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Mathematical properties of generalized Sturmian functions

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Abstract
We study some mathematical properties of generalized Sturmian functions which are solutions of a Schrödinger-like equation supplemented by two boundary conditions. These generalized functions, for any value of the energy, are defined in terms of the magnitude of the potential. One of the boundary conditions is imposed at the origin of the coordinate, where regularity is required. The second point is at large distances. For negative energies, bound-like conditions are imposed. For positive or complex energies, incoming or outgoing boundary conditions are imposed to deal with scattering problems; in this case, since scattering conditions are complex, the Sturmian functions themselves are complex. Since all of the functions solve a Sturm–Liouville problem, they allow us to construct a Sturmian basis set which must be orthogonal and complete: this is the case even when they are complex. Here we study some properties of generalized Sturmian functions associated with the Hulthén potential, in particular, the spatial organization of their nodes, and demonstrate explicitly their orthogonality. We also show that the overlap matrix elements, which are generally required in scattering or bound state calculations, are well defined. Many of these mathematical properties are expressed in terms of uncommon multivariable hypergeometric functions. Finally, applications to the scattering of a particle by a Yukawa and by a Hulthén potential serve as illustrations of the efficiency of the complex Hulthén–Sturmian basis.

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

1. Introduction

The applications in physics of Sturm–Liouville formulation appeared immediately after the principal theorems were demonstrated by Sturm and Liouville in 1836 and 1837. A large variety

of problems can be solved using this technique leading to a generalization of the Fourier method to expand general functions. In atomic physics studies, Sturmian functions were introduced by Shull and Löwdin [1] as a complete basis set to expand atomic wavefunctions. Later Rotenberg [2, 3] gave them the name *Sturmian* to emphasize their connection with the Sturm–Liouville theory. Glöckle and co-workers used Weinberg states (which are actually Sturmian functions) in scattering problems [4]. In 1968, Goscinsky [5] presented, in an Uppsala University internal report, a rigorous mathematical generalization of this basis set. This report was unknown to the atomic physics community until recently when Goscinsky and Avery presented it as an appendix in [6]. Originally, Goscinsky regarded Sturmian functions as solutions to the Schrödinger equation with a constant and externally defined energy, and considered the magnitude of the potential (the 'charges') as the eigenvalues [5, 6]. In his work, only negative energies were considered and no consideration over how to obtain the basis functions was done. Here we extend Goscinski's work by discussing some important issues related to Sturmian basis functions, mostly in connection with complex and positive energies and their applications to scattering problems.

When compared with hydrogenic functions, Sturmian basis functions present considerable advantages. One of them is that they are thickly crowded on a spatial region that can be adjusted to be the desired region of interest through the adequate choice of the energy and of different parameters appearing in the potentials. Bound-state hydrogenic wavefunctions, on the other hand, are widely spread in space, since the maximum value position is proportional to n^2; moreover, their innermost zeros are insensitive to the principal quantum number n. This accounts for the fact that these functions do not form a complete set; the continuum is required to describe the region between the origin and the first zero. Other properties (advantages) are best described according to whether the energy is taken positive, negative or complex.

Negative energy Sturmian functions, which asymptotically decrease exponentially, have been widely and efficiently used to perform *ab initio* calculations of N-electron atomic and molecular systems (see, for example, [7] and references therein). Their use substantially improves the convergence of the expansion for many configuration–interaction calculations, as shown, for instance, in [1, 8, 9].

Positive energy Sturmian functions, on the other hand, are useful for scattering problems, because one can generate functions having the same energy as the physical scattering particle (the same wave-number) and the same asymptotic boundary condition (for example, outgoing- or incoming-wave condition). Moreover, positive Sturmian functions with standing-wave boundary conditions form a continuum basis set with an infinite and continuum spectrum [10, 11]. Although a finite-size basis can be developed such that the spectrum discretizes, regularization of the wavefunctions often leads to potentially divergent functions, unless the energy itself becomes complex. This makes them impractical to use in scattering problems.

Complex energy Sturmian functions can be obtained by performing a complex scaling rotation. As an example of applications in scattering problems, we can mention those of Piraux's group using the J-matrix method. Such functions are used within time-independent and time-dependent approaches to solve the Schrödinger equation for calculations of single and double photoionization of helium [12] as well as ionization–excitation of neutral atoms [13].

Sturmian basis sets obtained for general potentials are very scarce in the literature because there are only a few two-body potentials that admit closed-form solutions. Some examples were discussed by Rawitscher [14–17], and by Macek and Ovchinnikov [18, 19]. However, the most widely used Sturmian functions (most of the references given above employ them) are called Coulomb Sturmian functions (CSF); they are obtained as discrete solutions of Schrödinger's equation with a pure Coulomb interaction. Since each one of these basis elements belongs to

a different charge eigenvalue, their individual asymptotic behavior is different, and hence they are not particularly appropriate and efficient.

Very recently our group extended the work of Rawistcher and proposed several methods [20–22] to generate discrete sets of functions having a unique behavior at large distances. The set possesses only asymptotically outgoing (or incoming) waves, all with the same wavenumber corresponding to the physical scattering energy; moreover, all the basis functions are required to be regular at the origin, and differ from each other by the number of nodes within the inner region. The energy is not the only parameter that determines the asymptotic behavior of the basis functions. In our attempt to generalize the use of Sturmian basis functions, we introduced generalized Sturmian functions (GSF) (see, for example, [14, 22, 23]), in which two potentials are included in the Schrödinger equation. One potential—called the *auxiliary potential*—is, in general, a long-range one that determines the asymptotic behavior of all the basis set elements. The other is a short-range potential—called the *generating potential*—which accounts for the dynamics of the inner region, where the two particles interact strongly with each other.

The proposal presented here is essentially an extension of the work of Goscinsky [5] to general energies (real positive and complex). When performing the extension, some doubts can arise regarding the validity of the solutions of a Sturm–Liouville problem, which involve not only positive (or complex) energies but also complex boundary conditions. One recurrent doubt is whether the GSF are $\mathcal{L}^2$, and whether they allow for well-defined matrix elements for different interaction potentials. Another issue regards completeness and whether GSF possess a nodal arrangement similar to that established by theory for real functions.

To address some of these issues, in this paper we present a comprehensive study which demonstrates that such matrix elements are indeed well defined and that the basis functions fulfill all expected properties of normal Sturmian functions (closure and orthogonality relations, nodal structure, etc). The whole investigation is exemplified with the solutions of the Hulthén potential.

In addition, we take the advantage of the fact that the Hulthén potential leads to analytic Sturmian functions to provide analytic expressions for several matrix elements. As we will write them in terms of multivariable hypergeometric functions, this study complements our investigations on multivariable hypergeometric functions connected with atomic physics problems [24–29].

The rest of the paper is arranged as follows. In section 2, we present the basic theory of Sturmian functions and some atomic physics applications. In section 3, we introduce Hulthén Sturmian functions and we provide analytic expressions for the orthogonality relation as well as for the overlap matrix elements; some properties related to the nodes of the basis functions are also discussed. In section 4, we exemplify the results by applying the method, and the proposed basis functions, to the study of a particle scattered by a Hulthén and a Yukawa potential. For the Hulthén case, expressions for Green's function, the scattering part of the wavefunction and the transition amplitude are provided analytically. In section 5, a brief summary is provided.

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

2. Generalized Sturmian functions

2.1. Basic theory

Generalized Sturmian radial functions are solutions of the non-homogeneous Schrödinger equation

$$[\mathcal{T}_l + \mathcal{U}(r) - E_s]\, S_{nl}(r) = -\beta_{nl}\, \mathcal{V}(r)\, S_{nl}(r), \tag{1}$$

where $\mathcal{T}_l = -\frac{1}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{l(l+1)}{2\mu r^2}$ is the kinetic energy, $\mathcal{U}(r)$ is the *auxiliary* potential, $\mathcal{V}(r)$ is a short-range *generating* potential which vanishes in the outer region $r > R_S$, μ is the reduced mass and l the angular momentum. In contrast to the traditional time-independent Schrödinger equation, where the magnitude of the potential is fixed and its solution leads to the energy eigenvalues, in equation (1) the energy E_s is a fixed parameter and the magnitude β_{nl} become the eigenvalues. Besides, two boundary conditions supplement the equation. We are seeking solutions that have a regular boundary condition at the origin $S_{nl}(r = 0) = 0$. If the auxiliary potential $\mathcal{U}(r)$ is a Coulomb potential, then the Kato cusp condition should also be imposed, as discussed in [30].

In the outer region $r > R_s$, where the second boundary condition is imposed, the radial equation (1) becomes

$$[\mathcal{T}_l + \mathcal{U}(r) - E_s]\, S_{nl}(r) = 0. \tag{2}$$

The solutions of the Sturmian equation then represent a particle of energy E_s moving under the influence of a potential $\mathcal{U}(r)$. For a short-range auxiliary potential $\mathcal{U}(r)$ (i.e. $\mathcal{U}(r)$ also vanishing in the outer region), the asymptotic solutions of (2) behave as $S_{nl}(r \to \infty) \propto \mathrm{e}^{-\kappa r}$ where $\kappa = \sqrt{-2\mu E_s}$ for negative energies $E_s < 0$, while $S_{nl}(r \to \infty) \propto \mathrm{e}^{\pm \mathrm{i}kr}$ where $k = \sqrt{2\mu E_s}$ for positive energies; the sign is associated with outgoing $(+)$ or incoming $(-)$ waves. For an auxiliary potential $\mathcal{U}(r)$ including a Coulomb contribution Z/r and a short-range potential, the asymptotic form for positive energies has to include the well-known logarithmic term, i.e. $S_{nl}(r \to \infty) \propto \mathrm{e}^{\pm \mathrm{i}(kr - \eta \ln(2kr))}$ where $\eta = Z\mu/k$ is the Sommerfeld parameter. Since E_s is a fixed parameter and the asymptotic equation (2) does not involve the eigenvalue, all basis functions $S_{nl}(r)$ have the same asymptotic behavior.

