\rho)=\frac{S_{m,\lambda}(\rho)}{\rho^{\frac{5}{2}}} \tag{33}$$

into (32) leads to

$$\left[-\frac{1}{2\mu}\frac{\partial^2}{\partial\rho^2}+\frac{\lambda(\lambda+4)+\frac{15}{4}}{2\mu\rho^2}+\mathcal{U}_{\rm int}(\rho)-E\right]S_{m,\lambda}(\rho)=-\beta_m\mathcal{V}_{\rm int}(\rho)S_{m,\lambda}(\rho), \tag{34}$$

which has the same form as equation (7) presented in section 2 (the difference appearing only in the definition of the $1/\rho^2$ term) and similar boundary conditions can then be used. The hyper-radial eigenfunctions $S_{m,\lambda}(\rho)$ form an orthogonal and complete set such that

$$\int {\rm d}\rho\, S_{m,\lambda}(\rho)\mathcal{V}_{\rm int}(\rho)S_{n,\lambda}(\rho)=\delta_{mn}, \tag{35a}$$

$$\sum_m S_{m,\lambda}(\rho')\mathcal{V}_{\rm int}(\rho)S_{m,\lambda}(\rho)=\delta(\rho-\rho'). \tag{35b}$$

Following Macek and Ovchinnikov [24], we define a set of Sturmian functions depending on the angular coordinates ω_5 as the eigenfunctions $\Omega_\nu(\omega_5)$ of the following angular Sturmian eigenvalue equation:

$$[\Lambda^2+2\mu\rho_\nu C(\omega_5)]\Omega_\nu(\omega_5)=\lambda(\lambda+4)\Omega_\nu(\omega_5), \tag{36}$$

where ρ_ν are the eigenvalues, while λ is an externally fixed parameter. These functions are connected to the adiabatic functions in the same way as the radial Sturmian functions are

connected to the eigenenergy functions corresponding to the same equation. For a given hyperradius R, the hyperspherical adiabatic basis functions $\varphi_s(R, \omega_5)$ are defined as eigenfunctions of the equation

$$[\Lambda^2 + 2\mu RC(\omega_5)]\varphi_s(R, \omega_5) = 2\mu\epsilon_s(R)R^2\varphi_s(R, \omega_5), \tag{37}$$

with eigenvalues $\epsilon_s(R)$; they define, for each value of s, a set of curves as a function of R. By comparison of equations (36) and (37), the resolution of the equation $2\mu\epsilon(\rho)\rho^2 = \lambda(\lambda + 4)$ provides the roots $\rho_\nu(\lambda)$. The Sturmian angular functions $\Omega_\nu(\omega_5)$ correspond to all those functions having energies associated with the externally fixed value λ and different angular Coulomb potentials $C(\omega_5)$.

As discussed in [24], the eigenfunctions $\Omega_\nu(\omega_5)$ satisfy the following orthogonality and closure relations:

$$\int \mathrm{d}\omega_5 C(\omega_5)\Omega_{a'}(\omega_5)\Omega_a(\omega_5) = \delta_{aa'} \tag{38a}$$

$$\sum_a \Omega_a\left(\omega_5'\right)\Omega_a(\omega_5)C(\omega_5) = \delta\left(\omega_5 - \omega_5'\right), \tag{38b}$$

where $\mathrm{d}\omega_5$ represents the five-dimensional volume element and $\delta\left(\omega_5 - \omega_5'\right)$ is the symbolic product of the delta functions corresponding to all five angular coordinates. Note that no complex conjugation appears in either (38*a*) or in (35*a*).

3.2.2. Hyperspherical GSF. With the intermediate Sturmians introduced above, we may now define a new set of hyperspherical generalized Sturmian functions (HGSF), denoted $\Phi_\eta(\rho, \omega_5)$, with outgoing (or incoming) asymptotic conditions. We ask these HGSF to satisfy the following equation:

$$\left[-\frac{1}{2\mu}\frac{1}{\rho^5}\frac{\partial}{\partial\rho}\left(\rho^5\frac{\partial}{\partial\rho}\right) + \frac{\Lambda^2}{2\mu\rho^2} + \frac{C(\omega_5)}{\rho} - E\right]\Phi_\eta(\rho, \omega_5) = -\gamma_\eta V_g(\rho)C(\omega_5)\Phi_\eta(\rho, \omega_5). \tag{39}$$

