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Mathematical methods in atomic physics

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Prefacio

Esta Tesis, desarrollada dentro de un régimen de cotutela entre la Universidad Nacional del Sur (Bahía Blanca, Argentina) y la Université de Lorraine (Metz, Francia), se presenta como parte de los requisitos para optar al grado Académico de Doctor en Física de la Universidad Nacional del Sur y de la Université de Lorraine, y no ha sido presentada previamente para la obtención de otro título en esta Universidad u otra. La misma contiene los resultados obtenidos en investigaciones llevadas a cabo en el ámbito del Departamento de Física (Universidad Nacional del Sur, Argentina) y del laboratorio Structure et Réactivité des Systèmes Moléculaires Complexes (Université de Lorraine, Francia) durante el período comprendido entre 13 de septiembre de 2011 y el 31 de enero de 2017, bajo la dirección del Dr. Gustavo Gasaneo (Universidad Nacional del Sur, Argentina) y del Dr. Lorenzo Ugo Ancarani (Université de Lorraine, Francia).

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Last but not the least, I would like to thank my family and friends for their support and encouragement in any new project I decide to undertake.

Thank you all very much.

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List of symbols

We present here a list of symbols appearing repeatedly through the chapters of this thesis, and indicate the number page of their first appearance.

Symbol	Description	First appearance (page)
ϕ_n^{STO}	Slater-type orbitals	17
ϕ_n^L	Laguerre-type functions	17
L_n^α	associated Laguerre Polynomials	17
${}_1F_1$	confluent hypergeometric function	17
$N_{n,\ell}$	normalization factor for ϕ_n^L	17
$(\alpha)_n$	Pochhammer symbol	18
Γ	Gamma function	18
$\delta_{m,n}$	Kronecker delta	18
δ	Dirac delta	18
F_2	Appell hypergeometric function	21
${}_2F_1$	Gauss hypergeometric function	21
$\mathbf{H_r}$	radial Hamiltonian	22
$\mathbf{T_r}$	radial kinetic energy operator	22
$\mathbf{H_r^C}$	one-dimensional Coulomb Hamiltonian	22
$A_n,\ B_n$	coefficients for recurrence relation	23
$F^{(s)},\ G^{(c)},\ H^{(\pm)}$	Coulomb wave functions	23
$M_{\chi,\mu/2},\ W_{\chi,\mu/2}$	Whittaker functions	23

Symbol	Description	First appearance (page)
η	Sommerfeld parameter	24
σ	phase shift (Coulomb potential)	24
$N_C,\ \widetilde{N}_C^{(\pm)}$	factors for $F^{(s)}$ and $H^{(\pm)}$ respectively	24
s_n	coefficients for $F^{(s)}$	25
ω	parameter	25
ψ	digamma function	28
${}_2\Theta_1^{(1)}$	two variable hypergeometric function	28
$\mathcal{G}_C^{(\pm)}$	Green's functions	37
$g_{n,q}^{(\pm)}$	coefficients for Green's functions	38
$\hat{h}^{(\pm)}$	coefficients for $\hat{H}^{(\pm)}$	39
$\hat{H}^{(\pm)}$	function for J-Matrix method	39
Φ_1	Horn's hypergeometric series	52
$\mathcal{V}_a,\ \mathcal{V}_g$	auxiliary and generating potentials	55
$S_{n,\ell}$	Generalized Sturmian functions	55
$\lambda_{n,\ell}$	eigenvalues of $S_{n,\ell}$	55
$S_{n,0}$	Hulten Sturmian functions	57
$\lambda_{n,0},\ \widetilde{\lambda}_{n,0}$	eigenvalues of $S_{n,0}$	57
N_n^S	factor for $S_{n,0}$	58
$P_n^{(a,b)}$	Jacobi's polynomials	61
Z_{QS}	parameter (charge) for Quasi-Sturmian functions	67
$Q_n^{(\pm)}$	Quasi-Sturmian functions	69
$\mathcal{Q}_n^{as}$	coefficient for the asymptotic behavior of $Q_n^{(\pm)}$	69

Symbol	Description	First appearance (page)
$Q_n^{STO(\pm)}$	Slater Quasi-Sturmian functions	71
$Q_n^{L(\pm)}$	Laguerre Quasi-Sturmian functions	78
$\mathcal{Q}_n^{STO\,as}$	coefficient for the asymptotic behavior of $Q_n^{STO(\pm)}$	73
$\mathcal{Q}_n^{L\,as}$	coefficient for the asymptotic behavior of $Q_n^{L(\pm)}$	78
$\widetilde{C},\ C$	functions representing a variable charge	88, 90

Abstract

Two and three-body scattering problems are of crucial relevance in atomic physics as they allow to describe different atomic collision processes. Nowadays, the two-body cases can be solved with any degree of numerical accuracy. Scattering problem involving three charged particles are notoriously difficult but something similar –though to a lesser extent- can be stated.

The aim of this work is to contribute to the understanding of three-body Coulomb scattering problems from an analytical point of view. This is not only of fundamental interest, it is also useful to better master numerical approaches that are being developed within the collision community. To achieve this aim we propose to approximate scattering solutions with expansions on sets of appropriate functions having closed form. In so doing, we develop a number of related mathematical tools involving Coulomb functions, homogeneous and non-homogeneous second order differential equations, and hypergeometric functions in one and two variables.

First we deal with the two-body radial Coulomb wave functions, and review their main properties. We extend known results to give in closed form the Laguerre expansions coefficients of the irregular solutions, and establish a new connection between the coefficients corresponding to the regular solution and Meixner-Pollaczek polynomials. This relation allows us to obtain an orthogonality and closure relation for these coefficients considering the charge as a variable.

Then we explore two-variable hypergeometric functions. For some of them, such as Appell and confluent Horn functions, we find closed form for the derivatives with respect to their parameters.

We also study a particular set of two-body Generalized Sturmian functions constructed with a Hulthén generating potential. Contrary to the usual case in which Sturmian functions are numerically constructed, the Hulthén Sturmian functions can be given in closed form. Their mathematical properties can thus be analytically studied providing a unique tool to investigate scattering problems.

Next, we introduce a novel set of functions that we name Quasi-Sturmian functions. They constitute an alternative set of functions, given in closed form, to expand the sought after solution of two- and three-body scattering processes. Quasi-Sturmian functions are solutions of a non-homogeneous second order Schrödinger-like differential equation and have, by construction, the appropriate asymptotic behavior. We present different analytic expressions and explore their mathematical properties, linking and justifying the developed mathematical tools described above.

Finally we use the studied Hulthén Sturmian and Quasi-Sturmian functions to solve some particular two- and three-body scattering problems. The efficiency of these sets of functions is illustrated by comparing our results with those obtained by other methods.

Resumen

Los problemas de dispersión de partículas, como son los de dos y tres cuerpos, tienen una relevancia crucial en física atómica, pues permiten describir diversos procesos de colisiones. Hoy en día, los casos de dos cuerpos pueden ser resueltos con el grado de precisión numérica que se desee. Los problemas de dispersión de tres partículas cargadas son notoriamente más difíciles pero aún así algo similar, aunque en menor medida, puede establecerse.

El objetivo de este trabajo es contribuir a la comprensión de procesos Coulombianos de dispersión de tres cuerpos desde un punto de vista analítico. Esto no solo es de fundamental interés, sino que también es útil para dominar mejor los enfoques numéricos que se actualmente se desarrollan dentro de la comunidad de colisiones atómicas. Para lograr este objetivo, proponemos aproximar la solución del problema con desarrollos en series de funciones adecuadas y expresables analíticamente. Al hacer esto, desarrollamos una serie de herramientas matemáticas relacionadas con funciones Coulombianas, ecuaciones diferenciales de segundo orden homogéneas y no homogéneas, y funciones hipergeométricas en una y dos variables.

En primer lugar, trabajamos con las funciones de onda Coulombianas radiales y revisamos sus principales propiedades. Así, extendemos los resultados conocidos para dar expresiones analíticas de los coeficientes asociados al desarrollo, en serie de funciones de tipo Laguerre, de las funciones Coulombianas irregulares. También establecemos una nueva conexión entre los coeficientes asociados al desarrollo de la función Coulombiana regular y los polinomios de Meixner-Pollaczek. Esta relación nos permite deducir propiedades de ortogonalidad y clausura para estos coeficientes al considerar la carga como variable.

Luego, estudiamos las funciones hipergeométricas de dos variables. Para algunas de ellas, como las funciones de Appell o las confluentes de Horn, presentamos expresiones analíticas de sus derivadas respecto de sus parámetros.

También estudiamos un conjunto particular de funciones Sturmianas Generalizadas de dos cuerpos construidas considerando como potencial generador el potencial de Hulthén. Contrariamente al caso habitual, en el que las funciones Sturmianas se construyen numéricamente, las funciones Sturmianas de Hulthén poseen forma analítica. Sus propiedades matemáticas pueden ser analíticamente estudiadas proporcionando una herramienta única para comprender y analizar los problemas de dispersión y sus soluciones.

Además, proponemos un nuevo conjunto de funciones a las que llamamos funciones Quasi-Sturmianas. Estas funciones se presentan como una alternativa para expandir la solución buscada en procesos de dispersión de dos y tres cuerpos. Se definen como soluciones de una ecuación diferencial de tipo-Schrödinger, no homogénea. Por construcción, incluyen un comportamiento asintótico adecuado para resolver problemas de dispersión. Presentamos diferentes expresiones analíticas y exploramos sus propiedades matemáticas, vinculando y justificando los desarrollos realizados previamente.

Para finalizar, utilizamos las funciones estudiadas (Sturmianas de Hulthén y Quasi-Sturmianas) en la resolución de problemas particulares de dos y tres cuerpos. La eficacia de estas funciones se ilustra comparando los resultados obtenidos con datos provenientes de la aplicación de otras metodologías.

Résumé

Les problèmes de diffusion de particules, à deux et à trois corps, ont une importance cruciale en physique atomique, car ils servent à décrire différents processus de collisions. Actuellement, le cas de deux corps peut être résolu avec une précision numérique désirée. Les problèmes de diffusion à trois particules chargées sont connus pour être bien plus difficiles mais une déclaration similaire peut être affirmée.

L'objectif de ce travail est de contribuer, d'un point de vue analytique, à la compréhension des processus de diffusion Coulombiens à trois corps. Ceci a non seulement un intérêt fondamental, mais est également utile pour mieux maîtriser les approches numériques en cours d'élaboration au sein de la communauté de collisions atomiques. Pour atteindre cet objectif, nous proposons d'approcher la solution du problème avec des développements en séries sur des ensembles de fonctions appropriées et possédant une expression analytique. Nous avons ainsi développé un nombre d'outils mathématiques faisant intervenir des fonctions Coulombiennes, des équations différentielles de second ordre homogènes et non-homogènes, et des fonctions hypergéométriques à une et à deux variables.

Tout d'abord, nous traitons les fonctions d'onde Coulombiennes radiales et rappelons leurs principales propriétés. Nous étendons certains résultats connus en donnant, pour les fonctions Coulombiennes irrégulières, des expressions analytiques pour les coefficients associés au développement en série avec des fonctions de type Laguerre. Nous établissons également une nouvelle connexion entre les coefficients associés au développement de la fonction Coulombienne régulière et les polynômes de Meixner-Pollaczek. Cette relation nous permet de déduire des propriétés d'orthogonalité et de fermeture de ces coefficients en considérant la charge comme variable.

Ensuite, nous étudions les fonctions hypergéométriques à deux variables. Pour certaines d'entre elles, comme celles d'Appell ou les fonctions confluentes de Horn, nous présentons des expressions analytiques de leurs dérivées par rapport à leurs paramètres.

Nous étudions également un ensemble particulier de fonctions Sturmiennes

Généralisées à deux corps, construites en considérant le potentiel Hulthén comme potentiel générateur. Contrairement au cas habituel, dans lequel les fonctions Sturmiennes sont construites numériquement, les fonctions Sturmiennes de Hulthén possèdent une expression analytique. Leurs propriétés mathématiques peuvent ainsi être étudiées, fournissant un outil unique pour comprendre et analyser des problèmes de diffusion.

En outre, nous proposons un nouvel ensemble de fonctions que nous appelons fonctions Quasi-Sturmiennes. Ces fonctions, également présentées sous forme analytique, sont proposées comme une alternative pour développer la solution de problèmes de diffusion à deux et à trois corps. Elles sont définies comme des solutions d'une équation différentielle de type Schrödinger, non-homogène, et par construction possèdent un comportement asymptotique approprié. Nous présentons différentes expressions analytiques en explorant leurs propriétés mathématiques, reliant et justifiant ainsi les développements mathématiques décrits précédemment.

Enfin, nous utilisons les fonctions étudiées (Sturmiennes de Hulthén et Quasi-Sturmiennes) pour résoudre certains problèmes à deux et à trois corps. L'efficacité de ces fonctions est illustrée en comparant les résultats avec ceux obtenus par l'application d'autres méthodologies.

Abstract for general public

Two and three-body scattering problems are of crucial relevance in atomic physics as they allow one to describe different atomic collision processes. The aim of this thesis is to contribute to the understanding of three-body Coulomb scattering problems from an analytical (mathematical) point of view.

The kind of scattering processes we are interested in here may be sketched as follows. An electron approaches an atom or a molecule, and interacts within a reaction zone. It is then scattered and some of the target electrons may be ejected leaving behind a positive ion. These outgoing electrons enter an asymptotic region where the behavior of the particles is known. While such scattering processes can be measured experimentally, we focus here on a theoretical analysis within Quantum Mechanics. The collision dynamics is described by a many-particle wave function that satisfies a Schrödinger equation with particular boundary conditions. This is a difficult mathematical problem that can be tackled only with numerical methods. Most of them use basis functions, the choice of which is decisive for the efficiency of computations. This thesis focusses on the construction of appropriate basis functions, and a number of related mathematical properties.

One important theoretical issue for time-independent three-body scattering problems is how to impose the correct asymptotic behavior to the wave function. Many spectral methods use two-body basis functions that generally do not possess the correct behavior at large distances. One exception are Generalized Sturmian functions, defined as to take into account the interactions of the problem, thus making them an efficient basis set. We present and study here an alternative set of functions, expressible in closed form, to be used for the description of two- and three-body scattering processes.

We begin this thesis by dealing with two-body radial Coulomb wave functions, reviewing their main properties and extending known results. We provide in closed form a particular expansion of the irregular solutions, and establish a new connection between the coefficients of a series expansion of the regular solution and Meixner-Pollaczek

polynomials.

Then we explore two-variable hypergeometric functions. For some of them, such as Appell and confluent Horn functions, we find closed form for the derivatives with respect to their parameters.

We also study a particular set of two-body Generalized Sturmian functions: the Hulthén Sturmian functions. Contrary to the usual case in which Sturmian functions are numerically constructed, the Hulthén Sturmian functions can be given in closed form. Their mathematical properties can thus be analytically studied providing a unique tool to investigate scattering problems.

Next, we introduce a novel set of functions: the Quasi-Sturmian functions. They constitute an alternative set of functions, also given in closed form, to expand the sought after solution of two- and three-body scattering processes. Quasi-Sturmian functions are solutions of a non-homogeneous second order Schrödinger-like differential equation and have, by construction, an appropriate asymptotic behavior. We present different analytic expressions and explore their mathematical properties, linking and justifying the developed mathematical tools described above.

Finally we use the studied Hulthén Sturmian and Quasi-Sturmian functions to solve some particular two- and three-body scattering problems. The efficiency of these sets of functions is illustrated by comparing our results with those obtained by other methods.

Résumé de thèse vulgarisé pour le grand public

Les problèmes de diffusion à deux et à trois corps sont d'une importance cruciale en physique atomique car ils permettent de décrire différents processus de collision atomique. L'objectif de cette thèse est de contribuer à la compréhension des problèmes de diffusion Coulombiennes à trois corps d'un point de vue analytique (mathématique).

Le genre de processus de diffusion qui nous intéresse peut être esquissé de la manière suivante. Un électron s'approche d'un atome ou d'une molécule et interagit à l'intérieur d'une zone de réaction. Il est alors diffusé, et certains des électrons de la cible peuvent être éjectés en laissant derrière eux un ion positif. Les électrons sortants entrent alors dans une région asymptotique où le comportement des particules est connu. Bien que ces processus de diffusion puissent être mesurés expérimentalement, nous nous concentrerons ici sur une analyse théorique dans le cadre de la mécanique quantique. La dynamique de collision est décrite par une fonction d'onde à plusieurs particules qui satisfait à une équation de Schrödinger avec des conditions aux limites particulières. Il s'agit d'un problème mathématique difficile qui ne peut être abordé que par des méthodes numériques. La plupart d'entre elles utilise des fonctions de base dont le choix est décisif pour l'efficacité des calculs. Cette thèse porte sur la construction de fonctions de base appropriées et sur un certain nombre de propriétés mathématiques liées à ces fonctions.

Un point théorique important pour les problèmes de diffusion à trois corps est de savoir comment imposer à la fonction d'onde le comportement asymptotique correct. De nombreuses méthodes spectrales utilisent des fonctions de base à deux corps qui ne possèdent généralement pas le bon comportement à grandes distances. Une exception est donnée par les fonctions Sturmiennes Généralisés, définies en tenant compte des interactions du problème ce qui rend efficace la base. Nous présentons et étudions ici un ensemble alternatif de fonctions, exprimées sous forme analytique, qui peuvent être utilisées pour décrire des processus de diffusion à deux et à trois corps.

Tout d'abord, nous traitons les fonctions d'onde Coulombiennes radiales et rappelons leurs principales propriétés. Nous étendons certains résultats connus en donnant, pour les fonctions Coulombiennes irrégulières, un développement en série particulier, et établissons également une nouvelle connexion entre les coefficients associés au développement de la fonction Coulombienne régulière et les polynômes de Meixner-Pollaczek.

Ensuite, nous étudions les fonctions hypergéométriques à deux variables. Pour certaines d'entre elles, comme celles d'Appell ou les fonctions confluentes de Horn, nous présentons des expressions analytiques de leurs dérivées par rapport à leurs paramètres.

Nous étudions également un ensemble particulier de fonctions Sturmiennes Généralisées à deux corps, construites en considérant le potentiel Hulthén comme potentiel générateur. Contrairement au cas habituel, dans lequel les fonctions Sturmiennes sont construites numériquement, les fonctions Sturmiennes de Hulthén possèdent une expression analytique. Leurs propriétés mathématiques peuvent ainsi être étudiées, fournissant un outil unique pour comprendre et analyser des problèmes de diffusion.

En outre, nous proposons un nouvel ensemble de fonctions que nous appelons fonctions Quasi-Sturmiennes. Ces fonctions, également présentées sous forme analytique, sont proposées comme une alternative pour développer la solution de problèmes de diffusion à deux et à trois corps. Elles sont définies comme des solutions d'une équation différentielle de type Schrödinger, non-homogène, et par construction possèdent un comportement asymptotique approprié. Nous présentons différentes expressions analytiques en explorant leurs propriétés mathématiques, reliant et justifiant ainsi les développements mathématiques décrits précédemment.

Enfin, nous utilisons les fonctions étudiées (Sturmiennes de Hulthén et Quasi-Sturmiennes) pour résoudre certains problèmes à deux et à trois corps. L'efficacité de ces fonctions est illustrée en comparant les résultats avec ceux obtenus par l'application d'autres méthodologies.

Introduction

The use of basis functions to describe certain atomic and molecular processes is a standard strategy in Quantum Mechanics. It provides a theoretical approach to problems for which, in most cases, the analytical solution is not available. A very well known example is provided by the wave functions associated to the bound states of the hydrogen atom. These wave functions are given in terms of the energy and angular momentum eigenfunctions [1].

Scattering processes cannot be treated as easily as bound state problems, i.e. as an eigenvalue problem [2, 3]. Also, except for a few two-body problems, the solution is not known in closed form. In general, one can propose to expand the solution in terms of basis functions, but in this case it is not so clear which is the most appropriate one.

The methods that use basis functions to approximate the solution of a differential equation are known as spectral methods [4]. The J-matrix [5–8], the convergent close coupling [9–11], the exterior complex scaling [12–14], the configuration-interaction [15, 16] and the Sturmian methods [17–19] are examples of spectral methods used to describe different scattering problems. Basis functions are selected through mathematical or numerical considerations. A very important aspect to be considered when choosing a set of functions to represent the scattering solution is the expected asymptotic behavior of the wave function.

In bound states, the domain of the wave functions is a bounded region outside of which they asymptotically vanish. In contrast, for continuum states the domain is not bounded, hence their behavior cannot be neglected at large distances. For two charged particles, scattering problems can generally be solved and the asymptotic behavior properly imposed to the solution. For three charged particles, obtaining the correct asymptotic behavior of the resulting wave function has become a great challenge since the contributions of Rudge [20] and Peterkop [21]. These authors made a first description of the asymptotic form of the scattering solution (see also [22]). Later Kadyrov and co-workers extended the study of the asymptotic region and the behavior of the scattered wave [23–25].

Generalized Sturmian Functions [26, 27] are one example of basis functions defined taking into account the behavior of the particles at large values of the radial variable. They are constructed as the solutions of a Sturm-Liouville problem [2, 28] including some of the interactions of the problem under consideration (through an adequate choice of the so-called auxiliary potential and generating potential) and imposing as asymptotic condition the expected behavior of the scattering solution (up to a constant). Generalized Sturmian functions form an orthogonal and complete set of basis functions. Also they proved to be a computationally efficient basis set, as shown in the treatment of a the large variety of processes and systems (see references in [27]).

In most practical cases, Generalized Sturmian functions are obtained numerically, so it is not possible to study their particular properties following analytical procedures. Moreover, all the radial integrals that appear when solving scattering problems must be performed numerically. When one takes the Hulthén potential as the generating and/or the auxiliary potential, however, the resulting basis functions can be given in closed form [29]. Thus, their mathematical properties can be investigated and some integrals can be analytically solved.

The main purpose of this thesis work is to study basis functions convenient to represent the solution of two-body scattering problems in spherical coordinates and three-body problems using hyperspherical coordinates. We are interested in functions that can be given in closed form and include an appropriate asymptotic behavior. Thus, we can analytically explore the mathematical aspects and properties of these functions in the context of scattering processes.

We not only study the Hulthén Sturmian functions, which are very appropriate to solve some particular two-body scattering problems, but also, and as a central subject of this work, we introduce an alternative set of functions, that we name Quasi-Sturmian functions. They are defined as solutions of a non-homogeneous Schrödinger-like differential equation which, as in the case of Generalized Sturmian functions, includes some interactions of the problem and imposes an appropriate scattering behavior.

A disadvantage, compared to Generalized Sturmian functions, is that we do not have an orthogonality property for these functions. On the other hand, contrary to Generalized Sturmian functions, they can be presented in closed form for the case of Coulomb interactions. As a consequence it is possible to give analytical expressions for the matrix elements when solving two- and three-body scattering problems. Thus, these Quasi-Sturmian functions are helpful in studying the analytical properties of three-body wave functions, and also allow to improve convergence in numerical calculations.

In addition, the motivation of proposing a set of functions in closed form to study three-body scattering problems led us to review and study other functions, like Coulomb wave functions and two variable hypergeometric functions, which appeared while characterizing the Quasi-Sturmian functions.

At this point it is clear that the results of our research can be presented in two parts. A first one, more mathematical, in which we introduce and study the mathematical properties of Hulthén Sturmian functions, the proposed Quasi-Sturmian functions and other functions related to them. And a second one, related to a particular subject of Quantum Mechanics, in which we state the two- and three-body scattering problems and investigate their solution by using the functions proposed in the first part.

We start by introducing the one-variable functions that constitute the base of all constructions in the following chapters: Slater-type orbitals, Laguerre-type functions, Coulomb wave functions and Coulomb Green's functions. We review the main properties of Coulomb wave functions and analyse their series representation in terms of Laguerre-type functions; we present, as a novelty, the analytical expressions of the coefficients $h_n^{(\pm)}$ and c_n corresponding to the series expansion of the irregular Coulomb wave functions. Another contribution related to this subject is the connection we establish between the coefficients s_n associated to the regular Coulomb wave function and the Meixner-Pollaczek polynomials when considering the charge as a variable. The interest in series representations in terms of Laguerre-type functions is related to the fact that this strategy separates some parameters (charge and energy for example, appearing only in the coefficients) from the variable. Thus, the study of the parameters of the function reduces to the analysis of these coefficients.

The second chapter is dedicated to the study of two-variable hypergeometric functions in terms of their parameters. In particular we are interested in Appell functions [30]. Following the methodology exposed in [31], we present in closed form the derivatives of these functions with respect to their parameters. These results are part of a more extensive contribution [32] where the derivatives of eight two variable hypergeometric series with respect to their parameters are presented.

In the third chapter we review the definition and properties of Generalized Sturmian functions. In particular we study the Hulthén Sturmian functions for which analytical expressions can be found. The results we present here constitute the first part of a contribution in which we study the mathematical properties of these functions, and we show how to implement them to solve different two-body scattering problems [33].

The final chapter of the mathematical part is dedicated to study in detail the proposed

Quasi-Sturmian functions. In particular we analyse two different driven terms in the differential equation defining these functions: the two cases for which we can provide in closed form the Quasi-Sturmian functions. Hence, an analytical study of their properties and relations can be performed. In the last section of this chapter we investigate these functions considering one of the parameters involved as a variable. These kind of two variable Quasi-Sturmian functions is proposed in the last chapter to describe the coupling of the radial and angular variables appearing in three-body scattering problems.

Part of the results involving these new functions can be found in reference [34], in which we introduced the two sets of one-dimensional Quasi-Sturmian functions, presenting different analytical representations and their asymptotic behavior, and using them to solve a two-body scattering problem.

Quasi-Sturmian functions are also studied in reference [35], where the authors introduce and implement a set of Quasi-Sturmian functions to solve three-body scattering problems in parabolic coordinates.

As mentioned, in the second part of this work (the two last chapters) we present a general description of two- and three-body scattering problems, and the methodology used to approximate the solution in terms of Generalized Sturmian functions and Quasi-Sturmian functions.

First we analyse two-body scattering problems. Two different approaches are presented. The first one, using Generalized Sturmian functions, with the particular implementation of the Hulthén Sturmian functions to solve the scattering of a particle first by a Hulthén and then by a Yukawa potential. These two illustrations complete our study of Generalized Sturmian functions presented in reference [33]. The second approach uses Quasi-Sturmian functions to represent the scattering solution. As a particular example, we solve the problem of a particle under the influence of a combined attractive Coulomb potential plus a Yukawa potential (this example was published in reference [34]).

The last chapter is dedicated to the three-body case. We begin by introducing hyperspherical coordinates [36, 37]. The advantage of these coordinate system is that the asymptotic behavior of the scattering wave function, and consequently the behavior of Quasi-Sturmian functions, takes a simpler analytical form. As a particular case we describe the S-wave model (usually referred to as Temkin-Poet model [38, 39]) in which only the s-wave contribution of the two outgoing electrons' interaction is retained. This model serves as a test bed as it contains most of the physical and mathematical difficulties of the full problem and, at the same time, makes manipulations easier [40].

Finally, we conclude with a review of the results and contributions, and present some perspectives for our future work.

All numerical calculations and figures presented throughout this work were performed with the software MATHEMATICA [41], Also, unless otherwise indicated, we consider the indices in summations running from 0 to ∞.

Chapter 1

Coulomb Hamiltonian and Coulomb wave functions

1.1 Slater-type orbitals and Laguerre-type functions

For $n \in \mathbb{N} \cup \{0\}$, ℓ, $\beta \in \mathbb{R}$, ℓ, $\beta \geqslant 0$, we introduce the following functions:

◇ Slater-type orbital

$$\phi_n^{STO}(\ell, \beta; r) = e^{-\beta r}\, r^{\ell+1+n} \tag{1.1}$$

◇ Laguerre-type functions

$$\phi_n^{L}(\ell, \beta; r) = N_{n,\ell}\, e^{-\beta r}\, (2\beta r)^{\ell+1}\, L_n^{2\ell+1}(2\beta r) \tag{1.2a}$$

$$= \frac{1}{N_{n,\ell}\, \Gamma(2\ell+2)}\, e^{-\beta r}\, (2\beta r)^{\ell+1}\, {}_1F_1(-n, 2\ell+2; 2\beta r). \tag{1.2b}$$

This last definition includes a normalization factor

$$N_{n,\ell} = \sqrt{\frac{n!}{\Gamma(2\ell+2+n)}}, \tag{1.3}$$

and the associated Laguerre polynomials L_n^{α} [42–44], or alternatively, the confluent hypergeometric function of the first kind ${}_1F_1$ [42, 45, 46]. This hypergeometric function can be expressed as ($b \neq 0, -1, -2, \ldots$)

$$ {}_1F_1(a, b; z) = \sum_n \frac{(a)_n}{(b)_n} \frac{z^n}{n!} \tag{1.4}$$

where $(\alpha)_n$ is the Pochhammer symbol [47, 48]

$$(\alpha)_n = \alpha(\alpha+1)\dots(\alpha+n-1) \tag{1.5a}$$

also expressible, for $\alpha \neq 0, -1, -2...$, in terms of the Gamma functions [42]

$$(\alpha)_n = \frac{\Gamma(\alpha+n)}{\Gamma(\alpha)}. \tag{1.5b}$$

As a consequence of the Pochhammer's property

$$(-n)_j = 0 \quad \forall n, j \in \mathbb{N},\ j > n, \tag{1.6}$$

the series representations for ${}_1F_1(-n, 2\ell+2; 2\beta r)$ is actually a finite sum. Thus, Laguerre-type functions can be given in terms of Slater-type orbitals

$$\phi_n^L(\ell,\beta;r) = \sum_{j=0}^{n} c_{n,j}\, \phi_j^{STO}(\ell,\beta;r), \tag{1.7a}$$

$$c_{n,j} = \frac{1}{N_{n,\ell}\ \Gamma(2\ell+2)}\ \frac{(2\beta)^{\ell+1+j}\,(-n)_j}{j!\,(2\ell+2)_j}. \tag{1.7b}$$

Laguerre-type functions are the solutions of a Sturm-Liouville problem [2, 49, 50],

$$\frac{d^2}{dr^2}\phi_n^L(\ell,\beta;r) - \left[\frac{\ell(\ell+1)}{r^2} - \frac{2\beta(\ell+1+n)}{r} + \beta^2\right]\phi_n^L(\ell,\beta;r) = 0, \tag{1.8a}$$

$$\phi_n^L(\ell,\beta;0) = 0, \tag{1.8b}$$

$$\phi_n^L(\ell,\beta;r) \overset{r\to\infty}{\sim} 0. \tag{1.8c}$$

Therefore they satisfy an orthogonality and a closure relation,

$$\int_0^\infty \phi_p^L(\ell,\beta;r)\,\frac{1}{r}\,\phi_n^L(\ell,\beta;r)\,dr = \delta_{p,n} \tag{1.9a}$$

$$\sum_n \phi_n^L(\ell,\beta;r_1)\,\frac{1}{r_1}\,\phi_n^L(\ell,\beta;r_2) = \delta(r_1-r_2). \tag{1.9b}$$

In addition, they obey a three-terms recurrence relation

$$\frac{n+1}{N_{n+1,\ell}}\,\phi_{n+1}^L(\ell,\beta;r) = \frac{2(\ell+1+n-\beta r)}{N_{n,\ell}}\,\phi_n^L(\ell,\beta;r) - \frac{2\ell+1+n}{N_{n-1,\ell}}\,\phi_{n-1}^L(\ell,\beta;r) \tag{1.10}$$

setting, for $n = 0$, $N_{-1,\ell} = 1$, $\phi^L_{-1} \equiv 0$. This relation is a direct consequence of the three-terms recurrence relation satisfied by associated Laguerre polynomials [43].

In **Figure 1.1** we present three Laguerre-type functions taking $\ell = 1$, $\beta = 1.1$, and the indices $n = 3$ (full line), $n = 7$ (line with dots) and $n = 12$ (dashed line). We can observe the polynomial behavior in the inner region ($r < R_n$ for appropriate R_n) and corroborate the boundary conditions (1.8b) and (1.8c).

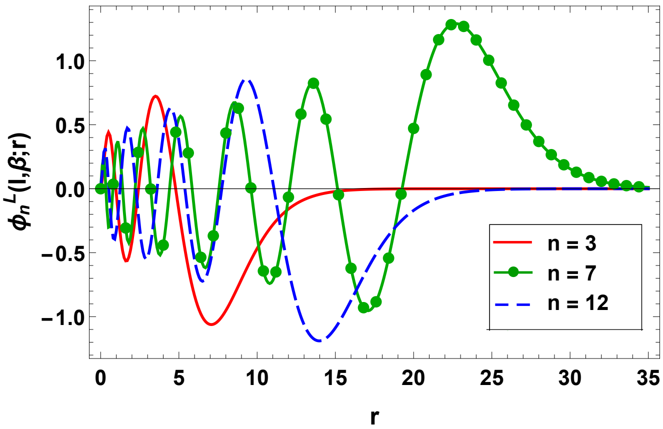

Figure 1.1: Laguerre-type functions corresponding to $n = 3$ (full line), $n = 7$ (line with dots) and $n = 12$ (dashed line). In all three cases we took $\ell = 1$ and $\beta = 1.1$.

1.1.1 Series expansions and integrals

Series expansion in terms of Laguerre-type functions

Throughout this thesis we study functions which are directly or somehow related to the Schrödinger equation. It means that they include, besides position variables, also the physical parameters involved in the dynamics of a quantum system: the mass μ, the charge Z, the angular momentum ℓ and the energy $E = \dfrac{k^2}{2\mu}$.

Any of these one variable functions can be expressed in a generalized Fourier expansion [2, 49–51]

$$f(Z, \mu, \ell, k; r) = \sum_n a_n \, \phi^L_n(\ell, \beta; r) \tag{1.11a}$$

since Laguerre-type functions, solutions of a Sturm-Liouville problem, form an orthogonal and complete basis set. The coefficients a_n are given by

$$a_n = \int_0^\infty \phi^L_n(\ell, \beta; r) \, \frac{1}{r} \, f(Z, \mu, \ell, k; r) \, dr. \tag{1.11b}$$

We consider generally the β parameter as independent of the ones involved in the system under study. Thus, except for the angular momentum ℓ, the other parameters appear only in the coefficients a_n of the series expansion. We have therefore a representation that separates Z, μ, k from the variable r, and the study of a function f in terms of these parameters is reduced to the analysis of the coefficients a_n. For this reason we present, for most of the functions studied, their coefficients in closed form. For example, in **Section 1.2.2** we will show that the coefficients corresponding to the sine-like Coulomb wave function are orthogonal polynomials when considering the charge as a variable.

The importance of separating out the parameters, and the particular interest in the charge Z, will be clarified in **Chapter 6**. The point is that in three-body problems the position variables are coupled, and to solve this difficulty we use functions (the Quasi-Sturmian functions introduced in **Section 4.3.7**) including one of the angular variables into a parametric Coulomb charge. Other strategies may be proposed to deal with this coupling, requiring the treatment of one function's variables as parameters of other function.

Another advantage of separating the parameters from the variables is that it facilitates the calculation of integrals with respect to the variable r (something necessary to solve the Schrödinger equation); indeed, a number of integrals involving Laguerre-type functions are available in reference textbooks.

Integrals involving Laguerre-type functions

In what follows, we perform two radial integrals appearing repeatedly in scattering problems.

The first one is called overlap integral,

$$\vartheta_{p,n} = \int_0^\infty \phi_p^L(\ell,\beta;r)\, \phi_n^L(\ell,\beta;r)\, dr. \tag{1.12a}$$

To calculate it we first rewrite (1.10) as

$$\begin{aligned}\phi_n^L(\ell,\beta;r) = {} & \frac{\ell+1+n}{\beta}\,\frac{1}{r}\,\phi_n^L(\ell,\beta;r) \\ & - \frac{N_{n,\ell}}{N_{n-1,\ell}}\,\frac{2\ell+1+n}{2\beta}\,\frac{1}{r}\,\phi_{n-1}^L(\ell,\beta;r) - \frac{N_{n,\ell}}{N_{n+1,\ell}}\,\frac{n+1}{2\beta}\,\frac{1}{r}\,\phi_{n+1}^L(\ell,\beta;r).\end{aligned}$$

Multiplying by $\frac{1}{r}\,\phi_p^L(\ell,\beta;r)$, integrating from $r=0$ to infinity, and using the orthogonal relation (1.9a), we obtain

$$\vartheta_{p,n} = \frac{\ell+1+n}{\beta}\,\delta_{p,n} - \frac{N_{n,\ell}}{N_{n-1,\ell}}\,\frac{2\ell+1+n}{2\beta}\,\delta_{p,n-1} - \frac{N_{n,\ell}}{N_{n+1,\ell}}\,\frac{n+1}{2\beta}\,\delta_{p,n+1}, \tag{1.12b}$$

or equivalently, in terms of p,

$$\vartheta_{p,n} = \frac{\ell+1+p}{\beta}\,\delta_{p,n} - \frac{N_{p+1,\ell}}{N_{p,\ell}}\,\frac{2\ell+2+p}{2\beta}\,\delta_{p+1,n} - \frac{N_{p-1,\ell}}{N_{p,\ell}}\,\frac{p}{2\beta}\,\delta_{p-1,n}. \tag{1.12c}$$

Another interesting integral is the analogous to (1.9a) but with different ℓ parameters for each function,

$$\begin{aligned}
\int_0^\infty & \phi_q^L(\ell_p,\beta;r)\,\frac{1}{r}\,\phi_n^L(\ell_m,\beta;r)\,dr \\
&\overset{(1.2)}{=} \frac{1}{N_{q,\ell_p}\,N_{n,\ell_m}\,\Gamma(2\ell_p+2)\,\Gamma(2\ell_m+2)}\,(2\beta)^{\ell_m+\ell_p+2} \\
&\qquad \times \int_0^\infty e^{-2\beta r}\,r^{\ell_m+\ell_p+1}\;{}_1F_1(-n,2\ell+2;2\beta r)\,{}_1F_1(-q,2\ell+2;2\beta r)\,dr \\
&\overset{(B.7)}{=} \frac{\Gamma(\ell_p+\ell_m+2)}{N_{q,\ell_p}\,N_{n,\ell_m}\,\Gamma(2\ell_p+2)\,\Gamma(2\ell_m+2)} F_2(\ell_p+\ell_m+2,-q,-n,2\ell_p+2,2\ell_m+2;1,1) \\
&\overset{(2.4)}{=} \frac{\Gamma(\ell_p+\ell_m+2)}{N_{q,\ell_p}\,N_{n,\ell_m}\,\Gamma(2\ell_p+2)\,\Gamma(2\ell_m+2)} \\
&\qquad \times \sum_{j=0}^{q} \frac{(\ell_p+\ell_m+2)_j(-q)_j}{(2\ell_p+2)_j\;j!}\;{}_2F_1(\ell_p+\ell_m+2+j,-n,2\ell_m+2;1)
\end{aligned} \tag{1.13}$$

The function F_2 appearing in an intermediate step of the previous calculation is one of the Appell hypergeometric functions [30, 46, 52]. Some properties and its derivatives with respect to the parameters are presented in **Chapter 2**. The function ${}_2F_1$ is the Gauss hypergeometric function [42, 43, 46] for which we have, if $|z|<1$ and $c \neq 0,-1,-2,...$, the series representation

$${}_2F_1\,(a,b,c;z) = \sum_n \frac{(a)_n\,(b)_n}{(c)_n}\frac{z^n}{n!}. \tag{1.14}$$

For the particular value $z=1$, and $\mathrm{Re}\,(c-a-b)>0$, we have

$${}_2F_1(a,b,c;1) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}, \tag{1.15}$$

so that the integral (1.13) becomes

$$\int_0^\infty \phi_q^L(\ell_p,\beta;r)\,\frac{1}{r}\,\phi_n^L(\ell_m,\beta;r)\,dr$$
$$= \frac{N_{n,\ell_m}\,\Gamma(\ell_p+\ell_m+2)}{N_{q,\ell_p}\,n!\,\Gamma(2\ell_p+2)} \sum_{j=0}^{q} \frac{(\ell_p+\ell_m+2)_j(-q)_j}{(2\ell_p+2)_j\;j!}\,(\ell_m-\ell_p-j)_n. \quad (1.16)$$

1.1.2 Matrix representation for the Coulomb Hamiltonian operator

In **Chapter 5** we will study the scattering of a particle by a radial potential V. The Schrödinger equation describing this process (using atomic units) includes a reduced radial Hamiltonian operator

$$\mathbf{H_r} = \mathbf{T_r} + V(r), \quad (1.17)$$

where $\mathbf{T_r}$ is the reduced radial kinetic energy operator,

$$\mathbf{T_r} = -\frac{1}{2\mu}\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{2\mu r^2} \quad (1.18)$$

(reduced here means that the scattering wave function is divided by r).

For the particular case of a Coulomb interaction between two particles of charges z_1, z_2, the potential is $V(r) = \dfrac{z_1 z_2}{r}$ and we label

$$\mathbf{H_r^C} = -\frac{1}{2\mu}\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{2\mu\, r^2} + \frac{z_1 z_2}{r} \quad (1.19)$$

the radial Coulomb Hamiltonian operator.

Yamani and Fishman [7] showed that the matrix representation of $[\mathbf{H_r^C} - E]$ in terms of not-normalized Laguerre-type functions

$$\varphi_n(\lambda\, r) = (\lambda\, r)^{\ell+1}\, e^{-\lambda\, r/2} L_n^{2\ell+1}(\lambda\, r)$$

is a tridiagonal matrix $\mathbf{J}$ (called J-matrix). The elements of this matrix are given by the integral

$$\mathbf{J}_{m,n} = \int_0^\infty \varphi_m(\lambda\, r)\,[\mathbf{H_r^C} - E]\,\varphi_n(\lambda\, r)\,dr.$$

Remark 1.1.1. In a general way, an operator $[\mathbf{O}]$ has a matrix representation in terms of two set of functions $\{\varphi_n(\omega)\}$, $\{\widetilde{\varphi}_n(\omega)\}$, $n \in \mathbb{N}\cup\{0\}$ and a weight function $w(\omega)$, with elements given by

$$\mathbf{O}_{m,n} = \int_{\Omega} w(\omega)\, \widetilde{\varphi}_n(\omega)\, [\mathbf{O}]\, \varphi_n(\omega)\, d\Omega.$$

Here ω represents the set of involved variables, Ω is the domain associated to these variables, and $d\Omega$ the corresponding differential.