Equation (1), together with the two boundary conditions, defines a Sturm–Liouville problem. Thus, according to the standard theory, the Sturmian functions conform a complete basis set [5]:

$$\sum_n S_{nl}(r')\, \mathcal{V}(r)\, S_{nl}(r) = \delta(r - r'), \tag{3}$$

and obey the following potential-weighted ($\mathcal{V}(r)$) orthogonality relation

$$\mathcal{V}_{n',n} = \mathcal{V}_{n,n}\delta_{n',n}, \tag{4}$$

where the general matrix elements are defined through

$$\mathcal{A}_{n',n} = \int_0^\infty S_{n'l}(r)\, A(r)\, S_{nl}(r)\, \mathrm{d}r; \tag{5}$$

this includes, as a subcase, the overlap matrix elements

$$\mathcal{O}_{n',n} = \int_0^\infty S_{n'l}(r) S_{nl}(r)\, \mathrm{d}r. \tag{6}$$

Note that no complex conjugation appears in these formulae, contrary to the case of the standard Hilbert space. As we will see, this makes a fundamental difference when dealing with Sturmian functions possessing scattering asymptotic conditions. The same applies for the closure relation.

2.2. Applications in atomic physics

Many advantages appear when using GSF in atomic physics. In this subsection, we briefly review the methodology for both bound and scattering states. For a given interaction potential $V(r)$, the aim is to solve the Schrödinger equation

$$[\mathcal{T}_l + V(r) - E]\, \Psi(r) = 0. \tag{7}$$

For bound states, the solution $\Psi_B(r)$ may be expanded as

$$\Psi_B(r) = \sum_n a_n S_{n,l}(r). \tag{8}$$

Upon replacement in (7), and using (1), we have

$$\sum_n a_n \left[V(r) - \mathcal{U}(r) - \beta_{nl}\mathcal{V}(r) - E + E_s\right] S_{nl}(r) = 0. \tag{9}$$

We may choose the auxiliary potential $\mathcal{U}(r)$ to be the interaction $V(r)$, so that the first two terms on (9) cancel each other. Projecting with basis functions $S_{n',l}(r)$ from the left, integrating on the coordinate, using the orthogonality relation (4) and the overlap matrix (6), we get

$$\sum_n [-\beta_{nl}\mathcal{V}_{n',n}\delta_{n'n} - (E - E_s)\mathcal{O}_{n'n}]a_n = 0, \tag{10}$$

which can be easily solved by standard matrix methods.

For scattering solutions, one may set the full solution as [31] $\Psi(r) = \Psi_0(r) + \Psi_{\rm sc}(r)$, where $\Psi_0(r)$ is an asymptotic solution which solves the simplified, potential-free, equation $[\mathcal{T}_l - E]\,\Psi_0(r) = 0$; the scattering part $\Psi_{\rm sc}(r)$ solves the non-homogeneous differential equation

$$[\mathcal{T}_l + V(r) - E]\,\Psi_{\rm sc}(r) = -V(r)\Psi_0(r). \tag{11}$$

Expanding $\Psi_{\rm sc}(r)$ and $V(r)\Psi_0(r)$ in Sturmian functions with externally fixed energy $E_s = E$

$$\Psi_{\rm sc}(r) = \sum_n a_n S_{n,l}(r) \tag{12}$$

$$V(r)\Psi_0(r) = \sum_n b_n \mathcal{V}(r) S_{n,l}(r), \tag{13}$$

and using equation (1), the radial Schrödinger equation is converted into

$$\sum_n a_n \left[V(r) - \mathcal{U}(r) - \beta_{nl}\mathcal{V}(r)\right] S_{n,l}(r) = -\sum_n b_n \mathcal{V}(r) S_{n,l}(r). \tag{14}$$

Choosing again $\mathcal{U}(r) = V(r)$, only the generating potential remains on the LHS. Projecting by the left by $S_{n',l}(r)$, we end up again with a matrix problem

$$\beta_{n'l} a_{n'} = b_{n'}. \tag{15}$$

The Sturmian basis functions transformed the operator $[\mathcal{T}_l + V(r) - E]$ into a diagonal matrix whose elements are simply the Sturmian eigenvalues. This can be seen in an alternative form. Equation (11) can be rewritten as

$$\Psi^{\pm}_{\rm sc}(r) = G^{\pm}_l V(r)\Psi_0(r) \tag{16}$$

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

$$[\mathcal{T}_l + V(r) - E]\,G^{\pm}_l(E, r, r') = \delta(r - r'), \tag{17}$$

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

$$G^{\pm}_l(E, r, r') = \sum_n g_{nl} S^{\pm}_{n,l}(r') S^{\pm}_{n,l}(r). \tag{18}$$

Replacing this expansion into (17), using equation (1) and taking $\mathcal{U}(r) = V(r)$, we find

$$-\sum_n g_{nl}\beta_{nl} S^{\pm}_{n,l}(r') S^{\pm}_{n,l}(r)\mathcal{V}(r) = \delta(r - r'). \tag{19}$$

Comparing this expression with the closure relation (3) we see that $g_{nl} = -1/\beta_{nl}$. 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 is directly given by the correct asymptotic behavior of the Sturmian functions. This is clear since (1) can be written as

$$-\frac{1}{\beta_{nl}} S^{\pm}_{n,l}(r) = G^{\pm}_{l} \mathcal{V}(r) S^{\pm}_{n,l}(r), \tag{20}$$

and thus the Sturmian functions are eigenfunctions of the operator $G^{\pm}_{l}\mathcal{V}(r)$ with eigenvalues $-1/\beta_{nl}$ [15–17].

It is clear that for both bound and scattering problems, the Schrödinger equation to be solved is considerably simplified when using GSF.

2.3. Some additional mathematical considerations

2.3.1. Orthogonality relation. The orthogonality relation (4) can be derived from the differential equation (1) satisfied by the Sturmian functions. However, this standard approach is generally presented for real functions with a real variable. In our case, due to the boundary conditions (for scattering problems) and due also to the fact that the energy might be complex, the solutions of the Sturm–Liouville problem are complex functions. Consequently, some doubts (see the next subsection) may appear regarding the mere existence of overlap matrix elements (and similarly for other matrix elements corresponding to potential interactions, e.g. the electromagnetic field). Another issue is the validity of the orthogonality and closure relations. In appendix B of a very interesting paper [10], the author mentioned that for positive energy, only Sturmian functions corresponding to Coulomb potentials are orthogonal and yield a delta function. Thus, it is reasonable to have some doubts regarding the orthogonality of the Sturmian basis functions $S_{n,l}(r)$ defined above. As mentioned before, starting from the differential equation it is easy to derive the following expression:

$$-2\mu\,(\beta_{nl} - \beta_{n'l}) \int_0^R S_{n'l}(r)\,\mathcal{V}(r)\,S_{nl}(r)\,\mathrm{d}r = \left[S_{nl}(r) \frac{\mathrm{d}S_{n'l}(r)}{\mathrm{d}r} - S_{n'l}(r) \frac{\mathrm{d}S_{nl}(r)}{\mathrm{d}r} \right]_R, \tag{21}$$

where the limit $R \to \infty$ should be taken. Now, at large distances $r > R_S$ where the generating potential vanishes, the asymptotic behavior of the Sturmian functions is such that the right-hand side of equation (21) is indeed zero. Thus, for $n \neq n'$ the functions must be orthogonal even in the case where the boundary conditions and the basis functions are complex. However, we believe it is instructive to explore the way the orthogonality is achieved. The underlying mathematical function generating the Kronecker symbol will therefore be investigated in section 3.1 for Hulthén Sturmian functions. This is of interest from the mathematical point of view and in connection with the theory of multivariable hypergeometric functions. The relation like the one to be obtained is similar to many of the formulae provided in, e.g., [32] and [33] which are extremely useful for many physical–mathematical developments [24–29].