The generating potential $V_g(\rho)$ has to be of short range, the range being associated with that of the perturbation $W(\rho, \omega_5)$. Asymptotically, all the basis functions will satisfy the equation

$$\left[-\frac{1}{2\mu}\frac{1}{\rho^5}\frac{\partial}{\partial\rho}\left(\rho^5\frac{\partial}{\partial\rho}\right) + \frac{\Lambda^2}{2\mu\rho^2} + \frac{C(\omega_5)}{\rho} - E\right]\Phi_\eta(\rho, \omega_5) = 0, \tag{40}$$

which includes the Coulomb interactions and the subsequent coupling produced even in the asymptotic region.

To build the HGSF, we propose the expansion

$$\Phi_\eta(\rho, \omega_5) = \sum_{m\nu} a_{m\nu}\frac{S_{m,\lambda}(\rho)}{\rho^{\frac{5}{2}}}\Omega_\nu(\omega_5). \tag{41}$$

Replacing into equation (39), and using equation (36), we obtain

$$\sum_{m\nu} a_{m\nu}\left[\left(\mathcal{U}_{\mathrm{int}}(\rho) + \beta_m\mathcal{V}_{\mathrm{int}}(\rho)\right) + \rho_\nu(\lambda)\frac{C(\omega_5)}{\rho^2} - \frac{C(\omega_5)}{\rho} - \gamma_\eta V_g(\rho)C(\omega_5)\right] \times S_{m,\lambda}(\rho)\Omega_\nu(\omega_5) = 0. \tag{42}$$

The non-separability of the term $C(\omega_5)/\rho$ enforces the generating potential $\mathcal{V}_{\mathrm{int}}(\rho)$ to be of long range. For that reason, we make the following choice:

$$\mathcal{U}_{\mathrm{int}}(\rho) = 0, \tag{43a}$$

$$\mathcal{V}_{\rm int}(\rho) = \frac{1}{\rho}. \tag{43b}$$

With these potentials, the Sturmian equation (34) defines a set of hyper-radial Coulomb Sturmian functions (HCSF) with an externally fixed centrifugal barrier fixed by λ,

$$S_{m,\lambda}(\rho) = \mathcal{N}_{m,\lambda}\, \mathrm{e}^{\mathrm{i}K\rho} (2\mathrm{i}K\rho)^{\lambda+5/2}\, {}_1F_1\left(-m, 2\lambda+5, -2\mathrm{i}K\rho\right), \tag{44}$$

where $E = K^2/2\mu$ and $\mathcal{N}_{m,\lambda}$ defines a normalization constant. These functions are equivalent to those given in appendix D of [36] but in hyperspherical coordinates. In this case, the eigencharges of equation (34) are given by $\beta_m = (m + \frac{5}{2} + \lambda)\mathrm{i}K/\mu$.

Projecting equation (42) over the basis functions, and using the orthogonality properties (38*a*) and (35*a*), we find

$$\sum_{m\nu} \left[\beta_m \delta_{mm'} \mathcal{O}_{\nu'\nu} + \left(\rho_\nu(\lambda) \left[\frac{1}{\rho^2} \right]_{mm'} - \delta_{mm'} - \gamma_\eta [V_g]_{mm'} \right) \delta_{\nu\nu'} \right] a_{m\nu} = 0, \tag{45}$$

where the overlap of the angular functions is given by the matrix

$$\mathcal{O}_{\nu'\nu} = \int \mathrm{d}\omega_5\, \Omega_{\nu'}(\omega_5)\Omega_\nu(\omega_5), \tag{46}$$

and the matrix elements $[A]_{mm'}$ are defined by one-dimensional integrals,

$$[A]_{mm'} = \int \mathrm{d}\rho\, S_{m,\lambda}(\rho) A(\rho) S_{m',\lambda}(\rho). \tag{47}$$

Solving equation (45) provides the expansion coefficients $a_{m\nu}$ and the eigenvalues γ_ν.