■

For further implementations, we give the expressions of the matrix elements $\mathbf{J}_{m,n}$ for an arbitrary μ (the mentioned authors have taken $\mu = 1$) and using our normalized Laguerre-type functions. Let $Z = z_1 z_2$ and $k^2 = 2\mu E$. Setting, for $n = 0, 1, 2, \ldots$,

$$A_n = \begin{cases} 1, & \text{if} \quad n = 0, \\ \dfrac{N_{n,\ell}}{N_{n-1,\ell}} \, \dfrac{(\beta^2 + k^2)(2\ell + 1 + n)}{4\mu\beta}, & \text{if} \quad n > 0, \end{cases} \tag{1.20a}$$

$$B_n(Z) = \frac{2\mu Z\beta + (\beta^2 - k^2)(\ell + 1 + n)}{2\mu\beta}, \tag{1.20b}$$

and using the properties of Laguerre-type functions (1.8), (1.9a), (1.10) and (1.12b), we obtain

$$\int_0^\infty \phi_p^L(\ell, \beta; r)\, [\mathbf{H}_\mathbf{r}^\mathbf{C} - E]\, \phi_n^L(\ell, \beta; r)\, dr = A_{n+1} \delta_{p,n+1} + B_n(Z)\, \delta_{p,n} + A_n\, \delta_{p,n-1}. \tag{1.21}$$

1.2 Coulomb wave functions

Solutions of the Coulomb equation

$$[\mathbf{H}_\mathbf{r}^\mathbf{C} - E] \Psi_C(\ell, k; r) = 0 \tag{1.22}$$

where $k^2 = 2\mu E$ and $E > 0$, are known as Coulomb wave functions [3, 42, 53]. As these continuum functions describe the scattering of a particle by a Coulomb potential, it is usual to consider a pair of independent solutions $F^{(s)}$, $G^{(c)}$ with sine-like (s) and cosine-like (c) asymptotic behavior, or equivalently two solutions $H^{(\pm)}$ having incoming $(-)$ / outgoing $(+)$ behavior at large distances. The function $F^{(s)}$ is the only one regular at the origin.

Analytical expressions for Coulomb wave functions can be given in terms of confluent hypergeometric functions of the first and second kind ${}_1F_1$, U or, equivalently, in terms of Whittaker functions $M_{\chi,\mu/2}$, $W_{\chi,\mu/2}$ [42, 45]. In **Appendix A** we present Whittaker functions and give detailed calculations of some integrals involving them.

We set

$$\eta(Z) = \frac{\mu Z}{k}, \tag{1.23a}$$

$$\sigma_C(\ell, Z) = \mathrm{Arg}[\Gamma(\ell + 1 + i\eta(Z))], \tag{1.23b}$$

$$N_C(\ell) = \frac{(2k)^{\ell+1}}{2} \frac{|\Gamma(\ell + 1 + i\eta(Z))|}{\Gamma(2\ell + 2)} e^{-\frac{\pi}{2}\eta(Z)}, \tag{1.23c}$$

$$\widetilde{N}_C^{(\pm)}(\ell) = e^{\frac{\pi}{2}\eta(Z)} e^{\pm i\left[\sigma_C(\ell,Z) - \ell\frac{\pi}{2}\right]}. \tag{1.23d}$$

The element η is usually called Sommerfeld parameter (it measures the strength of the Coulomb interaction for a given energy) and σ_C is the Coulomb phase shift. The solution

$$\begin{aligned} F^{(s)}(\ell, k; r) &= \frac{N_C(\ell)}{(2ik)^{\ell+1}} M_{i\eta(Z),\ell+\frac{1}{2}}(2ikr) \\ &= N_C(\ell)\, r^{\ell+1} e^{-ikr}\, {}_1F_1(\ell + 1 - i\,\eta(Z), 2\ell + 2; 2ikr), \end{aligned} \tag{1.24a}$$

is a real function, is regular at the origin and has a sine-like asymptotic behavior,

$$F^{(s)}(\ell, k; 0) = 0, \tag{1.24b}$$

$$F^{(s)}(\ell, k; r) \overset{r\to\infty}{\approx} \sin\left[kr - \eta(Z)\ln(2kr) - \frac{\pi}{2}\ell + \sigma_C(\ell, Z)\right]. \tag{1.24c}$$

The solution

$$G^{(c)}(\ell, k; r) = iN_C(\ell)\, M_{i\eta(Z),\ell+\frac{1}{2}}(2ikr) + \widetilde{N}_C^{(-)}(\ell)\, W_{i\eta(Z),\ell+\frac{1}{2}}(2ikr) \tag{1.25a}$$

is also a real function, is irregular at the origin and has a cosine-like asymptotic behavior,

$$G^{(c)}(\ell, k; r) \overset{r\to\infty}{\approx} \cos\left[kr - \eta(Z)\ln(2kr) - \frac{\pi}{2}\ell + \sigma_C(\ell, Z)\right]. \tag{1.25b}$$

Combining these two functions it is possible to give another pair of independent solutions $H^{(+)}$, $H^{(-)}$ having outgoing (+) or incoming (−) wave asymptotic behavior,

$$H^{(\pm)}(\ell, k; r) = G^{(c)}(\ell, k; r) \pm i\, F^{(s)}(\ell, k; r). \tag{1.26}$$

This pair of solutions simplify to

$$H^{(+)}(\ell,k;r) = \widetilde{N}_C^{(+)}(\ell)\, W_{-i\,\eta(Z),\ell+\frac{1}{2}}(-2ikr), \tag{1.27a}$$

$$H^{(-)}(\ell,k;r) = \widetilde{N}_C^{(-)}(\ell)\, W_{i\,\eta(Z),\ell+\frac{1}{2}}(2ikr) = \left[H^{(+)}(\ell,k;r)\right]^*, \tag{1.27b}$$

they are complex functions, both irregular at $r = 0$, and for $r \to \infty$ behave as

$$H^{(\pm)}(\ell,k;r) \overset{r\to\infty}{\approx} e^{\pm i\left[kr-\eta(Z)\ln(2kr)-\frac{\pi}{2}\ell+\sigma_C(\ell,Z)\right]}. \tag{1.28}$$

The following relations between the Coulomb wave functions exist

$$F^{(s)}(\ell,k;r) = \frac{H^{(+)}(\ell,k;r) - H^{(-)}(\ell,k;r)}{2i}, \tag{1.29a}$$

$$G^{(c)}(\ell,k;r) = \frac{H^{(+)}(\ell,k;r) + H^{(-)}(\ell,k;r)}{2}. \tag{1.29b}$$

1.2.1 Series representation in terms of Laguerre-type functions

We mentioned previously our particular interest in expressing functions as series expansions (1.11) in terms of Laguerre-type functions. In this subsection we review the results known for the sine-like Coulomb wave function and then extend the study to the other solutions providing closed form expressions for the coefficients (1.11b) corresponding to the series representation of $H^{(\pm)}$ and $G^{(c)}$.

For the sine-like Coulomb wave function $F^{(s)}$ the coefficients, indicated by s_n, have been presented and studied by Yamani and Fishman [7]. Their explicit form according to our notation is

$$s_n = (-1)^n \frac{N_C(\ell)}{N_{n,\ell}} \left(\frac{2\beta}{\beta^2+k^2}\right)^{\ell+1} \omega^{-n-i\eta(Z)}\, {}_2F_1\left(-n, \ell+1-i\eta(Z), 2\ell+2; 1-\omega^2\right) \tag{1.30}$$

where we have introduced the parameter

$$\omega = \frac{\beta+ik}{\beta-ik}, \qquad \zeta = \mathrm{Arg}(\omega). \tag{1.31}$$

The tridiagonal matrix associated to $[\mathbf{H}_\mathbf{r}^\mathbf{C} - E]$ introduced by Yamani and Fishman [7] and rewritten in (1.21), is equivalent to a three-terms recurrence relation for the coefficients s_n. To show this, we replace the series representation

$$F^{(s)}(\ell, k; r) = \sum_{n=0}^{\infty} s_n\, \phi_n^L(\ell, \beta; r) \tag{1.32}$$

into the Coulomb differential equation (1.22), multiply both sides from the left by $\phi_m^L(\ell, \beta; r)$, and integrate over r, to find

$$\begin{aligned}\int_0^\infty \sum_n s_n\, \phi_m^L(\ell, \beta; r) \left[\mathbf{H}_{\mathbf{r}}^{\mathbf{C}} - E\right] \phi_n^L(\ell, \beta; r)\, dr \\ = \sum_n s_n \int_0^\infty \phi_m^L(\ell, \beta; r) \left[\mathbf{H}_{\mathbf{r}}^{\mathbf{C}} - E\right] \phi_n^L(\ell, \beta; r)\, dr = 0.\end{aligned} \tag{1.33}$$

Now, using result (1.21), we obtain

$$\sum_{n=0}^{\infty} s_n \left[A_{n+1}\, \delta_{p,n+1} + B_n(Z)\, \delta_{p,n} + A_n\, \delta_{p,n-1}\right] = 0,$$

with A_n and B_n defined by (1.20). This expression gives us the three-terms recurrence relation

$$A_{n+1}\, s_{n+1} + B_n(Z)\, s_n + A_n\, s_{n-1} = 0, \quad n \geqslant 0, \tag{1.34}$$

setting, for $n = 0$, $s_{-1} = 0$. Thus, once we know the first element of the sequence (i.e., s_0) one can find all the coefficients s_n of expansion (1.32). For this reason we give its explicit form

$$\begin{aligned} s_0 &= \frac{N_C(\ell)}{N_{0,\ell}} \left(\frac{2\beta}{\beta^2 + k^2}\right)^{\ell+1} \omega^{-i\eta(Z)} \\ &= \frac{N_{0,\ell}}{2} \left|\Gamma(\ell + 1 + i\,\eta(Z))\right| e^{-\frac{\pi}{2}\eta(Z)}\, \omega^{-i\eta(Z)} \left(\frac{4\beta k}{\beta^2 + k^2}\right)^{\ell+1}. \end{aligned} \tag{1.35}$$

Remark 1.2.1. The recurrence relation can be also derived from the contiguous relations that Gauss hypergeometric functions satisfy [42, 43, 46]. In the deduction presented above, we made explicit the interchange of the series and the integral. For the irregular Coulomb functions this interchange is no longer valid.

■

We now turn to the series representation (1.11a) of functions $H^{(\pm)}$ and $G^{(c)}$ which are irregular at the origin. Since Laguerre-type functions are regular at the origin such expansions are convergent to zero at that point. Moreover, the fact that ℓ is an integer in physical problems makes calculations more complicated. We start by performing the integral

$$h_n^{(\pm)}(\ell) = \int_0^\infty \phi_n^L(\ell,\beta;r)\,\frac{1}{r}\,H^{(\pm)}(\ell,k;r)\,dr \tag{1.36}$$

to obtain a Laguerre expansion of the incoming/outgoing Coulomb wave $H^{(\pm)}$. The resulting series

$$\widetilde{H}^{(\pm)}(\ell,k;r) = \sum_n h_n^{(\pm)}(\ell)\,\phi_n^L(\ell,\beta;r)$$

converges pointwise to $H^{(\pm)}$ for $r > 0$, and as a consequence of the regularity of the Laguerre-type functions at $r = 0$ we have $\widetilde{H}^{(\pm)} = 0$. We made explicit the ℓ parameter dependence in the coefficients $h_n^{(\pm)}$ because particular attention must be paid for non-negative integer values of $2\ell+1$.

When dealing with Coulomb problems the angular momentum ℓ is a non-negative integer. In this case the corresponding Whittaker function appearing in the definition of $H^{(\pm)}$, given by formula (1.27), involves a limit process as described in **Appendix A**. For the calculation of the coefficients $h_n^{(\pm)}$, that is to say the integral (1.36), one needs to consider, separately, the following two cases. For $2\ell+1 \notin \mathbb{N}\cup\{0\}$,

$$\begin{aligned} h_n^{(+)}(\ell) \quad &= \quad \widetilde{N}_C^{(+)}(\ell)\int_0^\infty \phi_n(\ell,\beta;r)\,\frac{1}{r}\,W_{-i\,\eta(Z),\ell+\frac{1}{2}}(-2ikr)\,dr \\ &\overset{(A.5)}{=} \quad \frac{\widetilde{N}_C^{(+)}(\ell)\,\pi}{\sin[\pi(2\ell+1)]}\left\{\frac{2i\,\widetilde{N}_C^{(+)}(\ell)}{\Gamma(-\ell+i\eta(Z))}\,s_n + \frac{2\beta}{N_{n,\ell}\,\Gamma(2\ell+2)\Gamma(-2\ell)}\left(-\frac{\beta}{ik}\right)^{\ell}\right. \\ &\quad \left.\times\ \frac{1}{\beta-ik}F_2\left(1,-n,-\ell+i\eta(Z),2\ell+2,-2\ell;\frac{2\beta}{\beta-ik},-\frac{2ik}{\beta-ik}\right)\right\}, \end{aligned} \tag{1.37}$$

where F_2 is one of the Appell hypergeometric functions studied in **Chapter 2**. For $2\ell+1 \in \mathbb{N}\cup\{0\}$, we calculate a limit process,

$$h_n^{(+)}(\ell) = \lim_{\epsilon\to 0} h_n^{(+)}(\ell+\epsilon).$$

and use (A.10), to end up with much more cumbersome coefficients,

$$
\begin{aligned}
h_n^{(+)}(\ell) =& \frac{\widetilde{N}_C^{(+)}(\ell)}{N_{n,\ell}\,\Gamma(2\ell+2)} \left(\frac{\beta}{k} i\right)^{\ell} x \\
& \times \Bigg[\frac{\Gamma(2\ell+1)}{\Gamma(\ell+1+i\eta(Z))} \sum_{q=0}^{2\ell} \frac{(-\ell+i\eta(Z))_q}{(-2\ell)_q}\, y^q \,{}_2F_1(-n, q+1, 2\ell+2; x) \\
& + \frac{(-1)^{2\ell+1} y^{2\ell+1}}{\Gamma(-\ell+i\eta(Z))} \sum_{q=0}^{\infty} (\ell+1+i\eta(Z))_q \frac{y^q}{q!} \Big\{ {}_2F_1(-n, 2\ell+2+q, 2\ell+2; x) \\
& \times [\psi(q+1) - \mathrm{Log}\,(y) - \psi(\ell+1+q+i\eta(Z))] \\
& + \frac{n\,x}{4(\ell+1)^2} \Bigg[-q(1-x)^{n-1}\, {}_2\Theta_1^{(1)} \left(\begin{array}{c} 1,1\,|\,2\ell+2, -n+1, -q+1 \\ 2\ell+3\,|\,2, 2\ell+3 \end{array} \middle| ; x^*, x^* \right) \\
& + (2\ell+2+q)\;\; {}_2\Theta_1^{(1)} \left(\begin{array}{c} 1,1\,|\,2\ell+2, -n+1, 2\ell+3+q \\ 2\ell+3\,|\,2, 2\ell+3 \end{array} \middle| ; x, x \right) \Bigg] \Big\} \Bigg] .
\end{aligned}
\tag{1.38}
$$

Here ψ is the digamma function [42, 46], ${}_2\Theta_1^{(1)}$ is a generalized Kampé de Fériet hypergeometric function [defined in (2.2), when studying two variable hypergeometric functions] and we have introduced

$$
x = \frac{2\beta}{\beta - ik}, \quad y = -\frac{2ik}{\beta - ik}.
$$

Making use of the expression (1.37) found for the first case we present in **Figure 1.2** the real (left panel) and imaginary (right panel) parts of an approximation

$$
H_N^{(+)}(\ell, k; r) = \sum_{n=0}^{N} h_n^{(+)} \phi_n^L(\ell, \beta; r) \tag{1.39}
$$

of the outgoing Coulomb wave function $H^{(+)}$. We compare the results obtained taking $N = 25$ (full line) and $N = 35$ (line with dots) with the function $H^{(+)}$ (dashed line) given by formula (1.27). As expected, the more Laguerre functions we use, the more accurate is the approximation of $H^{(+)}$, and the range of accuracy increases.

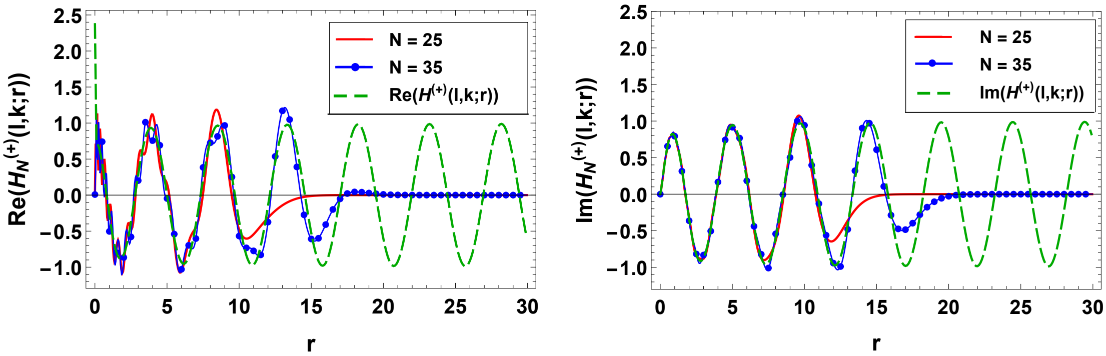

Figure 1.2: Real (left panel) and imaginary (right panel) parts of an approximation $H_N^{(+)}$ of the Coulomb wave function $H^{(+)}$, taking $N = 25$ (full line) and $N = 35$ (line with dots). We have fixed $Z = -1$, $\mu = 1$, $k = 1.23$, $\ell = 0.3$ and $\beta = 4$.

Using the series representation (2.4) of Appell function F_2 and the contiguous relations of Gauss hypergeometric functions [42, 43, 46], one can establish a sort of relation between three consecutive coefficients $h_n^{(+)}$. Contrary to the one satisfied by s_n, the relation for $h_n^{(+)}$ is not homogeneous; moreover, the resulting extra term is not simple. The fact that the recurrence relation for s_n in no longer valid for $h_n^{(+)}$ is connected with **Remark 1.2.1**: the series and the integral interchange performed with coefficients s_n in (1.33) can not be done with the expansion of $H^{(+)}$.

Although the coefficients $h_n^{(+)}$, $n > 0$, cannot be deduced from the first one $h_0^{(+)}$ in a simple manner, we present the expressions of $h_0^{(+)}$ just to show how they simplify. For $2\ell + 1 \notin \mathbb{N} \cup \{0\}$ one finds

$$h_0^{(+)}(\ell) = \frac{\widetilde{N}_C^{(+)}(\ell)\,\pi}{\sin[\pi(2\ell+1)]} \left\{ \frac{2i\,\widetilde{N}_C^{(+)}(\ell)}{\Gamma(-\ell+i\eta(Z))} s_0 + \frac{2\beta\,N_{0,\ell}}{\beta - ik} \left(-\frac{\beta}{ik}\right)^{\ell} \times \frac{1}{\Gamma(-2\ell)}\, {}_2F_1\left(1, -\ell+i\eta(Z), -2\ell; -\frac{2ik}{\beta-ik}\right) \right\},$$

and for $2\ell + 1 \in \mathbb{N} \cup \{0\}$ it becomes

$$h_0^{(+)}(\ell) = \widetilde{N}_C^{(+)}(\ell) N_{0,\ell} \left(\frac{\beta}{k} i\right)^{\ell} \frac{2\beta}{\beta - ik} \left\{ \frac{\Gamma(2\ell+1)}{\Gamma(\ell+1+i\eta(Z))} \sum_{q=0}^{2\ell} \frac{(-\ell+i\eta(Z))_q}{(-2\ell)_q} y^q + \frac{(-1)^{2\ell+1} y^{2\ell+1}}{\Gamma(-\ell+i\eta(Z))} \sum_{q=0}^{\infty} (\ell+1+i\eta(Z))_q \frac{y^q}{q!} \left[\psi(q+1) - \mathrm{Log}\,(y) - \psi(\ell+1+q+i\eta(Z))\right] \right\}.$$

The coefficients $h_n^{(-)}(\ell)$ corresponding to the expansion of $H^{(-)}$ are easily deduced by conjugation

$$h_n^{(-)}(\ell) = \left[h_n^{(+)}(\ell)\right]^*.$$

From the relation (1.29) between the Coulomb wave functions, we obtain

$$s_n = \frac{h_n^{(+)}(\ell) - h_n^{(-)}(\ell)}{2i}, \tag{1.40a}$$

$$c_n(\ell) = \frac{h_n^{(+)}(\ell) + h_n^{(-)}(\ell)}{2}, \tag{1.40b}$$

where we set $c_n(\ell)$ for the expansion coefficients of $G^{(c)}$. Relation (1.40b) allows us to deduce an expression for the $c_n(\ell)$ elements without performing the corresponding integrals. As in the case of the coefficients $h_n^{(\pm)}(\ell)$ a distinction must be made depending on the value of $2\ell+1$ (the irregular Whittaker function appearing in the definition (1.25a) is responsible for this situation). Clearly, to derive an expression for the case $2\ell+1 \in \mathbb{N}\cup\{0\}$ is really difficult, therefore we are not presenting it here. For $2\ell + 1 \notin \mathbb{N} \cup \{0\}$ the coefficients take the form

$$\begin{aligned} c_n(\ell) = \frac{2}{\sin[\pi(2\ell+1)]} \Bigg\{ &- \left[e^{\pi\eta(Z)} \sinh[\pi\eta(Z)] + \sin^2(\pi\ell)\right] s_n \\ &+ \frac{\pi\ \beta\ e^{\frac{\pi}{2}\eta(Z)}}{N_{n,\ell}|\Gamma(\ell+1+i\eta(Z))|} \frac{1}{\Gamma(2\ell+2)\Gamma(-2\ell)} \left(\frac{\beta}{k}\right)^{\ell} \frac{1}{\beta - ik} \\ &\times F_2\left(1, -n, -\ell + i\eta(Z), 2\ell+2, -2\ell; \frac{2\beta}{\beta - ik}, -\frac{2ik}{\beta - ik}\right)\Bigg\}. \end{aligned}$$

1.2.2 Connection with orthogonal polynomials

The three-terms recurrence relation (1.34) satisfied by coefficients s_n can be related to generalized Pollaczek [44, 46, 54] or Meixner-Pollaczek [55, 56] polynomials, depending on the element we consider as the variable. The connection with Pollaczek polynomials was established and deeply investigated by different authors [7, 57, 59, 60]. In this section we first review previous findings and then we present a novel interpretation of the s_n coefficients relating them to Meixner-Pollaczek polynomials.

It is convenient to multiply (1.34) by

$$\frac{4\mu\beta}{N_{n,\ell}\,(\beta^2 + k^2)}$$

to obtain the equivalent relation

$$\begin{aligned} (n+1)\,\frac{s_{n+1}}{N_{n+1,\ell}} &= 2\left[-\frac{2\mu\beta Z}{\beta^2+k^2} + \left(-\frac{\beta^2 - k^2}{\beta^2+k^2}\right)(\ell+1+n)\right]\frac{s_n}{N_{n,\ell}} \\ &\quad -(2\ell+1+n)\frac{s_{n-1}}{N_{n-1,\ell}}. \end{aligned} \tag{1.41}$$

Now we define a new coefficient

$$b_n = \frac{s_n/N_{n,\ell}}{s_0/N_{0,\ell}} = \frac{N_{0,\ell}}{N_{n,\ell}} \frac{s_n}{s_0}, \tag{1.42}$$

for which we have

$$b_{-1} = 0, \tag{1.43a}$$

$$b_0 = 1, \tag{1.43b}$$

$$(n+1)\, b_{n+1} = 2\left[-\frac{2\mu\beta Z}{\beta^2+k^2} + \left(-\frac{\beta^2-k^2}{\beta^2+k^2}\right)(\ell+1+n)\right] b_n - (2\ell+1+n)\, b_{n-1}. \tag{1.43c}$$

Generalized Pollaczek polynomials

Generalized Pollaczek polynomials P_n^λ form a set of orthogonal polynomials [44, 46, 54] characterized by the recurrence relation

$$P_{-1}^\lambda(x;a,b) = 0, \tag{1.44a}$$

$$P_0^\lambda(x;a,b) = 1, \tag{1.44b}$$

$$(n+1)P_{n+1}^\lambda(x;a,b) = 2[b+(n+\lambda+a)x]P_n^\lambda(x;a,b) - (n-1+2\lambda)P_{n-1}^\lambda(x;a,b) \tag{1.44c}$$

where

$$x = \cos\theta, \quad \theta \in (0,\pi), \qquad a \geqslant |b|, \qquad \lambda > -1. \tag{1.45}$$

In closed form they are given by a product of a complex exponential and a Gauss hypergeometric function ${}_2F_1$,

$$P_n^\lambda(x;a,b) = \frac{(2\lambda)_n}{n!}\, e^{in\theta}\, {}_2F_1(-n, \lambda+it, 2\lambda; 1-e^{-2i\theta}), \tag{1.46}$$

with

$$t = \frac{a\cos\theta + b}{\sin\theta} = \frac{ax+b}{\sqrt{1-x^2}}.$$

Notice that the variable $x = \cos\theta$ appears not only in the argument of the hypergeometric function but also in its second parameter.

The orthogonality property

$$\int_{-1}^{1} P_m^\lambda(x;a,b)\, P_n^\lambda(x;a,b)\, w_P(x)\, dx = \frac{\Gamma(2\lambda+n)}{n!(\lambda+n+a)}\, \delta_{m,n} \tag{1.47a}$$

is satisfied, with weight function

$$w_P(x) = \frac{1}{\pi} e^{(2\theta-\pi)t} (2\sin\theta)^{2\lambda-1} \left|\Gamma\left(\lambda + it\right)\right|^2 . \tag{1.47b}$$

When studying the J-Matrix method different authors [7, 57–59] have investigated the relation between generalized Pollaczek polynomials and the coefficients s_n associated to the expansion of the sine-like Coulomb wave function. Comparing (1.43) with (1.44) and identifying

$$a = \frac{\mu Z}{\beta}, \qquad b = -\frac{\mu Z}{\beta}, \qquad \lambda = \ell + 1, \qquad x = -\frac{\beta^2 - k^2}{\beta^2 + k^2} \tag{1.48}$$

the two recurrence relations coincide. The quantity t is related to the Sommerfeld parameter η defined by formula (1.23a),

$$t = -\eta(Z)$$

For b_n to be a generalized Pollaczek polynomial, the restrictions (1.45) must be satisfied. Since the parameters a, b must be independent of the variable, we must consider μ, Z, β as fixed values, and then we have k as the (implicit) variable and to have the complete x domain it suffices to take $k > 0$. The condition on λ is verified for $\ell > -2$. Finally, as we are considering μ, β fixed and positive, the conditions on a and b impose $Z > 0$. It means that the coefficients s_n are related to generalized Pollaczek polynomials only for repulsive Coulomb potentials.

Thus, for $\mu, Z, \beta > 0$, $\ell > -2$ and $k \in (0, +\infty)$ we have

$$b_n = P_n^{\lambda}(x; a, b),$$

or equivalently, using (1.42),

$$s_n = \frac{N_{n,\ell}}{N_{0,\ell}}\, s_0\, P_n^{\ell+1}\left(-\frac{\beta^2 - k^2}{\beta^2 + k^2}; \frac{\mu Z}{\beta}, -\frac{\mu Z}{\beta}\right) \tag{1.49a}$$

$$\overset{(1.46)}{=} \frac{N_{0,\ell}}{N_{n,\ell}}\, s_0\, e^{in\theta}\, {}_2F_1\left(-n, \ell + 1 - i\eta(Z), 2\ell + 2; 1 - e^{-2i\theta}\right). \tag{1.49b}$$

Let us notice that, for $\beta, k > 0$ and $\theta \in (0, \pi)$,

$$\cos\theta = -\frac{\beta^2 - k^2}{\beta^2 + k^2} \qquad \Longrightarrow \qquad \sin\theta = \frac{2\beta k}{\beta^2 + k^2}$$

and then

$$e^{i\theta} = -\frac{\beta^2 - k^2}{\beta^2 + k^2} + i\frac{2\beta k}{\beta^2 + k^2} = -\frac{\beta - ik}{\beta + ik}.$$

In (1.31) we have introduced a parameter ω related to the previous identity,

$$e^{i\theta} = -\omega^{-1} = e^{(\pi-\zeta)i}.$$

Then (1.49b) can be rewritten as

$$s_n = \frac{N_{0,\ell}}{N_{n,\ell}} s_0 (-1)^n e^{-in\zeta} {}_2F_1\left(-n, \ell + 1 - i\eta(Z), 2\ell + 2; 1 - e^{2i\zeta}\right), \qquad (1.50)$$

which is equivalent to expression (1.30).

With this particular choice of the variable and the parameters, the weight function (1.47b) becomes

$$\begin{aligned} w_P(k) &= \frac{1}{\pi} e^{-\pi\eta(Z)} \omega^{-i\,2\eta(Z)} \left(\frac{4\beta k}{\beta^2 + k^2}\right)^{2\ell+1} \left|\Gamma\left(\ell + 1 - i\,\eta(Z)\right)\right|^2 \\ &\overset{(1.35)}{=} \frac{\Gamma(2\ell+2)}{\pi} \frac{\beta^2 + k^2}{\beta k} s_0^2 \end{aligned} \qquad (1.51)$$

and, from (1.49a), the orthogonality property (1.47a) in terms of the coefficients $s_n = s_n(k)$ reads

$$\int_0^{+\infty} s_n(k)\, s_m(k)\, \frac{1}{\beta^2 + k^2}\, dk = \frac{\pi}{4\beta(\ell + 1 + n) + 4\mu Z}\, \delta_{m,n},$$

for $\ell > -2$, $\beta, \mu, Z > 0$.

Remark 1.2.2. We have seen that for the case of an attractive Coulomb potential ($Z < 0$), the restriction $a \geqslant |b|$ fails and the coefficients s_n are no longer related to Pollaczek polynomials. Yamani and Reinhardt [57] proposed a new set of polynomials that they called “attractive Coulomb-Pollaczek” polynomials. Ten years later, Bank and Ismail [60] presented a complete study of these polynomials and their properties. In both attractive and repulsive cases, the charge Z is considered as a parameter and the momentum k (or the energy E through the relation $2\mu E = k^2$) is the implicit polynomial variable.

■

Remark 1.2.3. The choice of the parameters (1.48) is not unique, but it can be shown that other choices lead to equivalent expressions of the same polynomials.

■

Meixner-Pollaczek polynomials

Meixner-Pollaczek polynomials [55, 56] are orthogonal polynomials defined by

$$P_n^\lambda(x;\theta) = \frac{(2\lambda)_n}{n!}\, e^{in\theta}\, {}_2F_1\left(-n, \lambda + ix, 2\lambda; 1 - e^{-2i\theta}\right). \tag{1.52a}$$

for

$$x \in \mathbb{R}, \qquad \theta \in (0,\pi), \qquad \lambda > 0. \tag{1.52b}$$

Let us remark that the variable x is only present in the second parameter of the hypergeometric function. The recurrence relation characterizing these polynomials is

$$P_{-1}^\lambda(x;\theta) = 0, \tag{1.53a}$$

$$P_0^\lambda(x;\theta) = 1, \tag{1.53b}$$

$$(n+1)P_{n+1}^\lambda(x;\theta) = 2\left[x\sin\theta + (n+\lambda)\cos\theta\right]P_n^\lambda(x;\theta) - (n+2\lambda-1)P_{n-1}^\lambda(x;\theta). \tag{1.53c}$$

The orthogonality property requires a weight function

$$w_M(x) = e^{(2\theta-\pi)x}|\Gamma(\lambda+ix)|^2 \tag{1.54}$$

thus

$$\int_{-\infty}^{+\infty} P_m^\lambda(x;\theta)P_n^\lambda(x;\theta)w_M(x)\,dx = 2\pi\frac{\Gamma(2\lambda+n)}{(2\sin\theta)^{2\lambda}\,n!}\delta_{m,n}. \tag{1.55}$$

Now we compare (1.43) and (1.53). Setting

$$x = -\eta(Z) \overset{(1.23a)}{=} -\frac{\mu Z}{k}, \qquad \lambda = \ell + 1$$

and ω as in (1.31), we find

$$\cos(\pi-\zeta) = -\frac{\beta^2-k^2}{\beta^2+k^2}, \qquad \sin(\pi-\zeta) = \frac{2\beta k}{\beta^2+k^2}$$

and we conclude that, taking $\theta = \pi - \zeta$, relation (1.43) for the coefficients b_n becomes the one characterizing Meixner-Pollaczek polynomials.

From (1.52b) we have the restrictions

$$\begin{aligned} &\ell > -1, \\ &\theta \in (0,\pi) \quad \Longrightarrow \quad \sin\theta = \sin(\pi-\zeta) = \frac{2\beta k}{\beta^2+k^2} > 0, \\ &\eta(Z) \in \mathbb{R}. \end{aligned}$$

Thus for $\ell > -1, \mu, \beta, k > 0$ and $Z \in \mathbb{R}$ we find

$$b_n = P_n^{\lambda}(-\eta(Z); \pi - \zeta)$$

or equivalently, using (1.42),

$$s_n = \frac{N_{n,\ell}}{N_{0,\ell}}\, s_0\, P_n^{\ell+1}\left(-\eta(Z); \pi-\zeta\right) \tag{1.56a}$$

$$\overset{(1.52a)}{=} \frac{N_{0,\ell}}{N_{n,\ell}}\, s_0\, (-1)^n\, e^{-in\zeta}\, {}_2F_1\left(-n, \ell+1-i\eta(Z), 2\ell+2; 1-e^{2i\zeta}\right). \tag{1.56b}$$

Even if we finally arrive at the same expression found in (1.50), this constitutes an alternative interpretation for the s_n coefficients as functions of the charge $Z \in \mathbb{R}$, including both attractive and repulsive Coulomb potentials in the same family.

Moreover, these "charge" functions satisfy two interesting properties. First of all, an orthogonality property consequence of the orthogonality known for the Meixner-Pollaczek polynomials. Rewritten in terms of the parameters of the Coulomb problem, the weight function (1.54) becomes

$$\begin{aligned} w_M(Z) &= \omega^{-2i\eta(Z)} e^{-\pi\eta(Z)} |\Gamma(\ell+1-i\eta(Z))|^2 \\ &\overset{(1.35)}{=} 4\,\Gamma(2\ell+2)\left(\frac{\beta^2+k^2}{4\beta k}\right)^{2\ell+2} s_0^2 \end{aligned}$$

and, from (1.56a) and the orthogonality property (1.55), we obtain an orthogonality relation for the coefficients $s_n = s_n(Z)$,

$$\int_{-\infty}^{+\infty} s_n(Z)\, s_m(Z)\, dZ = \frac{\pi k}{2\mu}\, \delta_{m,n}, \tag{1.57}$$

taking $\ell > -1$, $\beta, \mu, k > 0$. Second, as a consequence of their relation with

Meixner-Pollaczek polynomials, these coefficients form a complete basis set. Thus,

$$\sum_n s_n(Z_1)s_n(Z_2) = \frac{\pi k}{2\mu}\,\delta(Z_1 - Z_2). \tag{1.58}$$

In **Figure 1.3**, we plot as a function of the charge Z, three coefficients s_n: $n = 2$ (full line), $n = 3$ (dashed line) and $n = 4$ (line with dots). Notice the polynomial behavior of these coefficients in an " inner" region $|Z| < Z_n$, for an appropriate Z_n, and the fact that they vanish in the "asymptotic" region $|Z| > Z_n$.

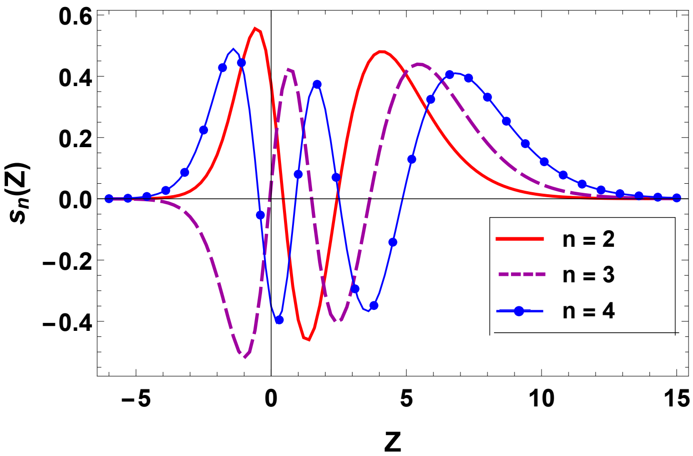

Figure 1.3: Plot of three consecutive coefficients s_n as a function of the charge Z. We take $n = 2$ (full line), $n = 3$ (dashed line) and $n = 4$ (line with dots). The values of the parameters are $\mu = 1.7, k = 1.25, \ell = 1.3$ and $\beta = 2.4$.

This novel interpretation of the coefficients as orthogonal functions with the charge as the variable invites us to explore the sine-like Coulomb wave function in terms of the charge. The closure relations (1.9b) and (1.58) allow us to perform the following integrals over Z for the regular Coulomb wave function. The first one gives a completeness relation with respect to the radial variable,

$$\begin{aligned}
&\int_{-\infty}^{\infty} F^{(s)}(Z,\ell,k;r_1)\,\frac{1}{r_1}\,F^{(s)}(Z,\ell,k;r_2)\,dZ \\
&\overset{(1.32)}{=} \frac{1}{r_1}\int_{-\infty}^{\infty}\sum_n s_n(Z)\,\phi_n^L(\ell,\beta;r_1)\sum_m s_m(Z)\,\phi_m^L(\ell,\beta;r_2)\,dZ \\
&\overset{(1.57)}{=} \frac{\pi k}{2\mu}\,\sum_m \phi_m^L(\ell,\beta;r_1)\,\frac{1}{r_1}\,\phi_m^L(\ell,\beta;r_2) \\
&\overset{(1.9b)}{=} \frac{\pi k}{2\mu}\,\delta(r_1 - r_2),
\end{aligned} \tag{1.59a}$$

while the second one establishes the same relation when considering the charge as the variable,

$$\begin{aligned}
&\int_0^\infty F^{(s)}(Z_1,\ell,k;r)\,\frac{1}{r}F^{(s)}(Z_2,\ell,k;r)\,dr \\
&\qquad\overset{(1.32)}{=} \int_0^\infty \sum_n s_n(Z_1)\,\phi_n^L(\ell,\beta;r)\,\frac{1}{r}\,\sum_m s_m(Z_2)\,\phi_m^L(\ell,\beta;r)\,dr \\
&\qquad\overset{(1.9a)}{=} \sum_m s_m(Z_1)s_m(Z_2) \\
&\qquad\overset{(1.58)}{=} \frac{\pi k}{2\mu}\,\delta(Z_1-Z_2). \qquad (1.59b)
\end{aligned}$$

These integrals were deduced in [61] in a different context, where the authors proposed to consider a set $\{S_{\gamma,\ell}(x)\}_{\gamma\in\mathbb{R}}$ of charge Coulomb Sturmian functions that happen to be regular Coulomb wave functions with the charge as the index.

Remark 1.2.4. The integral (1.59b) can not be performed using (B.7) because one of the conditions required is not satisfied.

■

1.3 The Coulomb Green's functions

The Coulomb Green's functions are solutions of

$$\left[\mathbf{H}_{\mathbf{r}}^{\mathbf{C}} - E\right]\mathcal{G}_C(\ell;r,r') = \delta(r-r'), \qquad (1.60)$$

with particular boundary conditions.

Different analytical expressions have been presented for these functions in both coordinate and momentum space [62–65]. Series expansions in terms of Coulomb Sturmian and Generalized Sturmian functions have also been proposed [66–69].

We are interested here in solutions which are regular at $r=0$ and have incoming or outgoing wave asymptotic behavior ($r\to\infty$). The Coulomb Green's function, in this case, can be expressed as the product of the two independent solutions (1.24) and (1.27) of the corresponding homogeneous equation,

$$\mathcal{G}_C^{(\pm)}(\ell;r,r') = \mp\frac{\mu}{ik}\frac{\Gamma(\ell+1\pm i\eta(Z))}{(2l+1)!}\,M_{\mp i\eta(Z);\,\ell+1/2}(\mp 2ikr_<)W_{\mp i\eta(Z);\,\ell+1/2}(\mp 2ikr_>). \qquad (1.61)$$

Hostler [63] studied this expression and deduced an alternative representation,

$$\mathcal{G}_C^{(\pm)}(\ell;\ r,\ r') = 2\mu\sqrt{r\,r'}\int_0^\infty dy\, e^{\pm ik(r+r')\cosh(y)}\left[\coth\left(\frac{y}{2}\right)\right]^{\mp 2i\eta(Z)}\ I_{2\ell+1}(\mp 2ik\sqrt{r\,r'}\sinh(y)), \tag{1.62}$$

where $I_{2\ell+1}$ is a Bessel function [42].

It is possible to give a series representation of $\mathcal{G}_C$ also in terms of Laguerre-type functions,

$$\mathcal{G}_C^{(\pm)}(\ell; r, r') = \sum_{n,q} g_{n,q}^{(\pm)}\, \phi_n^L(\ell,\beta;r)\, \phi_q^L(\ell,\beta;r'). \tag{1.63}$$

The coefficients $g_{n,q}^{(\pm)}$ are formally given by

$$g_{n,q}^{(\pm)} = \int_0^\infty \int_0^\infty \frac{1}{r}\,\phi_n^L(\ell,\beta;r)\,\frac{1}{r'}\,\phi_q^L(\ell,\beta;r')\mathcal{G}_C^{(\pm)}(\ell;r,r')\,dr\,dr', \tag{1.64}$$

and, independently of the boundary conditions, they satisfy a recurrence relation consequence of the tridiagonal matrix representation (1.21) of the operator $[\mathbf{H_r^C} - E]$ in terms of Laguerre-type functions. Replacing the series (1.63) in (1.60), multiplying by the left both sides of the equation by

$$\frac{1}{r}\,\phi_m^L(\ell,\beta;r)\,\frac{1}{r'}\,\phi_p^L(\ell,\beta;r')$$

and integrating over r and r', we obtain

$$A_{n+1}\,g_{n+1,q} + B_n(Z)\,g_{n,q} + A_n\,g_{n-1,q} = \delta_{n,q}, \tag{1.65}$$

where A_n and B_n are given by formulas (1.20), and for $n = 0$ we take $g_{-1,q} = 0$.