An interesting fact to be noticed is that the orthogonality relation is associated with the definition of a family of orthogonal polynomials defined on a finite-range coordinate, as now discussed. For short-range potentials $\mathcal{U}(r)$, for example, we can write the Sturmian functions as $S_{nl}(r) = \mathrm{e}^{\mathrm{i}kr} s_{nl}(r)$. For $r > R_S$, $S_{nl}(r)$ must behave as $\mathrm{e}^{\mathrm{i}kr}$ while at the origin as r^{l+1}. Thus, the functions $s_{nl}(r)$ behave as r^{l+1} at the origin and go to 1 for large values of the coordinate. We do not pretend to demonstrate this here but, according to the studies performed by our group, we know that the functions $s_{nl}(r)$ are polynomials. The nodal structure, the way nodes arrange and other properties support our affirmation. Moreover, we may use a new variable $x = g(r)$ such that the range $r \in [0, \infty]$ converts into $x \in [0, 1]$, x being associated with the

range of the generating potential $\mathcal{V}(r)$. With such polynomials, the orthogonality relation may be written as

$$\int_0^\infty S_{n'l}(r)\mathcal{V}(r)S_{nl}(r)\,\mathrm{d}r = \int_0^1 s_{n'l}(x)s_{nl}(x)w(x)\,\mathrm{d}x \propto \delta_{n'n} \tag{22}$$

with a given weight function $w(x)$ related to $\mathcal{V}(g^{-1}(x))$ and to the cut-off function appearing in $\mathcal{V}(r)$. This is also supported by our previous work [22, 34] where we used a numerical discretization, finite differences, to solve the Sturmian equation by transforming it into a difference equation. The discretization, and the boundary conditions imposed, lead to a set of orthogonal polynomials. For all hypergeometric-type polynomials it is possible to demonstrate that the obtained polynomials are the 'hyperquantized' version [35] of other families of polynomials. This has a general character. Some examples have been discussed in publications in connection with the angular Sturmian function in hyperspherical coordinates [34, 35], with the Coulomb potential [36, 37] and with general potentials [34].

The definition and investigation of these polynomials is part of our current investigations and is very important as they provide the tool to perform highly accurate integrations by quadrature for all the matrix elements required in collision and structure calculations. In addition, the existence of polynomials of different orders provides a natural nodes order (on the complex plane); this can be useful to order the Sturmian functions themselves in applications of structure or collision problems (of course, one should also investigate which of the basis functions are the most useful for the problem being solved).

2.3.2. Overlap matrix elements. Overlap integrals (6) appear in many types of calculations, both in scattering and structure problems. When dealing with scattering problems, the Sturmian functions correspond to positive energy states. We will now show that even in this case, the overlap integrals $\mathcal{O}_{n',n}$ and also other matrix elements $\mathcal{A}_{n',n}$ with some operator $A(r)$ (e.g. an electromagnetic field) are well defined.

The first thing to be noticed in connection with the definition of these matrix elements is that because there is no complex conjugation when using Sturmian functions, oscillating exponential factors such as $\mathrm{e}^{\mathrm{i}kr}$ will be present in the integrand (for energy eigenfunctions they cancel each other). Secondly, for values of r larger than a given point R_S all the basis functions are proportional to $\mathrm{e}^{\mathrm{i}kr}$ (this is for short-range auxiliary potentials; see section 2.1). This allows us to split the integral (6) as follows:

$$\mathcal{O}_{n',n} = \int_0^{R_S} S_{n'l}(r)S_{nl}(r)\,\mathrm{d}r + \int_{R_S}^\infty \mathrm{e}^{2\mathrm{i}kr}\,\mathrm{d}r. \tag{23}$$

Since the Sturmian functions are well behaved in the whole finite range $[0, R_S]$, the first integral is always well defined. The second integral can be performed analytically by introducing an integrating factor $\mathrm{e}^{-\epsilon r}$:

$$\int_{R_S}^\infty \mathrm{e}^{(2\mathrm{i}k-\epsilon)r}\,\mathrm{d}r = \frac{\mathrm{e}^{(-\epsilon+2\mathrm{i}k)R_S}}{\epsilon - 2\mathrm{i}k}, \tag{24}$$

where the limit $\epsilon \to 0$ yields a perfectly defined result $-\mathrm{e}^{2\mathrm{i}kR_S}/(2\mathrm{i}k)$. Thus, the whole overlap integral $\mathcal{O}_{n',n}$ is well defined for positive energies. A similar analysis applies to matrix elements $\mathcal{A}_{n'n}$ containing extra positive powers of r^p ($p \geqslant 0$). This is in contrast with what would happen for energy eigenfunctions. With the complex conjugation required, the oscillating exponential factors cancel out and the integration between R_S and ∞ would diverge, leading to not well-defined overlap integrals.

A similar analysis can be performed when the auxiliary potential is a Coulomb potential $\mathcal{U}(r) = Z/r$. The logarithmic phase appearing in the asymptotic form of the Sturmian functions can also be integrated leading also to well-defined limits.

3. The Hulthén Sturmian functions: mathematical properties

Consider the Hulthén potential (it is a particular case of Eckart's potential)

$$\mathcal{V}(r) = \mathcal{V}_0 \frac{\mathrm{e}^{-r/a}}{1 + c\,\mathrm{e}^{-r/a}} = \mathcal{V}_0 \frac{x}{1 + cx}, \tag{25}$$

where $a > 0$ is the screening parameter, $c = -1$ and $\mathcal{V}_0 < 0$; $x = \mathrm{e}^{-r/a}$ in the second equality. The Hulthén potential is of short range: it behaves as a Coulomb potential ($-Z/r$ if one takes $\mathcal{V}_0 = -Z/a$) at small distances and decreases exponentially for large values of r. In contrast with the Coulomb case, the Hulthén potential allows only for a finite number of bound states.

For $l = 0$, the energy eigensolutions are known analytically [38]. Those, regular at the origin, are given by $x^{\alpha}\,{}_2F_1(\alpha - \gamma, \alpha + \gamma, 2\alpha + 1; x)$ with $\alpha^2 = -2\mu E a^2$ and $\gamma = \mathrm{i}a\sqrt{2\mu(\mathcal{V}_0 + E)}$; ${}_2F_1$ is the Gauss hypergeometric function. For positive energies, $\alpha = \pm \mathrm{i}ka$; outgoing behavior ($\mathrm{e}^{\mathrm{i}kr}$) is obtained for $\alpha = -\mathrm{i}ka$. Bound states correspond to $\alpha - \gamma = -n$ (the hypergeometric series reduces to a polynomial of order n in $x = \mathrm{e}^{-r/a}$); hence, $\kappa = \kappa_n = (\mu\mathcal{V}_0 a)/n - n/(2a)$ and the energy $E_n = -\kappa_n^2/(2\mu)$ is quantized ($n = 1, 2, \ldots$).

Valid Sturmian $l = 0$ functions for outgoing (the incoming case can be treated similarly) scattering conditions can be chosen—in r and x formulations—as

$$S_n(r) = N_n\,\mathrm{e}^{\mathrm{i}kr}\,{}_2F_1(-n, -2\mathrm{i}ak + n, -2\mathrm{i}ak + 1, \mathrm{e}^{-r/a}) = N_n\,\mathrm{e}^{\mathrm{i}kr}\,{}_2F_1(-n, B_n, C_n, \mathrm{e}^{-r/a}), \tag{26a}$$

$$s_n(x) = N_n x^{-\mathrm{i}ka} p_n(x), \tag{26b}$$

where $B_n = -2\mathrm{i}ka + n$, $C_n = -2\mathrm{i}ka + 1$ is a fixed value and $p_n(x) = {}_2F_1(-n, B_n, C_n, x)$ are polynomials of order n; for further use, we set $A_n = -n$. In (26*a*), the normalization constant

$$N_n = \frac{(-2\mathrm{i}ak + n)!}{(-2\mathrm{i}ak)!}\sqrt{\frac{(-2\mathrm{i}ak + 2n)}{n!\Gamma(n)a\mathcal{V}_0(-2\mathrm{i}ak + n)}} \tag{27}$$

is such that the functions generate the closure relation (3). The Sturmian functions, as well as energy eigenfunctions, result from looking for the roots of the Gauss function with respect to one of its parameters for $r = 0$; in that way, one can fix either the energy or the magnitude of the potential. Even when these two sets are similar, they contain completely different physical information. One of the main differences is, e.g., that Sturmian functions form a discrete spectra even for positive energies.

At large distances, $x = \mathrm{e}^{-r/a} \to 0$ so that ${}_2F_1(-n, -2\mathrm{i}ak + n, -2\mathrm{i}ak + 1, \mathrm{e}^{-r/a}) \to 1$, and the asymptotic behavior $S_{nl}(r \to \infty) \propto \mathrm{e}^{\pm \mathrm{i}kr}$ is fulfilled. At short distances, for $r \to 0$ the argument of the Gauss function $x \to 1$. To satisfy regularity at the origin, the whole function must vanish, requiring thus the zeros of the Gauss function in terms of its parameters. This leads to an infinite number of eigenvalues:

$$\beta_n^{(0)} = -\frac{n(-2\mathrm{i}ak + n)}{2\mu a^2 \mathcal{V}_0} \qquad (n = 1, 2, \ldots) \tag{28}$$

transforming the Gauss function into a polynomial of order n in the variable x.