The boundary conditions for the Sturmian functions are such that they vanish at $\rho = 0$. The centrifugal barrier defined in terms of λ is introduced through the angular equation; it provides the Sturmian functions $S_{m,\lambda}(\rho)$ a behavior ρ^λ close to the origin, making the integrals $[1/\rho^2]_{m'm}$ well defined. Note that the parameter λ is externally fixed and is not the eigenvalue of equation (36). It is included in the angular equation with the purpose of giving a well-defined definition for the hyper-radial integrals (47). It is also worth mentioning that the HCSF closed form leads to analytical expressions for the matrix elements (47) allowing for their high precision evaluation.

The HGSF built in this way have the following important properties:

$$\int \mathrm{d}\mathbf{v}\, \Phi_{\eta'}(\rho, \omega_5)\Phi_\eta(\rho, \omega_5) V_g(\rho) C(\omega_5) = \delta_{\eta\eta'} \tag{48a}$$

$$\sum_\eta \Phi_\eta(\rho', \omega_5')\Phi_\eta(\rho, \omega_5) V_g(\rho) C(\omega_5) = \delta(\rho - \rho')\delta(\omega_5 - \omega_5'), \tag{48b}$$

where $\mathrm{d}\mathbf{v} = \rho^5\, \mathrm{d}\rho \sin^2\alpha \cos^2\alpha\, \mathrm{d}\alpha\, \mathrm{d}\hat{\mathbf{X}}\, \mathrm{d}\hat{\mathbf{x}}$. Note again that no complex conjugation is used in (48*a*).

The HGSF $\Phi_\eta(\rho, \omega_5)$ are the generalization of the Sturmian functions introduced by Macek and Ovchinnikov to the whole set of hyperspherical coordinates. The study of the properties of these functions themselves is of interest due to the fact that they contain most of the physics of the collision problem; different types of asymptotic behavior can be imposed on them, as indicated in section 2. The exponential term $\mathrm{e}^{\mathrm{i}K\rho}$ of (44) provides the outgoing behavior to function $\Phi_\eta(\rho, \omega_5)$ of (41), while the polynomial of (44) combined with the angular functions allows for the construction of the Peterkop-type asymptotic behavior in the region where all the particles are far from each other.

3.3. Solving the driven equation

When dealing with two electrons and a heavy nucleus, the driven Schödinger equation (31) results

$$\left[T + \frac{C(\omega_5)}{\rho} - E\right]\Psi_{sc}(\rho, \omega_5) = -W(\rho, \omega_5)\Psi_0(\rho, \omega_5), \tag{49}$$

where $W(\rho, \omega_5)$ depends on the election of the initial channel $\Psi_0(\rho, \omega_5)$. One of the requirements of the standard scattering theory is that the interaction on the right-hand-side of (49) must be of short range. Two main reasons are associated with this condition. One is a mathematical issue: if the interaction $W(\rho, \omega_5)$ is of long range, the kernel of the associated integral equation is not compact. The second reason is that if $W(\rho, \omega_5)$ is of long range, this function enforces given asymptotic behavior on the solution of (49). Conversely, if $W(\rho, \omega_5)$ is of short range, after a given ρ value, the driven term of (49) will be zero and then an asymptotic solution possessing pure outgoing (or incoming) behavior of the homogeneous equation will be allowed for $\Psi_{sc}(\rho, \omega_5)$.

To solve equation (49), we can expand $\Psi_{sc}(\rho, \omega_5)$ and $W(\rho, \omega_5)\Psi_0(\rho, \omega_5)$ on the HGSF basis,

$$\Psi_{sc}(\rho, \omega_5) = \sum_\eta \psi_\eta \Phi_\eta(\rho, \omega_5) \tag{50}$$

$$W(\rho, \omega_5)\Psi_0(\rho, \omega_5) = \sum_\eta c_\eta V_g(\rho) C(\omega_5)\Phi_\eta(\rho, \omega_5). \tag{51}$$

Replacing in (49), projecting on the left with the basis functions and using (48*a*), we obtain

$$\sum_\eta \gamma_\eta \delta_{\eta\eta'}\psi_\eta = c_{\eta'}, \tag{52}$$

that is, the same matrix form as found for the two-body problem (see equation (15) of section 2). Similarly, the range of the generating potential $V_g(\rho)$ is clearly associated with the range of $W(\rho, \omega_5)$ through expansion (51).