Taking $\mu = 1$ and using not-normalized Laguerre-type functions, the previous relation reduces to the one given by Heller in reference [62], a paper in which the author also deduced a closed form for the coefficients $g_{n,q}^{(+)}$ corresponding to the Coulomb Green's function having outgoing asymptotic behavior. The analogous expression for a general μ and our normalized ϕ_q^L is

$$g_{n,q}^{(\pm)} = \frac{2\mu}{k}\ s_{n_<}\ \hat{h}_{n_>}^{(\pm)}, \tag{1.66}$$

where $n_< = \min(n,q)$, $n_> = \max(n,q)$. Clearly, we have the symmetry property

$$g_{n,q}^{(\pm)} = g_{q,n}^{(\pm)}.$$

The elements s_n are the coefficients (1.30) of the series expansion of the Coulomb wave function having sine-like asymptotic behavior, and

$$\hat{h}_n^{(\pm)} = -\frac{n!}{N_{n,\ell}}\left(\frac{\beta^2+k^2}{4\beta k}\right)^{\ell}\frac{\Gamma(\ell+1\pm i\eta(Z))}{|\Gamma(\ell+1\pm i\eta(Z))|}\frac{e^{\frac{\pi}{2}\eta(Z)}\;\omega^{i\eta(Z)}\;(-\omega)^{\pm(n+1)}}{\Gamma(\ell+2+n\pm i\eta(Z))} \times\; {}_2F_1(-\ell\pm i\eta(Z), n+1, \ell+2+n\pm i\eta(Z); \omega^{\pm 2}). \tag{1.67}$$

These are the coefficients of the series representation of a function

$$\hat{H}^{(\pm)}(\ell,\beta;r) = \sum_n \hat{h}_n^{(\pm)}\;\phi_n^L(\ell,\beta;r) \tag{1.68}$$

solution of the boundary value problem

$$\left[\mathbf{H}_{\mathbf{r}}^{\mathbf{C}} - E\right]\hat{H}^{(\pm)}(\ell,\beta;r) = b\,\frac{1}{r}\,\phi_0^L(\ell,\beta;r), \tag{1.69a}$$

$$\hat{H}^{(\pm)}(\ell,\beta;0) = 0, \tag{1.69b}$$

$$\hat{H}^{(\pm)}(\ell,\beta;0) \overset{r\to\infty}{\sim} e^{\pm i\left[kr-\eta(Z)\ln(2kr)-\frac{\pi}{2}\ell+\sigma_C(\ell,Z)\right]}. \tag{1.69c}$$

The constant b is chosen to obtain the proposed asymptotic behavior. The coefficients $\hat{h}_n^{(\pm)}$ were presented by Yamani and Fishman [7], and then studied by Broad [58, 59], considering $\mu = 1$ and using not-normalized Laguerre-type functions. They also obtained a recurrence relation for $\hat{h}_n^{(\pm)}$ by replacing (1.68) in (1.69a), multiplying both sides by ϕ_n^L and integrating over r. Making use of (1.21), for the case of a general μ and taking our normalized Laguerre-type functions, the recurrence relation reads

$$A_1\,\hat{h}_1^{(\pm)} + B_0(Z)\,\hat{h}_0^{(\pm)} = b, \tag{1.70a}$$

$$A_{n+1}\,\hat{h}_{n+1}^{(\pm)} + B_n(Z)\,\hat{h}_n^{(\pm)} + A_n\,\hat{h}_{n-1}^{(\pm)} = 0, \qquad n \geqslant 1, \tag{1.70b}$$

Notice that, except for the first two elements, this is exactly the relation found for the coefficients s_n of the Laguerre representation of the sine-like Coulomb wave function (1.34).

In **Chapter 4** we will see that $\hat{H}^{(\pm)}$ happens to be one of the Quasi-Sturmian functions we study in this thesis, and we shall present different analytical expressions for it.

1.4 Chapter summary

In this chapter we have presented and reviewed some properties of the functions constituting the base of our further investigations.

First we have introduced Slater-type orbitals and Laguerre-type functions, commonly used as basis sets to represent wave functions in the context of scattering problems. Here we will use them to generate the Quasi-Sturmian functions we will study in **Chapter 4**. The matrix representation of the Coulomb Hamiltonian operator in terms of Laguerre-type functions is tridiagonal, and this property originates the J-Matrix method [5–8]. In our work, this feature will be responsible for the recurrence relations we will deduce for the Quasi-Sturmian functions.

Then, we have presented the Coulomb wave functions and Coulomb Green's functions, reviewing their definition and some of their properties. For the sine-like Coulomb wave function, we have referred to the analytical expression of the coefficients s_n, introduced by Yamani and Fishman [7], corresponding to the series expansion in terms of Laguerre-type functions. We pointed out the three-term recurrence relation they satisfy, consequence of the tridiagonal matrix form of the Coulomb Hamiltonian operator. We have also examined the existing relation between s_n and Pollaczek polynomials, and have extended known results. On one side, we have contributed with analytical expressions for the coefficients of the Laguerre expansion of the irregular solutions of the Coulomb Hamiltonian, $G^{(c)}$ and $H^{(\pm)}$, and we have observed that the known recurrence relation for s_n is no longer valid for the new coefficients. On the other, we have established a novel relation between the coefficients s_n and Meixner-Pollaczek polynomials. This connection came from considering the charge as the variable, and it allowed us to explore new properties of these coefficients, finding an orthogonality and a closure relation with respect to the charge.

Chapter 2

Two variables hypergeometric functions

Since they appear throughout the thesis work, we have developed a special interest in hypergeometric functions in one and two variables. For example, in the previous chapter we have expressed Coulomb wave functions in terms of one variable hypergeometric functions M and W (Whittaker's functions). We have also found that the expressions of the series expansions coefficients of irregular Coulomb wave functions involve a two variable hypergeometric function F_2 (Appell's function). In the next chapter, we will see that Hulthén Sturmian functions are expressed in terms of Gauss hypergeometric functions, and that some related matrix elements involve two variable hypergeometric functions. In **Chapter 4**, the starting point of our investigation on Quasi-Sturmian functions is the solution of a non-homogeneous differential equation that happens to be a two variable hypergeometric function, noted $\Theta^{(1)}$. The latter is a Kampé de Fériet function that appears also when performing the derivative of the confluent hypergeometric function ${}_1F_1$ with respect to its parameters [70].

Furthermore, we have mentioned in **Section 1.1.1** that in some cases it may be important to know the behavior of a function with respect to its parameters rather than the variables. In the case of one variable hypergeometric functions ${}_pF_q$, a detailed mathematical study of their derivatives with respect to their parameters was presented in references [31, 70, 71]. Such derivatives were expressed in terms of two variable hypergeometric functions which happened to be closely related to the solution of Coulomb scattering problems [14, 72–75]. Although we do not go deeper in this subject here, several generating functions for angular Quasi-Sturmian functions can be derived from Appell functions. This fact adds interest to explore their derivatives with respect to the parameters. In this chapter, we extend and generalize the methodology presented in references [31, 70, 71]; we provide formulas to calculate the derivatives of two variables hypergeometric functions with respect to their parameters.

Starting with the four Appell hypergeometric functions F_1, F_2, F_3 and F_4 [30, 46, 76], we describe the procedure and give the expressions for their first derivative with respect to each of the parameters involved. This procedure makes use of series expansions in terms of Gauss hypergeometric functions, and then exploits the expressions presented in reference [31]. This will provide us, in most cases, with a systematic way of writing the nth derivatives with respect to the parameters in terms of generalized Kampé de Fériet functions, noted ${}_2\Theta_1^{(n)}$, whose definition and properties were presented in reference [31]. An extension to some other two variables hypergeometric series is also briefly outlined. The results presented in this chapter are part of a manuscript submitted for publication [32].

We assume hereafter that all variables and parameters are complex numbers. Also, unless otherwise indicated, in all summations the index runs from 0 to ∞.

Let us first recall some results of reference [31] which we shall need below. Consider the series representation (1.14) of the Gauss hypergeometric function ${}_2F_1(a, b, c; z)$; it is assumed that $|z| < 1$, and that c is neither zero nor a negative integer. The derivatives with respect to the parameters a or c of the function ${}_2F_1\,(a, b, c; z)$ can be written as

$$\frac{d}{da}\,{}_2F_1(a,b,c;z) = \frac{z}{a}\,\frac{a\,b}{c}\,{}_2\Theta_1^{(1)}\left(\begin{array}{c} 1,1|a,a+1,b+1 \\ a+1|2,c+1 \end{array}\middle|\,;z,z\right), \tag{2.1a}$$

$$\frac{d}{dc}\,{}_2F_1(a,b,c;z) = -\frac{z}{c}\,\frac{a\,b}{c}\,{}_2\Theta_1^{(1)}\left(\begin{array}{c} 1,1|c,a+1,b+1 \\ c+1|2,c+1 \end{array}\middle|\,;z,z\right), \tag{2.1b}$$

where ${}_2\Theta_1^{(1)}$ stands for a two-variables Kampé de Fériet function [30] defined as

$${}_2\Theta_1^{(1)}\left(\begin{array}{c} a_1,a_2|b_1,b_2,b_3 \\ c_1|d_1,d_2 \end{array}\middle|\,;z_1,z_2\right) = \sum_{m,n} \frac{(a_1)_m (a_2)_n (b_1)_m}{(c_1)_m}\,\frac{(b_2)_{m+n}(b_3)_{m+n}}{(d_1)_{m+n}(d_2)_{m+n}}\,\frac{z_1^m}{m!}\,\frac{z_2^n}{n!}. \tag{2.2}$$

Since ${}_2F_1(a, b, c; z) = {}_2F_1(b, a, c; z)$, the derivative with respect to b may be obtained by interchanging a and b in (2.1a).

2.1 Derivative of Appell hypergeometric functions with respect to their parameters

The Appell hypergeometric functions are two-variable (say, z_1 and z_2) functions extensively studied from their mathematical point of view. Amongst their known properties one finds compact expressions for the derivatives with respect to z_1 and/or z_2.

In some cases one may be interested, instead of the variables, in one parameter of the function, say α. Then one should consider the study of Appell functions as one variable functions of this parameter α. The derivatives with respect to such parameter become an important tool since they allow, for example, to write a Taylor expansion around a given value α_0.

2.1.1 Function F_2

For presentation convenience we shall start with the Appell F_2 function which is defined by the two-variable series

$$F_2(a, b_1, b_2, c_1, c_2; z_1, z_2) = \sum_{m,n} \frac{(a)_{m+n}(b_1)_m(b_2)_n}{(c_1)_m(c_2)_n} \frac{z_1^m}{m!} \frac{z_2^n}{n!}, \quad |z_1| + |z_2| < 1, \tag{2.3}$$

where we assume that c_1 and c_2 are neither zero nor negative integers. One may also express the F_2 function as a series about $z_1 = 0$, for fixed z_2

$$F_2(a, b_1, b_2, c_1, c_2; z_1, z_2) = \sum_{k} \frac{(a)_k(b_1)_k}{(c_1)_k} \, {}_2F_1(a + k, b_2, c_2; z_2) \frac{z_1^k}{k!}. \tag{2.4}$$

Using the derivatives of the Gauss hypergeometric function with respect to its second (respectively third) parameter (i.e., relations (2.1a), respectively (2.1b)), we find

$$\begin{aligned}
&\frac{d}{db_2} F_2(a, b_1, b_2, c_1, c_2; z_1, z_2) \\
&= z_2 \frac{a}{c_2} \sum_{k} \frac{(a+1)_k(b_1)_k}{(c_1)_k} \, {}_2\Theta_1^{(1)} \left(\begin{matrix} 1, 1|b_2, b_2 + 1, a + k + 1 \\ b_2 + 1|2, c_2 + 1 \end{matrix} \middle| ; z_2, z_2 \right) \frac{z_1^k}{k!} \\
&= z_2 \frac{a}{c_2} \sum_{k,m,n} (a+1)_{k+m+n} \frac{(b_2+1)_{m+n}}{(2)_{m+n}(c_2+1)_{m+n}} \frac{(b_1)_k}{(c_1)_k} \frac{(1)_m(b_2)_m}{(b_2+1)_m} (1)_n \frac{z_1^k}{k!} \frac{z_2^m}{m!} \frac{z_2^n}{n!},
\end{aligned} \tag{2.5a}$$

$$\begin{aligned}
&\frac{d}{dc_2}F_2(a,b_1,b_2,c_1,c_2;z_1,z_2)\\
&=-\,z_2\,\frac{a\,b_2}{c_2^2}\sum_k \frac{(a+1)_k(b_1)_k}{(c_1)_k}\;{}_2\Theta_1^{(1)}\left(\begin{array}{c}1,1|c_2,a+k+1,b_2+1\\ c_2+1|2,c_2+1\end{array}\middle|\;;z_2,z_2\right)\frac{z_1^k}{k!}\\
&=-\,z_2\,\frac{a\,b_2}{c_2^2}\sum_{k,m,n}(a+1)_{k+m+n}\frac{(b_2+1)_{m+n}}{(2)_{m+n}(c_2+1)_{m+n}}\frac{(b_1)_k}{(c_1)_k}\frac{(1)_m(c_2)_m}{(c_2+1)_m}(1)_n\frac{z_1^k}{k!}\frac{z_2^m}{m!}\frac{z_2^n}{n!}.
\end{aligned} \tag{2.5b}$$

In each case, the second equality is obtained by using the identity

$$\frac{1}{(a+k)}=\frac{1}{a}\,\frac{(a)_k}{(a+1)_k}. \tag{2.6}$$

Thus the derivative of the Appell function is expressed either as an infinite series of functions ${}_2\Theta_1^{(1)}$ or, equivalently, as a triple infinite summation.

Making use of the symmetry relation

$$F_2(a,b_1,b_2,c_1,c_2;z_1,z_2)=F_2(a,b_2,b_1,c_2,c_1;z_2,z_1)$$

we have similar expressions for the derivatives with respect to b_1 and c_1 where in the above one interchanges (z_1,b_1,c_1) with (z_2,b_2,c_2).

Next, we consider the derivative with respect to the parameter a which appears in the numerator of the series (2.3) with combined index $m+n$ or, alternatively, in a more cumbersome manner in expansion (2.4). For this case we use a different approach, based on the derivative of the Pochhammer symbol [47, 48]

$$\frac{d}{da}(a)_{n+m}=(a)_{n+m}[\psi(a+n+m)-\psi(a)]=(a)_{n+m}\sum_{k=0}^{m+n-1}\frac{1}{a+k},$$

the second equality coming from the recurrence relation of the digamma function

$$\psi\left(z+n\right)=\frac{1}{z+n-1}+\frac{1}{z+n-2}+\ldots+\frac{1}{z+1}+\psi(z+1)$$

[equation (6.3.6) of [42]]. Note that for $n=m=0$ this derivative is obviously zero. It is convenient to split the sum in two parts,

$$\frac{d}{da}(a)_{n+m}=(a)_{n+m}\left[\sum_{k=0}^{m-1}\frac{1}{a+k}+\sum_{k=0}^{n-1}\frac{1}{a+m+k}\right].$$

The derivative of F_2 with respect to a can therefore be written as

$$\begin{aligned}
&\frac{d}{da}F_2(a,b_1,b_2,c_1,c_2;z_1,z_2)\\
&=\sum_{m,n}(a)_{n+m}\frac{(b_1)_m(b_2)_n}{(c_1)_m(c_2)_n}\frac{z_1^m}{m!}\frac{z_2^n}{n!}\left[\sum_{k=0}^{m-1}\frac{1}{a+k}+\sum_{k=0}^{n-1}\frac{1}{a+m+k}\right]\\
&=\sum_n\frac{(b_2)_n}{(c_2)_n}\frac{z_2^n}{n!}\sum_m\frac{(b_1)_{m+1}}{(c_1)_{m+1}}\frac{z_1^{m+1}}{(m+1)!}(a)_{n+m+1}\sum_{k=0}^{m}\frac{1}{a}\frac{(a)_k}{(a+1)_k}\\
&\quad+\sum_m\frac{(b_1)_m}{(c_1)_m}\frac{z_1^m}{m!}\sum_n\frac{(b_2)_{n+1}}{(c_2)_{n+1}}\frac{z_2^{n+1}}{(n+1)!}(a)_{n+m+1}\sum_{k=0}^{n}\frac{1}{a}\frac{(a)_{m+k}}{(a+1)_{m+k}},
\end{aligned}$$

where for the second equality we shifted the index m (respectively n), and we made use of relation (2.6). Using then the rearrangement series technique [77]

$$\sum_{p=0}^{\infty}\sum_{k=0}^{p}\mathcal{B}(k,p)=\sum_{p=0}^{\infty}\sum_{k=0}^{\infty}\mathcal{B}(k,p+k), \tag{2.7}$$

we obtain two separate triple infinite summations

$$\begin{aligned}
&\frac{d}{da}F_2(a,b_1,b_2,c_1,c_2;z_1,z_2)\\
&=z_1\frac{b_1}{c_1}\sum_{k,m,n}(a+1)_{n+m+k}\frac{(b_1+1)_{m+k}}{(c_1+1)_{m+k}(2)_{m+k}}\frac{(1)_k\,(a)_k}{(a+1)_k}(1)_m\frac{(b_2)_n}{(c_2)_n}\frac{z_1^k}{k!}\frac{z_1^m}{m!}\frac{z_2^n}{n!}\\
&\quad+z_2\frac{b_2}{c_2}\sum_{k,m,n}(a+1)_{n+m+k}\frac{(b_2+1)_{n+k}}{(c_2+1)_{n+k}(2)_{n+k}}\frac{(a)_{m+k}}{(a+1)_{m+k}}(1)_k\frac{(b_1)_m}{(c_1)_m}(1)_n\frac{z_2^k}{k!}\frac{z_2^n}{n!}\frac{z_1^m}{m!},
\end{aligned}$$

and each of this triple summations can also be expressed as single series of ${}_2\Theta_1^{(1)}$ functions.

2.1.2 Function F_1

We now turn to the F_1 function which is defined as

$$F_1(a,b_1,b_2,c;z_1,z_2)=\sum_{m,n}\frac{(a)_{m+n}(b_1)_m(b_2)_n}{(c)_{m+n}}\frac{z_1^m}{m!}\frac{z_2^n}{n!},\quad |z_1|<1,|z_2|<1, \tag{2.8}$$

and we assume that c is neither zero nor a negative integer. As a series around the $z_1=0$ point, for fixed z_2, one has

$$F_1(a,b_1,b_2,c;z_1,z_2)=\sum_k\frac{(a)_k(b_1)_k}{(c)_k}\,{}_2F_1(a+k,b_2,c+k;z_2)\,\frac{z_1^k}{k!}. \tag{2.9}$$

Using expression (2.1a) we get

$$\begin{aligned}
\frac{d}{db_2} F_1(a,b_1,b_2,&c;z_1,z_2)\\
&= z_2\,\frac{a}{c}\sum_k \frac{(a+1)_k (b_1)_k}{(c+1)_k}\; {}_2\Theta_1^{(1)}\left(\begin{array}{c} 1,1|b_2,b_2+1,a+k+1 \\ b_2+1|2,c+k+1 \end{array}\middle|\, ;z_2,z_2\right)\frac{z_1^k}{k!}\\
&= z_2\,\frac{a}{c}\sum_{k,m,n}\frac{(a+1)_{k+m+n}}{(c+1)_{k+m+n}}\,\frac{(b_2+1)_{m+n}}{(2)_{m+n}}\,(b_1)_k\,\frac{(1)_m (b_2)_m}{(b_2+1)_m}\,(1)_n\,\frac{z_1^k}{k!}\,\frac{z_2^m}{m!}\,\frac{z_2^n}{n!}, \qquad (2.10)
\end{aligned}$$

and similarly for the derivative with respect to b_1 by interchanging (z_1, b_1) with (z_2, b_2), since

$$F_1(a,b_1,b_2,c;z_1,z_2) = F_1(a,b_2,b_1,c;z_2,z_1).$$

For the derivative with respect to the first parameter a and c, we first use the identity

$$F_2(a,b_1,b_2,c,a;z_1,z_2) = (1-z_2)^{-b_2}\, F_1\left(b_1, a-b_2, b_2, c; z_1, \frac{z_1}{1-z_2}\right)$$

from which

$$F_1(a,b_1,b_2,c;z_1,z_2) = \left(\frac{z_1}{z_2}\right)^{b_2} F_2\left(b_1+b_2, a, b_2, c, b_1+b_2; z_1, 1-\frac{z_1}{z_2}\right). \qquad (2.11)$$

Then, applying the expressions (2.5) found previously for F_2, one easily finds

$$\begin{aligned}
\frac{d}{da} F_1(a,b_1,b_2,&c;z_1,z_2)\\
&= \left(\frac{z_1}{z_2}\right)^{b_2} \frac{d}{da} F_2\left(b_1+b_2, a, b_2, c, b_1+b_2; z_1, 1-\frac{z_1}{z_2}\right)\\
&= \left(\frac{z_1}{z_2}\right)^{b_2} z_1\,\frac{b_1+b_2}{c}\sum_k \frac{(b_1+b_2+1)_k (b_2)_k}{(b_1+b_2)_k}\,\frac{1}{k!}\left(1-\frac{z_1}{z_2}\right)^k\\
&\quad\times\; {}_2\Theta_1^{(1)}\left(\begin{array}{c} 1,1|a,a+1,b_1+b_2+1+k \\ a+1|2,c+1 \end{array}\middle|\, ;z_1,z_1\right) \qquad (2.12a)\\
&= \left(\frac{z_1}{z_2}\right)^{b_2} z_1\,\frac{b_1+b_2}{c}\sum_{k,m,n}(b_1+b_2+1)_{k+m+n}\,\frac{(a+1)_{m+n}}{(2)_{m+n}(c+1)_{m+n}}\,\frac{(b_2)_k}{(b_1+b_2)_k}\\
&\quad\times\;\frac{(1)_m (a)_m}{(a+1)_m}\,(1)_n\,\frac{1}{k!}\left(1-\frac{z_1}{z_2}\right)^k\frac{z_1^m}{m!}\,\frac{z_1^n}{n!}, \qquad (2.12b)
\end{aligned}$$

$$
\begin{aligned}
&\frac{d}{dc}F_1(a,b_1,b_2,c;z_1,z_2)\\
&\quad=\left(\frac{z_1}{z_2}\right)^{b_2}\frac{d}{dc}F_2\left(b_1+b_2,a,b_2,c,b_1+b_2,z_1,1-\frac{z_1}{z_2}\right)\\
&\quad=-\left(\frac{z_1}{z_2}\right)^{b_2}z_1\,\frac{(b_1+b_2)\,a}{c^2}\sum_k\frac{(b_1+b_2+1)_k(b_2)_k}{(b_1+b_2)_k}\,\frac{1}{k!}\left(1-\frac{z_1}{z_2}\right)^k\\
&\qquad\times\ {}_2\Theta_1^{(1)}\left(\begin{array}{c}1,1|c,b_1+b_2+1+k,a+1\\ c+1|2,c+1\end{array}\middle|;z_1,z_1\right)\\
&\quad=-\left(\frac{z_1}{z_2}\right)^{b_2}z_1\,\frac{(b_1+b_2)\,a}{c^2}\sum_{k,m,n}(b_1+b_2+1)_{k+m+n}\,\frac{(a+1)_{m+n}}{(2)_{m+n}(c+1)_{m+n}}\,\frac{(b_2)_k}{(b_1+b_2)_k}\\
&\qquad\times\ \frac{(1)_m(c)_m}{(c+1)_m}\,(1)_n\,\frac{1}{k!}\left(1-\frac{z_1}{z_2}\right)^k\frac{z_1^m}{m!}\,\frac{z_1^n}{n!}.
\end{aligned}
$$

2.1.3 Function F_3

Next, we consider the F_3 function which is defined as

$$
F_3(a_1,a_2,b_1,b_2,c;z_1,z_2)=\sum_{m,n}\frac{(a_1)_m(a_2)_n(b_1)_m(b_2)_n}{(c)_{m+n}}\,\frac{z_1^m}{m!}\,\frac{z_2^n}{n!},\quad |z_1|<1,|z_2|<1,\quad (2.13)
$$

and assume that c is neither zero nor a negative integer. Using the series around the $z_1=0$ point, for fixed z_2,

$$
F_3(a_1,a_2,b_1,b_2,c;z_1,z_2)=\sum_k\frac{(a_1)_k(b_1)_k}{(c)_k}\,{}_2F_1(a_2,b_2,c+k;z_2)\,\frac{z_1^k}{k!},
$$

and following the same procedure (i.e., using result (2.1a)) we obtain

$$
\begin{aligned}
&\frac{d}{da_2}F_3(a_1,a_2,b_1,b_2,c;z_1,z_2)\\
&\quad=z_2\,\frac{b_2}{c}\sum_k\frac{(a_1)_k(b_1)_k}{(c+1)_k}\,\frac{z_1^k}{k!}\,{}_2\Theta_1^{(1)}\left(\begin{array}{c}1,1|a_2,a_2+1,b_2+1\\ a_2+1|2,c+k+1\end{array}\middle|;z_2,z_2\right)\\
&\quad=z_2\,\frac{b_2}{c}\sum_{k,m,n}\frac{1}{(c+1)_{k+m+n}}\,\frac{(a_2+1)_{m+n}(b_2+1)_{m+n}}{(2)_{m+n}}\,(a_1)_k(b_1)_k\frac{(1)_m(a_2)_m}{(a_2+1)_m}\,(1)_n\,\frac{z_1^k}{k!}\,\frac{z_2^m}{m!}\,\frac{z_2^n}{n!}.
\end{aligned}
$$

Since a_2 and b_2 play a similar role in the definition of F_3, the derivative with respect to b_2 is the same as the above by simply interchanging a_2 with b_2. Moreover, since

$$
F_3(a_1,a_2,b_1,b_2,c;z_1,z_2)=F_3(a_2,a_1,b_2,b_1,c;z_2,z_1)
$$

the derivative with respect to a_1 (and similarly to b_1) are the above by interchanging (z_1, a_1, b_1) with (z_2, a_2, b_2).

For the derivative with respect to c, the calculation is longer, as c appears with an index $m+n$ in (2.13). In this case we must use

$$\frac{d}{dc}\frac{1}{(c)_{n+m}} = -\frac{1}{(c)_{n+m}}\left[\sum_{k=0}^{m-1}\frac{1}{c+k} + \sum_{k=0}^{n-1}\frac{1}{c+m+k}\right],$$

and proceed as with the derivative with respect to a of function F_2.

2.1.4 Function F_4

Finally, the Appell function F_4 is defined as

$$F_4(a,b,c_1,c_2;z_1,z_2) \;=\; \sum_{m,n}\frac{(a)_{m+n}(b)_{m+n}}{(c_1)_m(c_2)_n}\,\frac{z_1^m}{m!}\,\frac{z_2^n}{n!}, \qquad |\sqrt{z_1}|+|\sqrt{z_2}|<1, \tag{2.14}$$

where we assume that c_1 and c_2 are neither zero nor a negative integer. Alternatively, as a series around the $z_1 = 0$ point, for fixed z_2, one has

$$F_4(a,b,c_1,c_2;z_1,z_2) = \sum_k \frac{(a)_k(b)_k}{(c_1)_k}\,{}_2F_1(a+k,b+k,c_2;z_2)\,\frac{z_1^k}{k!}.$$

Applying result (2.1b) one easily finds

$$\begin{aligned}
&\frac{d}{dc_2}F_4(a,b,c_1,c_2;z_1,z_2)\\
&\quad= -\,z_2\,\frac{a\,b}{c_2^2}\sum_k\frac{(a+1)_k(b+1)_k}{(c_1)_k}\,\frac{z_1^k}{k!}\;{}_2\Theta_1^{(1)}\left(\begin{array}{c}1,1|c_2,a+k+1,b+k+1\\ c_2+1|2,c_2+1\end{array}\middle|\,;z_2,z_2\right)\\
&\quad= -\,z_2\,\frac{a\,b}{c_2^2}\sum_{k,m,n}(a+1)_{k+m+n}(b+1)_{k+m+n}\frac{1}{(2)_{m+n}(c_2+1)_{m+n}}\frac{1}{(c_1)_k}\\
&\qquad\times\frac{(1)_m(c_2)_m}{(c_2+1)_m}\,(1)_n\,\frac{z_1^k}{k!}\,\frac{z_2^m}{m!}\,\frac{z_2^n}{n!},
\end{aligned}$$

and a similar expression for the derivative with respect to c_1, by interchanging (z_1, c_1) with (z_2, c_2), since

$$F_4(a,b,c_1,c_2;z_1,z_2) = F_4(a,b,c_2,c_1;z_2,z_1).$$

For the derivative with respect to a (and similarly with respect to b, by permutation), the calculation is longer, as a appears with an index $m+n$ in (2.14). We can proceed as with the derivative with respect to a of function F_2, and we end up with two triple infinite summations.

2.2 nth derivative and properties

Similarly to the case of the first derivatives of the Gaussian hypergeometric function ${}_2F_1$ for which one introduces a two-variable ${}_2\Theta_1^{(1)}$ function, for the nth derivative it is convenient to introduce a hypergeometric function in $n+1$ variables [31]

$$\begin{aligned}
&{}_2\Theta_1^{(n)}\left(\begin{array}{c} a_1, a_2, \ldots, a_{n+1} | \, b_1, b_2, \ldots, b_{n+2} \\ c_1, \ldots, c_n | \, d_1, d_2 \end{array} \middle| ; z_1, \ldots, z_{n+1}\right) \\
&= \sum_{m_1} \cdots \sum_{m_{n+1}} (a_1)_{m_1} (a_2)_{m_2} \ldots (a_{n+1})_{m_{n+1}} \frac{(b_1)_{m_1} (b_2)_{m_1+m_2} \ldots (b_{n+1})_{m_1+m_2+\ldots+m_{n+1}}}{(c_1)_{m_1} (c_2)_{m_1+m_2} \ldots (c_n)_{m_1+m_2+\ldots+m_n}} \\
&\times \frac{(b_{n+2})_{m_1+m_2+\ldots+m_{n+1}}}{(d_1)_{m_1+m_2+\ldots+m_{n+1}} (d_2)_{m_1+m_2+\ldots+m_{n+1}}} \frac{z_1^{m_1} z_2^{m_2} \ldots z_{n+1}^{m_{n+1}}}{m_1! m_2! \ldots m_{n+1}!}. \qquad (2.15)
\end{aligned}$$

In terms of these new functions (which are also Kampé de Fériet functions [31]), the nth derivatives of the Gaussian hypergeometric function with respect to the parameters read

$$\begin{aligned}
&\frac{d^n}{da^n} \, {}_2F_1(a, b, c; z) \\
&\quad = \frac{(b)_n}{(c)_n} z^n \, {}_2\Theta_1^{(n)}\left(\begin{array}{c} 1, 1, \ldots, 1 | \, a, a+1, \ldots, a+n, b+n \\ a+1, \ldots, a+n | \, n+1, c+n \end{array} \middle| ; z, \ldots, z\right), \qquad (2.16a)
\end{aligned}$$

$$\begin{aligned}
&\frac{d^n}{dc^n} \, {}_2F_1(a, b, c; z) \\
&\quad = (-1)^n \frac{n!}{c^n} \frac{ab}{c} z \, {}_2\Theta_1^{(n)}\left(\begin{array}{c} 1, 1, \ldots, 1 | \, c, c, \ldots, c, a+1, b+1 \\ c+1, \ldots, c+1 | \, 2, c+1 \end{array} \middle| ; z, \ldots, z\right). \qquad (2.16b)
\end{aligned}$$

Thus, applying the same procedure as described in the previous section, the nth derivative of the Appell functions with respect to their parameters are given by $n+2$ infinite summations. In most cases, they can be obtained straightforwardly, and expressed as a single sum of these ${}_2\Theta_1^{(n)}$ functions. However, for the derivatives of F_2 (respectively F_3 or F_4) with respect to a (respectively, c or a), the generalization of the results to nth order is not as compact.

For example, from (2.9) one immediately finds

$$\begin{aligned}
&\frac{d^n}{db_2^n} F_1(a, b_1, b_2, c; z_1, z_2) \\
&\qquad = z_2^n \sum_k \frac{(a)_{n+k} (b_1)_k}{(c)_{n+k}} \frac{z_1^k}{k!} \\
&\qquad \times {}_2\Theta_1^{(n)} \left(\begin{array}{c} 1, 1, \ldots, 1 |\, b_2, b_2+1, \ldots, b_2+n, a+n+k \\ b_2+1, \ldots, b_2+n |\, n+1, c+n+k \end{array} \middle| ; z_2, \ldots, z_2 \right).
\end{aligned}$$

To obtain the nth derivative of F_1 with respect to a or c it is convenient to use relation (2.11). Thus, for example for the parameter a we have

$$\begin{aligned}
&\frac{d^n}{da^n} F_1(a, b_1, b_2, c; z_1, z_2) \\
&\qquad = \left(\frac{z_1}{z_2} \right)^{b_2} \frac{d^n}{da^n} F_2 \left(b_1 + b_2, a, b_2, c, b_1 + b_2; z_1, 1 - \frac{z_1}{z_2} \right) \\
&\qquad = \left(\frac{z_1}{z_2} \right)^{b_2} \frac{1}{(c)_n} z_1^n \sum_k \frac{(b_1+b_2)_{n+k} \, (b_2)_k}{(b_1+b_2)_k \, k!} \left(1 - \frac{z_1}{z_2} \right)^k \\
&\qquad \times {}_2\Theta_1^{(n)} \left(\begin{array}{c} 1, 1, \ldots, 1 |\, a, a+1, \ldots, a+n, b_1+b_2+n+k \\ a+1, \ldots, a+n |\, n+1, c+n \end{array} \middle| ; z_1, \ldots, z_1 \right).
\end{aligned}$$

The ${}_2\Theta_1^{(n)}$ functions follow some recurrence relations and possess alternative series representations [31], which may be useful in certain cases. For $n = 1$, for example,

$$\begin{aligned}
&{}_2\Theta_1^{(1)} \left(\begin{array}{c} a_1, a_2 |\, b_1, b_2, b_3 \\ c_1 |\, d_1, d_2 \end{array} \middle| ; z_1, z_2 \right) \\
&= \sum_{m_1} \frac{(a_1)_{m_1} (b_1)_{m_1} (b_2)_{m_1} (b_3)_{m_1}}{(c_1)_{m_1} (d_1)_{m_1} (d_2)_{m_1}} \frac{z_1^{m_1}}{m_1!} \, {}_3F_2 \left(a_2, b_2 + m_1, b_3 + m_1; d_1 + m_1, d_2 + m_1; z_2 \right) \\
&= \sum_{m_2} \frac{(a_2)_{m_2} (b_2)_{m_2} (b_3)_{m_2}}{(d_1)_{m_2} (d_2)_{m_2}} \frac{z_2^{m_2}}{m_2!} \, {}_4F_3 \left(a_1, b_1, b_2 + m_2, b_3 + m_2; c_1, d_1 + m_2, d_2 + m_2; z_1 \right).
\end{aligned}$$

Thus the derivatives of the Appell functions with respect to the parameters can be written in alternative forms which may result to be more practical. For example, for the F_1

function we have

$$
\begin{aligned}
&\frac{d}{db_1}\, F_1(a,b_1,b_2,c;z_1,z_2)\\
&\qquad = z_1\,\frac{a}{c}\sum_{k,m}\frac{(a+1)_{k+m}}{(c+1)_{k+m}}\,(b_2)_k\frac{(1)_m(b_1)_m}{(2)_m}\,\frac{z_2^k}{k!}\,\frac{z_1^m}{m!}\\
&\qquad\quad \times\ {}_3F_2(1,b_1+1+m,a+1+k+m,2+m,c+1+k+m;z_1)\\
&\qquad = z_1\,\frac{a}{c}\sum_{k,m}\frac{(a+1)_{k+m}}{(c+1)_{k+m}}\,(b_2)_k\frac{(1)_m(b_1+1)_m}{(2)_m}\,\frac{z_2^k}{k!}\,\frac{z_1^m}{m!}\\
&\qquad\quad \times\ {}_4F_3(1,b_1,b_1+1+m,a+1+k+m,b_1+1,2+m,c+1+k+m;z_1).
\end{aligned}
$$

It is also possible to express such derivative in terms of Gauss hypergeometric functions

$$
\begin{aligned}
&\frac{d}{db_1}\, F_1(a,b_1,b_2,c;z_1,z_2)\\
&\qquad = z_1\,\frac{a}{c}\sum_{m,n}\frac{(a+1)_{m+n}(b_1+1)_{m+n}}{(c+1)_{m+n}(2)_{m+n}}\,\frac{(b_1)_m}{(b_1+1)_m}\,z_1^{m+n}\\
&\qquad\quad \times\ {}_2F_1(a+1+m+n,b_2,c+1+m+n;z_2). \qquad (2.17)
\end{aligned}
$$

As a consequence, if one should be interested in mixed derivatives such as $\dfrac{d^2F_1}{db_1\,db_2}$, relation (2.17) could be used together with relation (2.1a). One obtains straightforwardly a double infinite summation of ${}_2\Theta_1^{(1)}$ functions or, alternatively, a quadruple infinite summation.

Remark 2.2.1. In some subcases one may easily recover previously published results. As an example, consider the derivative with respect to a of the F_1 function in the case $z_1 = z_2$; by inspection of result (2.12a), only the $k = 0$ term survives in the summation and the derivative is given as a single ${}_2\Theta_1^{(1)}$ function. At the same time, the Appell function F_1 is known to reduce to a Gauss hypergeometric function,

$$F_1(a,b_1,b_2,c;z_1,z_1) = {}_2F_1(a,b_1+b_2,c;z_1),$$

so that the derivative

$$\frac{d}{da}F_1(a,b_1,b_2,c;z_1,z_1) = \frac{d}{da}\,{}_2F_1(a,b_1+b_2,c;z_1)$$

is also directly provided by (2.1a) as presented in reference [31]. The results obviously coincide.

■

2.3 Extension to other two-variables hypergeometric series

Following the procedure presented in the previous sections the derivatives with respect to the parameters of other two variables Horn hypergeometric series [46, 52] can be studied. The idea is to first express them as a single sum of ${}_2F_1$ (possibly ${}_1F_1$, or even ${}_pF_q$) functions, and then apply the expressions for the derivative of these one variable hypergeometric functions in terms of Kampé de Fériet functions.

Amongst Horn functions, we are particularly interested in the two variable confluent hypergeometric series Φ_1 [52] since it appears in one of the representations of the Slater Quasi-Sturmian functions studied in **Chapter 4** [see equation (4.15)]. The function Φ_1 has the following alternative representations

$$\Phi_1(a,b,c;z_1,z_2) = \sum_{m,n} \frac{(a)_{m+n}(b)_m}{(c)_{m+n}} \frac{z_1^m}{m!} \frac{z_2^n}{n!}, \qquad |z_1| < 1 \tag{2.18a}$$

$$= \sum_{n} \frac{(a)_n}{(c)_n} \frac{z_2^n}{n!} {}_2F_1(a+n,b,c+n;z_1) \tag{2.18b}$$

$$= \sum_{m} \frac{(a)_m(b)_m}{(c)_m} \frac{z_1^m}{m!} {}_1F_1(a+m,c+m;z_2). \tag{2.18c}$$

From the series (2.18b) one can obtain the nth derivative with respect to the b parameter applying directly formula (2.16a). The derivative with respect to a presents the same difficulty found when calculating the derivative with respect to the first parameter of the Appell F_2 function, while the situation with the parameter c is equivalent to the one found with the fifth parameter of the Appell F_3 function. Thus they can be calculated proceeding as described in those two cases.

For the confluent hypergeometric series Ψ_1 one has the equivalent expressions

$$\Psi_1(a,b,c_1,c_2;z_1,z_2) = \sum_{m,n} \frac{(a)_{m+n}(b)_m}{(c_1)_m(c_2)_n} \frac{z_1^m}{m!} \frac{z_2^n}{n!}, \qquad |z_1| < 1 \tag{2.19a}$$

$$= \sum_{m} \frac{(a)_m(b)_m}{(c_1)_m} \frac{z_1^m}{m!} {}_1F_1(a+m,c_2;z_2) \tag{2.19b}$$

$$= \sum_{n} \frac{(a)_n}{(c_2)_n} \frac{z_2^n}{n!} {}_2F_1(a+n,b,c_1;z_1). \tag{2.19c}$$

If one is interested in its derivative with respect to the parameter c_2 one can use the series representation (2.19b) in terms of the confluent hypergeometric function ${}_1F_1$ whose nth derivative was presented in reference [31]. But if one needs the derivative with respect to b or c_1 it is more convenient to calculate them from the series (2.19c) applying (2.16a) or (2.16b). Once again, the derivative with respect to a can be calculated as done in the case of the derivative with respect to the first parameter of the F_2 function.

More details on the nth derivative of these, and other, two variable hypergeometric series can be found in [32].

2.4 Chapter summary

We have studied the derivatives to any order n, with respect to their parameters, of the four Appell hypergeometric functions. They can be written as $n + 2$ infinite summations. To perform these derivatives we have expressed the Appell functions in terms of single series of one variable Gauss hypergeometric functions. Then, we took advantage of the compact expressions, obtained previously with a differential equation approach [31], for their nth derivatives with respect to parameters. Hence, for most parameters, the nth derivatives can be easily written as single sums of a generalized multivariable Kampé de Fériet function, noted ${}_2\Theta_1^{(n)}$.

For the parameters that could not be treated following this strategy, we have performed the first derivative of the function by derivating the corresponding Pochhammer symbol and making some algebraic manipulations. These cases can not be easily generalized to the nth order.