Each Sturmian function (26*a*) is the product of an oscillating exponential $\mathrm{e}^{\mathrm{i}kr}$ multiplied by a polynomial of order n (this is generally the case for generating potentials of short range, as mentioned in section 2.3). In our case, the polynomials have a variable x which varies from 0 to 1. However, moving the energy to the complex plane, one may transform the exponential variable $\mathrm{e}^{\mathrm{i}kr}$ into an oscillatory exponentially decreasing function; the upper half-plane corresponds to the outgoing behavior. Moreover, for negative energy, i.e. choosing a pure imaginary $k = \mathrm{i}\kappa$ (simple analytic continuation), the oscillatory exponential becomes a decaying exponential $\mathrm{e}^{-\kappa r}$. Thus, for any value of complex energy (on the appropriated

half-plane), the Sturmian functions $S_n(r)$ are defined as the product of a decaying exponential times a bound polynomial. In figures 1(a) and (b), we have plotted as a function of r, the real and imaginary parts of the first four $S_n(r)$ with $E = 0.5$, $\mu = 1$, $a = 4$ and $\mathcal{V}_0 = 1$. It can be observed that they differ mostly within the range of the Hulthén potential (plotted in figure 1(a)) and then all acquire the asymptotic behavior imposed by the energy, the outgoing wave boundary condition and the auxiliary potential (identically zero in this case). This illustrates how the basis functions are ideally suited to expand correctly the asymptotic domain. The study of the polynomials is deferred to subsection 3.2 where the nodal structure of the basis functions is investigated.

The eigenvalues of the problem are the magnitudes $\beta_n^{(0)}$ of the Hulthén potential. What we have illustrated is that there exists an infinite and discrete number of potential magnitudes $\beta_n^{(0)}$ supporting a state with a given externally fixed energy value E.

The same basic equation results if we allow the auxiliary potential to be a Hulthén potential with the same range as the generating potential. While the eigenfunctions remain the same, there is a shift in the eigenvalues given by the magnitude $\mathcal{U}_0$ of the auxiliary potential:

$$\beta_n = \beta_n^{(0)} - \mathcal{U}_0. \tag{29}$$

This result will be employed when we exemplify, in section 4.1, the assertions of section 2.2 with the scattering of a particle by a Hulthén potential.

3.1. The orthogonality relation

According to the study we performed in section 2.3, we only need an expression for $\mathcal{V}_{n,n}$; however, we will derive an expression for the general matrix elements $\mathcal{V}_{n',n}$, and in particular for $c = -1$. The purpose of this is to simply verify, in an alternative way, the fulfillment of the orthogonality. In addition, we want to explore the type of mathematical functions representing this orthogonality, i.e. the way the Kronecker symbol is generated.

Using the variable x we have for the matrix elements $\mathcal{V}_{n',n}$

$$\mathcal{V}_{n',n} = a\mathcal{V}_0 N_{n'} N_n \int_0^1 {}_2F_1(A_{n'}, B_{n'}, C_{n'}; x)\ {}_2F_1(A_n, B_n, C_n; x) x^{-2ika}(1-x)^{-1}\mathrm{d}x. \tag{30}$$

The apparent divergence at $x = 1$ (i.e. $r = 0$) is removed because of the regularity condition $S_n(r = 0) = 0$. To evaluate $\mathcal{V}_{n',n}$ we use the series definition of the Gauss hypergeometric functions, and find

$$\mathcal{V}_{n',n} = a\mathcal{V}_0 N_{n'} N_n \sum_{l,m} \frac{(A_{n'})_l\,(B_{n'})_l}{(C_{n'})_l\,l!} \frac{(A_n)_m\,(B_n)_m}{(C_n)_m\,m!} \int_0^1 x^{-2ika+l+m}(1-x)^{-1}\,\mathrm{d}x. \tag{31}$$

With the well-known expansion [32]

$$(1-x)^{-1} = \sum_{s=0}^{\infty} \frac{(1)_s}{s!}(x)^s,$$

the integral $\mathcal{V}_{n',n}$ is then given by a triple series

$$\mathcal{V}_{n',n} = a\mathcal{V}_0 N_{n'} N_n \sum_{l,m,s} \frac{(A_{n'})_l\,(B_{n'})_l}{(C_{n'})_l\,l!} \frac{(A_n)_m\,(B_n)_m}{(C_n)_m\,m!} \frac{(1)_s}{s!} J_{l,m,s}(a,k), \tag{32}$$

where

$$J_{l,m,s}(a,k) = \int_0^1 \mathrm{d}x\, x^{-2ika+l+m+s}. \tag{33}$$

For $l+m+s \geqslant 0$, we have

$$J_{l,m,s}(a,k) = \frac{1}{-2\mathrm{i}ka+l+m+s+1} = \frac{(-2\mathrm{i}ka+1)_{l+m+s}}{(-2\mathrm{i}ka+1)\,(-2\mathrm{i}ka+2)_{l+m+s}}. \tag{34}$$

Thus, $\mathcal{V}_{n',n}$ may be written as

$$\mathcal{V}_{n',n} = \frac{a\mathcal{V}_0 N_{n'} N_n}{-2\mathrm{i}ak+1}\,\Theta\left(\begin{matrix}A_{n'}B_{n'}|A_nB_n|1|-2\mathrm{i}ka+1\\ C_{n'}|C_n|-|-2\mathrm{i}ka+2\end{matrix}\;|\;1,1,1\right), \tag{35}$$

where the three-variable hypergeometric function Θ is defined as

$$\Theta\left(\begin{matrix}A_{n'}B_{n'}|A_nB_n|D|E\\ C_{n'}|C_n|-|F\end{matrix}\;|\;x,y,z\right) = \sum_{l,m,s}\frac{(A_{n'})_l\,(B_{n'})_l}{(C_{n'})_l}\,\frac{(A_n)_m\,(B_n)_m}{(C_n)_m}\,(D)_s\,\frac{(E)_{l+m+s}}{(F)_{l+m+s}}\,\frac{x^l}{l!}\,\frac{y^m}{m!}\,\frac{z^s}{s!}. \tag{36}$$

An alternative representation can be obtained using the property

$$(A)_{l+m+s} = (A+s)_{l+m}\,(A)_s \tag{37}$$

to replace the expressions $(-2\mathrm{i}ka+1)_{l+m+s}$ and $(-2\mathrm{i}ka+2)_{l+m+s}$ in (34) and obtain

$$\mathcal{V}_{n',n} = \frac{a\mathcal{V}_0 N_{n'} N_n}{-2\mathrm{i}ak+1}\sum_s\frac{(-2\mathrm{i}ka+1)_s}{(-2\mathrm{i}ka+2)_s}\sum_{l,m}\frac{(A_{n'})_l\,(B_{n'})_l}{(C_{n'})_l}\,\frac{(A_n)_m\,(B_n)_m}{(C_n)_m}\,\frac{(-2\mathrm{i}ka+1+s)_{l+m}}{(-2\mathrm{i}ka+2+s)_{l+m}}\,\frac{1^l}{l!}\,\frac{1^m}{m!} \tag{38}$$

which results in a single series

$$\mathcal{V}_{n',n} = \frac{a\mathcal{V}_0 N_{n'} N_n}{-2\mathrm{i}ak+1}\sum_s\frac{(-2\mathrm{i}ka+1)_s}{(-2\mathrm{i}ka+2)_s}\,F^{122}_{111}\left(\begin{matrix}-2\mathrm{i}ka+1+s;A_{n'}B_{n'};A_nB_n\\ -2\mathrm{i}ka+2+s;C_{n'};C_n\end{matrix}\Big|\,1,1\right) \tag{39}$$

of the relatively more familiar two-variable hypergeometric function [33]

$$F^{122}_{111}\left(\begin{matrix}D;A_{n'}B_{n'};A_nB_n\\ E;C_{n'};C_n\end{matrix}\;|\;x,y\right) = \sum_{l,m}\frac{(A_{n'})_l\,(B_{n'})_l}{(C_{n'})_l}\,\frac{(A_n)_m\,(B_n)_m}{(C_n)_m}\,\frac{(D)_{l+m}}{(E)_{l+m}}\,\frac{x^l}{l!}\,\frac{y^m}{m!}. \tag{40}$$

We should underline here that since the coefficient $A_n = -n$ the summations over l and m are truncated. This means that $\mathcal{V}_{n',n}$ reduces to a single infinite series over s, and a double finite summation.

A further alternative, more *evaluation oriented*, representation can be derived by making use of the identity [39]

$${}_2F_1(\alpha,\beta,\gamma;x) = (1-x)^{-\alpha}\;{}_2F_1\left(\alpha,\gamma-\beta,\gamma;\frac{x}{x-1}\right), \tag{41}$$

to recast the integral as

$$\begin{aligned}\mathcal{V}_{n',n} = a\mathcal{V}_0 N_{n'} N_n\int_0^1 {}_2F_1\left(A_{n'},C_{n'}-B_{n'},C_{n'};\frac{x}{x-1}\right){}_2F_1\left(A_n,C_n-B_n,C_n;\frac{x}{x-1}\right)\\ \times x^{-2\mathrm{i}ka}(1-x)^{n'+n-1}\,\mathrm{d}x.\end{aligned} \tag{42}$$

Inserting the series representation of the Gauss hypergeometric, we find

$$\begin{aligned}\mathcal{V}_{n',n} = a\mathcal{V}_0 N_{n'} N_n\sum_{l,m}\frac{(-n')_l(1-n')_l}{(C_{n'})_l l!}\,\frac{(-n)_m\,(1-n)_m}{(C_n)_m\,m!}\,(-1)^{l+m}\\ \times\beta(1-2\mathrm{i}ak+l+m,n'+n-l-m),\end{aligned} \tag{43}$$

where the Euler beta function [38] is given by

$$\beta(1-2\mathrm{i}ak+l+m,n'+n-l-m) = \int_0^1 x^{-2\mathrm{i}ak+l+m}\,(1-x)^{n'+n-1-l-m}\,\mathrm{d}x. \tag{44}$$

This expression can be quickly evaluated with commercial software.