The reason behind the obtained diagonal representation of $(H - E)$ is connected with the definition of Green's function, similar to the two-body case (section 2.2). The three-body Coulomb Green's function satisfies the following hyperspherical equation:

$$\left[-\frac{1}{2\mu}\frac{1}{\rho^5}\frac{\partial}{\partial\rho}\left(\rho^5\frac{\partial}{\partial\rho}\right) + \frac{\Lambda^2}{2\mu\rho^2} + \frac{C(\omega_5)}{\rho} - E\right]G(\rho', \omega_5', \rho, \omega_5) = \delta(\rho - \rho')\delta(\omega_5 - \omega_5'), \tag{53}$$

and we propose the following expansion in terms of HGSF:

$$G(\rho', \omega_5', \rho, \omega_5) = \sum_\eta g_\eta \Phi_\eta(\rho', \omega_5')\Phi_\eta(\rho, \omega_5). \tag{54}$$

Replacing into (53), we obtain

$$\sum_\eta g_\eta[-\gamma_\eta V_g(\rho)C(\omega_5)]\Phi_\eta(\rho', \omega_5')\Phi_\eta\,(\rho, \omega_5) = \delta(\rho - \rho')\delta(\omega_5 - \omega_5'), \tag{55}$$

and by comparison with the closure relation (48*b*), we deduce

$$g_\eta = -\frac{1}{\gamma_\eta}. \tag{56}$$

Green's function built in this way will possess the correct asymptotic behavior in the region where the generating potential is negligible.

The HGSF $\Phi_\eta(\rho, \omega_5)$ can be constructed so as to provide $\Psi_{sc}(\rho, \omega_5)$ with outgoing (or incoming) asymptotic behavior. Expansion (50) is then restricted to the region where the interaction $W(\rho, \omega_5)$ is not negligible, exactly as happened in the two-body problem. The main task of the whole problem is then to solve the Sturmian equation (39). If we employ expansion (41) together with the HCSF defined by (44), all HGSF will possess outgoing behavior. Thus, a complex rotation of the coordinate, as described in section 2.2 for the two-body case, can be easily implemented. Similarly, the exterior complex rotation can be performed on the Sturmian equation (39) rather than on the driven equation (49).

4. Summary

In this paper, we have presented the theory, based on GSF, necessary to deal with scattering problems for two and three particles.

For the simple case of two particles, we showed how to build the scattering part of the solution in terms of Sturmian functions which are defined in terms of an auxiliary and a generating potential. We showed that the operator $(H - E)$ can be reduced to a diagonal matrix whose elements are given by the Sturmian eigenvalues, i.e. the magnitudes of the generating potential. The range of the latter is adjusted to match that of the driven term of the scattering non-homogeneous equation; this makes the basis particularly efficient as exemplified with Hulthén Sturmian functions. The auxiliary potential provides all basis functions pure outgoing behavior, as the sought scattering function itself. Consequently, an exterior complex rotation of the coordinate can be performed. The use of Sturmian basis functions avoids all the problem appearing in the standard ECS theory discussed in [22]. We showed also that the ECS theory is a particular case of the Sturmian approach.

For three-body problems, we defined a strategy similar to the one discussed for two-body problems, although the mathematical approach is more elaborate. We constructed six-dimensional Sturmian functions in hyperspherical coordinates. As for the two-body case, the Sturmian equation includes a generating and an auxiliary potential, the latter defining the asymptotic behavior of all the basis functions. The generating potential, being of short range, is again adjusted to the range of the driven term of the scattering Schrödinger equation. The hyperspherical Sturmian functions are constructed in terms of some intermediate Sturmian functions. For the angular part, we use the functions presented and discussed by Macek and Ovchinnikov [24], while for the hyper-radial coordinate, we use closed form Coulomb Sturmian functions. Similar to the two-body case, the constructed basis functions lead to a diagonal matrix representation of the three-body operator $(H - E)$. The fact that all the hyper-radial basis functions possess pure outgoing behavior allows again for an exterior complex rotation of the hyper-radius ρ. Thus, it is possible to show that the present Sturmian approach includes the exterior complex rotation approach as a particular case, the procedure to show the equivalence of the methods being similar to the one presented for the two-body case.

The calculations of cross sections and application to different three-body scattering processes will soon be presented elsewhere.

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