The methodology presented, which makes part of a more extensive study [32], can be extended – in the same systematic way – to the study of the derivative with respect to their parameters of other two variable, or three variable, hypergeometric functions. The starting point is to express such series as a sum of ${}_2F_1$ (possibly ${}_1F_1$, or even ${}_pF_q$) functions, and then apply the expressions presented in [31, 70, 71] for the derivatives of these one-variable hypergeometric functions with respect to their parameters. We have illustrated this idea in the last section of this chapter, for the case of Horn hypergeometric series Φ_1 and Ψ_1.

Chapter 3

Generalized Sturmian functions

In this chapter we briefly introduce Generalized Sturmian functions and their main properties. We analyse the particular case of Hulthén Sturmian functions because they can be given in closed form, so that integrals related to scattering problems can be analytically solved. The results presented in this chapter, together with the implementation displayed in **Section 5.2**, are part of a published work [33].

3.1 General considerations

Generalized Sturmian functions [26, 27] form a set of basis functions (index n) used to expand the solution of different bound and scattering problems. For the two-body case, they are defined as the solution of the Schrödinger-like differential equation

$$[\mathbf{T_r} + \mathcal{V}_a(r) - E]S_{n,\ell}(r) = -\lambda_{n,\ell}\,\mathcal{V}_g(r)\,S_{n,\ell}(r), \tag{3.1}$$

where $\mathbf{T_r} = -\frac{1}{2\mu}\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{2\mu r^2}$, and the parameters μ, ℓ appearing in this kinetic operator can be conveniently chosen to coincide with the reduced mass and the angular momentum, and E is the energy of the problem under consideration. The functions $\mathcal{V}_a$ and $\mathcal{V}_g$ are called auxiliary and generating potential respectively. Usually $\mathcal{V}_g$ is a short-range potential which means that there exist $R \in \mathbb{R}$ such that

$$\mathcal{V}_g(r) \sim 0, \quad \forall\ r > R.$$

Together with two appropriate boundary conditions, equation (3.1) becomes a Sturm-Liouville problem [2, 28, 49, 50], with eigenvalues $\lambda_{n,\ell}$. The eigenfunctions $S_{n,\ell}$

form then a complete basis set with the closure relation

$$\sum_n S_{n,\ell}(r_1)\,\mathcal{V}_g(r_1)\,S_{n,\ell}(r_2) = V_n\,\delta(r_1 - r_2), \tag{3.2}$$

and they satisfy an orthogonality relation

$$\int_0^\infty S_{m,\ell}(r)\,\mathcal{V}_g(r)\,S_{n,\ell}(r)\,dr = V_n\,\delta_{m,n}, \tag{3.3a}$$

where

$$V_n = \int_0^\infty S_{n,\ell}(r)\,\mathcal{V}_g(r)\,S_{n,\ell}(r)\,dr. \tag{3.3b}$$

As usual for the Schrödinger equation, the boundary conditions for Sturmian functions are imposed at the origin and in the asymptotic region ($r > R$) where the generating potential vanishes. The first one is

$$S_{n,\ell}(0) = 0. \tag{3.4}$$

In the region $r > R$ the equation for Generalized Sturmian functions becomes

$$[\mathbf{T_r} + \mathcal{V}_a(r) - E]S_{n,\ell}(r) = 0, \tag{3.5}$$

and is independent of the index n; thus all functions $S_{n,\ell}$ describe, in the asymptotic region, the behavior of a particle of energy E moving under the influence of a potential $\mathcal{V}_a$ [see **Figure 3.2**] . For an auxiliary potential also vanishing in the asymptotic region, i.e. $\mathcal{V}_a(r) = 0$ in equation (3.5), the solutions $S_{n,\ell}$ represent then a free particle in this region and have the following asymptotic form,

$$\begin{aligned} S_{n,\ell}(r) &\overset{r\to\infty}{\propto} e^{-\kappa r}, \quad \kappa = \sqrt{-2\mu E}, \qquad \text{if } E < 0,\\ S^{(\pm)}_{n,\ell}(r) &\overset{r\to\infty}{\propto} e^{\pm ikr}, \quad k = \sqrt{2\mu E}, \qquad \text{if } E > 0. \end{aligned}$$

Here we introduce the notation $S^{(\pm)}_{n,\ell}$ to make explicit the incoming $(-)$ or outgoing $(+)$ wave behavior at large values of r.

For an auxiliary potential including a Coulomb term plus a short-range potential,

$$\mathcal{V}_a(r) = \frac{Z}{r} + \widetilde{\mathcal{V}}_a(r),$$

equation (3.5) becomes the Coulomb equation (1.22). Thus the behavior of the $S_{n,\ell}$

functions coincides with the one of the Coulomb wave functions introduced in **Section 1.2**.

Remark 3.1.1. As explained in reference [26], the asymptotic behavior is reached once the generating potential vanishes (say at $r = R$). Thus, independently of the index n, all functions $S_{n,\ell}$ have the same asymptotic behavior (up to a complex constant that may depend on n). In other words, these functions are not linearly independent in the region $r > R$. We will see in the following chapter that this is not the case with our proposed Laguerre and Slater Quasi-Sturmian function Q_n, each of which is constructed with a different generating potential that vanishes farther of the origin as the index n increases.

■

Remark 3.1.2. Notice that for positive energies Generalized Sturmian functions are complex functions. Nevertheless, properties (3.2) and (3.3) remain valid without taking the complex conjugated of one of the basis functions because they are general properties of Sturm-Liouville theory.

■

3.2 The Hulthén Sturmian functions

The Hulthén potential [29], a particular case of Eckart's potential, is defined as

$$\mathcal{V}(r) = v_0 \, \frac{e^{-\frac{r}{\alpha}}}{1 - e^{-\frac{r}{\alpha}}}, \tag{3.6}$$

where $a > 0$, $v_0 < 0$ are fixed real parameters. It is a short-range potential that behaves as a Coulomb potential near the origin (taking $v_0 = \frac{z_1 z_2}{\alpha}$) and decreases exponentially for large values of r.

For $\ell = 0$, Hulthén Sturmian functions can be given in closed form. Taking

$$\mathcal{V}_a(r) \equiv 0, \qquad \mathcal{V}_g(r) = v_g \, \frac{e^{-\frac{r}{\alpha}}}{1 - e^{-\frac{r}{\alpha}}}, \tag{3.7}$$

the differential equation (3.1) defining them becomes

$$\left[-\frac{1}{2\mu} \frac{d^2}{dr^2} + \lambda_{n,0} \, v_g \, \frac{e^{-\frac{r}{\alpha}}}{1 - e^{-\frac{r}{\alpha}}} - E \right] S^{(+)}_{n,0}(r) = 0 \tag{3.8a}$$

and we consider the outgoing scattering boundary conditions

$$S_{n,0}^{(+)}(0) \quad = \quad 0, \tag{3.8b}$$
$$S_{n,0}^{(+)}(r) \quad \overset{r\to\infty}{\propto} \quad e^{ikr}. \tag{3.8c}$$

We now make brief a review of the procedure presented in [29] to find the solution of the eigenvalue problem. First we perform a change of variable

$$x = e^{-\frac{r}{\alpha}}$$

and propose

$$S_{n,0}^{(+)}(x) = N_n^S\, x^{-ik\alpha}\, y(x). \tag{3.9}$$

We introduce a normalization coefficient N_n^S in such a way that the closure relation (3.2) holds; its analytical expression is given below. With this proposal, one obtains an equation for the function $y(x)$

$$\left[x(1-x)\frac{d^2}{dx^2} + [1 - 2ik\alpha - (1-2ik\alpha)x]\frac{d}{dx} - 2\mu a^2 v_g\, \lambda_{n,0}\right] y(x) = 0,$$

which is a Gauss hypergeometric differential equation, whose general form is

$$\left[x(1-x)\frac{d^2}{dx^2} + [C - (A+B+1)x]\frac{d}{dx} - AB\right] y(x) = 0.$$

Its solution, regular at the origin, is the Gauss hypergeometric function $y(x) = {}_2F_1(A, B, C; x)$,and therefore,

$$S_{n,0}^{(+)}(r) = N_n^S\, e^{ikr}\, {}_2F_1\left(A, B, C; e^{-\frac{r}{\alpha}}\right).$$

The parameter $C = 1 - 2ik\alpha$ can be immediately identified, while for A and B we have the system

$$\begin{cases} A + B = -2ik\alpha, \\ AB = 2\mu\alpha^2 v_g\, \lambda_{n,0}, \end{cases} \tag{3.10}$$

whose solution is

$$A = -ik\alpha \pm i\alpha\sqrt{k^2 + 2\mu v_g\, \lambda_{n,0}}, \qquad B = -ik\alpha \mp i\alpha\sqrt{k^2 + 2\mu v_g\, \lambda_{n,0}}. \tag{3.11}$$

The asymptotic condition is clearly verified since

$$S_{n,0}^{(+)}(r) \overset{\mathbf{r}\to\infty}{\sim} N_n^S\, e^{ikr}. \tag{3.12}$$

The condition of regularity at $r=0$ is responsible for the discretization of the eigenvalues. At $r=0$ we have

$$0 = {}_2F_1(A,B,C;1) = \frac{\Gamma(C)\,\Gamma(C-A-B)}{\Gamma(C-A)\,\Gamma(C-B)}$$

which implies that either $C-A=-m$ or $C-B=-m$, $m=0,1,2,\ldots$. With the first option,

$$C-A=-m \quad \Longrightarrow \quad \begin{cases} A = m+1-2ik\alpha \\ B = -(m+1) \end{cases} \tag{3.13}$$

while the other option ($C-B=-m$) interchanges the roles of A and B. Setting $m+1=n$, and taking into account that ${}_2F_1(A,B,C;x) = {}_2F_1(B,A,C;x)$, in both cases we finally obtain the same result for the Hulthén Sturmian functions, namely

$$S_{n,0}^{(+)}(r) = N_n^S\, e^{ikr}\, {}_2F_1\left(-n, n-2ik\alpha, 1-2ik\alpha; e^{-\frac{r}{\alpha}}\right), \quad n=1,2,3,\ldots \tag{3.14a}$$

$$= N_n^S\, e^{ikr} \sum_{q=0}^{n} \frac{(-n)_q\,(n-2ik\alpha)_q}{(1-2ik\alpha)_q}\, \frac{\left(e^{-\frac{r}{\alpha}}\right)^q}{q!}. \tag{3.14b}$$

The eigenvalues result from equating (3.11) with (3.13),

$$\lambda_{n,0} = -\frac{n(n-2ik\alpha)}{2\mu\,\alpha^2\,v_g}. \tag{3.15}$$

The Hulthén Sturmian functions $S_{n,0}^{(+)}$ were displayed in reference [26] as an example of Sturmian functions having outgoing boundary condition. The authors took advantage of the analytical expressions of these functions and their eigenvalues to illustrate the efficiency of the numerical method proposed to generate Generalized Sturmian functions.

In **Figure 3.1** we plot the real part (full line) and imaginary part (line with dots) of a Hulthén Sturmian function taking $n=5$, $k=0.9$, $v_g=-3$, $\alpha=1$. The corresponding generating Hulthén potential is shown with a dashed line.

In **Figure 3.2** we plot the real part of normalized Hulthén Sturmian functions

$$\overline{S}_{n,0}^{(+)}(r) = \frac{1}{N_n^S} S_{n,0}^{(+)}(r)$$

for three different indices: $n = 3$ (full line), $n = 8$ (line with dots) and $n = 15$ (line with diamonds). The dashed line corresponds to the real part of the outgoing wave e^{ikr} that characterizes the asymptotic behavior.

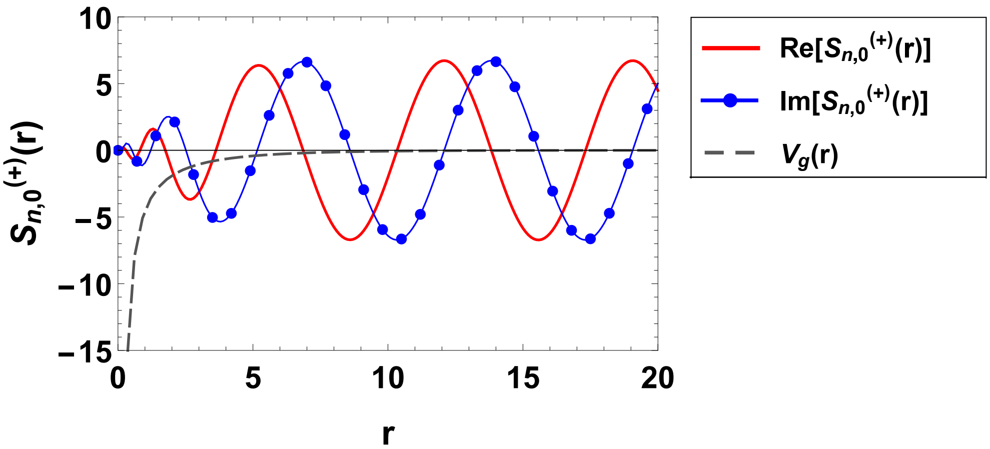

Figure 3.1: Real and imaginary parts (full line and line with dots respectively) of a Hulthén Sturmian function with outgoing scattering condition. We fix $n = 5$, $k = 0.9$, $v_g = -3$, $\alpha = 1$. The dashed line corresponds to the generating Hulthén potential.

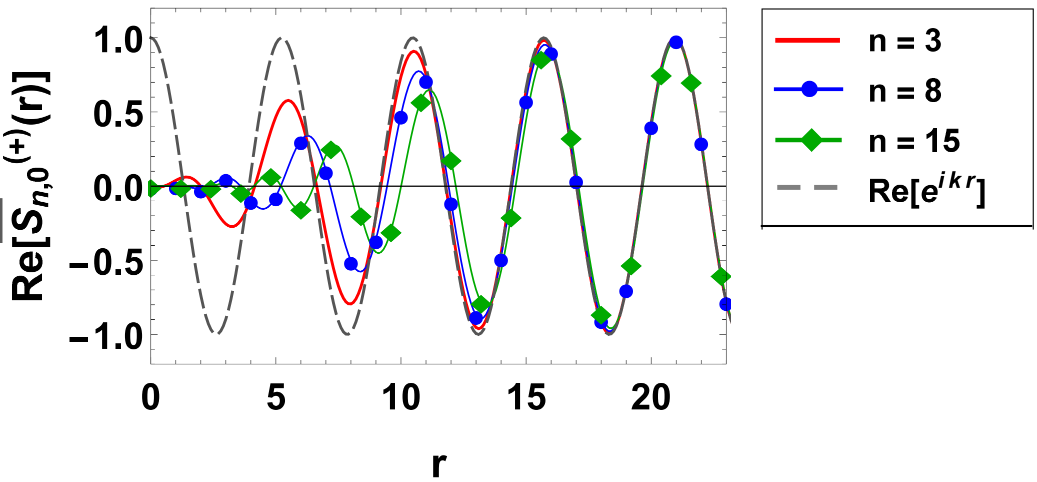

Figure 3.2: Real part of $\overline{S}_{n,0}^{(+)}$ for different values of n and parameters $k = 1.2$, $v_g = -1.8$, $\alpha = 3$. The dashed line represents the real part of the asymptotic behavior e^{ikr}.

As mentioned in **Remark 3.1.1**, these plots illustrate the fact that in the region where the generating potential vanishes all Sturmian functions reach an asymptotic behavior, unique up to a complex constant depending on the index n.

Remark 3.2.1. The hypergeometric function appearing in the expression of Hulthén Sturmian functions is related to a Jacobi polynomial $P_n^{(a,b)}$ [42] taking the parameters $a = -2ik\alpha$, $b = -1$ and the variable $z = 1 - 2x$, $x = e^{-\frac{r}{\alpha}}$. Hence, we have the equivalent form

$$S_{n,0}^{(+)}(r) = N_n^S \frac{n!}{(1-2ik\alpha)_n} e^{ikr} P_n^{(-2ik\alpha,-1)}(1 - 2e^{-\frac{r}{\alpha}}). \tag{3.16}$$

■

As indicated at the beginning of this section, we choose the magnitude N_n^S such that the functions generate the closure relation (3.2). To find its value we start from the following relation for the Jacobi polynomials [78]

$$\sum_n \frac{n!(a+b+2n+1)\Gamma(a+b+n+1)}{\Gamma(a+n+1)\,\Gamma(b+n+1)} P_n^{(a,b)}(x)\, P_n^{(a,b)}(y)$$
$$= 2^{a+b+1}(1-x)^{-\frac{a}{2}}(1+x)^{-\frac{b}{2}}(1-y)^{-\frac{a}{2}}(1+y)^{-\frac{b}{2}}\,\delta(x-y) \tag{3.17}$$

valid for $x, y \in (-1, 1)$ and $\mathrm{Re}(a), \mathrm{Re}(b) > -1$. Setting

$$x = 1 - 2e^{-\frac{r_1}{\alpha}}, \qquad y = 1 - 2e^{-\frac{r_2}{\alpha}},$$

and using (3.16) we find

$$\sum_n \frac{n!(2n-2ik\alpha)\Gamma(n-2ik\alpha)}{\Gamma(n+1-2ik\alpha)\,\Gamma(n)} \left[\frac{(1-2ik\alpha)_n}{N_n^S\, n!}\right]^2 S_{n,0}^{(+)}(r_1)\, S_{n,0}^{(+)}(r_2)$$
$$= 2(1-e^{-\frac{r_1}{\alpha}})^{\frac{1}{2}}(1-e^{-\frac{r_2}{\alpha}})^{\frac{1}{2}}\ \delta(-2e^{-\frac{r_1}{\alpha}} + 2e^{-\frac{r_2}{\alpha}}). \tag{3.18}$$

Now we make use of some properties of Dirac delta δ that can be found in §15 of [79] or in [80]. The Dirac delta satisfies

$$\delta(f(x)) = \sum_n \frac{\delta(x - x_n)}{|f'(x_n)|}$$

for x_n such that $f(x_n) = 0$, $f'(x_n) \neq 0$. Taking $f(r_2) = -2e^{-\frac{r_1}{\alpha}} + 2e^{-\frac{r_2}{\alpha}}$, we have

$$f(r_2) = 0 \iff r_2 = r_1,$$

$$|f'(r_1)| = \frac{2}{\alpha} e^{-\frac{r_1}{\alpha}}.$$

Then, using $\delta(x) = \delta(-x)$,

$$\delta(-2e^{-\frac{r_1}{\alpha}} + 2\,e^{-\frac{r_2}{\alpha}}) = \frac{\alpha}{2e^{-\frac{r_1}{\alpha}}}\,\delta(r_1 - r_2).$$

From the property

$$h(x)\delta(x - x_0) = h(x_0)\delta(x - x_0),$$

and taking $h(r_2) = (1 - e^{-\frac{r_2}{\alpha}})^{\frac{1}{2}}$ we find

$$(1 - e^{-\frac{r_2}{\alpha}})^{\frac{1}{2}}\,\delta(r_1 - r_2) = (1 - e^{-\frac{r_1}{\alpha}})^{\frac{1}{2}}\,\delta(r_1 - r_2).$$

Combining these two results, and using the recurrence property of the Gamma function, identity (3.18) becomes

$$\sum_n \frac{n\,(2n - 2ik\alpha)}{n - 2ik\alpha}\left[\frac{(1 - 2ik\alpha)_n}{N_n^S\,n!}\right]^2 S_{n,0}^{(+)}(r_1)\,S_{n,0}^{(+)}(r_2) = \alpha\,\frac{1 - e^{-\frac{r_1}{\alpha}}}{e^{-\frac{r_1}{\alpha}}}\,\delta(r_1 - r_2),$$

or, equivalently, in terms of the Hulthén potential (3.7)

$$\sum_n \frac{n\,(2n - 2ik\alpha)}{(n - 2ik\alpha)\,\alpha\,v_g}\left[\frac{(1 - 2ik\alpha)_n}{N_n^S\,n!}\right]^2 S_{n,0}^{(+)}(r_1)\,\mathcal{V}_g(r_1)\,S_{n,0}^{(+)}(r_2) = \delta(r_1 - r_2).$$

By comparing with the closure relation (3.2) we immediately deduce

$$N_n^S = \frac{(1 - 2ik\alpha)_n}{n!}\sqrt{\frac{2n\,(n - ik\alpha)}{\alpha\,v_g\,(n - 2ik\alpha)}}. \tag{3.19}$$

As a consequence of this choice for the normalization coefficient N_n^S we can assert that the integral (3.3) related to the orthogonality property happens to be $V_n = 1$. To show it we start from the closure relation (3.2) for the $\ell = 0$ Hulthén Sturmian functions $S_{n,0}^{(+)}$. We multiply both sides of this identity by $S_{m,0}^{(+)}(r_1)$ and integrate over the r_1 variable,

$$\sum_n S_{n,0}^{(+)}(r_2)\int_0^\infty S_{n,0}^{(+)}(r_1)\,\mathcal{V}_g(r_1)\,S_{m,0}^{(+)}(r_1)\,dr_1 = \int_0^\infty S_{m,0}^{(+)}(r_1)\,\delta(r_1 - r_2)\,dr_1.$$

The integral on the left vanishes for all $n \neq m$ and equals V_m for $n = m$. On the other hand, the integral on the right equals $S_{m,0}^{(+)}(r_2)$. Then

$$S_{m,0}^{(+)}(r_2)\,V_m = S_{m,0}^{(+)}(r_2), \quad \forall\ r_2,$$

from which we conclude that $V_m = 1$.

Remark 3.2.2. Notice that the initial formula (3.17) requires $\mathrm{Re}(b) > -1$, which is not satisfied in the present situation (we took $b = -1$). Generally in textbooks one finds for Jacobi polynomials the condition $\mathrm{Re}(a), \mathrm{Re}(b) > -1$, even when it is not necessary (but it suffices). One example is the orthogonality relation. Clearly in the situation we are studying, as a consequence of the orthogonality property satisfied by the Hulthén Sturmian functions (3.3) and their relation with Jacobi polynomials (3.16), the Jacobi polynomials $P_n^{(-2ik\alpha,-1)}(1 - 2e^{-\frac{r}{\alpha}})$ are indeed orthogonal.

■

To illustrate the validity of the result $V_n = 1$, we performed numerically the integral (3.3b) for various n values. The V_n values obtained for two sets of parameters are presented in **Table 3.1**.

Parameters: $\alpha = 1, v_g = -1, k = 1.2$		Parameters: $\alpha = 2, v_g = -1.8, k = 1.7$	
n	$V_n = \int_0^\infty dr\,[S_{n,0}^{(+)}(r)]^2\,\mathcal{V}_g(r)$	n	$V_n = \int_0^\infty dr\,[S_{n,0}^{(+)}(r)]^2\,\mathcal{V}_g(r)$
1	1.	1	1.
3	1.	3	1.
8	1.	8	$1. + 8.21272 \times 10^{-6}\,i$
16	$0.999993 + 1.16476 \times 10^{-5}\,i$	16	$1. + 1.34232 \times 10^{-4}\,i$

Table 3.1: Verification of the assertion $V_n = 1$ for two different set of parameters.

Remark 3.2.3. If we take the auxiliary potential also as a Hulthén potential

$$\mathcal{V}_a(r) = v_a\,\frac{e^{-\frac{r}{\alpha}}}{1 - e^{-\frac{r}{\alpha}}},$$

equation (3.1) defining the Sturmian functions becomes

$$\left[-\frac{1}{2\mu}\frac{d^2}{dr^2} + \left(\frac{v_a}{v_g} + \widetilde{\lambda}_{n,0}\right) v_g\,\frac{e^{-\frac{r}{\alpha}}}{1 - e^{-\frac{r}{\alpha}}} - E\right] S_{n,0}^{(+)}(r) = 0. \tag{3.20}$$

Clearly the eigenfunctions are exactly the Hulthén Sturmian functions (3.14), but now the eigenvalues are shifted

$$\widetilde{\lambda}_{n,0} = \lambda_{n,0} - \frac{v_a}{v_g}. \tag{3.21}$$

■

3.3 Integrals involving Hulthén Sturmian functions

When dealing with two- and three-body scattering problems different integrals are generally needed.

The overlap integral

$$\int_0^\infty S^{(+)}_{n,0}(r)\, S^{(+)}_{m,0}(r)\, dr$$

is not convergent but we can perform, using (3.14b), the following integral,

$$\begin{aligned}
&\lim_{\epsilon\to 0^+} \int_0^\infty e^{-\epsilon\, r} S^{(+)}_{n,0}(r)\, S^{(+)}_{m,0}(r)\, dr \\
&\quad = N_n^S\, N_m^S \sum_{q=0}^{n} \sum_{p=0}^{m} \frac{(-n)_q\,(n-2ik\alpha)_q}{(1-2ik\alpha)_q\, q!}\, \frac{(-m)_p\,(m-2ik\alpha)_p}{(1-2ik\alpha)_p\, p!} \lim_{\epsilon\to 0^+} \int_0^\infty e^{-\frac{(\epsilon\alpha+q+p-2ik\alpha)r}{\alpha}}\, dr \\
&\quad = N_n^S\, N_m^S \sum_{q=0}^{n} \sum_{p=0}^{m} \frac{(-n)_q\,(n-2ik\alpha)_q}{(1-2ik\alpha)_q\, q!}\, \frac{(-m)_p\,(m-2ik\alpha)_p}{(1-2ik\alpha)_p\, p!}\, \frac{\alpha}{q+p-2ik\alpha}.
\end{aligned} \tag{3.22}$$

Writing

$$\frac{1}{q+p-2ik\alpha} = \frac{(-2ik\alpha)_{q+p}}{(-2ik\alpha)\,(1-2ik\alpha)_{q+p}},$$

we obtain

$$\begin{aligned}
&\lim_{\epsilon\to 0^+} \int_0^\infty e^{-\epsilon\, r} S^{(+)}_{n,0}(r)\, S_{m,0}(r)\, dr \\
&\quad = -\frac{N_n^S\, N_m^S}{2ik}\, F^{1:2;2}_{1:1;1}\left[\begin{array}{lccc} -2ik\alpha : & -n, n-2ik\alpha; & -m, m-2ik\alpha; & \\ & & & 1,1 \\ 1-2ik\alpha : & 1-2ik\alpha; & 1-2ik\alpha; & \end{array}\right],
\end{aligned} \tag{3.23}$$

where the two variable hypergeometric function $F^{1:2;2}_{1:1;1}$ has the series representation [52]

$$\begin{aligned}
&F^{1:2;2}_{1:1;1}\left[\begin{array}{lccc} D: & A_1, B_1; & A_2, B_2; & \\ & & & x_1, x_2 \\ E: & C_1; & C_2; & \end{array}\right] \\
&\quad = \sum_{q,p} \frac{(A_1)_q (B_1)_q}{(C_1)_q}\, \frac{(A_2)_p (B_2)_p}{(C_2)_p}\, \frac{(D)_{q+p}}{(E)_{q+p}}\, \frac{x_1^q}{q!}\, \frac{x_2^p}{p!}.
\end{aligned} \tag{3.24}$$

The next two integrals include Laguerre-type functions ϕ_n^L and they will be useful in a three-body scattering model problem we present in **Chapter 6**. Using the polynomial expression (3.14b) for the Hulthén Sturmian functions and definition (1.2a) in the integral formula (B.4), one finds

$$\begin{aligned}\int_0^\infty & \phi_q^L(\ell,\beta;r)\,\frac{1}{r^p}\,S_{n,0}^{(+)}(r)\,dr \\ &= \frac{N_n^S}{N_{q,\ell}^L}\,\frac{\Gamma(\ell+2-p)}{\Gamma(2\ell+2)}\,(2\beta)^{p-1}\sum_{j=0}^{n}\frac{(-n)_j\,(n-2ik\alpha)_j}{(1-2ik\alpha)_j\,j!}\left(\frac{2\beta\alpha}{\alpha(\beta-ik)+j}\right)^{\ell+2-p} \\ &\times\;{}_2F_1\left(-q,\ell+2-p,2\ell+2;\frac{2\beta\alpha}{\alpha(\beta-ik)+j}\right), \end{aligned} \tag{3.25}$$

where the Gauss hypergeometric function reduces to a polynomial of order q.

In addition, using the Taylor series for the Hulthén potential

$$\mathcal{V}_g(r) = v_g\sum_s\left(e^{-\frac{r}{\alpha}}\right)^{s+1} \tag{3.26}$$

and again formulas (3.14b) and (B.4), one obtains

$$\begin{aligned}\int_0^\infty & \phi_q^L(\ell,\beta;r)\,\mathcal{V}_g(r)\,S_{n,0}^{(+)}(r)\,dr \\ &= \frac{N_n^S}{N_{q,\ell}^L}\,\frac{\Gamma(\ell+2)}{\Gamma(2\ell+2)}\,\frac{v_g}{2\beta}\sum_{j=0}^{n}\frac{(-n)_j\,(n-2ik\alpha)_j}{(1-2ik\alpha)_j\,j!} \\ &\times\sum_s\left(\frac{2\beta a}{a(\beta-ik)+j+s+1}\right)^{\ell+2}{}_2F_1\left(-q,\ell+2,2\ell+2;\frac{2\beta\alpha}{\alpha(\beta-ik)+j+s+1}\right). \end{aligned} \tag{3.27}$$

Finally we perform an integral involving a spherical Bessel function $j_0(x) = \dfrac{\sin(x)}{x}$ [42]. Expressing the sine function in terms of complex exponential functions, making a change of variable $x = e^{-\frac{r}{\alpha}}$ and using (3.14a), the mathematical integral (B.5) yields

$$\int_0^\infty S_{n,0}^{(+)}(r)\,\mathcal{V}_g(r)\,kr j_0(kr)\,dr = -\frac{kN_n^S}{2\mu\lambda_{n,0}} \tag{3.28}$$

Remark 3.3.1. Even if we have shown that for the particular choice of the coefficient N_n^S we obtain

$$V_{m,n} = \int_0^\infty dr\,S_{m,0}^{(+)}(r)\,\frac{v_g\,e^{-\frac{r}{\alpha}}}{1-e^{-\frac{r}{\alpha}}}\,S_{n,0}^{(+)}(r) = \delta_{m,n},$$

this integral can be analytically performed. The procedure is described in [33] and the resulting expression is

$$V_{m,n} = N_n^S N_m^S \frac{\alpha v_g}{1-2ik\alpha} \sum_s \frac{(1-2ik\alpha)_s}{(2-2ik\alpha)_s} \times F^{1:2;2}_{1:1;1}\left[\begin{array}{llll} 1-2ik\alpha+s: & -n, n-2ik\alpha; & -m, m-2ik\alpha; & \\ & & & 1,1 \\ 2-2ik\alpha+s: & 1-2ik\alpha; & 1-2ik\alpha; & \end{array}\right] \tag{3.29}$$

where $F^{1:2;2}_{1:1;1}$ is given by formula (3.24).

■

3.4 Chapter summary

This chapter was dedicated to introducing Generalized Sturmian functions. They are generated from a Sturm-Liouville problem with appropriate boundary conditions, making them an efficient basis set to describe two-body problems. These orthogonal basis set is usually obtained numerically.

We present in this chapter a particular case in which Generalized Sturmian functions can be presented in closed form: using a Hulthén potential as generating potential. Besides reviewing the deduction of these functions, we contribute with analytical expressions for their normalization constant and some related integrals involving them, usually appearing in scattering problems. The results presented here constitute the first part of reference [33], a paper in which we studied these functions from an analytical and numerical point of view, and used them to solve two-body scattering problems. The implementation of these functions, not only in two- but also in three-body scattering problems, will be presented in the last two chapters of this thesis.

Chapter 4

Quasi-Sturmian functions

Quasi-Sturmian functions constitute our proposal as an alternative set of functions useful to describe two- and three-body scattering problems. Like Generalized Sturmian functions, they are constructed to possess an appropriate asymptotic behavior and, in some very interesting cases, they present the great advantage of having closed form expressions. In this chapter we introduce Quasi-Sturmian functions and study their properties. Part of the results presented here can be found in reference [34].

4.1 Definition and general characteristics

We name Quasi-Sturmian functions the solutions of the non-homogeneous differential equation

$$[\mathbf{T_r} + \mathcal{V}_a(r) - E]\, Q_n(r) = \mathcal{V}_g(r)\phi_n(r). \tag{4.1}$$

where $n \in \mathbb{N} \cup \{0\}$, and the operator $\mathbf{T_r}$ is given in (1.18).

This Schrödinger-like radial equation is similar to the one defining Generalized Sturmian functions (3.1): it has the same left hand side, but a completely different right hand side (hereafter referred to as driven term). Rather than the eigenvalues multiplied by the eigenfunctions, we have some chosen functions ϕ_n. This is the reason for calling the solutions Q_n Quasi-Sturmian functions. We maintain the notation $\mathcal{V}_a$ and $\mathcal{V}_g$ used to define Generalized Sturmian functions: $\mathcal{V}_a$ may be considered as an auxiliary potential, but $\mathcal{V}_g$ is no longer responsible for generating the set of functions Q_n. That role will be played by the driven functions ϕ_n.

If in the driven term we have a set of linearly independent functions $\{\phi_n\}$, $n = 0, 1, 2...$, then the resulting Quasi-Sturmian functions are also linearly independent. To prove it, suppose there exists one Quasi-Sturmian function that can be expressed as a linear combination of other Quasi-Sturmian functions,

$$Q_m(r) = \sum_{i=0}^{M} a_i \, Q_{n_i}(r).$$

Now, from the definition (4.1) we have

$$[\mathbf{T_r} + \mathcal{V}_a(r) - E] \, Q_m(r) = \mathcal{V}_g(r)\phi_m(r),$$

and, on the other hand,

$$[\mathbf{T_r} + \mathcal{V}_a(r) - E] \sum_{i=0}^{M} a_i \, Q_{n_i}(r) = \sum_{i=0}^{M} a_i \, \mathcal{V}_g(r)\phi_{n_i}(r).$$

Thus we find

$$\phi_m(r) = \sum_{i=0}^{M} a_i \, \phi_{n_i}(r),$$

which is an absurd if functions ϕ_n are linearly independent. As a consequence, Quasi-Sturmian functions are linearly independent if functions ϕ_n are so.

In order to provide Quasi-Sturmian functions in closed form and study their properties, we must choose in (4.1) appropriate driven functions ϕ_n, as well as potentials $\mathcal{V}_a$ and $\mathcal{V}_g$.

For the driven term we propose two different functions ϕ_n: the Slater-type orbitals ϕ_n^{STO} and the Laguerre-type functions ϕ_n^{L} both introduced in **Section 1.1**. Since we wish to use Quasi-Sturmian functions to describe scattering problems, we consider hereafter the case $E > 0$.

For $\mathcal{V}_a$ we take a Coulomb potential corresponding to a charge Z_{QS}, and $\mathcal{V}_g$ is the weight function associated to Laguerre-type functions,

$$\mathcal{V}_a(r) = \frac{Z_{QS}}{r}, \qquad \mathcal{V}_g(r) = \frac{1}{r}.$$

Notice that with this auxiliary potential, and considering $E > 0$, the homogeneous equation associated to (4.1) is the Coulomb equation (1.22) described in **Section 1.2**.

Contrary to the usual situation for Generalized Sturmian functions, $\mathcal{V}_g$ is no longer a short range potential, but the whole driven term is still of short range. Indeed, as a consequence of the decaying exponential factor appearing in both Slater-type orbitals and

Laguerre-type functions, the two driven terms we are considering

$$\frac{1}{r}\,\phi_n^{STO}(\ell,\beta;r) \qquad \text{and} \qquad \frac{1}{r}\,\phi_n^{L}(\ell,\beta;r) \tag{4.2}$$

vanish in the region $r > R_n$, for some n-dependent value $R_n > 0$. In other words, in the asymptotic region (R_n, ∞), the differential equation (4.1) becomes the Coulomb equation, and the Quasi-Sturmian solution Q_n behaves proportionally to a Coulomb wave function. In particular, we are interested in solutions regular at the origin and with the incoming $(-)$ or outgoing $(+)$ wave behavior (1.28). Summarizing, the Quasi-Sturmian functions we present in this chapter are solutions of the boundary value problem

$$\left[\mathbf{T_r} + \frac{Z_{QS}}{r} - E\right] Q_n^{(\pm)}(r) = \frac{1}{r}\,\phi_n(r), \tag{4.3a}$$

$$Q_n^{(\pm)}(0) = 0, \tag{4.3b}$$

$$Q_n^{(\pm)}(r) \quad \overset{r\to\infty}{\sim} \quad \mathcal{Q}_n^{as}\, e^{\pm i\left[kr - \eta(Z_{QS})\ln(2kr) + \sigma_C(\ell, Z_{QS}) - \frac{\pi}{2}\ell\right]}. \tag{4.3c}$$

The parameters η and σ_C were defined in (1.23a) and (1.23b) respectively.

The asymptotic coefficients $\mathcal{Q}_n^{as}$ depend on the index n and on the parameters appearing in the equation, i.e., ℓ, E and Z_{QS}. For both driven terms (4.2) we are able to express $\mathcal{Q}_n^{as}$ in closed form and show their independence of the $(\pm)$ sign. Moreover these coefficients happen to be real numbers.

An interesting thing to notice is that since the driven terms we are considering are real functions, the imaginary part of the Quasi-Sturmian solution is actually one of the Coulomb wave functions with charge $Z = Z_{QS}$. Taking into account the imposed boundary conditions (4.3b) and (4.3c) together with the fact that the asymptotic coefficients $\mathcal{Q}_n^{as}$ are real, the imaginary part of any of the Quasi-Sturmian functions differs from the sine-like Coulomb wave function by a real factor. Specifically

$$\operatorname{Im}\left[Q_n^{(\pm)}(\ell,\beta;r)\right] = \pm \mathcal{Q}_n^{as} F^{(s)}(\ell,k;r), \tag{4.4}$$

where the function $F^{(s)}$ is defined in (1.24). This will be illustrated in **Figure 4.2** for the case of a Slater-type orbital in the driven term and in **Figure 4.4** for the case of a Laguerre-type function.

In addition, we have $Q_n^{(-)} = \left[Q_n^{(+)}\right]^*$. Then, from (4.4) we immediately deduce

$$F^{(s)}(\ell, k; r) = \frac{1}{2\,i\,\mathcal{Q}_n^{as}} \left[Q_n^{(+)}(\ell, \beta; r) - Q_n^{(-)}(\ell, \beta; r)\right]. \tag{4.5}$$

This is valid for any $n \in \mathbb{N} \cup \{0\}$, which means that the way to express $F^{(s)}$ in terms of the set of functions $\{Q_n^{(+)}, Q_n^{(-)}\}_{n=0,1,2...}$ is not unique.

Remark 4.1.1. The range R_n of the driven terms (4.2) depends on n through the power r^n, as illustrated in **Figure 1.1** for the case of Laguerre-type functions. As indicated in **Remark 3.1.1**, the situation is therefore very different from that of Generalized Sturmian functions since the latter are related to a unique generating potential and thus to a unique range. Quasi-Sturmian functions (specifically their real part) are not all proportional to the same asymptotic function in a fixed region (R, ∞) as it was the case with Generalized Sturmian functions. As mentioned, they reach their asymptotic behavior at gradually larger R_n values, thus forming a linearly independent set in $(0, \infty)$. We will come back to this characteristic when describing **Figure 4.2** and **Figure 4.4**.

■

Remark 4.1.2. Taking $\phi_n(r) = \phi_n^L(\ell, \beta; r)$ and $n = 0$ in (4.3) one obtains the boundary value problem (1.69), introduced in the context of Coulomb Green's functions. Its solution is $\hat{H}^{(\pm)}$, except for a factor in the asymptotic behavior amplitude.

In virtue of relation (1.7),

$$\phi_0^L(\ell, \beta; r) = c_{0,0}\, \phi_0^{STO}(\ell, \beta; r),$$

the solutions $Q_0^{STO(\pm)}$ and $Q_0^{L(\pm)}$, resulting from taking Slater-type orbitals and Laguerre-type functions, respectively, as driven term in (4.3a), satisfy

$$c_{0,0}\, Q_0^{STO(\pm)}(\ell, \beta; r) = Q_0^{L(\pm)}(\ell, \beta; r) = \mathcal{Q}_0^{L\,as}\, \hat{H}^{(\pm)}(\ell, \beta; r). \tag{4.6}$$

Hence, our Quasi-Sturmian functions $Q_n^{(\pm)}$ can be viewed as a generalization to any index n of the function $\hat{H}^{(\pm)}$ proposed by Yamani and Fishman [7] (and further by Broad [58, 59]) to be used in the J-Matrix method. Moreover, the constant b appearing in equation (1.69) happens to be

$$b = \frac{1}{\mathcal{Q}_0^{L\,as}}.$$

■

Remark 4.1.3. Having a real functions as driven term in the Quasi-Sturmian problem (4.3) has another consequence: combining Quasi-Sturmian functions with incoming (+) and outgoing (-) wave behavior we can provide Quasi-Sturmian functions with cosine-like asymptotic behavior.

$$Q_n^{(c)}(\ell, \beta; r) = \frac{1}{2}\left[Q_n^{(+)}(\ell, \beta; r) + Q_n^{(-)}(\ell, \beta; r)\right].$$

■

Remark 4.1.4. The functions ϕ_n^{STO} and ϕ_n^{L} can be used to expand more general functions f. Suppose we are interested in solving the non-homogeneous equation

$$\left[\mathbf{T_r} + \frac{Z}{r} - E\right] F(r) = f(r).$$

As explained in reference [75], it suffices to express, for example

$$f(r) = \frac{1}{r}\sum_n a_n \phi_n^L(\ell, \beta; r),$$

to deduce directly the solution

$$F(r) = \sum_n a_n Q_n^{L(\pm)}(\ell, \beta; r), \tag{4.7}$$

taking Z as the charge of each Quasi-Sturmian function. Alternatively, one can express f in terms of ϕ_n^{STO} and obtain a solution F given by (4.7) with $Q_n^{STO(\pm)}$ replacing $Q_n^{L(\pm)}$.

■

4.2 Slater Quasi-Sturmian functions

Slater Quasi-Sturmian functions are solutions of the differential equation (4.3a) with a Slater-type orbital ϕ_n^{STO} in the driven term together with boundary conditions (4.3b) and (4.3c). We denote them as $Q_n^{STO(\pm)}$.