Table 1. $\mathcal{V}_{n,n}/(N_nN_n)$ elements for $n = 1, \ldots, 6$.

Equation (39)	Equation (43)	Numerical
−5.000 01E-2 + 1.500 00E-1i	−5.000 00E-2 + 1.500 00E-1i	−5.000 00E-2 + 1.500 00E-1i
−2.999 99E-2 − 1.000 01E-2i	−3.000 00E-2 − 1.000 00E-2i	−3.000 00E-2 − 1.000 00E-2i
−2.307 25E-4 − 1.315 38E-2i	−2.307 69E-4 − 1.315 38E-2i	−2.307 69E-4 − 1.315 38E-2i
6.139 91E-3 − 4.322 94E-3i	6.139 92E-3 − 4.323 01E-3i	6.139 92E-3 − 4.323 01E-3i
4.958 09E-3 + 9.182 12E-4i	4.958 17E-3 + 9.181 84E-4i	4.958 17E-3 + 9.181 84E-4i
2.448 44E-3 + 2.804 82E-3i	2.448 54E-3 + 2.804 86E-3i	2.448 53E-3 + 2.804 86E-3i

Table 2. $\mathcal{V}_{n,n+1}/(N_nN_{n+1})$ for $n = 1, \ldots, 5$.

Equation (39)	Equation (43)	Numerical
5.58E-8	0.0	<1.0E-17
5.28E-8	0.0	<1.0E-17
7.661E-8	0.0	<1.0E-17
9.49E-8	0.0	<1.0E-17
1.16E-7	0.0	<1.0E-17

In table 1, respectively 2, we give the first six diagonal (respectively five subdiagonal) matrix elements $\mathcal{V}_{n',n}/(N_{n'}N_n)$ evaluated in three different manners: (i) using expression (43); (ii) using expression (39) with 4000 terms; and (iii) with a conventional numerical radial integration. We took $a = 1$ and $E = 0.5$. Generally subdiagonal elements (and farther away from the diagonal) are, for a given matrix size, easier to evaluate since they require fewer terms to add up in the analytical summation and have less oscillations to deal with in the numerical integration. In all cases, the most reliable set was the one obtained with (43), with identically zero off-diagonal elements (table 2). The direct numerical integration yielded diagonal elements in agreement with both analytical methods and a ratio of roughly 14 orders of magnitude between diagonal and off-diagonal elements (ideally zero). While the three methodologies work, we found expression (43) to be the most accurate and also time efficient to implement; the other two yield values correct up to the fourth digit for diagonal terms. The accuracy of expression (39) depends obviously on the number of terms in the infinite summation; convergence was observed to be very slow.

The above investigation verified the potential-weighted orthogonality (4) between Hulthén basis functions.

3.2. Nodal structure

We now turn our attention to the polynomials $p_n(x)$ which are Jacobi polynomials. As we did not encounter any study on the placement of their nodes when the parameters are complex, we present below an exploratory study which is by no means exhaustive. The first four polynomials are shown in figures 2(*a*) and (*b*), respectively in real and imaginary parts. The whole set has a node at $x = 1$, which corresponds to the regularity condition in $r = 0$. Since they constitute a complete basis set, a given $p_n(x)$ must have exactly n nodes and be bound for any $x \in [0, 1]$.

We start by analyzing the behavior of the nodes when we depart from bound states, which imply real coefficients, and start to consider complex energies. We observed that when the phase of k is gradually rotated from $\pi/2$ (bound states) to 0 (non-decaying outgoing waves) the number of nodes for a given n does not vary; however, they migrate continuously to the lower half-plane of the complex plane. The node at the origin ($r = 0$, $x = 1$) remains even when

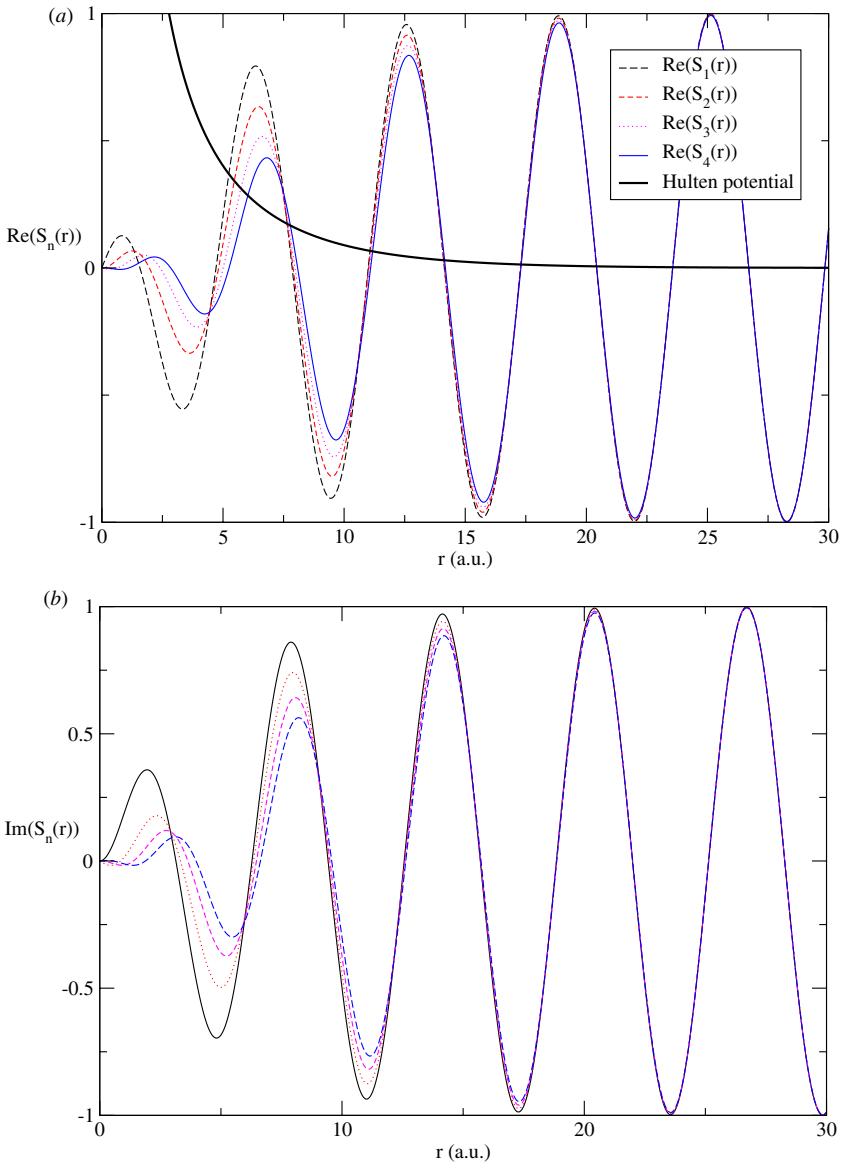

Figure 1. $S_{n,0}(r)$ $(n = 1 - 4)$ for angular momentum $l = 0$, range $a = 4$ and energy $E = 0.5$. The Hulthén potential with $\mathcal{V}_0 = 1$ (thicker line) is also shown. The whole set of functions has the same asymptotic behavior.

the phase of k changes; this is to be expected since the Sturmian functions were discretized enforcing the regularity there. The remaining nodes acquire a negative imaginary part that gets more pronounced as the k phase tends to zero and their real parts shift slightly toward smaller x, as can be seen in figure 3.

We have also studied, for a given k, the placement (ordering) of the $p_n(x)$ nodes in the complex plane. Though the general theory [40] is developed strictly for real polynomials, the real parts of our complex $p_n(x)$ nodes still comply with the ordering properties. That is to