In the following subsections we describe two different ways to obtain $Q_n^{STO(\pm)}$ in closed form. The first one consists in expressing this function as a combination of one particular solution of the non-homogeneous equation and a solution of the corresponding homogeneous equation. The second one makes use of the Coulomb Green's function introduced in **Section 1.3**.

4.2.1 A particular solution for the differential equation

We can express the solution $Q_n^{STO(\pm)}$ as the sum of two functions: a solution of the homogeneous equation plus a particular solution of the non-homogeneous equation. This is,

$$Q_n^{STO(\pm)}(\ell,\beta;r) = A_n^{(\pm)}\,\Phi^{(H)}(r) + \Phi_n^{(P)}(r), \tag{4.8}$$

where $A_n^{(\pm)}$ is a convenient coefficient, and the labels H and P stand for "homogeneous" and "particular".

Since we are interested in solutions regular at the origin, for the solution of the homogeneous equation the only option is to take the sine-like Coulomb wave function,

$$\Phi^{(H)}(r) = F^{(s)}(\ell,k;r),$$

whose explicit form and asymptotic behavior are given by (1.24) with $Z = Z_{QS}$.

A particular solution of the non-homogeneous equation (4.3a), presented in reference [75], reads

$$\begin{aligned}\Phi_n^{(P)}(r) = &-\frac{2\mu}{(n+1)(2\ell+2+n)}\,e^{ikr}\,r^{\ell+n+2}\\ &\times\,\Theta^{(1)}\left(\begin{array}{c} n+1,1\,|\,2\ell+2+n,\ell+2+n+i\eta(Z_{QS}) \\ \ell+2+n+i\eta(Z_{QS})\,|\,2+n,2\ell+3+n\end{array}\right|;-(\beta+ik)\,r,-2ikr\Bigg)\end{aligned} \tag{4.9}$$

where $\Theta^{(1)}$ is a two variables Kampé de Fériet hypergeometric function [30],

$$\Theta^{(1)}\left(\begin{array}{c} a_1,a_2\,|\,b_1,b_2 \\ c_1\,|\,d_1,d_2\end{array}\right|;x_1,x_2\Bigg) = \sum_{m,n}\frac{(a_1)_m\,(a_2)_n}{(c_1)_m}\frac{(b_1)_m\,(b_2)_{m+n}}{(d_1)_{m+n}\,(d_2)_{m+n}}\,\frac{x_1^m}{m!}\,\frac{x_2^m}{n!}. \tag{4.10}$$

It has been introduced and discussed in connection with the derivatives of regular confluent hypergeometric functions with respect to their parameters [70]. Later, in references [72, 75], this function appeared in the context of two-body Coulomb problems with sources. In these two works, as well as in reference [73], the authors presented different expressions for $\Theta^{(1)}$, the study of its convergence, and the form of its asymptotic behavior in the case of two-body problems.

Let us notice that at $r = 0$ we have $\Phi_n^{(P)}(0) = 0$. Since the chosen homogeneous solution $\Phi^{(H)}$ is also regular at the origin, condition (4.3b) is satisfied for the Slater

Quasi-Sturmian functions $Q_n^{STO(\pm)}$.

The procedure to choose the adequate $A_n^{(\pm)}$ value in order to obtain the desired asymptotic behavior (4.3c) is presented in reference [72]. Setting

$$ {}_2F_1 = {}_2F_1\left(n+1, 2\ell+2+n, \ell+2+n+i\eta(Z_{QS}); \frac{\beta+ik}{2ik}\right), \tag{4.11a}$$

$$ f_n = |\,{}_2F_1\,|, \tag{4.11b}$$

$$ \theta_n = \mathrm{Arg}(\,{}_2F_1\,), \tag{4.11c}$$

$$ N_{source}(n,\ell) = -2\mu\,\frac{(1)_n\,(2\ell+2)_n}{(2\ell+2)_{2n+2}}\,\frac{f_n}{N_C(\ell+1+n)}, \tag{4.11d}$$

$$ a_1 = kr - \eta(Z_{QS})\ln(2kr) - \frac{\pi}{2}\,\ell + \sigma_C(\ell, Z_{QS}), \tag{4.11e}$$

$$ a_2 = -\frac{\pi}{2}(2+n) + \sigma_C(\ell+1+n, Z_{QS}) - \theta_n - \sigma_C(\ell, Z_{QS}), \tag{4.11f}$$

one obtains, for the case we are studying, the coefficient

$$ A_n^{(\pm)} = \pm i\, N_{source}(n,\ell)e^{\mp i a_2}, $$

and the asymptotic behavior of Slater Quasi-Sturmian functions reads

$$ Q_n^{STO(\pm)}(\ell,\beta;r) \overset{r\to\infty}{\sim} N_{source}(n,\ell)\,\cos(a_2)\,e^{\pm i a_1}. $$

Thus, we have an expression for the asymptotic coefficient

$$ \mathcal{Q}_n^{STO\,as} = N_{source}(n,\ell)\,\cos(a_2), \tag{4.12}$$

which, as mentioned in the general characteristics, happens to be a real number independent of the $(\pm)$ sign.

4.2.2 The solution using the Coulomb Green's function

The solution of the boundary value problem (4.3a) with a Slater-type orbital in the driven term can be obtained also through the Coulomb Green's function introduced in **Section 1.2**. In this case the resulting expression satisfies automatically the boundary conditions because they are imposed to the Green's function. Formally we have

$$ Q_n^{STO(\pm)}(\ell,\beta;r) = \int_0^\infty \mathcal{G}_C^{(\pm)}(\ell;\ r,\ r')\,\frac{1}{r'}\,\phi_n^{STO}(\ell,\beta;r')\,dr'. \tag{4.13}$$

Using expression (1.62), performing a change of variables and after some intermediate steps, one finds the integral representation

$$Q_n^{STO(\pm)}(\ell,\beta;r) = \frac{2\mu(2\ell+2)_n}{(\beta \mp ik)^{n+1}}\, r^{\ell+1}\, e^{-\beta r} \times \int_0^1 z^n (1-z)^{\ell \pm i\eta(Z_{QS})} (1-\omega^{\pm 1} z)^{\ell \mp i\eta(Z_{QS})} e^{z[\beta \pm ik]r}\, {}_1F_1\left(-n, 2\ell+2; X\right)\, dz, \tag{4.14a}$$

where $\omega = \dfrac{\beta + ik}{\beta - ik}$ was introduced in (1.31), and

$$X = -\frac{r(1-z)(1-\omega^{\pm 1}z)(\beta \mp ik)}{z}. \tag{4.14b}$$

The confluent hypergeometric function appearing in (4.14a) is actually a polynomial

$${}_1F_1\left(-n, 2\ell+2; X\right) = \sum_{q=0}^{n} \frac{(-n)_q}{(2\ell+2)_q\, q!} \left(-\frac{r(1-z)(1-\omega^{\pm 1}z)(\beta \mp ik)}{z}\right)^q .$$

With this expression the integration over the variable z can be directly performed using (B.3). Taking into account the properties of the Pochhammer symbol one finally obtains

$$Q_n^{STO(\pm)}(\ell,\beta;r) = \frac{2\mu(2\ell+2)_n\, n!}{(\beta \mp ik)^{n+1}(\ell+1 \pm i\eta(Z_{QS}))_{n+1}}\, r^{\ell+1}\, e^{-\beta r} \tag{4.15}$$

$$\times \sum_{p=0}^{n} \frac{(\ell+1 \pm i\eta(Z_{QS}))_p}{(2\ell+2)_p} \frac{[r\,(\beta \mp ik)]^p}{p!} \times \Phi_1\left(n-p+1, -p-\ell \pm i\eta(Z_{QS}), n+2+\ell \pm i\eta(Z_{QS}); \omega^{\pm 1}, r(\beta \pm ik)\right), \tag{4.16}$$

in terms of one of the Horn's two-variable series Φ_1 [52]. We introduced this function when studying the derivatives of two variable hypergeometric functions with respect to their parameters [see formula (2.18a)]. Making use of its series representation (2.18c), the Slater Quasi-Sturmian function becomes

$$
\begin{aligned}
Q_n^{STO(\pm)}(\ell,\beta;r) = {} & \frac{2\mu(2\ell+2)_n\, n!}{(\beta\mp ik)^{n+1}(\ell+1\pm i\eta(Z_{QS}))_{n+1}}\, r^{\ell+1}\, e^{-\beta r} \\
& \times \sum_{p=0}^{n} \frac{(\ell+1\pm i\eta(Z_{QS}))_p}{(2\ell+2)_p} \frac{[r(\beta\mp ik)]^p}{p!} \\
& \times \sum_{q} \frac{(n-p+1)_q(-p-\ell\pm i\eta(Z_{QS}))_q}{(n+2+\ell\pm i\eta(Z_{QS}))_q} \frac{\omega^{\pm q}}{q!} \\
& \times\ {}_1F_1\left(n-p+1+q, n+2+\ell\pm i\eta(Z_{QS})+q; r(\beta\pm ik)\right). \quad (4.17)
\end{aligned}
$$

Even if we have already found an expression for the asymptotic coefficient [see formula (4.12)], it is possible to give an equivalent one deduced from the asymptotic behavior of the confluent hypergeometric function [42] appearing in (4.17). After some algebraic simplifications, one finds the expected behavior (4.3c) with the coefficient

$$
\begin{aligned}
\mathcal{Q}_n^{STO\,as} &= \omega^{-i\eta(Z_{QS})} e^{-\frac{\pi}{2}\eta(Z_{QS})} \frac{\mu(2\ell+2)_n}{k(\beta-ik)^n} \left|\Gamma(\ell+1\pm i\eta(Z_{QS}))\right| \left(\frac{2k}{\beta^2+k^2}\right)^{\ell+1} \\
& \times {}_2F_1\left(-n, \ell+1+i\eta(Z_{QS}), 2\ell+2; 1-\omega^{-1}\right), \quad (4.18)
\end{aligned}
$$

which is independent of the $\pm$ choice. To verify that it is in fact a real number it suffices to note that $\omega^{-i\eta(Z_{QS})}$ is real and to use one of the linear transformation formulas for the Gauss hypergeometric function [formula (15.3.4) in reference [42]] to find that

$$
\begin{aligned}
& \left[(\beta-ik)^{-n}\, {}_2F_1\left(-n, \ell+1+i\eta(Z_{QS}), 2\ell+2; 1-\omega^{-1}\right)\right]^* \\
& \qquad = (\beta-ik)^{-n}\, {}_2F_1\left(-n, \ell+1+i\eta(Z_{QS}), 2\ell+2; 1-\omega^{-1}\right).
\end{aligned}
$$

The equivalence between expressions (4.12) and (4.18) can be deduced by expressing the cosine function as a combination of complex exponentials.

4.2.3 Series representation in terms of Laguerre-Type functions

It is possible to give the analytic form of the coefficients

$$
a_{n,q}^{(\pm)} = \int_0^\infty dr\, \phi_q^L(\ell,\beta;r)\, \frac{1}{r}\, Q_n^{STO(\pm)}(r)
$$

corresponding to the series representation of $Q_n^{STO\,(\pm)}(r)$ in terms of Laguerre-type functions,

$$Q_n^{STO(\pm)}(r) = \sum_q a_{n,q}^{(\pm)} \, \phi_q^L(\ell, \beta; r).$$

From (4.17) and using (B.7) we obtain

$$\begin{aligned}
a_{n,q}^{(\pm)} =& \frac{2\mu\Gamma(2\ell+2)}{(2\beta)^{\ell+1}} \, \frac{N_{q,\ell}\,(2\ell+2)_q}{q!} \, \frac{(2\ell+2)_n \, n!}{(\beta \pm ik)^{n+1}(\ell+1 \pm i\eta(Z_{QS}))_n} \\
&\times \sum_{p=0}^{n} \frac{(\ell+1+i\eta(Z_{QS}))_p}{p!} \left(\frac{\beta \mp ik}{2\beta}\right)^p \\
&\times \sum_j \frac{(-n+p+1)_j \, (-\ell-p \pm i\eta(Z_{QS}))_j}{(\ell+2+n \pm i\eta(Z_{QS}))_j} \, \frac{\omega^{\pm j}}{j!} \\
&\times F_2\left(2\ell+2+p, -q, n-p+j+1, 2\ell+2, \ell+2+n+j \pm i\eta(Z_{QS}); 1, \frac{\beta \pm ik}{2\beta}\right).
\end{aligned}$$

An algebraic manipulation of this expression leads to the equivalent form

$$\begin{aligned}
a_{n,q}^{(\pm)} =& \frac{2\mu\Gamma(2\ell+2)}{(2\beta)^{\ell+1}} \, \frac{N_{q,\ell}}{q!} \, \frac{(2\ell+2)_n \, n!}{(\beta \mp ik)^{n+1}(\ell+1 \pm i\eta(Z_{QS}))_n} \\
&\times \sum_{p=0}^{n} \frac{(\ell+1+i\eta(Z_{QS}))_p}{p!} \left(\frac{\beta \mp ik}{2\beta}\right)^p \sum_{s=0}^{q} \frac{(-q)_s(2\ell+2+p)_s}{(2\ell+2)_s \, s!} \\
&\times F_1\left(n-p+1, -\ell-p \pm i\eta(Z_{QS}), 2\ell+2+p+s, \ell+2+n \pm i\eta(Z_{QS}); \omega, \frac{\beta \pm ik}{2\beta}\right),
\end{aligned}$$

where we have finite sums instead of full series. Once again we end up with expressions involving two of the Appell functions studied in **Chapter 2**. Other representations in terms of the more familiar Gaussian hypergeometric function can be obtained using alternative formulations for the two variable hypergeometric functions F_1 or F_2.

Remark 4.2.1. The coefficients

$$a_{n,q}^{(\pm)} = \int_0^\infty dr \, \phi_q^L(\ell, \beta; r) \, \frac{1}{r} \, \Phi_n^{(P)}(r)$$

corresponding to the Laguerre expansion of the particular solution (4.9) can also be given in closed form. Starting with some of the representations presented in reference [75] for the function $\Theta^{(1)}$ one obtains different expressions in terms of Appell functions. The resulting formulas are not easy to manipulate, neither numerically nor analytically. However they may be of interest if one wants to study $\Phi_n^{(P)}$ in terms of its parameters, as explained in **Section 1.1.1**.

■

4.2.4 Illustration

Let us illustrate numerically some of the obtained results. We have calculated, using the integral representation (4.14a), Slater Quasi-Sturmian functions for several n values, and for the following values of the parameters

$$Z_{QS} = -1,\ \mu = 1,\ k = 1.1,\ \ell = 0,\ \beta = 0.8.$$

Figure 4.1 shows the result for $n = 3$, together with the corresponding driven term of the differential equation defining this function, i.e., $\frac{1}{r}\,\phi_n^{STO}(\ell,\beta;r)$ [see equation (4.3a)]. The plot illustrates that, as mentioned at the beginning of the chapter, Quasi-Sturmian functions reach their asymptotic behavior once the driven term vanishes.

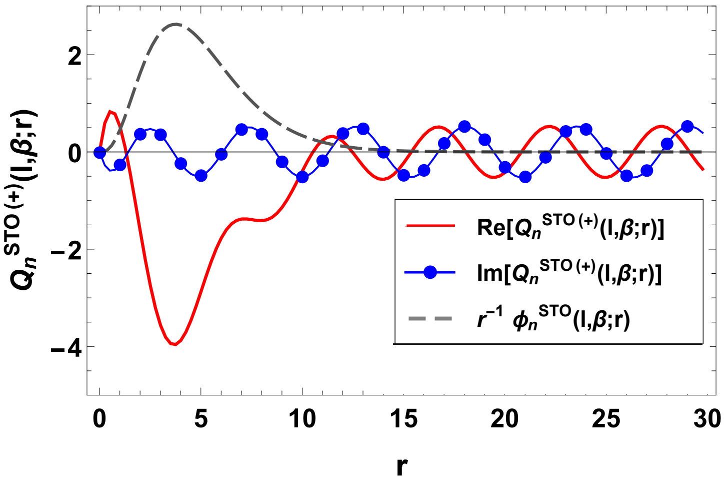

Figure 4.1: Real and imaginary parts of a Slater Quasi-Sturmian function $Q_n^{STO(+)}$ taking $n = 3$ and $Z_{QS} = -1$, $\mu = 1$, $k = 1.1$, $\ell = 0$, $\beta = 0.8$. The dashed line represents the corresponding driven term $r^{-1}\,\phi_n^{STO}(\ell,\beta;r)$.

In **Figure 4.2** (left panel) we plot the real part of the "normalized" Slater Quasi-Sturmian functions

$$\overline{Q}_n^{STO(+)}(\ell,\beta;r) = \frac{1}{Q_n^{STO\,as}}\,Q_n^{STO(+)}(\ell,\beta;r) \tag{4.19}$$

for two different values of the index n. The expected asymptotic behavior, given by

$$f_{as}(r) = e^{\pm i\left[kr-\eta(Z_{QS})\ln(2kr)+\sigma_C(\ell,Z_{QS})-\frac{\pi}{2}\ell\right]}, \tag{4.20}$$

is also shown. Clearly, as n increases, the asymptotic behavior is gradually reached, an attribute mentioned in **Remark 4.1.1**. The plot presented in the right panel corresponds to the imaginary part of the same $\overline{Q}_n^{STO(+)}$. It illustrates identity (4.4): the imaginary part coincides with the sine-like Coulomb wave function $F^{(s)}$ with charge $Z = Z_{QS}$.

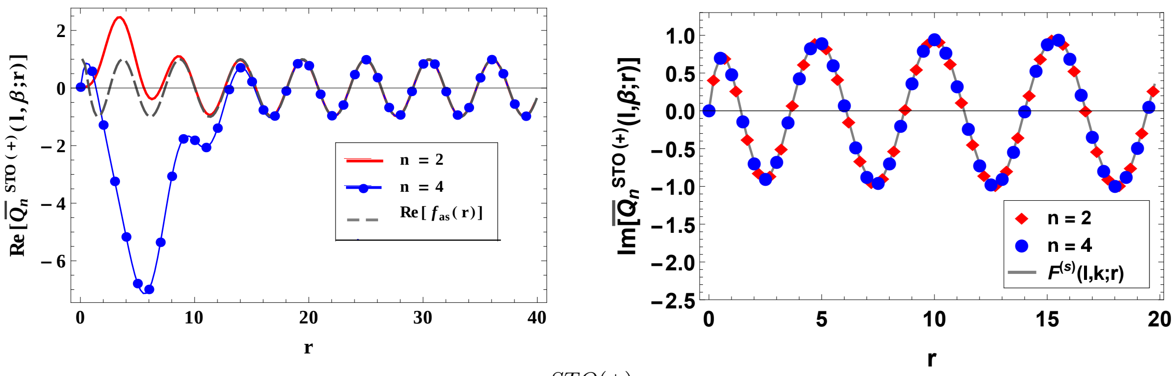

Figure 4.2: Left panel: real part of $\overline{Q}_n^{STO(+)}$, defined by (4.19), for $n = 2$ (solid line) and $n = 4$ (line with dots). The dashed line represents the real part of f_{as}, defined by (4.20). Right panel: imaginary part of $\overline{Q}_n^{STO(+)}$ for $n = 2$ (diamonds) and $n = 4$ (dots). The full line corresponds to $F^{(s)}$ with $Z = Z_{QS}$. In both cases we take $Z_{QS} = -1$, $\mu = 1$, $k = 1.1$, $\ell = 0$, $\beta = 0.8$.

4.3 Laguerre Quasi-Sturmian functions

Laguerre Quasi-Sturmian functions are solutions of the differential equation (4.3a) for the particular case of a Laguerre-type function as driven term, together with boundary conditions (4.3b) and (4.3c). We denote these Laguerre Quasi-Sturmian solutions as $Q_n^{L(\pm)}$.

As a consequence of the relation between Slater-type orbitals and Laguerre-type functions established in (1.7), the functions $Q_n^{L(\pm)}$ are a linear finite combination of Slater Quasi-Sturmian functions. This is a particular case of the situation described in **Remark 4.1.4**. Thus, we have a first closed form for the functions $Q_n^{L(\pm)}$ and the corresponding asymptotic coefficients, in terms of Slater Quasi-Sturmian functions

$$Q_n^{L(\pm)}(\ell, \beta; r) = \sum_{j=0}^{n} c_{n,j}^L \, Q_j^{STO\,(\pm)}(\ell, \beta; r), \tag{4.21a}$$

$$\mathcal{Q}_n^{L\,as} = \sum_{j=0}^{n} c_{n,j}^L \, \mathcal{Q}_j^{STO\,as}, \tag{4.21b}$$

with $c_{n,j}^L$ defined in (1.7b). Using expression (4.18) we can perform the second sum to obtain

$$\mathcal{Q}_n^{L\,as} = \frac{2\mu}{k}\, s_n, \tag{4.22}$$

where s_n, defined in (1.30), are the coefficients associated to the Laguerre expansion of the regular Coulomb wave function.

In terms of the Green's function, we have the following alternative representation

$$Q_n^{L(\pm)}(\ell,\beta;r) = \int_0^\infty \mathcal{G}_C^{(\pm)}(\ell;\ r,\ r')\, \frac{1}{r'}\, \phi_n^L(\ell,\beta;r')\, dr'. \tag{4.23}$$

From (1.62), after some algebraic manipulations, one finds

$$\begin{aligned} Q_n^{L(\pm)}(\ell,\beta;r) =& \frac{2\mu\, N_{n,\ell}}{\beta \mp ik}\, (2\beta r)^{\ell+1} e^{-\beta r} \\ &\times \int_0^1 (1-z)^{\ell \pm i\eta(Z_{QS})} (1-\omega^{\pm1}\, z)^{\ell \mp i\eta(Z_{QS})} (1-z-\omega^{\pm1}\, z)^n \\ &\quad \times e^{z(\beta \pm ik)r}\, L_n^{2\ell+1}\left(\frac{(1-z)(1-\omega^{\pm1}\, z)}{1-z-\omega^{\pm1}\, z}\, 2\beta r \right) dz. \end{aligned} \tag{4.24}$$

4.3.1 Series representation in terms of Laguerre-type functions

The coefficients of the series expansion

$$Q_n^{L(\pm)}(\ell,\beta;r) = \sum_q a_{n,q}^{(\pm)}\, \phi_q^L(\ell,\beta;r) \tag{4.25}$$

are given by

$$\begin{aligned} a_{n,q}^{(\pm)} &= \int_0^\infty \phi_q^L(\ell,\beta;r)\, \frac{1}{r}\, Q_n^{L(\pm)}(r)\, dr \\ &\overset{(4.23)}{=} \int_0^\infty \int_0^\infty \frac{1}{r}\, \phi_q^L(\ell,\beta;r)\, \mathcal{G}_C^{(\pm)}(\ell;\ r,\ r')\, \frac{1}{r'}\, \phi_n^L(\ell,\beta;r')\, dr\, dr'. \end{aligned}$$

This is exactly the expression for the coefficients $g_{n,q}^{(\pm)}$ of the series representation of the Green's function given by formulas (1.64), (1.66). Then, we have found

$$Q_n^{L(\pm)}(\ell,\beta;r) = \sum_j g_{n,j}^{(\pm)}\, \phi_j^L(\ell,\beta;r) \tag{4.26a}$$

$$= \frac{2\mu}{k}\, \hat{h}_n^{(\pm)} \sum_{j=0}^{n} s_j\, \phi_j^L(\ell,\beta;r) + \frac{2\mu}{k}\, s_n \sum_{j=n+1}^{\infty} \hat{h}_j^{(\pm)}\, \phi_j^L(\ell,\beta;r). \tag{4.26b}$$

Notice that for $n = 0$ (4.26b) yields

$$Q_0^{L(\pm)}(\ell, \beta; r) = \frac{2\mu}{k}\, s_0 \sum_{j=0}^{\infty} \hat{h}_j^{(\pm)}\, \phi_j^L(\ell, \beta; r) = \frac{2\mu}{k}\, s_0\, \hat{H}^{(\pm)}(\ell, \beta; r)$$

which is the proportionality relation (4.6) established in **Remark 4.1.2**.

In addition, from (4.26a) and (1.63) we find the following relation between Coulomb Green's functions and Laguerre Quasi-Sturmian functions,

$$\mathcal{G}_C^{(\pm)}(\ell; r, r') = \sum_n Q_n^{L(\pm)}(\ell, \beta; r)\, \phi_n^L(\ell, \beta; r'). \tag{4.27}$$

4.3.2 Illustration

We have calculated, using the integral formula (4.24), several Laguerre Quasi-Sturmian functions with different n values and parameters. In **Figure 4.3** we show their real and imaginary parts. Clearly, the Quasi-Sturmian functions achieve their asymptotic behavior when the driven term $\frac{1}{r}\phi_n^L(\ell, \beta; r)$ (dashed line) vanishes.

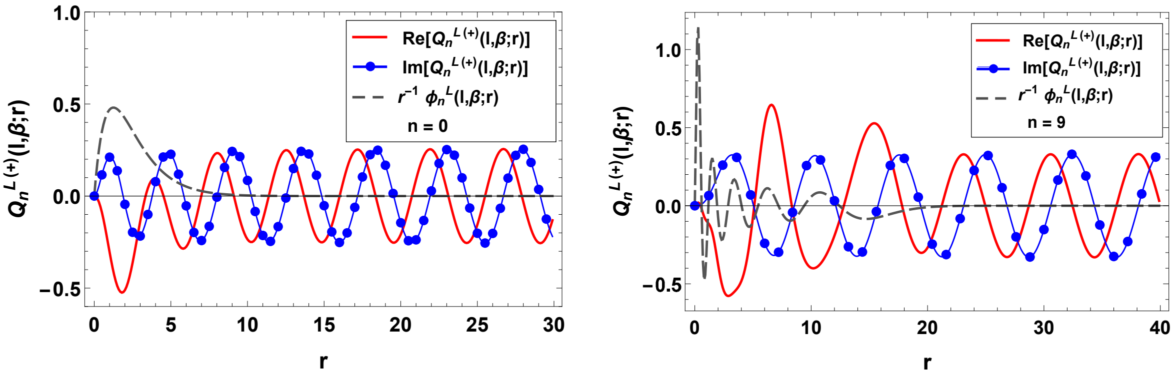

Figure 4.3: Real (solid line) and imaginary (line with dots) part of two different Laguerre Quasi-Sturmian function. Left panel: $n = 0$, $\ell = 1$, $\beta = 0.8$, $\mu = 1$, $Z_{QS} = -2$, $k = 1.25$. Right panel: $n = 9$, $\ell = 2$, $\beta = 1.4$, $\mu = 1$, $Z_{QS} = -1$, $k = 0.8$. The dashed line represents the corresponding generating Laguerre-type driven term.

Figure 4.4 corresponds to the real and imaginary parts of "normalized" outgoing Laguerre Quasi-Sturmian functions

$$\overline{Q}_n^{L(+)}(\ell, \beta; r) = \frac{1}{\mathcal{Q}_n^{L\,as}} Q_n^{L(+)}(\ell, \beta; r)$$

for $Z_{QS} = -1$, $\mu = 1$, $k = 1.3$, $\ell = 2$, $\beta = 1.1$. The left panel shows the real part of $\overline{Q}_n^{L(+)}$

taking $n = 2$, $n = 11$ and $n = 16$. We can observe how the asymptotic behavior of the real part is gradually reached as n increases, as explained in **Remark 4.1.1**. In the right panel we compare the imaginary part of $\overline{Q}_n^{L(+)}$ with the regular Coulomb wave function $F^{(s)}$. This plot illustrates the fact that imaginary part of Quasi-Sturmian functions coincides (up to a real factor) with the sine-like Coulomb wave function [identity (4.4)].

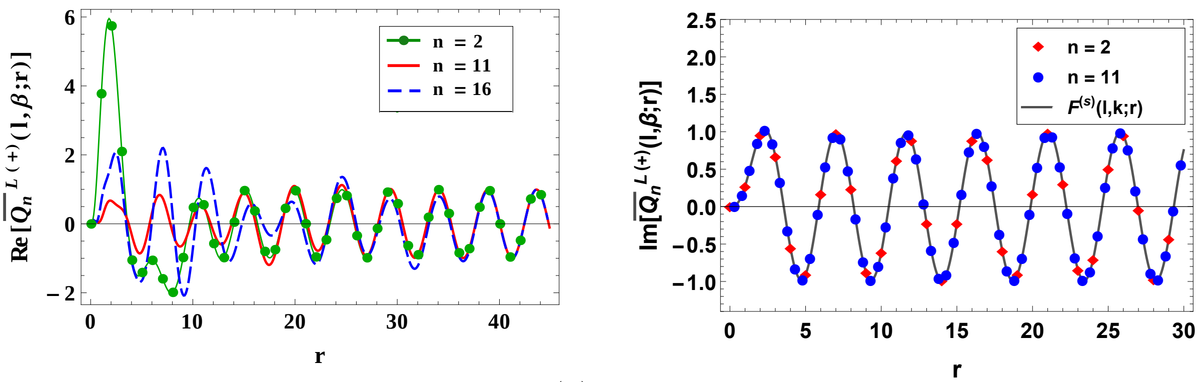

Figure 4.4: Left panel: real part of $\overline{Q}_n^{L(+)}(\ell, \beta; r)$ for $n = 2$ (line with dots), $n = 11$ (full line) and $n = 16$ (dashed line). Right panel: imaginary part of $\overline{Q}_n^{L(+)}(\ell, \beta; r)$ for $n = 2$ (diamonds) and $n = 11$ (dots). The full line corresponds to the Coulomb wave function $F^{(s)}(\ell, k; r)$. In both cases we take $Z_{QS} = -1$, $\mu = 1$, $k = 1.3$, $\ell = 2$, $\beta = 1.1$.

4.3.3 Integrals involving Laguerre Quasi-Sturmian functions

In this section we calculate analytically four integrals involving Laguerre Quasi-Sturmian functions. These kind of integrals usually appear in scattering problems as we will see in the last two chapters of this thesis. The key to perform the calculation is the use of the Laguerre expansion (4.26a).

We start with

$$\begin{aligned}\int_0^\infty \phi_q^L(\ell, \beta; r)\, \frac{1}{r}\, Q_n^{L\,(\pm)}(\ell, \beta; r)\, dr &= \sum_j g_{n,j}^{(\pm)} \int_0^\infty \phi_q^L(\ell, \beta; r)\, \frac{1}{r}\, \phi_j^L(\ell, \beta; r)\, dr \\ &= g_{n,q}^{(\pm)}. \end{aligned} \tag{4.28}$$

Next, we introduce the notation $Q_{m,n}^{(\pm)}$ for the the Quasi-Sturmian functions with an ℓ parameter depending on an index m, $\ell = \ell_m$. And we perform

$$
\begin{aligned}
&\int_0^\infty \phi_q^L(\ell_p,\beta;r)\,\frac{1}{r}\,Q_{m,n}^{L\,(\pm)}(\ell_m,\beta;r)\,dr \\
&\quad = \sum_s g_{n,s}^{(\pm)} \int_0^\infty \phi_q^L(\ell_p,\beta;r)\,\frac{1}{r}\,\phi_s^L(\ell_m,\beta;r)\,dr \\
&\quad \overset{(1.16)}{=} \frac{\Gamma(\ell_p+\ell_m+2)}{N_{q,\ell_p}\,\Gamma(2\ell_p+2)} \sum_s \frac{N_{s,\ell_m}}{s!}\, g_{n,s}^{(\pm)} \sum_{j=0}^{q} \frac{(\ell_p+\ell_m+2)_j(-q)_j}{(2\ell_p+2)_j\; j!}\,(\ell_m-\ell_p-j)_s.
\end{aligned} \tag{4.29}
$$

Now, for the case where the weight function is not present we cannot use the orthogonality relation of the Laguerre-type functions, and we have

$$
\begin{aligned}
&\int_0^\infty \phi_q^L(\ell,\beta;r)\,Q_n^{L\,(\pm)}(\ell,\beta;r)\,dr \\
&\quad = \sum_j g_{n,j}^{(\pm)} \int_0^\infty \phi_q^L(\ell,\beta;r)\,\phi_j^L(\ell,\beta;r)\,dr \\
&\quad \overset{(1.12c)}{=} \sum_j g_{n,j}^{(\pm)} \left(\frac{\ell+1+q}{\beta}\,\delta_{q,j} - \frac{N_{q+1,\ell}}{N_{q,\ell}}\,\frac{2\ell+2+q}{2\beta}\,\delta_{q+1,j} - \frac{N_{q-1,\ell}}{N_{q,\ell}}\,\frac{q}{2\beta}\,\delta_{q-1,j} \right) \\
&\quad = \frac{\ell+1+q}{\beta}\,g_{n,q}^{(\pm)} - \frac{N_{q+1,\ell}}{N_{q,\ell}}\,\frac{2\ell+2+q}{2\beta}\,g_{n,q+1}^{(\pm)} - \frac{N_{q-1,\ell}}{N_{q,\ell}}\,\frac{q}{2\beta}\,g_{n,q-1}^{(\pm)}.
\end{aligned} \tag{4.30}
$$

Finally, the integral of two Quasi-Sturmian functions yields

$$
\begin{aligned}
&\int_0^\infty Q_n^{(\pm)}(\ell,\beta;r)\,\frac{1}{r}\,Q_p^{(\pm)}(\ell,\beta;r)\,dr \\
&\qquad = \int_0^\infty \left(\sum_j g_{n,j}^{(\pm)}\; \phi_j^L(\ell,\beta;r) \right) \frac{1}{r} \left(\sum_i g_{p,i}^{(\pm)}\; \phi_i^L(\ell,\beta;r) \right) dr \\
&\qquad = \sum_j \; g_{n,j}^{(\pm)}\; g_{j,p}^{(\pm)}.
\end{aligned} \tag{4.31}
$$

Clearly, we are interchanging series and integrals without proving that the property can actually be applied. For this reason, we have performed some numerical verifications by comparing the results obtained by direct integration with the analytical expressions we found. For the first and third integrals [formula (4.28) and (4.30)], the comparison showed an excellent agreement. The fourth one [formula (4.31)] will be tested in **Section 4.3.7**, because this integral happens to be related to the derivative with respect to one of the parameters of the Laguerre Quasi-Sturmian functions. The numerical comparison for the second integral [formula (4.29)] is presented in **Table 4.1** for outgoing Quasi-Sturmian functions and the following values of the parameters: $Z=-2,\ \mu=1,\ k=1.8,\ \beta=2.6.$

The table compares, for different (ℓ_p, q, ℓ_m, n) values, the results obtained by numerically performing the integral with those of the corresponding analytical double series, noted $\Upsilon_{\ell_p,q;\ell_m,n}$.

ℓ_p	q	ℓ_m	n	$\int_0^\infty \phi_q^L(\ell_p,\beta;r)\,\frac{1}{r}\,Q_n^{L\,(+)}(\ell_m,\beta;r)\,dr$	$\Upsilon_{\ell_p,q;\ell_m,n}$
5.5	5	7.5	2	$-0.00264972+0.0054675\,i$	$-0.00264956+0.0054675\,i$
11.5	8	19.5	11	$0.000203239-0.00397045\,i$	$0.00020364-0.0039705\,i$
13.5	12	7.5	18	$-0.0305365-0.0306694\,i$	$-0.0305365-0.0306694\,i$
21.5	19	29.5	15	$0.0105045+0.00941789\,i$	$0.0105272+0.00965439\,i$

Table 4.1: Numerical verification of identity (4.29) for different indices ℓ_p, q, ℓ_m, n, and parameters $Z=-2, \mu=1$, $k=1.8$, $\beta=2.6$.

For all cases considered, the identity (4.29) is well satisfied. The small difference appearing in the last line of the table is related to the fact that the integrand becomes very oscillating, causing an increase of the numerical error.

4.3.4 Recurrence relations

From the recurrence relation (1.65) established for the coefficients $g_{n,q}$, and taking $Z=Z_{QS}$, one can deduce a relation for the Laguerre Quasi-Sturmian functions. Multiplying both sides of (1.65) by ϕ_q^L and making a formal summation over q we obtain

$$A_{n+1}\sum_q g_{n+1,q}^{(\pm)}\;\phi_q^L(\ell,\beta;r)+B_n(Z_{QS})\sum_q g_{n,q}^{(\pm)}\;\phi_q^L(\ell,\beta;r)$$
$$+A_n\sum_q g_{n-1,q}^{(\pm)}\;\phi_q^L(\ell,\beta;r)=\sum_q \delta_{n,q}\,\phi_q^L(\ell,\beta;r),$$

where A_n and B_n are given by formula (1.20). According to (4.26a), the series on the left hand side corresponds to Laguerre Quasi-Sturmian functions while the series on the right hand side reduces to ϕ_n^L. Hence, we have

$$A_{n+1}\,Q_{n+1}^{L(\pm)}(\ell,\beta;r)+B_n(Z_{QS})\,Q_n^{L(\pm)}(\ell,\beta;r)+A_n\,Q_{n-1}^{L(\pm)}(\ell,\beta;r)=\phi_n^L(\ell,\beta;r) \qquad (4.32)$$

taking, for the case $n = 0$, $Q^{L(\pm)}_{-1} \equiv 0$. As an alternative to the integral (4.24) or series (4.26) representations, the recurrence formula (4.32) may be useful to generate numerically a large number of Laguerre Quasi-Sturmian functions.

4.3.5 The Christoffel-Darboux formula

For orthogonal polynomials p_n with weight function w defined on the interval $[a, b]$, one has the Christoffel-Darboux formula (Theorem 5.2.4 in [43])

$$\sum_{k=0}^{n} \frac{p_k(x)p_k(y)}{h_k} = \frac{a_n}{a_{n+1}} \frac{p_{n+1}(x)p_n(y) - p_{n+1}(y)p_n(x)}{(x-y)h_n},$$

where a_k is the leading coefficient of p_k and $h_k = \int_a^b p_k^2(x)\, w(x)\, dx$.

Such general result is a consequence of the recurrence relation these polynomials satisfy. For Laguerre Quasi-Sturmian functions we found a non-homogeneous recurrence relation so we can expect an analogous formulation. Indeed, it is possible to express

$$Q^{L(\pm)}_{n+1}(\ell, \beta; r_1)\, Q^{L(\pm)}_{n}(\ell, \beta; r_2) - Q^{L(\pm)}_{n+1}(\ell, \beta; r_2)\, Q^{L(\pm)}_{n}(\ell, \beta; r_1) \tag{4.33}$$

as a combination of the first n Laguerre Quasi-Sturmian. To do so, we first rewrite relation (4.32) as

$$Q^{L(\pm)}_{n+1}(\ell, \beta; r) = \frac{1}{A_{n+1}}\, \phi^L_n(\ell, \beta; r) - \frac{B_n(Z_{QS})}{A_{n+1}}\, Q^{L(\pm)}_{n}(\ell, \beta; r) - \frac{A_n}{A_{n+1}}\, Q^{L(\pm)}_{n-1}(\ell, \beta; r), \tag{4.34}$$

and then replace $Q^{L(\pm)}_{n+1}$ in (4.33)

$$\begin{aligned}
&Q^{L(\pm)}_{n+1}(\ell, \beta; r_1)\, Q^{L(\pm)}_{n}(\ell, \beta; r_2) - Q^{L(\pm)}_{n+1}(\ell, \beta; r_2)\, Q^{L(\pm)}_{n}(\ell, \beta; r_1) \\
&\quad = \frac{1}{A_{n+1}} \left[\phi_n(\ell, \beta; r_1) Q^{L(\pm)}_{n}(\ell, \beta; r_2) - \phi^L_n(\ell, \beta; r_2) Q^{L(\pm)}_{n}(\ell, \beta; r_1)\right] \\
&\quad\quad + \frac{A_n}{A_{n+1}} \left[Q^{L(\pm)}_{n}(\ell, \beta; r_1)\, Q^{L(\pm)}_{n-1}(\ell, \beta; r_2) - Q^{L(\pm)}_{n}(\ell, \beta; r_2)\, Q^{L(\pm)}_{n-1}(\ell, \beta; r_1)\right].
\end{aligned}$$

The second term on the right hand side has the same form of the initial one, so we can use again (4.34) now to replace $Q^{L(\pm)}_{n}$ and find

$$
\begin{aligned}
&Q_{n+1}^{L(\pm)}(\ell,\beta;r_1)\,Q_n^{L(\pm)}(\ell,\beta;r_2)-Q_{n+1}^{L(\pm)}(\ell,\beta;r_2)\,Q_n^{L(\pm)}(\ell,\beta;r_1)\\
&\quad=\frac{1}{A_{n+1}}\left[\phi_n(\ell,\beta;r_1)\,Q_n^{L(\pm)}(\ell,\beta;r_2)-\phi_n^L(\ell,\beta;r_2)\,Q_n^{L(\pm)}(\ell,\beta;r_1)\right]\\
&\qquad+\frac{A_n}{A_{n+1}}\left\{\frac{1}{A_n}\left[\phi_{n-1}(\ell,\beta;r_1)\,Q_{n-1}^{L(\pm)}(\ell,\beta;r_2)-\phi_{n-1}^L(\ell,\beta;r_2)\,Q_{n-1}^{L(\pm)}(\ell,\beta;r_1)\right]\right.\\
&\qquad\quad\left.+\frac{A_{n-1}}{A_n}\left[Q_{n-1}^{L(\pm)}(\ell,\beta;r_1)\,Q_{n-2}^{L(\pm)}(\ell,\beta;r_2)-Q_{n-1}^{L(\pm)}(\ell,\beta;r_2)\,Q_{n-2}^{L(\pm)}(\ell,\beta;r_1)\right]\right\}.
\end{aligned}
$$

Again we obtain a term on which we can apply (4.34). Repeating the procedure $n-2$ more times we finally find

$$
\begin{aligned}
&Q_{n+1}^{L(\pm)}(\ell,\beta;r_1)\,Q_n^{L(\pm)}(\ell,\beta;r_2)-Q_{n+1}^{L(\pm)}(\ell,\beta;r_2)\,Q_n^{L(\pm)}(\ell,\beta;r_1)\\
&\quad=\frac{1}{A_{n+1}}\sum_{j=0}^{n}\left[\phi_j(\ell,\beta;r_1)\,Q_j^{L(\pm)}(\ell,\beta;r_2)-\phi_j^L(\ell,\beta;r_2)\,Q_j^{L(\pm)}(\ell,\beta;r_1)\right].
\end{aligned}
\tag{4.35}
$$

Consequences of this formula

From the asymptotic behavior of Quasi-Sturmian functions [formulas (4.3c) and (4.22)] and of Laguerre-type functions [formula (1.8c)], for large values of r_2 the left hand side of equation (4.35) becomes

$$
\begin{aligned}
&Q_{n+1}^{L(\pm)}(\ell,\beta;r_1)\,Q_n^{L(\pm)}(\ell,\beta;r_2)-Q_{n+1}^{L(\pm)}(\ell,\beta;r_2)\,Q_n^{L(\pm)}(\ell,\beta;r_1)\\
&\quad\overset{r_2\to\infty}{\sim}\frac{2\mu}{k}\left[Q_{n+1}^{L(\pm)}(\ell,\beta;r_1)\,s_n-s_{n+1}\,Q_n^{L(\pm)}(\ell,\beta;r_1)\right]\,e^{\pm i\left[k\,r_2-\eta(Z_{QS})\ln(2k\,r_2)+\sigma_C(\ell,Z_{QS})-\frac{\pi}{2}\ell\right]},
\end{aligned}
$$

while for the right hand side we find

$$
\begin{aligned}
&\phi_j(\ell,\beta;r_1)\,Q_j^{L(\pm)}(\ell,\beta;r_2)-\phi_j^L(\ell,\beta;r_2)\,Q_j^{L(\pm)}(\ell,\beta;r_1)\\
&\qquad\qquad\overset{r_2\to\infty}{\sim}\frac{2\mu}{k}\phi_j(\ell,\beta;r_1)\,s_j\,e^{\pm i\left[k\,r_2-\eta(Z_{QS})\ln(2k\,r_2)+\sigma_C(\ell,Z_{QS})-\frac{\pi}{2}\ell\right]}.
\end{aligned}
$$

The $r_2\to\infty$ limit of both sides of identity (4.35) yields therefore

$$
Q_{n+1}^{L(\pm)}(\ell,\beta;r)=\frac{s_{n+1}}{s_n}\,Q_n^{L(\pm)}(\ell,\beta;r)\;+\frac{1}{A_{n+1}\,s_n}\sum_{j=0}^{n}s_j\,\phi_j^L(\ell,\beta;r).
\tag{4.36}
$$

If we repeatedly apply this identity on itself we obtain, in a first step,

$$Q_{n+1}^{L(\pm)}(\ell,\beta;r) = \frac{s_{n+1}}{s_{n-1}}\, Q_{n-1}^{L(\pm)}(\ell,\beta;r) + \frac{1}{A_n}\frac{s_{n+1}}{s_n\, s_{n-1}} \sum_{j=0}^{n-1} s_j\, \phi_j^L(\ell,\beta;r) + \frac{1}{A_{n+1}\, s_n} \sum_{j=0}^{n} s_j\, \phi_j^L(\ell,\beta;r).$$

and finally

$$Q_{n+1}^{L(\pm)}(\ell,\beta;r) = \frac{s_{n+1}}{s_0}\, Q_0^{L(\pm)}(\ell,\beta;r) + \sum_{j=0}^{n} D_j^n\, \phi_j^L(\ell,\beta;r), \tag{4.37a}$$

$$D_j^n = s_{n+1}\, s_j \sum_{p=j}^{n} \frac{1}{A_{p+1}\, s_{p+1} s_p}. \tag{4.37b}$$

The coefficients s_n and A_n, as well as the Laguerre-type functions ϕ_n^L, are quite easy to evaluate. In **Chapter 1** we have shown that s_n and ϕ_n^L are related to orthogonal polynomials. Hence formula (4.37) provides probably the simplest form to evaluate any Laguerre Quasi-Sturmian function $Q_n^{L(\pm)}$ once we have $Q_0^{L(\pm)}$.

Result (4.37) has itself another consequence. Using the series representation (4.26b), the left hand side of (4.37a) can be expressed as

$$Q_{n+1}^{L(\pm)}(\ell,\beta;r) = \frac{2\mu}{k}\hat{h}_{n+1}^{(\pm)} \sum_{j=0}^{n} s_j\, \phi_j^L(\ell,\beta;r) + \frac{2\mu}{k} s_{n+1} \sum_{j=n+1}^{\infty} \hat{h}_j^{(\pm)}\, \phi_j^L(\ell,\beta;r)$$

while the right hand side reads

$$\begin{aligned}
&\frac{s_{n+1}}{s_0}\, Q_0^{L(\pm)}(\ell,\beta;r) + \sum_{j=0}^{n} D_j^n\, \phi_j^L(\ell,\beta;r)\\
&\quad = \frac{2\mu}{k} s_{n+1} \sum_{j} \hat{h}_j^{(\pm)} \phi_j^L(\ell,\beta;r) + \sum_{j=0}^{n} D_j^n\, \phi_j^L(\ell,\beta;r)\\
&\quad = \frac{2\mu}{k} s_{n+1} \sum_{j=0}^{n} \left[\hat{h}_j^{(\pm)} + \frac{k}{2\mu}\, s_j \sum_{p=j}^{n} \frac{1}{A_{p+1}\, s_{p+1}\, s_p}\right] \phi_j^L(\ell,\beta;r) + \frac{2\mu}{k} s_{n+1} \sum_{j=n+1}^{\infty} \hat{h}_j^{(\pm)} \phi_j^L(\ell,\beta;r).
\end{aligned}$$

Equating these two expressions we obtain

$$\hat{h}_{n+1}^{(\pm)} \sum_{j=0}^{n} s_j\, \phi_j^L(\ell,\beta;r) = s_{n+1} \sum_{j=0}^{n} \left[\hat{h}_j^{(\pm)} + \frac{k}{2\mu}\, s_j \sum_{p=j}^{n} \frac{1}{A_{p+1}\, s_{p+1}\, s_p}\right] \phi_j^L(\ell,\beta;r),$$

and, due to the linear independence of the Laguerre-type functions, we find a relation for the coefficients s_n, $\hat{h}_n^{(\pm)}$,

$$\hat{h}_{n+1}^{(\pm)}\, s_j - \hat{h}_j^{(\pm)}\, s_{n+1} = \frac{k}{2\mu}\, s_{n+1}\; s_j \sum_{p=j}^{n} \frac{1}{A_{p+1}\, s_{p+1}\, s_p}, \qquad j \leqslant n. \tag{4.38}$$

If $j = n$, this identity simplifies to

$$\hat{h}_{n+1}^{(\pm)}\, s_n - \hat{h}_n^{(\pm)}\, s_{n+1} = \frac{k}{2\mu\, A_{n+1}},$$

which is a formula introduced by Heller in reference [62]. Hence, relation (4.38) constitutes a generalization of such identity to any combination of indices n, j.

4.3.6 Laguerre Quasi-Sturmian functions and Coulomb wave functions

It is possible to provide a relation between the sine-like Coulomb wave function $F^{(s)}$ introduced in **Section 1.2** and $Q_n^{L(\pm)}$. Using the series representation (1.32) for $F^{(s)}$, the recurrence relations (4.32) and (1.34) for Quasi-Sturmian function and coefficients s_n, respectively, and taking $Z = Z_{QS}$, we deduce

$$\begin{aligned}
F^{(s)}(\ell, k; r) &\overset{(1.32)}{=} \sum_n s_n\, \phi_n^L(\ell, \beta; r) \\
&\overset{(4.32)}{=} \lim_{N\to\infty} \Big\{ s_0\, B_0(Z)\, Q_0^{L(\pm)}(\ell, \beta; r) + s_0\, A_1\, Q_1^{L(\pm)}(\ell, \beta; r) \\
&\qquad + \sum_{n=1}^{N} s_n \Big[A_{n+1}\, Q_{n+1}^{L(\pm)}(\ell, \beta; r) + B_n(Z)\, Q_n^{L(\pm)}(\ell, \beta; r) \\
&\qquad + A_n\, Q_{n-1}^{L(\pm)}(\ell, \beta; r)\Big]\Big\} \\
&= \lim_{N\to\infty} \Big\{ s_0\, B_0(Z)\, Q_0^{L(\pm)}(\ell, \beta; r) + s_1\, A_1\, Q_0^{L(\pm)}(\ell, \beta; r) \\
&\qquad + \sum_{n=1}^{N-1} s_{n+1}\, A_{n+1}\, Q_n^{L(\pm)}(\ell, \beta; r) \\
&\qquad + \sum_{n=1}^{N} s_n\, B_n(Z)\, Q_n^{L(\pm)}(\ell, \beta; r) + \sum_{n=1}^{N+1} s_{n-1}\, A_n\, Q_n^{L(\pm)}(\ell, \beta; r)\Big\}
\end{aligned}$$

Thus, using (1.34), we finally obtain

$$F^{(s)}(\ell, k; r) = \lim_{n\to\infty} A_{n+1} \Big[s_n\, Q_{n+1}^{L(\pm)}(\ell, \beta; r) - s_{n+1}\, Q_n^{L(\pm)}(\ell, \beta; r)\Big]. \tag{4.39}$$

To illustrate this result we plot in **Figure 4.5** the exact sine-like Coulomb wave function $F^{(s)}$ and its approximation

$$F_N^{(s)}(\ell,k;r) = A_{N+1}\left[s_N\, Q_{N+1}^{L(+)}(\ell,\beta;r) - s_{N+1}\, Q_N^{L(+)}(\ell,\beta;r)\right], \qquad (4.40)$$

in terms of outgoing Laguerre Quasi-Sturmian functions. As expected, an increment on N improves the quality and extends the radial range of the approximation $F_N^{(s)}$.

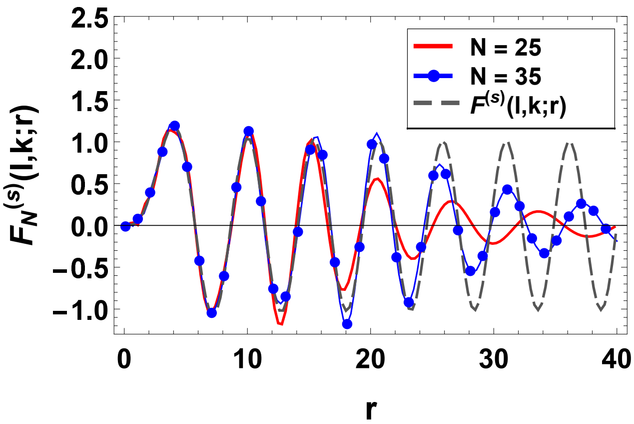

Figure 4.5: Plot of $F_N^{(s)}$, defined in (4.40), as a function of r, using $N = 25$ (full line) and $N = 35$ (line with dots). The dashed line corresponds to the regular Coulomb wave function $F^{(s)}$. Parameters: $Z = -1$, $\mu = 1$, $k = 1.25$, $\ell = 2$, $\beta = 0.8$.

4.3.7 Quasi-Sturmian functions with a variable charge

In order to use the functions $Q_n^{L(\pm)}$ to describe three-body scattering problems we present and study in this section a generalization of Laguerre Quasi-Sturmian functions. We no longer consider the charge Z_{QS} as a fixed parameter but as a function $\widetilde{C} = \widetilde{C}(\omega_5)$ of a set of variables ω_5. This situation of having a variable charge in a Coulomb potential appears when studying three-body scattering problems in hyperspherical coordinates, where ω_5 represents collectively the five angular variables of the coordinate system [see **Chapter 6**]. A great advantage of these angular-dependent Quasi-Sturmian functions is that their asymptotic behavior may be chosen to match that of three-body scattering wave functions described by Peterkop [21].

Hereafter, we present Laguerre Quasi-Sturmian functions with a general variable charge $\widetilde{C}$ and replace the radial variable r by the hyperradial variable ρ (used in hyperpherical coordinates). The boundary value problem defining these functions is

$$\left[-\frac{1}{2\mu}\frac{d^2}{d\rho^2}+\frac{\ell(\ell+1)}{2\mu\,\rho^2}+\frac{\widetilde{C}(\omega_5)}{\rho}-E\right]Q_n^{L(\pm)}(\ell,\beta,\omega_5;\rho)=\frac{1}{\rho}\,\phi_n^L(\ell,\beta;\rho), \tag{4.41a}$$

$$Q_n^{(\pm)}(\ell,\beta,\omega_5;0)=0, \tag{4.41b}$$

$$Q_n^{(\pm)}(\ell,\beta,\omega_5;\rho)\overset{\rho\to\infty}{\sim}\mathcal{Q}_n^{as}(\omega_5)\,e^{\pm i\left[k\rho-\eta(\widetilde{C}(\omega_5))\ln(2k\rho)+\sigma_C(\ell,\widetilde{C}(\omega_5))-\frac{\pi}{2}\ell\right]}. \tag{4.41c}$$

for $n\in\mathbb{N}\cup\{0\}$, $Z\in\mathbb{R}$, $\mu,E\in\mathbb{R}^+$ and $\ell\in\mathbb{R}^+\cup\{0\}$. The parameters η and σ_C were set in (1.23a) and (1.23b) respectively.

Clearly, analytical expressions for these Quasi-Sturmian functions and all related properties can be obtained simply by replacing Z_{QS} with the ω_5-dependent charge $\widetilde{C}$ in the formulas presented for the Laguerre Quasi-Sturmian functions $Q_n^{L(\pm)}$. The integral representation (4.24) becomes

$$\begin{aligned}Q_n^{L(\pm)}(\ell,\beta,\omega_5;\rho)=&\frac{2\mu\,N_{n,\ell}}{\beta\mp ik}\,(2\beta\rho)^{\ell+1}e^{-\beta\rho}\\&\times\int_0^1 dz\,(1-z)^{\ell\pm i\eta(\widetilde{C}(\omega_5))}(1-\omega^{\pm1}\,z)^{\ell\mp i\eta(\widetilde{C}(\omega_5))}(1-z-\omega^{\pm1}\,z)^n\\&\times e^{z(\beta\pm ik)\rho}\,L_n^{2\ell+1}\left(\frac{(1-z)(1-\omega^{\pm1}\,z)}{1-z-\omega^{\pm1}\,z}\,2\beta\rho\right),\end{aligned} \tag{4.42}$$

and the closed form for the asymptotic coefficient $\mathcal{Q}_n^{L\,as}$ can be obtained from (4.22). The series representation (4.26a) in terms of Laguerre-type functions reads now

$$Q_n^{L(\pm)}(\ell,\beta,\omega_5;\rho)=\sum_{j=0}^{\infty}g_{n,j}^{(\pm)}(\omega_5)\,\phi_j^L(\ell,\beta;\rho). \tag{4.43}$$

with $g_{n,j}^{(\pm)}$ defined by (1.66) but taking $Z=\widetilde{C}(\omega_5)$ in the expressions for s_n and $\hat{h}_n^{(\pm)}$. These ω_5-dependent coefficients $g_{n,j}^{(\pm)}$ satisfy the pseudo-recurrence relation (1.65),

$$A_{n+1}\,g_{n+1,j}^{(\pm)}(\omega_5)+B_n(\widetilde{C}(\omega_5))\,g_{n,j}^{(\pm)}(\omega_5)+A_n\,g_{n-1,j}^{(\pm)}(\omega_5)=\delta_{n,q}. \tag{4.44a}$$

As an immediate consequence, relation (4.32) becomes

$$\begin{aligned}A_{n+1}\,Q_{n+1}^{L(\pm)}(\ell,\beta,\omega_5;\rho)+B_n(\widetilde{C}(\omega_5))\,Q_n^{L(\pm)}(\ell,\beta,\omega_5;\rho)&\\+A_n\,Q_{n-1}^{L(\pm)}(\ell,\beta,\omega_5;\rho)=\phi_n^L(\ell,\beta;\rho)&\end{aligned} \tag{4.44b}$$

taking again, for the case $n=0$, $Q_{-1}^{L(\pm)}\equiv 0$.

Illustration

In order to present some illustrations of these Quasi-Sturmian functions, we introduce

$$C(\alpha) = \begin{cases} -\dfrac{Z-1}{\cos\alpha} - \dfrac{Z}{\sin\alpha}, & \text{for } 0 < \alpha < \dfrac{\pi}{4}, \\ \\ -\dfrac{Z}{\cos\alpha} - \dfrac{Z-1}{\sin\alpha}, & \text{for } \dfrac{\pi}{4} \leqslant \alpha < \dfrac{\pi}{2}. \end{cases} . \tag{4.45}$$

For the moment, the function C has no particular meaning, but in **Chapter 6** we will see that this is the variable charge corresponding to an approximation (the first term in a multipolar expansion) of the three-body Coulomb potential.

Using the integral representation (4.42) and taking as variable charge the function C, we present in **Figure 4.6** a plot of the real part of two α-dependent Laguerre Quasi-Sturmian function $Q_n^{L(+)} = Q_n^{L(+)}(\ell, \beta, \alpha; \rho)$. The plot is presented in spherical coordinates ($r_1 = \rho\cos\alpha$, $r_2 = \rho\sin\alpha$).

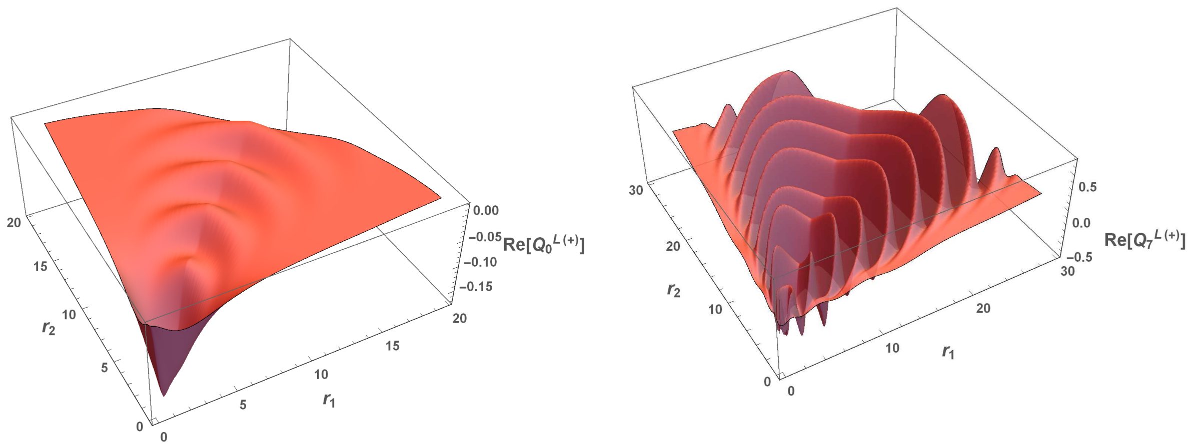

Figure 4.6: Real part of two α-dependent Laguerre Quasi-Sturmian function $Q_n^{L(+)}$ as functions of spherical coordinates (r_1, r_2) for $n = 0$ (left panel) and $n = 7$ (right panel). In both cases we fixed $\ell = 1$, $\beta = 0.8$, $\mu = 1$, $Z = 2$, $k = 1.25$.

In **Figure 4.7** we plot, as a function of α, the real and imaginary parts of two different coefficients $g_{n,q}^{(+)}$ calculated using formula (1.66) with the function C instead of Z. We observe that these coefficients are regular at the end points of the interval $(0, \frac{\pi}{2})$ even if the function C is not defined at these points. Also, for increasing values of the indices the coefficients oscillate more and the oscillations accumulate near the end points of the domain.

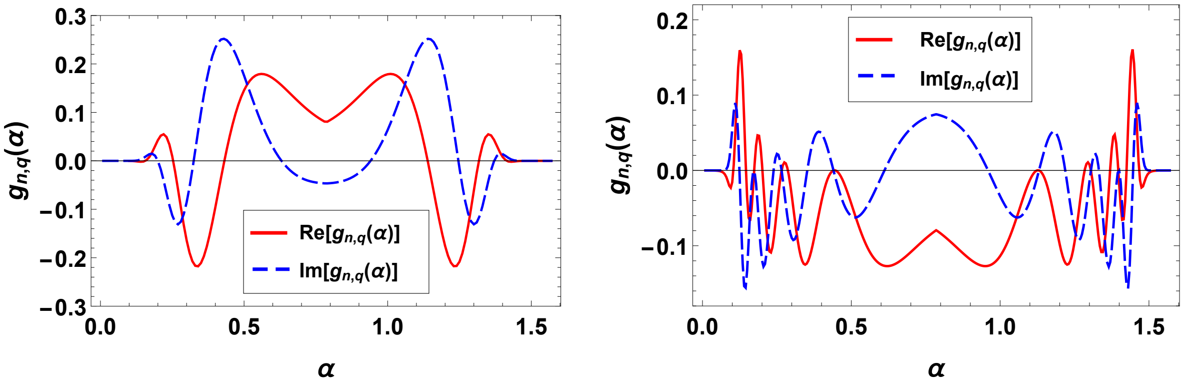

Figure 4.7: Real (solid line) and imaginary (dashed line) parts of two coefficients $g^{(+)}_{n,q}$ as a function of α: $n = 3$, $q = 8$ (left panel) and $n = 12, q = 9$ (right panel). We take $Z = 2, \mu = 1, k = 1.2, \ell = 1, \beta = 1.7$.

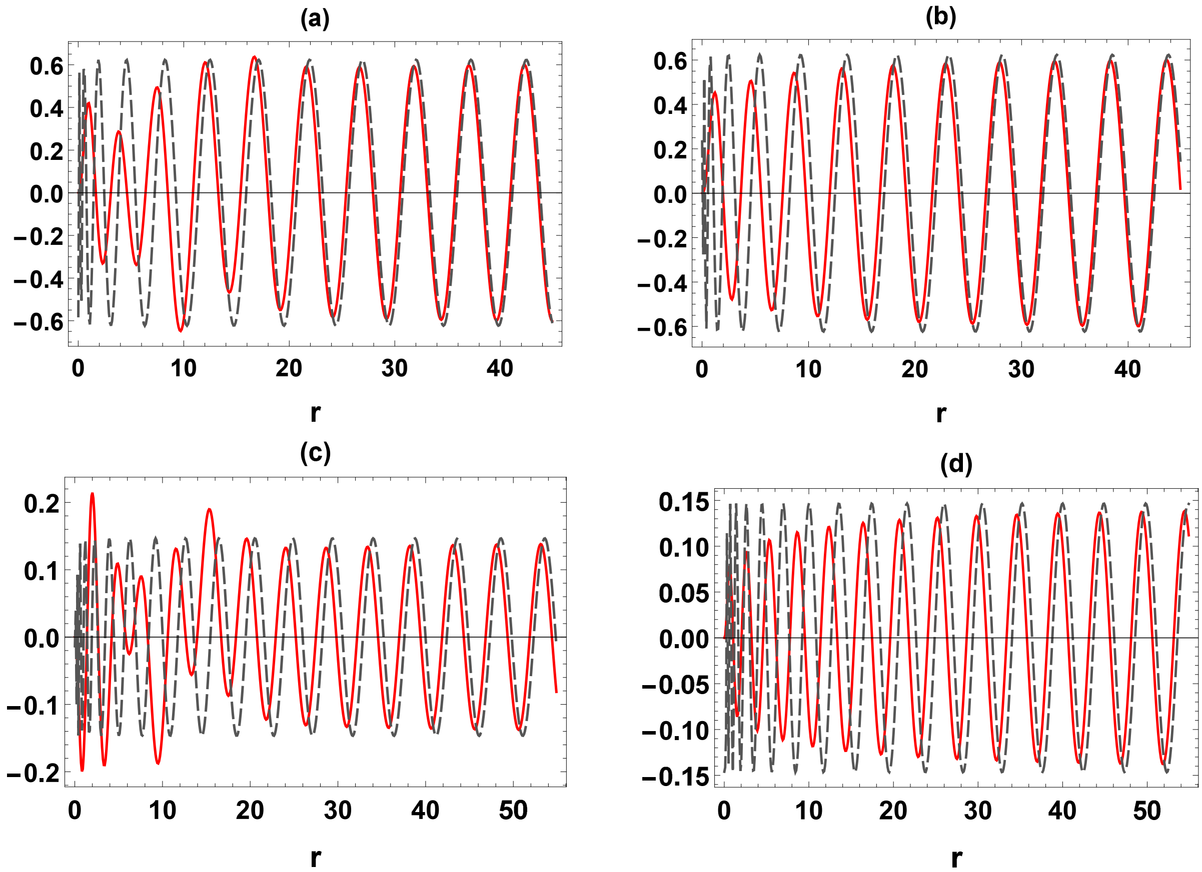

Figure 4.8: Panels (a) and (b): the full line represents the real and imaginary parts (respectively) of an α-dependent Quasi-Sturmian function $Q^{L(+)}_n$ as a function of ρ, fixing $\alpha = \frac{\pi}{4}$. The dashed line corresponds to the real and imaginary parts of its asymptotic behavior (4.3c). Panels (c) and (d) represent the same functions, but for $\alpha = \frac{\pi}{12}$. In all cases we take $n = 5$, $\ell = 2$, $\beta = 0.9$, $\mu = 1$, $Z = 2$, $k = 1.1$.

Finally we focus on the asymptotic behavior of the α-dependent Quasi-Sturmian functions. We present in **Figure 4.8** two radial sections of the function with fixed index $n = 5$. Panels (a) and (b) show, with solid line, the real and imaginary parts, respectively, of $Q_n^{L(+)}$ as a function of ρ and taking $\alpha = \dfrac{\pi}{4}$ as a constant. The dashed line corresponds to the real [panel (a)] and imaginary [panel (b)] parts of the asymptotic behavior (4.3c), calculated taking $Z_{QS} = C\left(\dfrac{\pi}{4}\right)$. Panels (c) and (d) present similar information but for a fixed $\alpha = \dfrac{\pi}{12}$. We clearly observe that for a α value close to the end points, the function C increases in magnitude, and the asymptotic behavior (4.3c) is reached at larger hyperradial distances.

Derivatives with respect to α

For the variable charge C defined by (4.45) we can explore the derivatives with respect to α of the coefficients $g_{n,j}^{(\pm)}$ and of the Quasi-Sturmian $Q_n^{L(\pm)}$.

From the series representation (4.43) we immediately obtain

$$\frac{\partial}{\partial\alpha} Q_n^{L(\pm)}(\ell,\beta,\alpha;\rho) = \sum_{j=0}^{\infty} \left[\frac{d}{d\alpha}\, g_{n,j}^{(\pm)}(\alpha)\right] \phi_j^L(\ell,\beta;\rho), \tag{4.46}$$

and from the pseudo-recurrence relations (4.44a) and (4.44b) we find

$$A_{n+1}\frac{d}{d\alpha}\, g_{n+1,j}^{(\pm)}(\alpha) + B_n(C(\alpha))\frac{d}{d\alpha}\, g_{n,j}^{(\pm)}(\alpha) + A_n\frac{d}{d\alpha}\, g_{n-1,j}^{(\pm)}(\alpha) = -\left[\frac{d}{d\alpha}\, C(\alpha)\right] g_{n,j}^{(\pm)}(\alpha), \tag{4.47a}$$

$$A_{n+1}\frac{\partial}{\partial\alpha}\, Q_{n+1}^{L(\pm)}(\ell,\beta,\alpha;\rho) + B_n(C(\alpha))\frac{\partial}{\partial\alpha}\, Q_n^{L(\pm)}(\ell,\beta,\alpha;\rho) + A_n\frac{\partial}{\partial\alpha}\, Q_{n-1}^{L(\pm)}(\ell,\beta,\alpha;\rho) = -\left[\frac{d}{d\alpha}\, C(\alpha)\right] Q_n^{L(\pm)}(\ell,\beta,\alpha;\rho) \tag{4.47b}$$

for A_n and B_n defined in (1.20).

A very interesting relation can be deduced following simple manipulations. Let us take the derivative with respect to α of both sides of the differential equation (4.41a) defining the α-dependent Quasi-Sturmian functions,

$$\left[-\frac{1}{2\mu}\frac{d^2}{d\rho^2} + \frac{\ell(\ell+1)}{2\mu\,\rho^2} + \frac{C(\alpha)}{\rho} - E\right]\frac{\partial}{\partial\alpha}Q_n^{L(\pm)}(\ell,\beta,\alpha;\rho) = -\left[\frac{d}{d\alpha}C(\alpha)\right]\frac{1}{\rho}\, Q_n^{L(\pm)}(\ell,\beta,\alpha;\rho). \tag{4.48}$$

On the other hand we take the differential equation (4.41a) for an index j, multiply both sides by

$$-\left[\frac{d}{d\alpha}C(\alpha)\right]\, g_{n,j}^{(\pm)}(\alpha)$$

and perform a formal summation over j to obtain

$$\left[-\frac{1}{2\mu}\frac{d^2}{d\rho^2}+\frac{\ell(\ell+1)}{2\mu\,\rho^2}+\frac{C(\alpha)}{\rho}-E\right]\left[-\frac{d}{d\alpha}C(\alpha)\right]\sum_{j=0}^{\infty} g_{n,j}^{(\pm)}(\alpha)Q_j^{L(\pm)}(\ell,\beta,\alpha;\rho)$$
$$= -\left[\frac{d}{d\alpha}C(\alpha)\right]\frac{1}{\rho}\sum_{j=0}^{\infty} g_{n,j}^{(\pm)}(\alpha)\,\phi_j^L(\ell,\beta;\rho). \quad (4.49)$$

From (4.43) we find that the right hand side is identical to that of equation (4.48): (4.48) and (4.49) are then the same differential equation. Supposing further that the solutions of both satisfy the same boundary conditions, we obtain

$$\frac{\partial}{\partial\alpha}Q_n^{L(\pm)}(\ell,\beta,\alpha;\rho) \quad = \quad -\left[\frac{d}{d\alpha}C(\alpha)\right]\sum_{j=0}^{\infty} g_{n,j}^{(\pm)}(\alpha)Q_j^{L(\pm)}(\ell,\beta,\alpha;\rho) \quad (4.50a)$$
$$\stackrel{(4.43)}{=} \quad -\left[\frac{d}{d\alpha}C(\alpha)\right]\sum_{p=0}^{\infty}\left[\sum_{j=0}^{\infty} g_{n,j}^{(\pm)}(\alpha)g_{j,p}^{(\pm)}(\alpha)\right]\phi_p^L(\ell,\beta;\rho). \quad (4.50b)$$

Besides, a series representation in terms of a basis set is unique. Thus equations (4.46) and (4.50b) imply

$$\frac{d}{d\alpha}\,g_{n,p}^{(\pm)}(\alpha) = -\left[\frac{d}{d\alpha}C(\alpha)\right]\sum_{j=0}^{\infty} g_{n,j}^{(\pm)}(\alpha)g_{j,p}^{(\pm)}(\alpha). \quad (4.51)$$

Finally, using relation (4.31), we obtain

$$\frac{d}{d\alpha}\,g_{n,p}^{(\pm)}(\alpha) = -\left[\frac{d}{d\alpha}C(\alpha)\right]\int_0^{\infty} Q_n^{(\pm)}(\ell,\beta,\alpha;\rho)\,\frac{1}{\rho}\,Q_p^{(\pm)}(\ell,\beta,\alpha;\rho)\,d\rho. \quad (4.52)$$

This is not a formal proof, but we can verify this assertion numerically. For the values of the parameters $Z=2, \mu=1$, $k=1.5$, $\ell=1$, $\beta=2.4$ and the indices $p=5$ and $n=2$, we evaluate numerically the α dependent quantities

$$\mathrm{Int}_{p,n}(\alpha) = \int_0^{\infty} Q_p^{(\pm)}(\ell,\beta,\alpha;\rho)\,\frac{1}{\rho}\,Q_n^{(\pm)}(\ell,\beta,\alpha;\rho)\,d\rho,$$
$$\mathrm{Der}_{p,n}(\alpha) = -\frac{\dfrac{d}{d\alpha}\,g_{p,n}^{(\pm)}(\alpha)}{\dfrac{d}{d\alpha}C(\alpha)},$$

and measure the relative error through

$$\mathcal{E}_{p,n}(\alpha) = \left| \frac{\mathrm{Der}_{p,n}(\alpha) - \mathrm{Int}_{p,n}(\alpha)}{\mathrm{Der}_{p,n}(\alpha)} \right|.$$

The obtained results are presented in **Table 4.2**. Clearly identity (4.52) is verified. We notice that the relative error $\mathcal{E}_{p,n}$ increases for values of α approaching the end points of the interval $\left(0, \frac{\pi}{2}\right)$. This is due to the fact that near these end points the coefficients $g^{(\pm)}_{p,n}$ concentrate most of their oscillations, as observed in **Figure 4.7**. We can also verify that, as expected, the symmetry of the function C with respect to $\alpha = \frac{\pi}{4}$ is present in these expressions.

α	$\mathrm{Int}_{p,n}(\alpha)$	$\mathrm{Der}_{p,n}(\alpha)$	$\mathcal{E}_{p,n}(\alpha)$
$\frac{\pi}{20}$	-0.00554295 - 0.0146246 i	-0.00543316 - 0.0146222 i	0.00704029
$\frac{\pi}{10}$	0.150919 + 0.0727451 i	0.150011 + 0.0729142 i	0.00553815
$\frac{\pi}{4} - 0.001$	-0.172925 + 0.0528128 i	-0.172526 + 0.0527495 i	0.00223454
$\frac{\pi}{4} + 0.001$	-0.172925 + 0.0528128 i	-0.172526 + 0.0527495 i	0.00223454

Table 4.2: Verification of identity (4.52) for different values of α and parameters $p = 5,\ n = 2,\ Z = 2, \mu = 1,\ k = 1.5,\ \ell = 1,\ \beta = 2.4$.

Remark 4.3.1. Notice that even if $\frac{d}{d\alpha}C(\alpha)$ is not defined for $\alpha = \frac{\pi}{4}$, the limit for $\alpha \to \frac{\pi}{4}$ of the ratio $\mathrm{Der}(\alpha)$ exists. This is a consequence of the symmetry of the functions C and $g^{(\pm)}_{n,p}(\alpha)$ with respect to $\alpha = \frac{\pi}{4}$.

■

4.4 Chapter summary

We have defined and studied Quasi-Sturmian functions. These functions, like Generalized Sturmian functions, are useful to describe two- and three-body scattering solutions because they can be constructed with an appropriate asymptotic behavior.

When considering the auxiliary potential as a Coulomb potential, and Slater-type orbitals or Laguerre-type functions as driven functions, Quasi-Sturmian functions can be given in closed form.

To start, different analytical expressions for one variable Quasi-Sturmian functions and their asymptotic behavior have been presented. This allowed us to study them from an analytical point of view, something we cannot do with most of Generalized Sturmian functions, which are numerically generated. We have explored the mathematical properties of Laguerre Quasi-Sturmian functions, establishing different useful relations between them and Laguerre-type functions. Most noteworthy is the pseudo-recurrence relation they satisfy. We have also shown that Laguerre and Slater Quasi-Sturmian functions are generalizations to any index n, of a particular function introduced by Yamani and Fishman to be used in the J-Matrix method.

Next, we have considered Quasi-Sturmian functions with a variable charge. Their advantage is that their asymptotic behavior can be chosen to coincide, in a hyperspherical framework, with the one expected in three-body scattering solutions. Analytical expressions for them, their asymptotic behavior and their derivative with respect to an angular parameter were given.

Some of the results exposed in this chapter can be found in reference [34], where we have made a first presentation of one variable Quasi-Sturmian functions and we have used them to solve a two-body scattering problem. The application to three-body scattering problems will be discussed in **Chapter 6**.

Chapter 5

Two-body scattering problems

In this chapter we show how to deal with two-body scattering problems using, as basis sets, Generalized Sturmian functions and Quasi-Sturmian functions. Atomic units are used throughout the chapter.

5.1 Statement of the problem

The dynamics of a particle of mass μ and energy $E = \dfrac{k^2}{2\mu} > 0$, under the influence of a general potential V, for a given angular momentum ℓ, is described by the Schrödinger equation (time-independent non-relativistic case) [3, 81]

$$[\mathbf{T} + V - E]\,\Psi = 0. \tag{5.1}$$

In spherical coordinates the kinetic energy $\mathbf{T}$ takes de form

$$\mathbf{T} = -\frac{1}{2\mu\, r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{2\mu\, r^2}\mathbf{L^2},$$

where $\mathbf{L^2}$ is the angular momentum operator, whose eigenfunctions are the spherical harmonics Y_ℓ^m [2, 28],

$$\mathbf{L}^2\, Y_\ell^m(\theta,\varphi) = \ell(\ell+1)\, Y_\ell^m(\theta,\varphi). \tag{5.2}$$

For a central potential $V = V(r)$ equation (5.1) becomes separable. Then, for fixed ℓ, m, one proposes

$$\Psi(\mathbf{r}) = \frac{1}{r}\Phi(r) Y_\ell^m(\theta,\varphi)$$

to obtain, using the angular equation (5.2), the reduced radial equation

$$[\mathbf{H_r} - E]\,\Phi(r) = 0, \tag{5.3}$$

where the reduced Hamiltonian operator $\mathbf{H_r} = \mathbf{T_r} + V$ was introduced in (1.17). Throughout the following sections we will focus on the solutions of the radial differential equation (5.3).

For scattering problems, we denote $\Psi^{(\pm)}$ and $\Phi^{(\pm)}$ the solution of the initial equation (5.1) and the reduced equation (5.3) respectively. The symbol $(\pm)$ indicates the chosen incoming $(-)$ or outgoing $(+)$ asymptotic wave behavior. The separation into initial Φ_0 plus scattering solution $\Phi_{sc}^{(\pm)}$

$$\Phi^{(\pm)}(r) = \Phi_0(r) + \Phi_{sc}^{(\pm)}(r), \tag{5.4}$$

is generally proposed. The potential V is also conveniently separated,

$$V(r) = V_0(r) + V_1(r), \tag{5.5}$$

where V_0 is the potential associated to the initial state Φ_0,

$$[\mathbf{T_r} + V_0(r) - E]\,\Phi_0(r) = 0, \tag{5.6}$$

and V_1 is the scattering potential. Replacing (5.4) and (5.5) into (5.1) one gets the following non-homogeneous differential equation for $\Phi_{sc}^{(\pm)}$

$$[\mathbf{H_r} - E]\,\Phi_{sc}^{(\pm)}(r) = F(r), \tag{5.7}$$

where we set $F(r) = -V_1(r)\Phi_0(r)$.

To solve the equation, we express its solution in terms of a set of basis functions $\{\varphi_n\}$,

$$\Phi_{sc}^{(\pm)}(r) = \sum_n a_n \varphi_n(r). \tag{5.8}$$

After inserting (5.8) into (5.7), we multiply by the left both sides of the equation with appropriate functions $\widetilde{\varphi}_q$ and a weight function w, and finally integrate over the interval $(0, +\infty)$. Thus we construct a matrix equation

$$\mathbf{O} \cdot \mathbf{a} = \mathbf{b}. \tag{5.9a}$$

The solution of this system is a vector **a** whose components are the coefficients a_n. The matrix **O** is the matrix representation of the Schrödinger operator describing the problem [see **Remark 1.1.1**]. Its elements $O_{q,n}$ are

$$O_{q,n} = \int_0^\infty \widetilde{\varphi}_q(r) w(r) \left[\mathbf{H_r} - E\right] \varphi_n(r)\, dr, \tag{5.9b}$$

and the components b_q of the vector **b** are given by

$$b_q = -\int_0^\infty \widetilde{\varphi}_q(r) w(r) V_1(r) \Phi_0(r)\, dr. \tag{5.9c}$$

If the basis set $\{\widetilde{\varphi}_q\}$ is orthonormal with weight function w, these coefficients correspond to a generalized Fourier expansion of $F(r) = -V_1(r)\Phi_0(r)$.

The boundary conditions depend on the particular problem to be solved. For example, when V behaves as a Coulomb potential $\frac{Z}{r}$ at large distances and V_1 is a short range potential, the boundary conditions, for a given angular momentum ℓ, become

$$\Phi^{(\pm)}_{sc}(0) = 0, \tag{5.10a}$$

$$\Phi^{(\pm)}_{sc}(r) \overset{r\to\infty}{\sim} \mathcal{A}\, e^{\pm i[kr - \eta(Z)\ln(2kr) - \frac{\pi}{2}\ell + \sigma_C(\ell,Z)]}, \tag{5.10b}$$

coinciding, up to a constant, with the asymptotic behavior of the Coulomb wave functions $H^{(\pm)}$ given in (1.28). The constant $\mathcal{A}$ is proportional to the transition amplitude for a given ℓ. If V is of short range, the asymptotic boundary condition (5.10b) simplifies to $e^{\pm ikr}$; this situation is illustrated in the next two sections.

Remark 5.1.1. If the basis functions φ_n, used in (5.8) to represent the scattering solution, behave in the asymptotic region proportionally to the expected behavior of $\Phi^{(\pm)}_{sc}$, it is straightforward to extract an expression for the transition amplitude. For example, in case of an expected Coulomb behavior at large distances as in (5.10b), if we take basis functions satisfying

$$\varphi_n(r) \overset{r\to\infty}{\sim} \mathcal{A}_n\, e^{\pm i[kr - \eta(Z)\ln(2kr) - \frac{\pi}{2}\ell + \sigma_C(\ell,Z)]},$$

we immediately deduce that

$$\mathcal{A} = \sum_n a_n\, \mathcal{A}_n.$$

■

5.2 Implementation of Generalized Sturmian functions

One possibility is to use Generalized Sturmian functions as basis functions. Their general description was presented in **Chapter 3**, and the results shown in this section form the second part of reference [33].