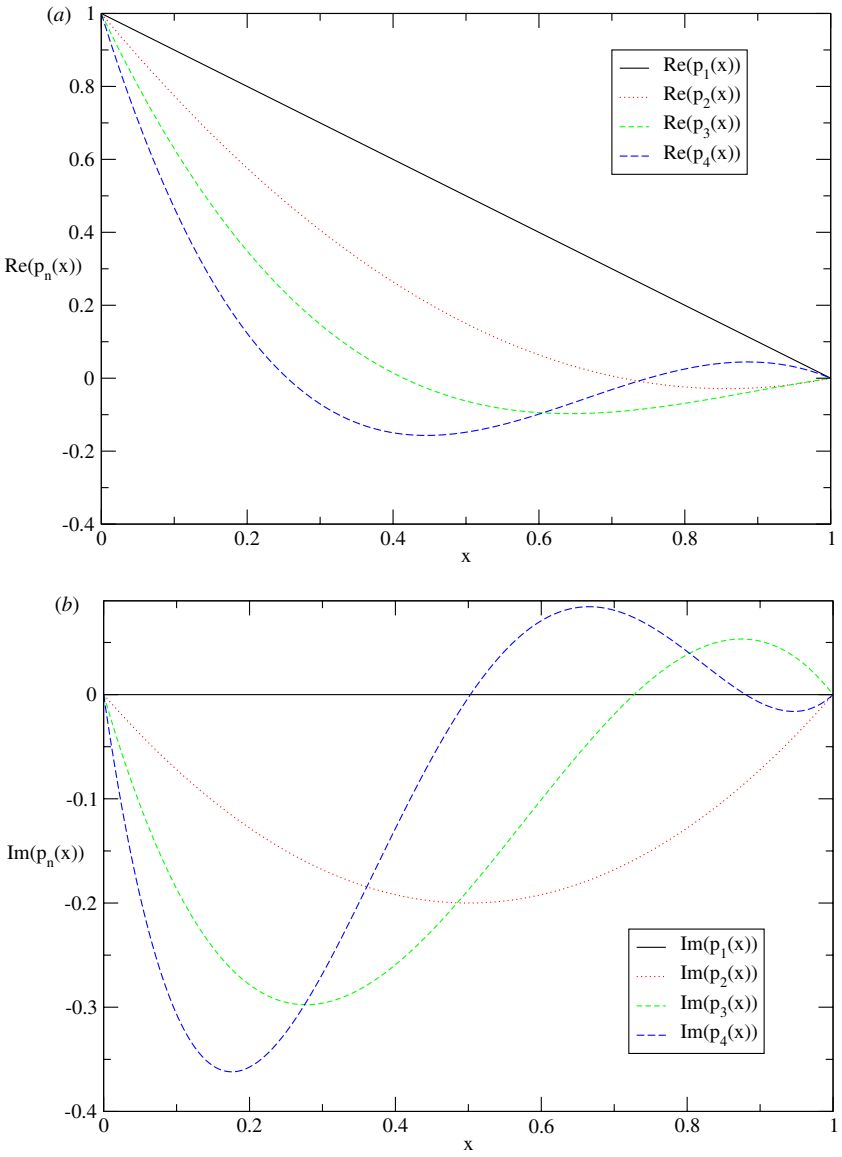

Figure 2. $p_n(x)$ for $n = 1, \ldots, 4$. The separate real and imaginary parts do not constitute two valid basis sets since some of their nodes may lie outside [0, 1]. For example, the polynomials $\Re(p_2(x))$ and $\Re(p_3(x))$ have the same number of nodes in the domain considered.

say, if $x_{n,j}$, $x_{n,j+1}$, with $j = 1, \ldots, n$, are the real parts of the nodes of a given $p_n(x)$, the real part of a node $x_{n+1,j+1}$ belonging to $p_{n+1}(x)$ will lie in between the previous two. This can be observed in figure 4, where we have plotted, for illustration, the complex nodes of the three polynomials with $n = 13, 14, 15$.

Finally, we analyzed the nodes of $\Re(p_n(x))$ and $\Im(p_n(x))$ as separate polynomials. Even though the zeros lie on the real axis, for some values of n there are nodes which were not confined to the valid x range [0, 1]. This single fact rules them out as valid basis sets in the

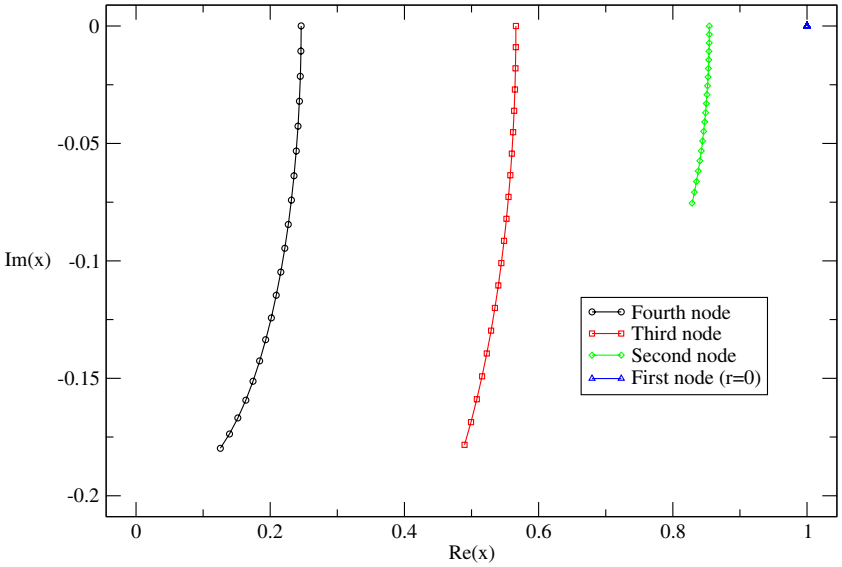

Figure 3. Position of the first four nodes in the complex plane as the phase of k is rotated from pure imaginary (nodes on the real axis) to real (nodes traveling gradually to the lower left).

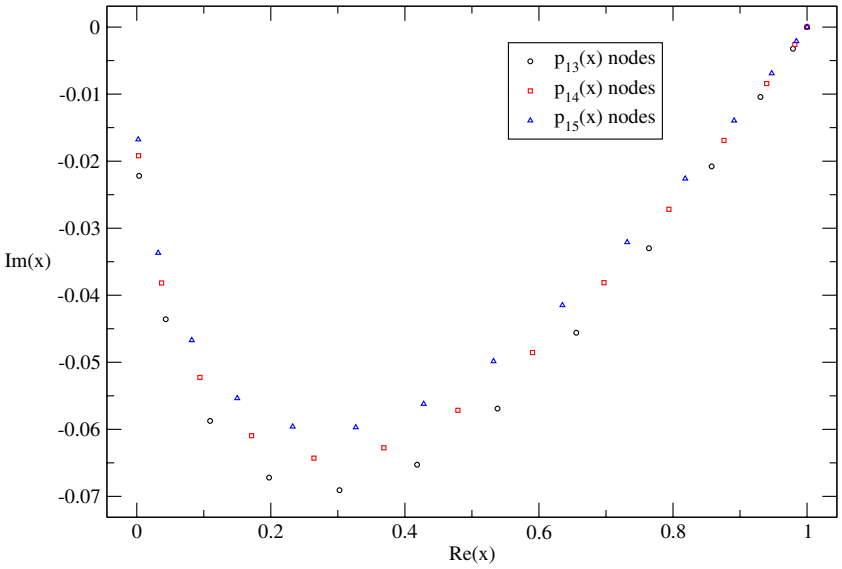

Figure 4. $p_n(x)$, with $n = 13, 14, 15$, in the complex plane. The real part of the nodes of polynomials with contiguous n are intercalated.

domain under study [40]. This can be seen in figure 2(a), where $\Re(p_2(x))$ and $\Re(p_3(x))$ have in [0, 1] the same number of nodes.

The behavior observed here for the Hulthén case is instructive in the sense that for general Sturmian functions associated with other potentials, we expect the nodal structure to be similar.

The nodes will be, for outgoing or incoming asymptotic behaviors, in the complex plane of the coordinate. Given the fact that the Sturmian functions are generally defined in terms of polynomials and that they have a natural order, there is then a one-to-one relation between the order and the number of nodes. This is of crucial importance when using the basis set in scattering calculations.

3.3. Overlap matrix elements

Analytic expressions can also be obtained for the overlap integrals $\mathcal{O}_{n',n}$. They allow us again to confirm the validity of the analysis presented in section 2.3, i.e. that they are well defined. To derive the results, and to allow for an easy extension for other matrix elements $\mathcal{A}_{n',n}$, we start from the more general integral

$$\tilde{\mathcal{O}}^{k',k}_{n',n} = N_{n'}N_n \int_0^\infty {}_2F_1\left(A'_{n'}, B'_{n'}, C'_{n'}; \mathrm{e}^{-\frac{r}{a}}\right) {}_2F_1\left(A_n, B_n, C_n; \mathrm{e}^{-\frac{r}{a}}\right) \mathrm{e}^{\mathrm{i}(k'+k)r-\varepsilon r}\,\mathrm{d}r, \tag{45}$$

where the primed coefficients $A'_{n'}$, $B'_{n'}$, $C'_{n'}$ are allowed to have $k' \neq k$ and where we have introduced an integrating factor $\mathrm{e}^{-\epsilon r}$. For $k = k'$ and $\varepsilon \to 0$, $\tilde{\mathcal{O}}^{k',k}_{n',n}$ reduces to $\mathcal{O}_{n',n}$ defined by (6). Using the series representation of both Gauss functions, we encounter again the integrals (33) where $s = 0$ and $-2\mathrm{i}ka$ is replaced by $-\mathrm{i}(k+k')a + \varepsilon a - 1$. Adapting the final result (39) obtained above for $\mathcal{V}_{n',n}$, and taking the limit $\varepsilon \to 0$, we immediately find

$$\mathcal{O}^{k',k}_{n',n} = N_{n'}N_n \frac{1}{-i(k'+k)}\, F^{122}_{111}\left(\begin{matrix}-\mathrm{i}(k'+k)a; A'_{n'} B'_{n'}; A_n B_n \\ -\mathrm{i}(k'+k)a+1; C'_{n'}; C_n\end{matrix}\middle| 1, 1\right). \tag{46}$$