Taking $\varphi_n(r) = S^{(\pm)}_{n,\ell}(r)$, the proposed solution (5.8) reads

$$\Phi^{(\pm)}_{sc}(r) = \sum_n a_n\, S^{(\pm)}_{n,\ell}(r). \tag{5.11}$$

Upon replacement in (5.7), and taking into account the differential equation (3.1) satisfied by the Generalized Sturmian functions, we find

$$\sum_n a_n[V(r) - \mathcal{V}_a(r) - \lambda_{n,\ell}\,\mathcal{V}_g(r)]S^{(\pm)}_{n,\ell}(r) = F(r). \tag{5.12}$$

If we further choose the auxiliary potential $\mathcal{V}_a$ to be the interaction potential V, only the generating potential remains on the left hand side of the equation. Taking $\widetilde{\varphi}_q(r) = S^{(\pm)}_{q,\ell}(r)$ and $w(r) = 1$ in (5.9), the matrix $\mathbf{O}$ becomes a diagonal matrix. Then the coefficients a_n are

$$a_n = -\frac{1}{\lambda_{n,\ell} V_n}\, b_n, \tag{5.13a}$$

where

$$V_n = \int_0^{+\infty} S^{(\pm)}_{n,\ell}(r)\,\mathcal{V}_g(r)\,S^{(\pm)}_{n,\ell}(r)\,dr, \tag{5.13b}$$

$$b_n = \int_0^{+\infty} S^{(\pm)}_{n,\ell}(r)\,F(r)\,dr = -\int_0^{+\infty} S^{(\pm)}_{n,\ell}(r)\,V_1(r)\Phi_0(r)\,dr. \tag{5.13c}$$

5.2.1 Scattering of a particle by a Hulthén potential

Let us consider the scattering of a particle under the influence of a Hulthén potential (3.6) and take only the angular momentum $\ell = 0$. As initial state we consider a free particle, hence

$$V_0 \equiv 0, \qquad V_1(r) = V(r) = v_0\,\frac{e^{-\frac{r}{\alpha}}}{1 - e^{-\frac{r}{\alpha}}} \tag{5.14a}$$

and

$$\Phi_0(r) = kr\,j_0(kr) = \sin(kr), \tag{5.14b}$$

where j_0 is a spherical Bessel function. For outgoing wave behavior, the non-homogeneous equation (5.7) becomes

$$\left[-\frac{1}{2\mu}\frac{d^2}{dr^2}+v_0\,\frac{e^{-\frac{r}{\alpha}}}{1-e^{-\frac{r}{\alpha}}}-E\right]\Phi_{sc}^{(+)}(r)=-v_0\,\frac{e^{-\frac{r}{\alpha}}}{1-e^{-\frac{r}{\alpha}}}\Phi_0(r), \tag{5.15}$$

and as boundary conditions we require

$$\Phi_{sc}^{(+)}(0)=0, \tag{5.16a}$$

$$\Phi_{sc}^{(+)}(r)\overset{r\to\infty}{\sim}\mathcal{A}\,e^{ikr}. \tag{5.16b}$$

Since these boundary conditions are exactly those of the Hulthén Sturmian functions presented in **Section 3.2**, it is natural to express the scattering solution as a combination of them, in particular, we may use the functions $S_{n,0}^{(\pm)}$ introduced in **Remark 3.2.3**, so that the scattering solution becomes

$$\Phi_{sc}^{(+)}(r)=\sum_{n=1}^{\infty}a_n\,S_{n,0}^{(+)}(r). \tag{5.17}$$

Taking as auxiliary potential the Hulthén potential (5.14a), i.e. $\mathcal{V}_a\equiv V$, we are in the situation described after equation (5.12). Thus we obtain from (5.13) the coefficients

$$a_n=\frac{1}{\widetilde{\lambda}_{n,0}V_n}\,v_0\int_0^{+\infty}S_{n,0}^{(+)}(r)\,\frac{e^{-\frac{r}{\alpha}}}{1-e^{-\frac{r}{\alpha}}}\,\sin(kr)\,dr\overset{(3.28)}{=}-\frac{v_0\,k\,N_n^S}{2\mu\,\lambda_{n,0}\,\widetilde{\lambda}_{n,0}},$$

where N_n^S is given by (3.19) and $V_n=1$ [see paragraph following formula (3.19)]. Since $v_a=v_0$, the eigenvalues $\widetilde{\lambda}_{n,0}$, given by (3.21), become

$$\widetilde{\lambda}_{n,0}=\lambda_{n,0}-1\overset{(3.15)}{=}-\frac{n(n-2k\alpha\,i)}{2\mu\,\alpha^2\,v_g}-1,$$

and the scattering solution reads

$$\Phi_{sc}^{(+)}(r)=-\frac{v_0\,k}{2\mu}\sum_{n=1}^{\infty}\frac{(N_n^S)^2}{\lambda_{n,0}(\lambda_{n,0}-1)}\,e^{ikr}\,{}_2F_1\left(-n,n-2k\alpha\,i,1-2k\alpha\,i;e^{-\frac{r}{\alpha}}\right).$$

Finally, as explained in **Remark 5.1.1**, taking the limit $r\to\infty$ we deduce the scattering transition amplitude $\mathcal{A}$ for the collision process. From

$$\Phi_{sc}^{(+)}(r)\overset{r\to\infty}{\sim}\left[-\frac{v_0\,k}{2\mu}\sum_{n=1}^{\infty}\frac{(N_n^S)^2}{\lambda_{n,0}(\lambda_{n,0}-1)}\right]e^{ikr}$$

we obtain

$$\mathcal{A} = -\frac{v_0\, k}{2\mu} \sum_{n=1}^{\infty} \frac{(N_n^S)^2}{\lambda_{n,0}(\lambda_{n,0}-1)}.$$

In reference [33] we have presented the value found for a particular choice of the physical parameters and compared it successfully with the result obtained by using an independent numerical procedure.

5.2.2 Scattering of a particle by a Yukawa potential

As another application we study the outgoing solution of

$$\left[-\frac{1}{2\mu}\frac{d^2}{dr^2} - \frac{e^{-\widetilde{\alpha}r}}{r} - E\right]\Phi_{sc}^{(+)}(r) = \frac{e^{-\widetilde{\alpha}r}}{r}\Phi_0(r) \tag{5.18}$$

which describes, again for $\ell = 0$, the scattering of a particle by a Yukawa potential

$$V(r) = -\frac{e^{-\widetilde{\alpha}r}}{r}. \tag{5.19}$$

The boundary conditions are those of the previous case [formulas (5.16)].

As in the previous example, we take for the initial state Φ_0 a free particle (5.14b), so that

$$V_0 \equiv 0, \qquad V_1(r) = V(r) = -\frac{e^{-\widetilde{\alpha}r}}{r}.$$

The proposed solution $\Phi_{sc}^{(+)}$ takes the form (5.17), where, this time, we use as basis functions, Hulthén Sturmian functions with auxiliary potential $\mathcal{V}_a \equiv 0$..

Since we are not choosing the auxiliary potential coinciding with the interaction potential, the matrix associated to the Schrödinger operator of this problem is not diagonal. Then the coefficients a_n cannot be calculated using (5.13); they are solution of the matrix equation (5.9) with

$$O_{q,n} = -\int_0^{\infty} S_{q,0}^{(+)}(r)\frac{e^{-\widetilde{\alpha}r}}{r}S_{n,0}^{(+)}(r)\, dr - \lambda_{n,0}\,\delta_{q,n}, \tag{5.20a}$$

$$b_q = \int_0^{\infty} S_{q,0}^{(+)}(r)\frac{e^{-\widetilde{\alpha}r}}{r}\Phi_0(r)\, dr, \tag{5.20b}$$

where we have taken $w \equiv 1$.

In reference [33] we have solved the scattering problem by setting the values of the parameters $\alpha = \widetilde{\alpha} = 1,\ v_0 = -1,\ \mu = 1,\ E = 0.5,\ \ell = 0$. The integrals (5.20) had to be numerically performed. We needed 60 terms in the expansion (5.17) to reproduce with a very good accuracy the scattering solution obtained by an independent numerical method. However, we also showed that 20 basis functions basically provide a good approximation of the solution.

According to **Remark 5.1.1**, the $\ell = 0$ transition amplitude, calculated with N terms, takes the form

$$\mathcal{A}^{(N)} = \sum_{n=1}^{N} a_n \, N_n^S .$$

With the first 20 terms of this series we obtained $\mathcal{A}^{(20)} = 0.389994 + 0.788451i$, while taking 60 terms we found $\mathcal{A}^{(60)} = 0.4085 + 0.7869i$.

5.3 Scattering solution in terms of Quasi-Sturmian functions

Similarly, but as an alternative, to Generalized Sturmian functions, we propose to express the solution of the general scattering equation (5.7)

$$\Phi_{sc}^{(\pm)}(r) = \sum_n a_n \, Q_n^{(\pm)}(\ell, \beta; r), \tag{5.21}$$

in terms of the Quasi-Sturmian functions presented in **Chapter 4**, with μ, ℓ and E given by the problem one wants to solve.

Consider first the functions $Q_n^{(\pm)}$ satisfying the differential equation (4.1). We apply the operator $[\mathbf{H_r} - E]$ to one of them to find

$$[\mathbf{H_r} - E] \, Q_n^{(\pm)}(\ell, \beta; r) = \mathcal{V}_g \phi_n(r) + [-\mathcal{V}_a(r) + V(r)] \, Q_n^{(\pm)}(\ell, \beta; r).$$

Taking $\mathcal{V}_a \equiv V$ and $\mathcal{V}_g$ equal to the weight function w of an orthonormal basis set $\{\phi_n\}$, the matrix $\mathbf{O}$ associated to the operator $[\mathbf{H_r} - E]$, introduced in (5.9b), becomes the identity for $\widetilde{\varphi}_n(r) = \phi_n(r)$. Thus, the coefficients a_n in (5.21) coincide with the generalized Fourier coefficients b_n given by (5.9c), associated to $F(r) = -V_1(r)\Phi_0(r)$. This option looks attractive. However, in the general case, Quasi-Sturmian functions are not known in closed form, so that no further analytical considerations can be made.

Alternatively, we may use the Laguerre Quasi-Sturmian functions studied in **Section**

4.3. In this case, using (4.3a), we obtain

$$[\mathbf{H_r} - E]\, Q_n^{L(\pm)}(\ell,\beta;r) = \frac{1}{r}\phi_n^L(\ell,\beta;r) + \left[-\frac{Z_{QS}}{r} + V(r)\right] Q_n^{L(\pm)}(\ell,\beta;r).$$

Choosing $\widetilde{\varphi}_q \equiv \phi_q^L$ and $w \equiv 1$ in (5.9), taking into account the orthogonality property (1.9a) of Laguerre-type functions, and using the series expansion (4.26a), the matrix elements $O_{q,n}$ and the components b_q become

$$O_{q,n} = \delta_{q,n} - Z_{QS}\; g_{n,q}^{(\pm)} + \int_0^\infty \phi_q^L(\ell,\beta;r)\, V(r)\, Q_n^{L(\pm)}(\ell,\beta;r)\, dr, \tag{5.22a}$$

$$b_q = -\int_0^\infty \phi_q^L(\ell,\beta;r) V_1(r)\Phi_0(r)\, dr. \tag{5.22b}$$

5.3.1 A particular two-body problem

To illustrate the efficiency of the proposed Quasi-Sturmian functions, we consider the scattering of a particle in a combined attractive Coulomb potential V_0 plus a Yukawa potential V_1,

$$V_0(r) = \frac{z_1 z_2}{r} \qquad (z_1 z_2 < 0), \tag{5.23a}$$

$$V_1(r) = -\frac{b\, e^{-ar}}{r} \qquad (a, b \in \mathbb{R},\ a, b > 0). \tag{5.23b}$$

We propose as initial solution Φ_0 the regular Coulomb wave function $F^{(s)}$ given by (1.24) that satisfies equation (1.22).

The scattering problem reads

$$\left[-\frac{1}{2\mu}\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{2\mu r^2} + \frac{z_1 z_2}{r} - \frac{b\, e^{-ar}}{r} - E\right] \Phi_{sc}^{(\pm)}(r) = \frac{b\, e^{-ar}}{r}\; F^{(s)}(\ell,k;r), \tag{5.24a}$$

$$\Phi_{sc}^{(\pm)}(0) = 0, \tag{5.24b}$$

$$\Phi_{sc}^{(\pm)}(r) \overset{r\to\infty}{\sim} \mathcal{A}\, e^{\pm i[kr - \eta(z_1 z_2)\ln(2kr) - \frac{\pi}{2}\ell + \sigma_C(\ell, z_1 z_2)]}. \tag{5.24c}$$

The following results have been presented in Section V of reference [34], where we have compared the solutions obtained with different numerical techniques. First, using a finite difference method, we have constructed a set of numerical Quasi-Sturmian functions, taking as generating potential the total potential $\mathcal{V}_g = V_0 + V_1$ and considering $\widetilde{\varphi}_q(r) = \phi_q^L(\ell,\beta;r)$. This choice led us to the trivial solution $a_n = b_n$ described at the beginning of

Section 5.3. Second, and for convergence rate comparisons, we have solved the problem using Generalized Sturmian functions (also numerically generated). Finally, we have employed the analytical Laguerre Quasi-Sturmian functions provided in **Section 4.3**.

Numerical Quasi-Sturmian functions

A linear system of equation as the one given by (5.9) was solved considering a set of Quasi-Sturmian functions numerically generated with a finite difference technique. Choosing the auxiliary potential to be the total potential

$$\mathcal{V}_a(r) = \frac{z_1 z_2}{r} - \frac{b\, e^{-ar}}{r},$$

and taking $\mathcal{V}_g(r) = \dfrac{1}{r}$, $\widetilde{\varphi}_q(r) = \phi_q^L(\ell,\beta;r)$ and $w(r) = 1$, the coefficients a_n in (5.21) coincide with b_n in (5.9c), and can be given in closed form

$$\begin{aligned} b_n &= -\int_0^\infty \phi_n^L(\ell,\beta;r)\,\frac{b\,e^{-ar}}{r}\; F^{(s)}(\ell,k;r)\,dr \\ &\overset{(B.8)}{=} -\frac{b\,N_C(\ell)}{N_{n,\ell}}\left(\frac{2\beta}{(a+\beta)^2+k^2}\right)^{\ell+1}\left(\frac{a-\beta-ik}{a+\beta-ik}\right)^{n}\left(\frac{a+\beta-ik}{a+\beta+ik}\right)^{i\eta(z_1z_2)} \\ &\quad\times\ {}_2F_1\left(-n,\ell+1+i\eta(z_1z_2),2\ell+2;-\frac{4\beta ki}{a^2-(\beta+ik)^2}\right). \end{aligned} \tag{5.25}$$

Analytical Laguerre Quasi-Sturmian functions

A set of Laguerre Quasi-Sturmian functions was also used to represent the scattering solution. We fixed the parameter Z_{QS} of the Quasi-Sturmian functions as the charge of the problem, $Z_{QS} = z_1 z_2$. Once again we took $\mathcal{V}_g(r) = \dfrac{1}{r}$, $\widetilde{\varphi}_q \equiv \phi_q^L$ and $w \equiv 1$, so that the coefficients b_n [formula (5.9c)] are those of the previous case, i.e., (5.25). The matrix elements $O_{q,n}$, given by formula (5.22a), are also analytical,

$$\begin{aligned} O_{q,n} &= \delta_{q,n} - \int_0^\infty \phi_q^L(\ell,\beta;r)\,\frac{b\ e^{-ar}}{r}\,Q_n^{L(\pm)}(\ell,\beta;r)\,dr \\ &= \delta_{q,n} - b\sum_{j=0}^{\infty} g_{n,j}^{(\pm)}\int_0^\infty \phi_q^L(\ell,\beta;r)\,\frac{e^{-ar}}{r}\,\phi_j^L(\ell,\beta;r)\,dr \\ &\overset{(B.9)}{=} \delta_{q,n} - \frac{b}{N_{q,\ell}\,\Gamma(2\ell+2)}\left(\frac{2\beta}{a+2\beta}\right)^{2\ell+2}\sum_{j=0}^{\infty} g_{n,j}^{(\pm)}\frac{1}{N_{j,\ell}}\left(\frac{a}{a+2\beta}\right)^{q+j} \\ &\qquad\times\ {}_2F_1\left(-q,\ -j;\ 2\ell+2;\ \left(\frac{2\beta}{a}\right)^2\right). \end{aligned} \tag{5.26}$$

For the particular choice $2\beta = a$, the hypergeometric function simplifies [see equation (1.15)], and we obtain

$$O_{q,n} = \delta_{q,n} - \frac{b\, N_{q,\ell}}{q!} \left(\frac{1}{2}\right)^{2\ell+2+q} \sum_{j=0}^{\infty} g^{(\pm)}_{n,j} \frac{(2\ell+2+j)_q}{N_{j,\ell}} \left(\frac{1}{2}\right)^{j}. \tag{5.27}$$

Fixing

$$b = 10, \quad a = 1.3, \quad z_1 z_2 = -2, \quad \mu = 1, \quad k = 1, \quad \ell = 0,$$

taking $\beta = 2a$ and truncating the summation in (5.26) at $j = 300$, only 15 Quasi-Sturmian functions were needed to approximate the scattering solution while 30 Generalized Sturmian functions were necessary to achieve the same accuracy. A comparison of the solutions obtained with different numerical techniques, as well as details of the computations, were presented in reference [34].

In **Figure 5.1** we plot the real and imaginary parts of the approximated scattering solution

$$\Phi^{N(+)}_{sc}(r) = \sum_{n=0}^{N} a_n\, Q^{L\,(+)}_n(\ell, \beta; r),$$

obtained by using expressions (5.25) and (5.26) to find the coefficients a_n, and the integral representation (4.24) to generate the Quasi-Sturmian functions $Q^{L(\pm)}_n$. The full line represents $\Phi^{N(+)}_{sc}$ taking $\beta = 2a$ and using 21 basis functions ($N = 20$). The dots correspond to taking $2\beta = a$, $N = 30$, and using formula (5.27) for the matrix elements. In this case more basis functions were needed to obtain a convergent series in (5.21), meaning that this choice of the parameter β is by far not optimal. This can also be observed through **Figure 5.2**, where we plot the modulus of coefficients a_n as a function of n, for the two situations considered: $\beta = 2a$ (dots) and $2\beta = a$ (diamonds). In the first case the coefficients become negligible for $n > 15$ while in the second case the coefficients can not be neglected up to $n = 55$. We conclude that, even if the analytical expression simplifies considerably, the choice $2\beta = a$ leads to a much slower convergence rate.

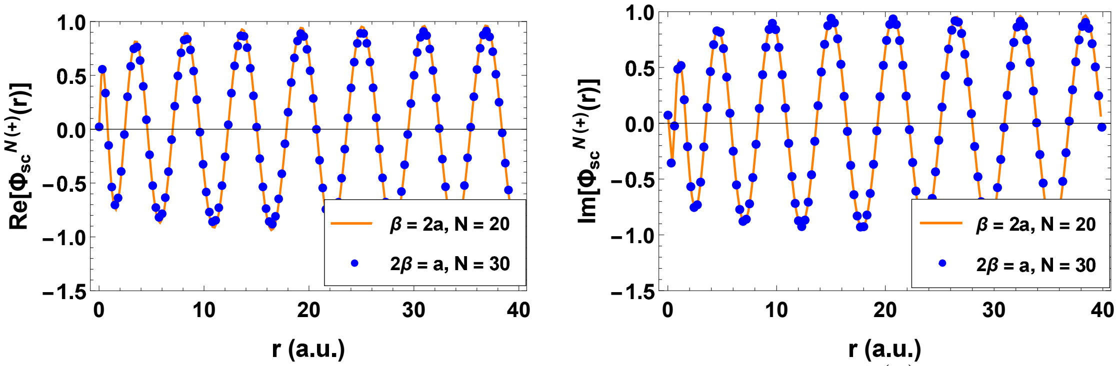

Figure 5.1: Real (left panel) and imaginary (right panel) parts of $\Phi_{sc}^{N(+)}$ as a function of r, taking $\beta = 2a$ with $N = 20$ and $2\beta = a$ with $N = 30$. Parameters: $b = 10$, $a = 1.3$, $z_1 z_2 = -2$, $\mu = 1$, $k = 1$, $\ell = 0$.

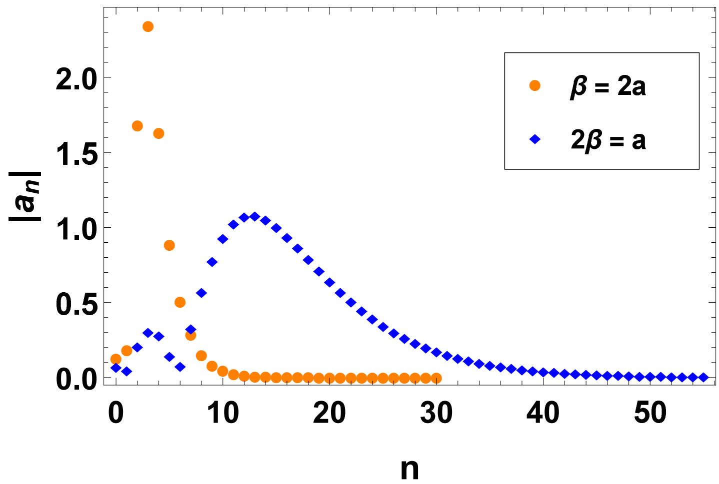

Figure 5.2: Modulus of the coefficients a_n as a function of n obtained for the approximated scattering solution $\Phi_{sc}^{N(+)}$ corresponding to $b = 10$, $a = 1.3$, $z_1 z_2 = -2$, $\mu = 1$, $k = 1$, $\ell = 0$. The dots are obtained when considering $\beta = 2a$ and the diamonds correspond to taking $2\beta = a$.

5.4 Chapter Summary

We described the procedure to solve a general two-body scattering problem by using, first, Generalized Sturmian functions and then, Quasi-Sturmian functions.

We have solved three different problems expanding the scattering solutions in terms of Hulthén Sturmian functions and Laguerre Quasi-Sturmian functions. Clearly, the fact that the basis functions have an appropriate asymptotic behavior represents a serious convergence advantage.

For a Coulomb plus Yukawa potential, the scattering problem was solved implementing a set of numerically generated Generalized Sturmian functions, as well as numerical and analytical Laguerre Quasi-Sturmian functions. All basis functions considered had the desired asymptotic behavior. For this particular problem, Quasi-Sturmian functions were the most efficient. Interestingly, for the analytical Quasi-Sturmian functions we were able to give in closed form the matrix elements and the components of the vector involved in the linear system to be solved. In this case, we have also tested the influence of the parameter controlling the spatial extension of the driven terms. We noted that even if a certain choice of the value of the parameter simplifies the expression of the matrix elements, the solution obtained was not optimal as it required many more functions in comparison to other choices of this parameter.

The results involving Hulthén Sturmian functions complete the second part of reference [33], while those related to Quasi-Sturmian functions were presented in reference [34].

Chapter 6

Three-body scattering problems

This chapter is dedicated to the study of three-body scattering problems by using different variants of Quasi-Sturmian functions as basis sets. We propose to use hyperspherical coordinates, and focus on the Temkin-Poet model problem. Atomic units are used.

6.1 Hyperspherical coordinates

In the laboratory reference frame, nine variables are needed to describe the motion of three particles: three variables to represent the motion of the center of mass and six variables to represent the internal motion.

Let $\mathbf{p}_i$ be the position of each particle of the system and m_i its mass, $i = 1, 2, 3$. The Jacobi vectors $\mathbf{r}_{ij}$ y $\mathbf{R}_{k,ij}$ are defined as follows

- ⋄ $\mathbf{r}_{ij}$ is the vector with starting point $\mathbf{p}_i$ and endpoint $\mathbf{p}_j$,
- ⋄ $\mathbf{R}_{k,ij}$ is the vector starting at the center of mass of the subsystem $\{\mathbf{p}_i,\ \mathbf{p}_j\}$, and ending at $\mathbf{p}_k$.

For example, fixing $k = 1$, $j = 2$, $i = 3$ we obtain the following picture.

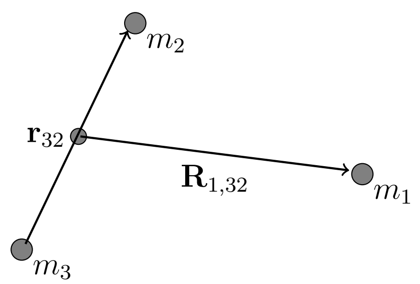

Figure 6.1: A pair of Jacobi vectors.

For fixed i, j, k, the normalization of the Jacobi vectors $\mathbf{r}_{ij}, \mathbf{R}_{k,ij}$ is given by

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

where

$$\mu_{ij} = \frac{m_1\, m_j}{m_i + m_j}, \qquad \text{and} \qquad \mu = \sqrt{\frac{m_1\, m_2\, m_3}{m_1 + m_2 + m_3}}$$

are the reduced mass of the subsystem $\{m_i,\, m_j\}$ and the reduced mass of the hole system $\{m_1, m_2, m_3\}$, respectively.

Leaving aside the motion of the center of mass, in the 6-dimensional space we define the hyperspherical coordinates [see formula (12.3.88) in reference [2], or references [36, 37]], consisting in one radial and five angular variables. The radial variable (named hyperradius) is defined by

$$\rho = x_k^2 + X_k^2 \tag{6.1}$$

and does not depend of the choice of i, j, k.

There are different ways to choose the angular coordinates [36], each of which gives an alternative coupling scheme of angular momenta and, as a consequence, to an alternative representation of the Schrödinger equation describing the three particles dynamics. We are going to consider the asymmetric hyperangular parametrization for which one of the angular variables is

$$\alpha = \arctan \left| \frac{X_k}{x_k} \right| \tag{6.2}$$

and the others are the polar angles $\theta_{\mathbf{x}_k},\ \varphi_{\mathbf{x}_k},\ \theta_{\mathbf{X}_k},\ \varphi_{\mathbf{X}_k}$ defining the orientations $\hat{\mathbf{x}}_k$ and $\hat{\mathbf{X}}_k$ of the Jacobi vectors in the center of mass reference frame. It is usual to indicate collectively the five angular variables by

$$\omega_5 = (\alpha, \theta_{\mathbf{x}_k}, \varphi_{\mathbf{x}_k}, \theta_{\mathbf{X}_k}, \varphi_{\mathbf{X}_k}).$$

From (6.1) and (6.2) we have

$$x_k = \rho \cos \alpha, \tag{6.3a}$$

$$X_k = \rho \sin \alpha. \tag{6.3b}$$

Let us fix $k = 1$, $j = 2$, $i = 3$. In the present work we consider m_3 much heavier than

m_1 and m_2, so that the reduced masses simplify

$$\mu = \sqrt{m_1\, m_2}, \qquad \mu_{32} = m_2,$$

the center of mass for the subsystem $\{\mathbf{r}_2, \mathbf{r}_3\}$ coincides with $\mathbf{p}_3$ and the Jacobi vectors scheme (**Figure 6.1**) transforms to the following one:

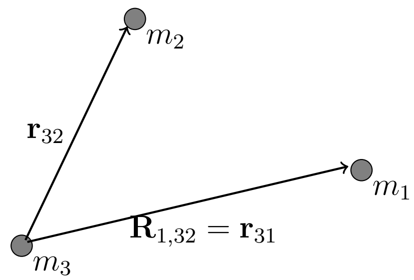

Figure 6.2: Jacobi vectors for $m_3 \gg \max(m_1, m_2)$.

In addition, for the case of two electrons and a nucleus we have $m_1 = m_2 = 1$ and

$$\mathbf{x}_1 = \mathbf{r}_{32}, \qquad \mathbf{X}_1 = \mathbf{R}_{1,32}.$$

Renaming $\mathbf{r}_{32} = \mathbf{r}_1$, $\mathbf{r}_{31} = \mathbf{r}_2$, we obtain for this particular case

$$r_1 = r_{32} = x_1 = \rho \cos\alpha, \tag{6.4a}$$

$$r_2 = R_{1,32} = X_1 = \rho \sin\alpha. \tag{6.4b}$$

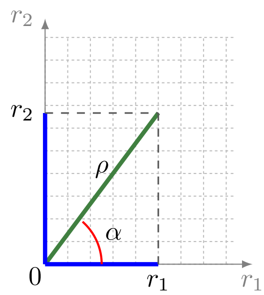

Figure 6.3: Relation between the spherical coordinates $(\mathbf{r}_1, \mathbf{r}_2)$ *and the hyperspherical pair* (ρ, α).

6.1.1 The Coulomb potential for three charged particles

In spherical coordinates the Coulomb interaction between three particles of charges Z, z_1, z_2 is

$$V(\mathbf{r}_1, \mathbf{r}_2) = \frac{z_1\, Z}{r_1} + \frac{z_2\, Z}{r_2} + \frac{z_1\, z_2}{|\mathbf{r}_1 - \mathbf{r}_2|}, \tag{6.5}$$

while in hyperspherical coordinates, and for $m_1 = m_2 = 1$, it becomes [2, 19, 37, 83]

$$V(\rho,\omega_5) = \frac{z_1\,Z}{\rho\,\cos\alpha} + \frac{z_2\,Z}{\rho\,\sin\alpha} + \frac{z_1\,z_2}{\rho\,\sqrt{1-\sin(2\alpha)\cos\theta_{12}}} = \frac{\widetilde{C}(\omega_5)}{\rho} \tag{6.6}$$

naming θ_{12} the angle between $\mathbf{r}_1$ and $\mathbf{r}_2$. The explicit form of the "charge" $\widetilde{C}$ can be found in reference [19].

For the last term in the spherical representation (6.5) we have the well known series expansion [50] in terms of Legendre polynomials P_n [43] (known as the multipole expansion)

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \sum_{n=0}^{\infty} \frac{1}{r_>} \left(\frac{r_<}{r_>}\right)^n \; P_n(\cos\theta_{12}),$$

where $r_< = \min(r_1, r_2)$, $r_> = \max(r_1, r_2)$.

As a first approach to the three-body scattering problem, it is usual to consider a model, known as Temkin-Poet model [38–40]. It results from keeping only the first term in the previous series, instead of the full Coulomb potential (6.5). The model potential in spherical coordinates reads

$$V(r_1, r_2) \sim \frac{z_1\,Z}{r_1} + \frac{z_2\,Z}{r_2} + \frac{z_1\,z_2}{r_>},$$

while in hyperspherical coordinates, for $m_1 = m_2 = 1$ thus using (6.4), it becomes

$$V(\rho,\alpha) \sim \frac{C(\alpha)}{\rho}, \tag{6.7a}$$

$$C(\alpha) = \frac{z_1\,Z}{\cos\alpha} + \frac{z_2\,Z}{\sin\alpha} + B(\alpha), \qquad B(\alpha) = \begin{cases} \dfrac{z_1\,z_2}{\cos(\alpha)}, & \text{for } \; 0 < \alpha < \dfrac{\pi}{4} \\[2ex] \dfrac{z_1\,z_2}{\sin(\alpha)}, & \text{for } \; \dfrac{\pi}{4} \leqslant \alpha < \dfrac{\pi}{2} \end{cases} . \tag{6.7b}$$

For the two-electron case, $z_1 = z_2 = -1$ and

$$C(\alpha) = \begin{cases} -\dfrac{Z-1}{\cos\alpha} - \dfrac{Z}{\sin\alpha}, & \text{for } 0 < \alpha < \dfrac{\pi}{4}, \\[2ex] -\dfrac{Z}{\cos\alpha} - \dfrac{Z-1}{\sin\alpha}, & \text{for } \dfrac{\pi}{4} \leqslant \alpha < \dfrac{\pi}{2}. \end{cases} \tag{6.7c}$$

Hereafter we assume $Z > 0$. Notice that C is a continuous function in $\left(0, \frac{\pi}{2}\right)$. At the endpoints $\alpha = 0$ and $\alpha = \frac{\pi}{2}$,

$$\lim_{\alpha\to 0^+} C(\alpha) = \lim_{\alpha\to\frac{\pi}{2}^-} C(\alpha) = -\infty,$$

which reflects the so-called electron-nucleus cusps ($r_1 = 0$ or $r_2 = 0$). In addition we have a symmetry with respect to $\alpha = \dfrac{\pi}{4}$,

$$C(\alpha) = C\left(\frac{\pi}{2} - \alpha\right), \qquad 0 < \alpha \leqslant \frac{\pi}{4}. \tag{6.8}$$

The derivative

$$\frac{d}{d\alpha} C(\alpha) = \begin{cases} -\dfrac{(Z-1)\sin\alpha}{\cos^2\alpha} + \dfrac{Z\cos\alpha}{\sin^2\alpha}, & \text{for } 0 < \alpha < \dfrac{\pi}{4} \\[2ex] -\dfrac{Z\sin\alpha}{\cos^2\alpha} + \dfrac{(Z-1)\cos\alpha}{\sin^2\alpha}, & \text{for } \dfrac{\pi}{4} < \alpha < \dfrac{\pi}{2} \end{cases} \tag{6.9}$$

is not defined in $\alpha = \dfrac{\pi}{4}$ but the one-sided limits for $\alpha \to \dfrac{\pi}{4}^{\pm}$ exist,

$$\lim_{\alpha\to\frac{\pi}{4}^-} -\frac{(Z-1)\sin\alpha}{\cos^2\alpha} + \frac{Z\cos\alpha}{\sin^2\alpha} = \sqrt{2}, \tag{6.10a}$$

$$\lim_{\alpha\to\frac{\pi}{4}^+} -\frac{Z\sin\alpha}{\cos^2\alpha} + \frac{(Z-1)\cos\alpha}{\sin^2\alpha} = -\sqrt{2}. \tag{6.10b}$$

The discontinuity at $\alpha = \frac{\pi}{4}$ does not exist in the real potential (6.5); it is an artifice that appears in the Temkin-Poet truncation of the multipole expansion.

6.1.2 The kinetic energy

In the hyperspherical coordinates system, the kinetic energy for a general reduced mass μ reads [2, 19, 37]

$$\mathbf{T}_{\rho,\omega_5} = -\frac{1}{2\mu}\left[\frac{1}{\rho^5}\frac{\partial}{\partial\rho}\rho^5\frac{\partial}{\partial\rho} - \frac{\mathbf{\Lambda}^{\mathbf{2}}_{\omega_5}}{\rho^2}\right]. \tag{6.11}$$

$\mathbf{\Lambda}^{\mathbf{2}}_{\omega_5}$ is the grand orbital angular momentum operator [2, 19] given by

$$\mathbf{\Lambda}^{\mathbf{2}}_{\omega_5} = -\frac{1}{\sin^2\alpha\,\cos^2\alpha}\frac{\partial}{\partial\alpha}\left(\sin^2\alpha\,\cos^2\alpha\,\frac{\partial}{\partial\alpha}\right) + \frac{\mathbf{j}^2}{\cos^2\alpha} + \frac{\mathbf{l}^2}{\sin^2\alpha}$$

with $\mathbf{j}^2$ and $\mathbf{l}^2$ the rotational and centrifugal angular momentum operators. The eigenfunctions of $\mathbf{\Lambda}^{\mathbf{2}}_{\omega_5}$ are the hyperspherical harmonics $\mathcal{Y}^{m_j,m_\ell}_{\lambda,j,\ell}$, and satisfy

$$\mathbf{\Lambda}^{\mathbf{2}}_{\omega_5}\,\mathcal{Y}^{m_j,m_\ell}_{\lambda,j,\ell}(\omega_5) = \lambda(\lambda+4)\mathcal{Y}^{m_j,m_\ell}_{\lambda,j,\ell}(\omega_5). \tag{6.12}$$

They can be expressed in closed form [36, 82]

$$\mathcal{Y}^{m_j,m_\ell}_{\lambda,j,\ell}(\omega_5) = H_{\lambda,j,\ell}(\alpha)Y^{m_j}_j(\hat{\mathbf{x}}_\mathbf{1})\,Y^{m_\ell}_\ell(\hat{\mathbf{X}}_\mathbf{1}).$$

Here $Y^{m_s}_s$ are spherical harmonics [2, 3], and $H_{\lambda,j,\ell}$ are given in terms of Jacobi polynomials $P^{(a,b)}_n$,

$$H_{\lambda,j,\ell}(\alpha) = \mathcal{N}_{\lambda,j,\ell}\,\cos^{j+1/2}(\alpha)\,\sin^{\ell+1/2}(\alpha)\,P^{(\ell+1/2,j+1/2)}_{(\lambda-j-\ell)/2}(\cos(2\alpha))$$

where $\mathcal{N}_{\lambda,j,\ell}$ is a normalization constant.

As mentioned, we are interested here in the Temkin-Poet model. This problem is also called S-wave model problem [83] because it coincides with the situation of performing a spherical average of the interelectronic term $1/r_{12}$, thus keeping only the s-wave ($\ell = j = 0$). In this case, the grand orbital angular momentum reduces to

$$\mathbf{\Lambda}^{\mathbf{2}}_{\alpha} = -\frac{1}{\sin^2(\alpha)\cos^2(\alpha)}\frac{\partial}{\partial\alpha}\left(\sin^2(\alpha)\cos^2(\alpha)\frac{\partial}{\partial\alpha}\right), \tag{6.13a}$$

and the kinetic energy for the model problem becomes

$$\mathbf{T}_{\rho,\alpha} = -\frac{1}{2\mu}\left[\frac{1}{\rho^5}\frac{\partial}{\partial\rho}\left(\rho^5\frac{\partial}{\partial\rho}\right) + \frac{1}{\rho^2}\,\frac{1}{\sin^2(\alpha)\cos^2(\alpha)}\frac{\partial}{\partial\alpha}\left(\sin^2(\alpha)\cos^2(\alpha)\frac{\partial}{\partial\alpha}\right)\right]. \tag{6.13b}$$

The eigenfunctions of $\mathbf{\Lambda}^{\mathbf{2}}_{\alpha}$ simplify to Jacobi polynomials $P^{(a,b)}_m$ usually expressed in terms of Gauss hypergeometric functions [2, 40],

$$\Omega_m(\alpha) = \frac{4(m+1)!}{\sqrt{\pi}\ \left(\frac{3}{2}\right)_m}\ P_m^{(\frac{1}{2},\frac{1}{2})}\left(1 - 2\sin^2\alpha\right)$$
$$= \frac{4(m+1)}{\sqrt{\pi}}\ {}_2F_1\left(-m, m+2, \frac{3}{2}, \sin^2\alpha\right).$$

The identity 15.1.16 of [42],

$${}_2F_1\left(a, 2-a, \frac{3}{2}; \sin^2 z\right) = \frac{\sin[2(a-1)z]}{(a-1)\sin(2z)},$$

allows one to give a simpler expression

$$\Omega_m(\alpha) = \frac{2}{\sqrt{\pi}}\frac{\sin[2(m+1)\alpha]}{\sin\alpha\ \cos\alpha}. \tag{6.14}$$

These orthogonal eigenfunctions satisfy

$$\mathbf{\Lambda}^{\mathbf{2}}_{\alpha}\,\Omega_m(\alpha) = 2m(2m+4)\Omega_m(\alpha), \tag{6.15a}$$
$$\int_0^{\frac{\pi}{2}} d\alpha\,\Omega_m(\alpha)\,\Omega_n(\alpha)\,\cos^2\alpha\,\sin^2\alpha = \delta_{m,n}. \tag{6.15b}$$

6.2 The Schrödinger equation

In hyperspherical coordinates the Schrödinger equation for a three-body scattering problem reads

$$[\mathbf{H}_{\rho,\omega_5} - E]\,\Psi^{(\pm)}(\rho,\omega_5) = 0. \tag{6.16}$$

Here $E = E_1 + E_2$ is the total energy of the system, and $\mathbf{H}_{\rho,\omega_5} = \mathbf{T}_{\rho,\omega_5} + V$. The kinetic energy $\mathbf{T}_{\rho,\omega_5}$ was introduced in (6.11), and from now on, we are going to consider V as the Coulomb potential given by formula (6.6).

As proposed in (5.4) for two-body scattering problems, we decompose the solution $\Psi^{(\pm)}$ as the sum

$$\Psi^{(\pm)}(\rho,\omega_5) = \Psi_0(\rho,\omega_5) + \Psi_{sc}^{(\pm)}(\rho,\omega_5), \tag{6.17}$$

where Ψ_0 is the initial state solution corresponding to a potential V_0,

$$[\mathbf{T}_{\rho,\omega_5} + V_0(\rho,\omega_5) - E]\Psi_0(\rho,\omega_5) = 0. \tag{6.18}$$

Then, setting $V_1 = V - V_0$, from equation (6.16) we find a non-homogeneous Schrödinger equation for the scattering function $\Psi_{sc}^{(\pm)}$

$$[\mathbf{T}_{\rho,\omega_5} + V(\rho,\omega_5) - E]\Psi_{sc}^{(\pm)}(\rho,\omega_5) = -V_1(\rho,\omega_5)\Psi_0(\rho,\omega_5). \tag{6.19a}$$

The boundary conditions associated to this equation are [20, 21, 83]

$$\Psi_{sc}^{(\pm)}(0,\omega_5) = 0, \tag{6.19b}$$

$$\Psi_{sc}^{(\pm)}(\rho,\omega_5) \overset{\rho\to\infty}{\sim} \mathcal{A}(\omega_5)\, \frac{e^{\pm i[K\rho - \eta(\widetilde{C}(\omega_5))\ln(2K\rho) + \sigma_C(\ell,\widetilde{C}(\omega_5)) - \ell\frac{\pi}{2}]}}{\rho^{5/2}}, \tag{6.19c}$$

where $\mathcal{A}$ is proportional to the scattering amplitude, K is the hyperspherical momentum related to the total energy of the system by $K^2 = 2\mu E$, and $\eta(\widetilde{C}(\omega_5))$ is the Sommerfeld parameter associated with the angular dependent charge $\widetilde{C}$.