Alternatively, we may express this result as a single series of ${}_3F_2$ hypergeometric functions

$$\begin{aligned}\mathcal{O}^{k',k}_{n',n} = N_{n'}N_n \frac{1}{-\mathrm{i}(k'+k)} \sum_l \frac{(A'_{n'})_l (B'_{n'})_l}{(C'_{n'})_l l!} \frac{(-\mathrm{i}(k'+k)a)_l}{(-\mathrm{i}(k'+k)a+1)_l} \\ \times {}_3F_2(A_n, B_n, -\mathrm{i}(k'+k)a + l, C_n, -\mathrm{i}(k'+k)a + 1 + l; 1).\end{aligned} \tag{47}$$

On the other hand, performing the integration term by term in (45), we get the double finite sum

$$\tilde{\mathcal{O}}^{k',k}_{n',n} = N_{n'}N_n \sum_{l,m} \frac{(A'_{n'})_l (B'_{n'})_l}{(C'_{n'})_l l!} \frac{(A_n)_m (B_n)_m}{(C_n)_m m!} \frac{a}{l + m + a\varepsilon - \mathrm{i}(k'+k)a}, \tag{48}$$

the two summations being truncated since $A_n = -n$ and $A'_{n'} = -n'$. Successive differentiations of (48) with respect to ε yield matrix elements with extra integer powers of r ($p \geqslant 0$):

$$\frac{\partial^p \tilde{\mathcal{O}}^{k',k}_{n',n}}{\partial \varepsilon^p} = (-1)^p N_{n'}N_n \int_0^\infty {}_2F_1(A'_{n'}, B'_{n'}, C'_{n'}; \mathrm{e}^{-\frac{r}{a}}) {}_2F_1(A_n, B_n, C_n; \mathrm{e}^{-\frac{r}{a}}) r^p\, \mathrm{e}^{\mathrm{i}(k'+k)r-\varepsilon r}\,\mathrm{d}r. \tag{49}$$

The integration is again easily performed, and taking the limit $\varepsilon \to 0$, we obtain

$$\left[\frac{\partial^p \tilde{\mathcal{O}}^{k',k}_{n',n}}{\partial \varepsilon^p}\right]_{\varepsilon\to 0} = N_{n'}N_n \sum_{l,m} \frac{(A'_{n'})_l (B'_{n'})_l}{(C'_{n'})_l l!} \frac{(A_n)_m (B_n)_m}{(C_n)_m m!} \frac{(-1)^p a^{p+1} p!}{[l + m - \mathrm{i}(k'+k)a]^{p+1}}. \tag{50}$$

Such expressions allow for a complete study of the Hulthén potential, which is one of the very few potentials having analytical solutions.

Matrix elements with positive powers r^p are mathematically well defined. This is due to the oscillatory character of the Sturmian functions, as stated in the introduction. However, in the following example k is taken as purely imaginary (bound states) and k' purely real for the sake of numerical simplicity.

Table 3. $\mathcal{O}^{k,k}_{n,n}/(N_nN_n)$ elements for $k = k' = 1$ and $n = 1, \ldots, 6$.

Equation (23)	Equation (46)
−1.500 00E-1 + 5.000 00E-2i	−1.500 00E-1 −5.000 00E-2i
2.000 00E-2 − 6.000 00E-2i	2.000 00E-2 − 6.000 00E-2i
3.946 15E-2 − 6.923 43E-4i	3.946 15E-2 − 6.923 08E-4i
1.729 22E-2 + 2.455 94E-2i	1.729 20E-2 + 2.455 97E-2i
−4.590 88E-3 + 2.479 09E-2i	−4.590 99E-3 + 2.479 08E-2i
−1.682 92E-2 + 1.469 15E-2i	−1.682 91E-2 + 1.469 12E-2i

Table 4. $\langle k', n \left| r^5 \right| k, n\rangle / (N_nN_n)$ for $k = i$ and $k' = 1$, and $n = 1, \ldots, 6$, evaluated with equation (50) and modulus of the relative error obtained by direct numerical integration.

Equation (50)	Modulus of the relative error with numerical integration
4.468 99 − 13.8484i	1.049E-7
7.694 86 − 10.5726i	1.376E-7
9.088 16 − 6.811 41i	1.540E-7
9.106 36 − 3.525 08i	1.792E-7
8.342 33 − 9.997 72E-1i	2.018E-7
7.223 51 + 7.961 83E-1i	2.405E-7

Overlap integrals were calculated numerically for the case $k' = k = 1$ and $a = 1$ and are presented in table 3 for $n = 1, \ldots, 6$; the direct numerical integration (23) and the hypergeometric representation (46) are seen to be in very close agreement. The validity of result (50) is illustrated through table 4. We evaluated the diagonal elements of the transition matrix $\langle k', n|r^5|k, n\rangle/(N_{n'}N_n)$ with $n = 1, \ldots, 6$ between two basis sets. One of them corresponds to purely bound states ($k = i$) and the other one to purely outgoing waves ($k' = 1$), both basis sets being generated with a Hulthén potential with range $a = 1.6$. Since the values obtained were identical to within eight figures, the table provides the values of the analytical expression and the absolute value of the difference with the numerical integration.

4. An application to scattering problems

4.1. The scattering of a particle by a Hulthén potential

In this section, we explicitly solve the scattering of a particle by a Hulthén potential $V(r) = V_0 \frac{e^{-r/a}}{1-e^{-r/a}}$. The result is of course very well known [38], but we will present here the closed form solution of the driven Schrödinger equation. We will also provide a closed form for Green's function. These results complement the information found in [38] for one of the very few potentials possessing analytical solutions.

According to the equations presented in section 2.2, we have for $l = 0$ the following representation of Green's function:

$$G_0^+(r', r) = \frac{2\mu a}{[(-2ika)!]^2} \sum_{n=1}^{\infty} \frac{[(n-2ika)!]^2}{(n-2iak)[n(n-2iak)+2\mu a^2 V_0 \mathcal{V}_0]} \frac{(2n-2ika)}{n!\Gamma(n)} \times e^{ikr'} {}_2F_1(-n, -2iak+n, -2iak+1; e^{-r'/a}) \times e^{ikr} {}_2F_1(-n, -2iak+n, -2iak+1; e^{-r/a}), \quad (51)$$

where $\mathcal{U}_0$ in (29) has been chosen equal to the weight V_0 of the interaction potential. This expression is valid for any energy in the complex plane. Here it is presented for positive energies, but through analytic continuation we can obtain the expression corresponding to any value of the energy. This is allowed by the fact that the Sturmian functions, being a discrete set, form a complete basis for any value of the energy. This representation is equivalent to the one given for the Coulomb potential [41, 42]. This confirms what we have stated before: energy and potential-magnitude eigenfunctions are different even when the mathematical functions are similar. Green's function (51) is defined as a summation over the discrete spectra of potential-magnitude eigenfunctions for all energies of the system. This differs considerably from the energy representation where the continuum part of the spectrum is also needed.

The scattering-driven equation to solve is given by (11) where the potential $V(r)$ is the Hulthén potential $\mathcal{V}(r)$ defined by (25). The initial state is taken as a free particle $\Psi_0(r) = krj_0(kr) = \sin(kr)$ where $j_0(x)$ is a spherical Bessel function of zeroth order. A closed form expression for the function $\Psi_{sc}(r)$ can be easily written, according to the presentation of section 2.2. Using (13) and (15), the coefficients a_n of equation (12) are given by

$$a_n = \frac{V_0}{\beta_n}\int_0^\infty S_n(r)\frac{\mathrm{e}^{-r/a}}{1-\mathrm{e}^{-r/a}}krj_0(kr)\,\mathrm{d}r. \tag{52}$$

The integral appearing in the definition of a_n can be evaluated analytically following a strategy similar to the one used in the previous sections. After some simplifications, we obtained the following quite simple representation:

$$\int_0^\infty S_n(r)\frac{\mathrm{e}^{-r/a}}{1-\mathrm{e}^{-r/a}}krj_0(kr)\,\mathrm{d}r = -\frac{kN_n}{2\mu\beta_n^{(0)}}, \tag{53}$$

where the eigenvalues $\beta_n^{(0)}$ are defined through equation (28).

The scattered part $\Psi_{sc}(r)$ is then explicitly given by

$$\Psi_{sc}(r) = -\frac{V_0 k}{2\mu}\sum_{n=1}^{\infty}\frac{1}{\beta_n\beta_n^{(0)}}N_n^2\,\mathrm{e}^{\mathrm{i}kr}{}_2F_1(-n, -2\mathrm{i}ak+n, -2\mathrm{i}ak+1; \mathrm{e}^{-r/a}). \tag{54}$$

Finally, taking the asymptotic limit $r \to \infty$, we find the scattering transition amplitude T_k for the collision process

$$\Psi_{sc}(r) \to \left(-\frac{V_0 k}{2\mu}\sum_{n=1}^{\infty}\frac{1}{\beta_n\beta_n^{(0)}}N_n^2\right)\mathrm{e}^{\mathrm{i}kr} = T_k\,\mathrm{e}^{\mathrm{i}kr}. \tag{55}$$

As an example, we evaluated the transition amplitude for $a = 1$, $k = 0.85$ and $V_0 = -1$ (an attractive potential). The value obtained with the expression of equation (55) is $0.370\,388 + 0.164\,27i$ which is in good agreement with the result of an independent numerical procedure: $0.370\,368 + 0.164\,102i$ and with that given in [38]. In this analytical example (the Hulthén potential), we were restricted to choose $\mathcal{U}(r) = V(r)$ and to use the same values of a in $\mathcal{U}(r)$, $V(r)$ and $\mathcal{V}(r)$. In the example shown in the following subsection, we had the freedom to choose the range of $\mathcal{V}(r)$ at the cost of dropping a fully analytical presentation.

4.2. The scattering of a particle by a Yukawa potential

As another application, we study the scattering of a particle by a Yukawa potential $V(r) = \mathrm{e}^{-\alpha r}/r$ ($\alpha > 0$). Expansions (12) and (13) were performed with the Hulthén Sturmian functions, having set the auxiliary potential to zero. The range parameter a of the generating Hulthén potential was chosen equal to that of the interaction potential. Under this condition,

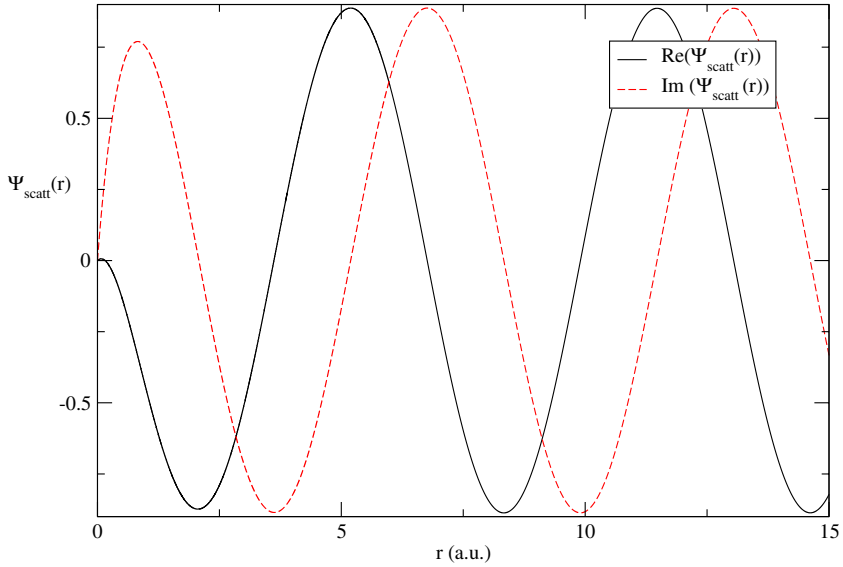

Figure 5. $l = 0$ partial wave for the Yukawa potential with $E = 0.5$ and $\alpha = 1$. The scattering function obtained with a Sturmian expansion is undistinguishable from the exact one (numerical).

the Yukawa potential range is slightly shorter due to the factor $1/r$ present in its expression. No other optimization was performed. The evaluation of the potential integrals $\mathcal{V}_{n',n}$ shows that the Sturmian set is effectively orthogonal. The integrals involving the Yukawa potential and the expansion of the driven term had to be done numerically (an analytical expression may be sought after).

Our results for the scattering wavefunction are plotted in figure 5 where we compare the exact wavefunction for $E = 0.5$, $l = 0$, $\alpha = 1$ and its expansion with 60 Sturmian basis elements. The differences are barely noticeable. This clearly shows that the complex, and regular at the origin, basis functions are able to expand the driven term even when this is purely real. Figure 6 shows the convergence of the real part of the $\Psi_{\rm sc}(r)$ expansion generated with 20, 40 and 60 basis functions; 20 basis functions basically provide the exact numerical solution, further elements giving full convergence.

The normalization of the function was fixed so that $\Psi_0(r) \to \sin(kr)$ for $r \to \infty$. This implies, for the overall function, $\Psi(r) = \Psi_0(r) + \Psi_{\rm sc}(r) \to {\rm e}^{{\rm i}\delta_0} \sin(kr + \delta_0)$ as $r \to \infty$, with δ_0 being the corresponding $l = 0$ phase shift for the interaction Yukawa potential. The obtained scattering amplitude is $0.4085 + 0.7869i$ which may be compared to the accurate value, $0.4086 + 0.7881i$, derived with a separate numerical procedure.

We emphasize that these results do not, by any means, constitute a deep study of convergence with respect to the parameters involved, as no optimization was performed. The chief application realm for the Sturmian theory is the three-body problem, for which two-body fully numerical methodologies do not extend in a straightforward way. The Sturmian functions contain the correct outgoing asymptotic behavior. This fact makes them suitable for expansions since the basis will only have to expand correctly a region of a few atomic units away from the origin. This is opposed to energy-type bases which need to expand both the near and asymptotic regions, thus requiring more elements and more computational resources.

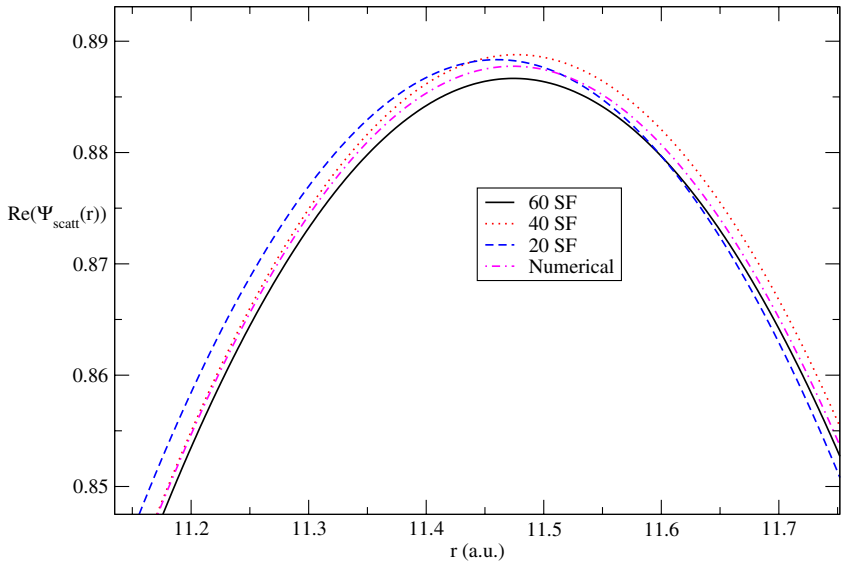

Figure 6. Crest detail of the real part of the scattering function for expansions taken with increasing number of basis elements ($l = 0,\ E = 0.5,\ \alpha = 1$).

5. Summary

Generalized Sturmian functions satisfying a Schrödinger-like equation, complemented with two-point boundary conditions, form a complete set of orthogonal functions for any auxiliary and generating potentials. The first one controls the asymptotic behavior of all the basis functions. The eigenvalues of the problem are the magnitude of the generating potential which controls most of the basis function properties. Interestingly, at large distances any type of boundary conditions can be enforced to the functions: incoming, outgoing or standing-wave behavior for positive energies, and exponentially decreasing behavior for negative energies. Even complex energies can be considered and similar behaviors at large distances can be imposed. In all cases, regularity at the origin was imposed as well.

The standard Sturm–Liouville theory is normally presented for real functions and in most cases orthogonality and closure issues are presented in that context. In this paper, we addressed the case of complex parameters and complex boundary conditions, with the purpose of clarifying some delicate aspects. We considered Sturmian functions corresponding to the $l = 0$ Hulthén potential for which analytical solutions exist (the results can be generalized—in principle—to any potential and any angular momentum l). Such a potential generates a set of orthogonal polynomials with a weight function involving the generating potential (the quadrature integration with respect to those polynomials is one of our current topics under investigation). The orthogonality was demonstrated by direct numerical integration and, also explicitly, by analytical evaluation. The corresponding integral was expressed in terms of a multivariable hypergeometric function or, alternatively, in terms of a finite sum more suitable for numerical implementations. We used both to numerically show that they yield the expected delta Kronecker-like behavior.

To the best of our knowledge, there are no studies of scattering-like (complex) basis functions, in particular with respect to the behavior of their nodes. Thus, we performed an

analysis for the Hulthén Sturmian functions, and found that the eigenvalues can be ordered as in the standard (real) theory. The trajectory of the nodes can be followed for the different energy values when they are moved to the complex plane (on the upper plane) from real negative to real positive. The corresponding complex polynomial set is orthogonal but, individually, the real and imaginary parts are not.

In addition, we studied analytically the overlap integrals and other matrix elements including extra powers of the coordinates. We managed to express all of them in terms of uncommon multivariable hypergeometric functions, and showed that they are well defined. Numerical validation of mathematical expressions was also presented.

Finally, to illustrate the efficiency of generalized Sturmian functions, we applied them to describe the scattering produced by a Hulthén and a Yukawa potential.

For the Hulthén case, we took advantage of the analyticity of the Hulthén Sturmian functions to derive various expressions which complement those given in standard collision theory [43] and mathematical physics books [38]. We provided a closed form expression for the $l = 0$ Green's function corresponding to any value of the energy. The expression makes use of the discrete character of the Sturmian spectra which allows for a diagonal representation in terms of a single series. We obtained a closed form expression for the solution of the driven equation corresponding to this potential, and for the corresponding transition amplitude. Analytical results were verified numerically with an independent numerical procedure and also with those given, e.g., in [38].

For the scattering by a Yukawa potential, our numerical application achieved a more than fair agreement with the exact solution, using a relatively low number of basis elements. The efficiency is related to the built-in correct asymptotic behavior of every basis element and to the appropriate choice of the generating potential range.

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