Considering a Temkin-Poet model, with kinetic energy $\mathbf{T}_{\rho,\alpha}$ given by (6.13b) and potential V as in (6.7), the non-homogeneous Schrödinger equation (6.19a) becomes

$$[\mathbf{T}_{\rho,\alpha} + V(\rho,\alpha) - E]\,\Psi_{sc}^{(\pm)}(\rho,\alpha) = F(\rho,\alpha), \tag{6.20}$$

for a general driven term $F(\rho,\alpha)$. To reduce this equation we express

$$\Psi_{sc}^{(\pm)}(\rho,\alpha) = \frac{\Phi_{sc}^{(\pm)}(\rho,\alpha)}{\rho^{5/2}\,\cos\alpha\,\sin\alpha}, \tag{6.21}$$

as to simplify the action of the grand orbital angular momentum (6.15), and then of the kinetic energy (6.13b),

$$\mathbf{\Lambda}^{\mathbf{2}}_{\alpha}\frac{\Phi_{sc}^{(\pm)}(\rho,\alpha)}{\rho^{5/2}\cos\alpha\,\sin\alpha} = -\frac{1}{\rho^{5/2}\cos\alpha\,\sin\alpha}\left[\frac{\partial^2}{\partial\alpha^2} + 4\right]\Phi_{sc}^{(\pm)}(\rho,\alpha), \tag{6.22a}$$

$$\frac{1}{\rho^5}\frac{\partial}{\partial\rho}\left(\rho^5\frac{\partial}{\partial\rho}\right)\frac{\Phi_{sc}^{(\pm)}(\rho,\alpha)}{\rho^{5/2}\,\cos\alpha\,\sin\alpha} = \frac{1}{\rho^{5/2}\cos\alpha\,\sin\alpha}\left[\frac{\partial^2}{\partial\rho^2} - \frac{15}{4}\frac{1}{\rho^2}\right]\Phi_{sc}^{(\pm)}(\rho,\alpha), \tag{6.22b}$$

$$\mathbf{T}_{\rho,\alpha}\,\frac{\Phi_{sc}^{(\pm)}(\rho,\alpha)}{\rho^{5/2}\cos\alpha\,\sin\alpha} = -\frac{1}{\rho^{5/2}\cos\alpha\,\sin\alpha}\,\frac{1}{2\mu}\left[\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho^2}\,\frac{\partial^2}{\partial\alpha^2} + \frac{1}{4\,\rho^2}\right]\Phi_{sc}^{(\pm)}(\rho,\alpha). \tag{6.22c}$$

Consequently, the Schrödinger equation (6.20) becomes

$$\frac{1}{\rho^{5/2}\cos\alpha\,\sin\alpha}\left[-\frac{1}{2\mu}\left(\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\alpha^2}\right)-\frac{1}{8\mu\rho^2}+\frac{C(\alpha)}{\rho}-E\right]\Phi_{sc}^{(\pm)}(\rho,\alpha)=F(\rho,\alpha). \tag{6.23}$$

In order to simplify the writing we name $\mathbf{H}_{\rho,\alpha}$ the reduced Coulomb Hamiltonian

$$\mathbf{H}_{\rho,\alpha}=-\frac{1}{2\mu}\left(\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\alpha^2}\right)-\frac{1}{8\mu\rho^2}+\frac{C(\alpha)}{\rho}. \tag{6.24}$$

With this, and from (6.19c) and (6.21), the reduced three-body scattering problem reads

$$[\mathbf{H}_{\rho,\alpha}-E]\;\Phi_{sc}^{(\pm)}(\rho,\alpha)=\rho^{5/2}\cos\alpha\,\sin\alpha\,F(\rho,\alpha), \tag{6.25a}$$

$$\Phi_{sc}^{(\pm)}(0,\alpha)=0, \tag{6.25b}$$

$$\Phi_{sc}^{(\pm)}(\rho,\alpha)\;\overset{\rho\to\infty}{\sim}\;\mathcal{A}_\alpha\,\cos\alpha\,\sin\alpha\;e^{\pm i[K\rho-\eta(C(\alpha))\ln(2K\rho)+\sigma_C(\ell,C(\alpha))-\ell\frac{\pi}{2}]}. \tag{6.25c}$$

6.3 The scattering wave function

To represent the solution of three-body problems several coordinates systems and expansions on different basis sets have been proposed in the literature. First, the basis should be chosen appropriately according to whether one is dealing with bound or continuum states. Second, the way the variables are coupled dictates the efficiency of a basis and, at the same time, the difficulty of its implementation. Hereafter, we consider only hyperspherical coordinates and focus on scattering problems.

The simplest expansion is to consider

$$\Psi^{(\pm)}(\rho,\omega_5)=\sum_{\nu,n}f_n(\rho)g_\nu(\omega_5),$$

which treats the angular and the hyperradial variables separately. This strategy is attractive from an implementation point of view, but it is known to be inadequate for non-separable differential equations such as the Schrödinger equation describing three-body scattering problems. Nevertheless, such a proposal have been considered in many studies [40, 83–88]. In particular, different Temkin-Poet model problems have been solved by expressing

$$\Psi_{sc}^{(\pm)}(\rho,\alpha)=\sum_{m,n}\frac{S_{m,n}^{(\pm)}(\rho)}{\rho^{5/2}}\,\Omega_m(\alpha),$$

using the Jacobi polynomials Ω_n, given by (6.14), as angular basis functions, and hyperradial functions $S^{(\pm)}_{m,n}$ such as Generalized Sturmian functions [40, 83, 84].

Other approaches, like those presented in references [19, 82, 89, 90], couple in a parametric form the angular and radial variables. To do it, the Schrödinger equation is expressed as

$$\left[-\frac{1}{2\mu}\frac{1}{\rho^5}\frac{\partial}{\partial\rho}\rho^5\frac{\partial}{\partial\rho} - \frac{\mathbf{\Lambda^2_{\omega_5}} + 2\mu\rho\,\widetilde{C}(\omega_5)}{\rho^2} - E\right]\Psi^{(\pm)}_{sc}(\rho,\omega_5) = 0.$$

To describe the angular part of the equation a set of Generalized Sturmian functions $\widetilde{\Omega}_\nu$ is constructed by solving

$$\left[\mathbf{\Lambda^2_{\omega_5}} - \lambda(\lambda+4)\right]\widetilde{\Omega}_\nu(\omega_5) = -2\mu\rho_\nu\widetilde{C}(\omega_5)\widetilde{\Omega}_\nu(\omega_5),$$

thus relating the radial variable with the eigenvalues ρ_ν of this problem (λ is an external fixed parameter). In references [19, 82, 90], the authors have solved scattering problems by generating hyperradial Generalized Sturmian functions $S^{(\pm)}_{\beta,\lambda}$, to finally represent the solution as

$$\Psi^{(\pm)}_{sc}(\rho,\omega_5) = \sum_{\beta,\nu}\frac{S^{(\pm)}_{\beta,\lambda}(\rho)}{\rho^{5/2}}\,\widetilde{\Omega}_\nu(\omega_5).$$

An important aspect to bare in mind is the asymptotic behavior of the scattering solution. We already explained, in the previous chapter, that a good strategy is to use basis functions including the expected behavior of the solution, as it was the case, for two-body problems, of Generalized Sturmian functions and Quasi-Sturmian functions.

For the three-body case, the Quasi-Sturmian functions presented in **Section 4.3.7** possess this characteristic, as one can see by comparing (4.41c) with (6.19c). Hence, one may conclude that functions

$$\varphi^{(\pm)}_{m,n}(\rho,\alpha) = \frac{1}{\rho^{5/2}}\,Q^{L\,(\pm)}_n(\ell_{QS},\beta,\omega_5;\rho)\,\mathcal{Y}^{m_j,m_\ell}_{\lambda,j,\ell}(\omega_5) \tag{6.26}$$

constitute an interesting option to represent the scattering solution. Applying the

Schrödinger operator to one of them we obtain

$$
\begin{aligned}
&[\mathbf{H}_{\rho,\omega_5} - E]\, \frac{1}{\rho^{5/2}}\, Q_n^{L(\pm)}(\ell_{QS},\beta,\omega_5;\rho)\; \mathcal{Y}_{\lambda,j,\ell}^{m_j,m_\ell}(\omega_5) \\
&\overset{(4.41a)}{=} \frac{1}{\rho^{5/2}} \left\{ \frac{1}{\rho}\, \phi_n^L(\ell_{QS},\beta;\rho)\, \mathcal{Y}_{\lambda,j,\ell}^{m_j,m_\ell}(\omega_5) \right. \\
&\qquad - \frac{1}{2\mu\rho^2} \left[\frac{\ell_{QS}(\ell_{QS}+1) - 15}{4} \right] Q_n^{L(\pm)}(\ell_{QS},\beta,\omega_5;\rho)\, \mathcal{Y}_{\lambda,j,\ell}^{m_j,m_\ell}(\omega_5) \\
&\qquad \left. - \frac{1}{2\mu\rho^2}\, \mathbf{\Lambda}^2_{\omega_5} \left[Q_n^{L(\pm)}(\ell_{QS},\beta,\omega_5;\rho)\, \mathcal{Y}_{\lambda,j,\ell}^{m_j,m_\ell}(\omega_5) \right] \right\}. \qquad (6.27)
\end{aligned}
$$

The application of the angular operator is by far not trivial and we do not go further in providing the resulting expression. Taking the limit $\rho \to \infty$, the three terms between braces go to zero faster than ρ^{-1}, indicating that the functions $\varphi_{m,n}^{(\pm)}$ given by (6.26) may be considered as approximated solutions of the Schrödinger equation (6.16) in the asymptotic region ($\rho > R$).

Another advantage of representing the scattering solution in terms of functions having the appropriate asymptotic behavior is that it facilitates the extraction of the transition amplitude, as explained in **Remark 5.1.1**.

For the Temkin-Poet model problem we investigate here, we present three different representations of the scattering solution using Quasi-Sturmian functions: one considering separate variables and separate indices, a second one coupling the indices of the basis functions and a third one coupling the variables by using Quasi-Sturmian functions with a variable charge.

First we describe the general strategy to solve the equation, which is an extension of the procedure implemented in **Section 5.1** for two-body scattering problems. We express $\Phi_{sc}^{(\pm)}$ in terms of a general set of basis functions $\{\varphi_{m,n}\}$

$$
\Phi_{sc}^{(\pm)}(\rho,\alpha) = \sum_{m,n} a_{m,n}\, \varphi_{m,n}(\rho,\alpha). \qquad (6.28)
$$

Inserting this double series into (6.25a), then multiplying, for each p and q, both sides of the equation by appropriate functions w and $\widetilde{\varphi}_{p,q}$, and finally integrating over the domain

$$
0 < \alpha < \frac{\pi}{2}, \quad 0 < \rho < \infty,
$$

we find a linear system $\mathbf{O} \cdot \mathbf{a} = \mathbf{b}$ for the unknown $a_{m,n}$. The elements $O_{p,q;m,n}$ and $b_{p,q}$

forming the matrix **O** and the vector **b** respectively, are

$$b_{p,q} = \int_0^{\frac{\pi}{2}} \int_0^{\infty} w(\rho,\alpha)\,\widetilde{\varphi}_{p,q}(\rho,\alpha)\;\rho^{5/2}\cos\alpha\,\sin\alpha\,F(\rho,\alpha)\,d\rho\,d\alpha, \tag{6.29a}$$

$$O_{p,q;m,n} = \int_0^{\frac{\pi}{2}} \int_0^{\infty} w(\rho,\alpha)\,\widetilde{\varphi}_{p,q}(\rho,\alpha)\,[\mathbf{H}_{\rho,\alpha} - E]\,\varphi_{m,n}(\rho,\alpha)\;d\rho\,d\alpha. \tag{6.29b}$$

The matrix **O** is what we called in **Remark 1.1.1** the matrix representation of the operator $[\mathbf{H}_{\rho,\alpha} - E]$.

Next we must choose the functions $\varphi_{m,n}$. The angular part of the scattering equation includes the grand orbital angular momentum whose eigenfunctions are given by (6.15). The eigenfunctions of the reduced form of this operator [see (6.22a)],

$$H_m(\alpha) = \cos(\alpha)\,\sin(\alpha)\,\Omega_m(\alpha) \overset{(6.14)}{=} \frac{2}{\sqrt{\pi}}\sin[2(m+1)\alpha], \tag{6.30}$$

are used hereafter to represent the angular part of the scattering solution. They satisfy

$$H_m(0) = H_m\left(\frac{\pi}{2}\right) = 0, \tag{6.31a}$$

$$\int_0^{\pi/2} H_p(\alpha)\,H_m(\alpha)\,d\alpha = \delta_{p,m}, \tag{6.31b}$$

$$\frac{d^2}{d\alpha^2}\,H_m(\alpha) = -4(m+1)^2\,H_m(\alpha). \tag{6.31c}$$

The hyperradial terms of the Schrödinger equation (6.23) are similar to the radial ones in the differential equation defining the Quasi-Sturmian functions [see (4.3a)]. Thus we propose to use incoming (−)/outgoing (+) Laguerre Quasi-Sturmian functions to describe the radial behavior of the scattering solution.

Now, as mentioned above, we explore three different possibilities with functions $\varphi_{m,n}$ in (6.28) associated to three variants of the Quasi-Sturmian functions;

A. $\varphi_{m,n}(\rho,\alpha) = Q_n^{L\,(\pm)}(\rho)H_m(\alpha)$,

B. $\varphi_{m,n}(\rho,\alpha) = Q_{m,n}^{L\,(\pm)}(\ell_m;\rho)H_m(\alpha)$,

C. $\varphi_{m,n}(\rho,\alpha) = Q_n^{L\,(\pm)}(\alpha;\rho)H_m(\alpha)$.

In each case, we present the resulting elements $O_{p,q;m,n}$ and $b_{p,q}$ defined in (6.29), as well as the asymptotic form of the obtained scattering solution.

Hereafter, the parameters μ, E and K are the reduced mass, the total energy and momentum of the scattering problem ($K^2 = 2\mu E$).

A. Separated variables

We first propose

$$\varphi_{m,n}(\rho,\alpha) = Q_n^{L\,(\pm)}(\ell,\beta;\rho)H_m(\alpha).$$

Each $Q_n^{L\,(\pm)}$ is the solution of the boundary value problem

$$\left[-\frac{1}{2\mu}\frac{d^2}{d\rho^2} + \frac{\ell(\ell+1)}{2\mu\rho^2} + \frac{Z_{QS}}{\rho} - E\right] Q_n^{L\,(\pm)}(\ell,\beta;\rho) = \frac{1}{\rho}\,\phi_n^L(\ell,\beta;\rho), \tag{6.33a}$$

$$Q_n^{L\,(\pm)}(\ell,\beta;0) = 0, \tag{6.33b}$$

$$Q_n^{L\,(\pm)}(\ell,\beta;\rho) \overset{\rho\to\infty}{\sim} \mathcal{Q}_n^{L\,as}\; e^{\pm i\left[K\rho-\eta(Z_{QS})\ln(2K\rho)+\sigma_C(\ell,Z_{QS})-\ell\,\frac{\pi}{2}\right]}, \tag{6.33c}$$

where the asymptotic coefficient $\mathcal{Q}_n^{L\,as}$ is given by (4.22). ℓ, Z_{QS} and β are real parameters that can be conveniently fixed, and the corresponding Sommerfeld parameter η and phase shift σ_C are defined by (1.23a) and (1.23b), respectively.

The linear system

Let us apply $[\mathbf{H}_{\rho,\alpha} - E]$ to one of these $\varphi_{m,n}$ functions. In a first step we have

$$\begin{aligned}
&[\mathbf{H}_{\rho,\alpha} - E]\;\varphi_{m,n}(\rho,\alpha) \\
&\quad = H_m(\alpha)\left[-\frac{1}{2\mu}\left(\frac{\partial^2}{\partial\rho^2}\right) - E\right] Q_n^{L(\pm)}(\ell,\beta;\rho) \\
&\quad\quad - \;Q_n^{L(\pm)}(\ell,\beta;\rho)\;\frac{1}{2\mu\rho^2}\frac{\partial^2}{\partial\alpha^2}H_m(\alpha) + \left[-\frac{1}{8\mu\rho^2} + \frac{C(\alpha)}{\rho}\right] Q_n^{L(\pm)}(\ell,\beta;\rho)H_m(\alpha).
\end{aligned}$$

Now taking into account (6.33a) and (6.31c) we obtain

$$\begin{aligned}
&[\mathbf{H}_{\rho,\alpha} - E]\,\varphi_{m,n}(\rho,\alpha) \\
&\quad = \frac{1}{\rho}\,\phi_n^L(\ell,\beta;\rho)H_m(\alpha) + \frac{16(m+1)^2-(2\ell+1)^2}{8\mu}\,\frac{1}{\rho^2}\,Q_n^{L(\pm)}(\ell,\beta;\rho)H_m(\alpha) \\
&\quad\quad + \frac{1}{\rho}\,[C(\alpha) - Z_{QS}]\,Q_n^{L(\pm)}(\ell,\beta;\rho)H_m(\alpha).
\end{aligned} \tag{6.34}$$

Choosing

$$w(\rho,\alpha) = \rho, \qquad \widetilde{\varphi}_{p,q}(\rho,\alpha) = \phi_q^L(\ell,\beta;\rho)\,H_p(\alpha),$$

the components $b_{p,q}$ in (6.29a) are

$$b_{p,q} = \int_0^{\frac{\pi}{2}} \int_0^{\infty} \phi_q^L(\ell,\beta;\rho)\, H_p(\alpha)\, F(\rho,\alpha)\rho^{7/2} \cos\alpha\, \sin\alpha\, d\rho\, d\alpha, \tag{6.35}$$

and the matrix elements (6.29b) become

$$\begin{aligned} O_{p,q;m,n} = &\int_0^{\frac{\pi}{2}} \int_0^{\infty} \phi_q^L(\ell,\beta;\rho)\, H_p(\alpha)\, \phi_n^L(\ell,\beta;\rho)\, H_m(\alpha)\, d\rho\, d\alpha \\ &+ \frac{16(m+1)^2 - (2\ell+1)^2}{8\mu} \int_0^{\frac{\pi}{2}} \int_0^{\infty} \phi_q^L(\ell,\beta;\rho)\, H_p(\alpha)\, \frac{1}{\rho}\, Q_n^{L(\pm)}(\ell,\beta;\rho) H_m(\alpha)\, d\rho\, d\alpha \\ &+ \int_0^{\frac{\pi}{2}} \int_0^{\infty} \phi_q^L(\ell,\beta;\rho)\, H_p(\alpha)\, [C(\alpha) - Z_{QS}]\, Q_n^{L(\pm)}(\ell,\beta;\rho) H_m(\alpha)\, d\rho\, d\alpha. \end{aligned} \tag{6.36}$$

Each of these three two-dimensional integrals can be expressed as the product of a radial and an angular integral. In the first two, the angular part reduces to a Kronecker delta $\delta_{p,m}$ because of the orthogonality property (6.31b). The angular integral involving the C function is performed in (B.12), and the radial integrals were solved in previous chapters. Setting

$$\begin{aligned} I_{q,n}^{(1)} &= \int_0^{\infty} \phi_q^L(\ell,\beta;\rho) \phi_n^L(\ell,\beta;\rho) d\rho \\ &\overset{(1.12b)}{=} \frac{\ell+1+n}{\beta}\, \delta_{q,n} - \frac{N_{n,\ell}}{N_{n-1,\ell}}\, \frac{2\ell+1+n}{2\beta}\, \delta_{q,n-1} - \frac{N_{n,\ell}}{N_{n+1,\ell}}\, \frac{n+1}{2\beta}\, \delta_{q,n+1} \end{aligned}$$

we obtain for the first integral

$$\int_0^{\frac{\pi}{2}} \int_0^{\infty} \phi_q^L(\ell,\beta;\rho) \phi_n^L(\ell,\beta;\rho) H_p(\alpha) H_m(\alpha)\, d\rho\, d\alpha = \delta_{p,m}\, I_{q,n}^{(1)}. \tag{6.37a}$$

For the second integral we use (4.28) to find

$$\int_0^{\frac{\pi}{2}} \int_0^{\infty} \phi_q^L(\ell,\beta;\rho)\, \frac{1}{\rho}\, Q_n^{L\,(\pm)}(\ell,\beta;\rho)\, H_p(\alpha)\, H_m(\alpha)\, d\rho\, d\alpha = g_{n,q}^{(\pm)}\, \delta_{p,m}. \tag{6.37b}$$

To perform the third integral we separate the radial part, calculated in (4.30),

$$\begin{aligned} I_{q,n}^{(3)} &= \int_0^{\infty} \phi_q^L(\ell,\beta;\rho)\, Q_n^{L\,(\pm)}(\ell,\beta;\rho)\, d\rho \\ &= \frac{\ell+1+q}{\beta}\, g_{n,q}^{(\pm)} - \frac{N_{q+1,\ell}}{N_{q,\ell}}\, \frac{2\ell+2+q}{2\beta}\, g_{n,q+1}^{(\pm)} - \frac{N_{q-1,\ell}}{N_{q,\ell}}\, \frac{q}{2\beta}\, g_{n,q-1}^{(\pm)}, \end{aligned}$$

and the angular part, calculated in (B.12). For m and p having the same parity we find

$$\begin{aligned} I^{(4)}_{p,m} &= \int_0^{\frac{\pi}{2}} C(\alpha)\, H_p(\alpha)\, H_m(\alpha)\, d\alpha \\ &= \frac{8}{\pi}\left\{ (Z-1) \sum_{j=|p-m|+1}^{p+m+2} (-1)^j \, \frac{\sin\left[(2j-1)\frac{\pi}{4}\right]}{2j-1} \right. \\ &\qquad \left. + \, Z \sum_{j=|p-m|+1}^{p+m+2} \frac{\cos\left[(2j-1)\frac{\pi}{4}\right]-1}{2j-1} \right\} \end{aligned} \tag{6.37c}$$

and the integral vanishes in all other cases. The third integral is thus given by

$$\int_0^{\frac{\pi}{2}} \int_0^{\infty} \phi^L_q(\ell,\beta;\rho)\, Q^{L\,(\pm)}_n(\rho)\; [C(\alpha) - Z_{QS}]\, H_p(\alpha)\, H_m(\alpha) d\rho\, d\alpha \\ = I^{(3)}_{q,n}\; I^{(4)}_{p,m} - Z_{QS}\; I^{(3)}_{q,n}\; \delta_{p,m}. \tag{6.37d}$$

Collecting (6.37a), (6.37b) and (6.37d) we arrive to a closed form for the matrix elements $O_{p,q;m,n}$,

$$O_{p,q;m,n} = \left(I^{(1)}_{q,n} + \frac{16(m+1)^2 - (2\ell+1)^2}{8\mu}\; g^{(\pm)}_{n,q} - Z_{QS}\, I^{(3)}_{q,n} \right) \delta_{p,m} + I^{(3)}_{q,n}\; I^{(4)}_{p,m}. \tag{6.38}$$

The asymptotic behavior

Using (6.33c) the asymptotic behavior of the scattering solution (6.28) reads

$$\Phi^{\pm}_{sc}(\alpha,\rho) \quad \overset{\rho\to\infty}{\sim} \quad e^{\pm i\left[K\rho - \eta(Z_{QS})\ln(2K\rho) + \sigma_C(\ell,Z_{QS}) - \ell\,\frac{\pi}{2}\right]} \sum_{m,n} a_{m,n}\, H_m(\alpha)\, \mathcal{Q}^{L\,as}_n.$$

Comparing this result with the expected asymptotic behavior of the reduced scattering wave function (6.25c), we find that it is not possible to extract an analytical expression for the amplitude $\mathcal{A}_\alpha$.

B. Laguerre Quasi-Sturmian depending on n and m

Instead of the previous $Q^{L\,(\pm)}_n$, for which the parameter ℓ takes any non-negative real value, we can choose the value of $\ell = \ell_m$, for each $m = 0, 1, 2, ...$, in such a way that the second term in (6.34) vanishes. This is,

$$16(m+1)^2 - (2\ell_m+1)^2 = 0 \quad \Longrightarrow \quad \ell_m = 2m + \frac{3}{2}. \tag{6.39}$$

Thus we have an alternative approximation of the reduced scattering solution

$$\Phi_{sc}^{(\pm)}(\rho,\alpha) = \sum_{m,n} a_{m,n}\, Q_{m,n}^{L\,(\pm)}(\ell_m,\beta;\rho)\, H_m(\alpha),$$

where $Q_{m,n}^{L\,(\pm)}$ is the incoming $(-)$/outgoing $(+)$ solution of

$$\left[-\frac{1}{2\mu}\frac{d^2}{d\rho^2} + \frac{\ell_m(\ell_m+1)}{2\mu\rho^2} + \frac{Z_{QS}}{\rho} - E\right] Q_{m,n}^{L\,(\pm)}(\ell_m,\beta;\rho) = \frac{1}{\rho}\,\phi_n^L(\ell_m,\beta;\rho), \tag{6.40a}$$

$$Q_{m,n}^{L\,(\pm)}(\ell_m,\beta;0) = 0, \tag{6.40b}$$

$$Q_{m,n}^{L\,(\pm)}(\ell_m,\beta;\rho) \overset{\rho\to\infty}{\sim} \mathcal{Q}_{m,n}^{L\,as}\, e^{\pm i\left[K\rho - \eta(Z_{QS})\ln(2K\rho) + \sigma_C(\ell_m,Z_{QS}) - \ell_m\frac{\pi}{2}\right]}. \tag{6.40c}$$

where η and σ_C are defined in (1.23a) and (1.23b) while Z_{QS} and β can be conveniently fixed.

The linear system

If we apply the operator $[\mathbf{H}_{\rho,\alpha} - E]$ to one of these functions

$$\varphi_{m,n}(\rho,\alpha) = Q_{m,n}^{L\,(\pm)}(\ell_m,\beta;\rho)\, H_m(\alpha)$$

we obtain

$$[\mathbf{H}_{\rho,\alpha} - E]\ \varphi_{m,n}(\rho,\alpha) = \frac{1}{\rho}\,\phi_n^L(\ell_m,\beta;\rho)H_m(\alpha) + \frac{1}{\rho}\ [C(\alpha) - Z_{QS}]\, Q_{m,n}^{L(\pm)}(\ell_m,\beta;\rho)H_m(\alpha).$$

In this case it is convenient to choose

$$w(\rho,\alpha) = 1, \quad \widetilde{\varphi}_{p,q}(\rho,\alpha) = \phi_q^L(\ell_p,\beta;\rho)\, H_p(\alpha)$$

so the matrix elements (6.29b) become

$$\begin{aligned} O_{p,q;m,n} =& \int_0^{\frac{\pi}{2}}\int_0^{\infty} \phi_q^L(\ell_p,\beta;\rho)\, H_p(\alpha)\,\frac{1}{\rho}\,\phi_n^L(\ell_m,\beta;\rho)\, H_m(\alpha)\, d\rho\, d\alpha \\ &+ \int_0^{\frac{\pi}{2}}\int_0^{\infty} \phi_q^L(\ell_p,\beta;\rho)\, H_p(\alpha)\,\frac{1}{\rho}\ [C(\alpha) - Z_{QS}]\, Q_{m,n}^{L(\pm)}(\ell_m,\beta;\rho)H_m(\alpha)\, d\rho\, d\alpha, \end{aligned} \tag{6.41}$$

while the components $b_{p,q}$ read

$$b_{p,q} = \int_0^{\frac{\pi}{2}} \int_0^{\infty} \phi_q^L(\ell_p, \beta; \rho)\, H_p(\alpha)\, F(\rho, \alpha) \rho^{5/2} \cos\alpha\, \sin\alpha\, d\rho\, d\alpha. \tag{6.42}$$

The first integral in (6.41) reduces to a product of two Kronecker delta. Only for $m = p$ the angular integral does not vanish, so that we have, for the radial integral, $\ell_m = \ell_p$ and we can apply thereafter the orthogonality property (1.9a), satisfied by Laguerre-type functions:

$$\begin{aligned} &\int_0^{\frac{\pi}{2}} \int_0^{\infty} \phi_q^L(\ell_p, \beta; \rho)\, \frac{1}{\rho}\, \phi_n^L(\ell_m, \beta; \rho) H_p(\alpha) H_m(\alpha)\, d\rho\, d\alpha \\ &\qquad = \left(\int_0^{\frac{\pi}{2}} H_p(\alpha)\, H_m(\alpha)\, d\alpha \right) \left(\int_0^{\infty} \phi_q^L(\ell_p, \beta; \rho)\, \frac{1}{\rho}\, \phi_n^L(\ell_m, \beta; \rho)\, d\rho \right) = \delta_{p,m}\, \delta_{q,n}. \end{aligned} \tag{6.43}$$

The second integral in (6.41) can be separated into two terms, one of them being

$$-Z_{QS} \left(\int_0^{\frac{\pi}{2}} H_p(\alpha)\, H_m(\alpha)\, d\alpha \right) \left(\int_0^{\infty} \phi_q^L(\ell_p, \beta; \rho)\, \frac{1}{\rho}\, Q_{m,n}^{(\pm)}(\ell_m, \beta; \rho)\, d\rho \right) \overset{(4.28)}{=} -Z_{QS}\, g_{q,n}^{(\pm)}\, \delta_{p,m},$$

Again, we have $m = p$ (otherwise the angular integral vanishes), then $\ell_p = \ell_m$ and then we can use result (4.28). To perform the other term,

$$\int_0^{\frac{\pi}{2}} \int_0^{\infty} \phi_q^L(\ell_p, \beta; \rho)\, \frac{1}{\rho}\, Q_{m,n}^{L\,(\pm)}(\ell_m, \beta; \rho)\, C(\alpha)\, H_p(\alpha)\, H_m(\alpha) d\rho\, d\alpha$$

we name

$$\begin{aligned} \mathcal{I}^{(1)}_{p,q,m,s} &= \int_0^{\infty} \phi_q^L(\ell_p, \beta; \rho)\, \frac{1}{\rho}\, \phi_s^L(\ell_m, \beta; \rho)\, d\rho \\ &\overset{(1.16)}{=} \frac{N_{s,\ell_m}\, \Gamma(\ell_p + \ell_m + 2)}{N_{q,\ell_p}\, s!\, \Gamma(2\ell_p + 2)} \sum_{j=0}^{q} \frac{(\ell_p + \ell_m + 2)_j (-q)_j}{(2\ell_p + 2)_j\; j!} (\ell_m - \ell_p - j)_s \end{aligned}$$

and use the series representation of the Laguerre Quasi-Sturmian functions (4.26a) to find

$$\begin{aligned} \mathcal{I}^{(2)}_{p,q,m,n} &= \int_0^{\infty} \phi_q^L(\ell_p, \beta; \rho)\, \frac{1}{\rho}\, Q_{m,n}^{L\,(\pm)}(\ell_m; \rho)\, d\rho \\ &= \sum_{s=0}^{\infty} g_{n,s}^{(\pm)} \int_0^{\infty} \phi_q^L(\ell_p, \beta; \rho)\, \frac{1}{\rho}\, \phi_s^L(\ell_m, \beta; \rho)\, d\rho \\ &= \sum_{s=0}^{\infty} g_{n,s}^{(\pm)}\; \mathcal{I}^{(1)}_{p,q,m,s}. \end{aligned}$$

Then, using (B.12) we obtain

$$\int_0^{\frac{\pi}{2}} \int_0^{\infty} \phi_q^L(\ell_p, \beta; \rho) \, \frac{1}{\rho} \, Q_{m,n}^{L\,(\pm)}(\ell_m, \beta; \rho) \, C(\alpha) \, H_p(\alpha) \, H_m(\alpha) d\rho \, d\alpha = \mathcal{I}_{p,q,m,n}^{(2)} \; I_{p,m}^{(4)}$$

with $I_{p,m}^{(4)}$ defined in (6.37c). We finally have an analytical expression for the elements of the linear system (6.29),

$$O_{p,q;m,n} = \left[\delta_{q,n} - Z_{QS} \, g_{q,n}^{(\pm)}\right] \; \delta_{p,m} + \mathcal{I}_{p,q,m,n}^{(2)} \; I_{p,m}^{(4)}. \tag{6.44}$$

The asymptotic behavior

As in the previous case, we can deduce an expression for the asymptotic behavior of the scattering solution by using the asymptotic form of the proposed Quasi-Sturmian functions (6.40c). We find,

$$\Phi_{sc}^{\pm}(\alpha, \rho) \quad \overset{\rho \to \infty}{\sim} \quad e^{\pm i\left[K\rho - \eta(Z_{QS}) \ln(2K\rho)\right]} \sum_{m,n} a_{m,n} \, H_m(\alpha) \, \mathcal{Q}_{m,n}^{L\,as} \, e^{\left[\sigma_C(\ell_m, Z_{QS}) - \ell_m \frac{\pi}{2}\right]},$$

and, again, we cannot obtain an analytical expression for the amplitude $\mathcal{A}_\alpha$ introduced in (6.25c).

C. Coupled variables

Another option for the functions $\varphi_{m,n}$ is to consider

$$\varphi_{m,n}(\rho, \alpha) = Q_n^{L\,(\pm)}(\ell, \beta, \alpha; \rho) H_m(\alpha). \tag{6.45}$$

where the Quasi-Sturmian functions $Q_n^{L\,(\pm)}$ depend on both variables, ρ and α. They are solution of (6.33a) but now with the angular function C instead of Z_{QS},

$$\left[-\frac{1}{2\mu} \frac{d^2}{d\rho^2} + \frac{\ell(\ell+1)}{2\mu\rho^2} + \frac{C(\alpha)}{\rho} - E\right] Q_n^{L\,(\pm)}(\ell, \beta, \alpha; \rho) = \frac{1}{\rho} \, \phi_n^L(\ell, \beta; \rho), \tag{6.46a}$$

$$Q_n^{L\,(\pm)}(\ell, \beta, \alpha; 0) = 0, \tag{6.46b}$$

$$Q_n^{L\,(\pm)}(\ell, \beta, \alpha; \rho) \quad \overset{\rho \to \infty}{\sim} \quad \mathcal{Q}_n^{L\,as}(\alpha) \; e^{\pm i\left[K\rho - \eta(C(\alpha)) \ln(2K\rho) + \sigma_C(\ell, C(\alpha)) - \ell \frac{\pi}{2}\right]}. \tag{6.46c}$$

where $\mathcal{Q}_n^{L\,as}$ is defined in (4.22). The α variable appears as a parameter of these coupled Quasi-Sturmian functions, a particular situation studied in **Section 4.3.7**. The

Sommerfeld parameter η [formula (1.23a)] and σ_C [formula (1.23b)] now depend on α through the function C; ℓ and β can be conveniently fixed.

The linear system

We apply the reduced Schrödinger operator to one of these φ_{mn} functions,

$$\begin{aligned}
&[\mathbf{H}_{\rho,\alpha} - E]\; Q_n^{L(\pm)}(\ell,\beta,\alpha;\rho)\, H_m(\alpha) \\
&\quad \overset{(4.41a)}{=} \frac{1}{\rho}\,\phi_n^L(\ell,\beta;\rho)\, H_m(\alpha) - \frac{4\ell(\ell+1)+1}{8\mu\rho^2}\, Q_n^{L(\pm)}(\ell,\beta,\alpha;\rho)\, H_m(\alpha) \\
&\qquad - \frac{1}{2\mu\rho^2}\frac{\partial^2}{\partial\alpha^2}\left[Q_n^{L(\pm)}(\ell,\beta,\alpha;\rho)\, H_m(\alpha)\right]. \qquad (6.47)
\end{aligned}$$

Choosing

$$w(\rho,\alpha) = \rho, \qquad \widetilde{\varphi}_{p,q}(\rho,\alpha) = \phi_q^L(\ell,\beta;\rho)\, H_p(\alpha),$$

the components $b_{p,q}$ given in (6.29a) coincide with the ones obtained in the first case when considering separate variables [i.e. equation (6.35)], while the matrix elements become

$$\begin{aligned}
O_{p,q;m,n} = &\int_0^{\frac{\pi}{2}}\int_0^{\infty} \phi_q^L(\ell,\beta;\rho)\phi_n^L(\ell,\beta;\rho)H_p(\alpha)H_m(\alpha)\, d\rho\, d\alpha \\
&- \frac{(2\ell+1)^2}{8\mu}\int_0^{\frac{\pi}{2}}\int_0^{\infty} \phi_q^L(\ell,\beta;\rho)\,\frac{1}{\rho}\, Q_n^{L\,(\pm)}(\ell,\beta,\alpha;\rho)\, H_p(\alpha)\, H_m(\alpha)\, d\rho\, d\alpha \\
&- \frac{1}{2\mu}\int_0^{\frac{\pi}{2}}\int_0^{\infty} \phi_q^L(\ell,\beta;\rho)\,\frac{1}{\rho}\, H_p(\alpha)\,\frac{\partial^2}{\partial\alpha^2}\left[Q_n^{L\,(\pm)}(\ell,\beta,\alpha;\rho)\, H_m(\alpha)\right] d\rho\, d\alpha. \qquad (6.48)
\end{aligned}$$

The first integral was already calculated in (6.37a), obtaining $\delta_{p,m} I^{(1)}_{q,n}$. To perform the integrals involving Quasi-Sturmian functions we use their expansion (4.43) in terms of Laguerre-type functions. Taking into account the orthogonality property of Laguerre-type functions (1.9a) we find

$$\begin{aligned}
&\int_0^{\frac{\pi}{2}}\int_0^{\infty} \phi_q^L(\ell,\beta;\rho)\,\frac{1}{\rho}\, Q_n^{L\,(\pm)}(\ell,\beta,\alpha;\rho)\, H_p(\alpha)\, H_m(\alpha)\, d\rho\, d\alpha \\
&\qquad = \int_0^{\frac{\pi}{2}} H_p(\alpha)\, H_m(\alpha)\, g^{(\pm)}_{n,q}(\alpha)\, d\alpha, \qquad (6.49)
\end{aligned}$$

$$\begin{aligned}
&\int_0^{\frac{\pi}{2}}\int_0^{\infty} \phi_q^L(\ell,\beta;\rho)\,\frac{1}{\rho}\, H_p(\alpha)\frac{\partial^2}{\partial\alpha^2}\left[Q_n^{L\,(\pm)}(\ell,\beta,\alpha;\rho)H_m(\alpha)\right] d\rho\, d\alpha \\
&\qquad = \int_0^{\frac{\pi}{2}} H_p(\alpha)\frac{\partial^2}{\partial\alpha^2}\left[g^{(\pm)}_{q,n}(\alpha)H_m(\alpha)\right] d\alpha. \qquad (6.50)
\end{aligned}$$

Applying the technique of integration by parts we obtain for this last integral,

$$\int_0^{\frac{\pi}{2}} H_p(\alpha)\frac{\partial^2}{\partial\alpha^2}\left[g^{(\pm)}_{q,n}(\alpha)H_m(\alpha)\right]d\alpha \overset{(B.17)}{=} S_{p,q;m,n} - 4(p+1)^2\int_0^{\frac{\pi}{2}} g^{(\pm)}_{q,n}(\alpha)\,H_p(\alpha)\,H_m(\alpha)\,d\alpha. \qquad (6.51)$$

where $S_{p,q;m,n}$ is the jump parameter (B.19).

Collecting the previous results, the matrix elements $O_{p,q;m,n}$ are given by

$$\begin{aligned} O_{p,q;m,n} &= I^{(1)}_{q,n}\,\delta_{p,m} - \frac{1}{2\mu}\,S_{p,q;m,n} \\ &+ \frac{16(p+1)^2-(2\ell+1)^2}{8\mu}\int_0^{\frac{\pi}{2}} H_p(\alpha)\,H_m(\alpha)\,g^{(\pm)}_{n,q}(\alpha)\,d\alpha. \end{aligned} \qquad (6.52)$$

In this case we do not have fully analytical expressions for these elements; the integral over α must be performed numerically.

The asymptotic behavior

Using the asymptotic behavior of these coupled Quasi-Sturmian functions [formula (6.46c)], the asymptotic form of the scattering solution reads

$$\Phi^{\pm}_{sc}(\alpha,\rho) \overset{\rho\to\infty}{\sim} e^{\pm i\left[K\rho-\eta(C(\alpha))\ln(2k\rho)+\sigma_C(\ell,C(\alpha))-\ell\,\frac{\pi}{2}\right]}\sum_{m,n} a_{m,n}\,H_m(\alpha)\,\mathcal{Q}^{L\,as}_n(\alpha)$$

where $\mathcal{Q}^{L\,as}_n$ – given by (4.22) with Z_{QS} replaced by the function C – depend on α. Comparing this expression with the form of the expected behavior (6.25c) we can provide an expression for $\mathcal{A}_\alpha$. From formulas (6.30) and (4.22) we obtain

$$\mathcal{A}_\alpha = \frac{1}{\cos\alpha\,\sin\alpha}\sum_{m,n} a_{m,n}\,H_m(\alpha)\,\mathcal{Q}^{L\,as}_n(\alpha).$$

6.4 An analytically solvable model problem

In references [83, 84] the authors have proposed to study a s-wave model problem consisting of equation (6.20) with the Coulomb interaction potential (6.7) replaced by

$$V(\rho) = \frac{\mathcal{C}}{\rho},$$

for which the Schrödinger equation becomes separable in hyperspherical coordinates. As driven term they took, for $\mathrm{Re}(s) > 1$ and $t \geqslant -1$,

$$f(\rho,\alpha) = \frac{e^{-s\,\rho}}{2}\,\rho^t \left(\frac{\sin(\rho\,\cos\alpha)}{\rho\cos\alpha}\,\frac{\sinh(\rho\sin\alpha)}{\rho\sin\alpha} + \frac{\sin(\rho\sin\alpha)}{\rho\sin\alpha}\,\frac{\sinh(\rho\cos\alpha)}{\rho\cos\alpha}\right) \tag{6.53}$$

which has the following series expansion in terms of H_n [83],

$$f(\rho,\alpha) = \frac{e^{-s\,\rho}}{\cos\alpha\sin\alpha}\sum_n c_n\,\rho^{2n+t}\,H_n(\alpha), \tag{6.54a}$$

$$c_n = \frac{\sqrt{\pi}\,\left[(-1)^n+1\right]}{8\,(n+1)\,2^{2n}\,\left(\frac{3}{2}\right)_n\,n!}. \tag{6.54b}$$

Note that only even values of n contribute, reflecting the driven term symmetry with respect to $\alpha = \frac{\pi}{4}$, i. e. with respect to r_1 and r_2.

The model problem consisted in searching the outgoing solution to the differential equation

$$\left[-\frac{1}{2\mu}\frac{\partial^2}{\partial\rho^2} - \frac{1}{2\mu\rho^2}\frac{\partial^2}{\partial\alpha^2} - \frac{1}{8\mu\rho^2} + \frac{\mathcal{C}}{\rho} - E\right]\Phi^{(+)}_{sc}(\rho,\alpha) = \rho^{5/2}\,\cos\alpha\,\sin\alpha\;f(\rho,\alpha) \tag{6.55}$$

with boundary conditions

$$\Phi^{(+)}_{sc}(0,\alpha) = 0 \tag{6.56a}$$

$$\Phi^{(+)}_{sc}(\rho,\alpha) \overset{\rho\to\infty}{\sim} \mathcal{A}_\alpha\cos\alpha\,\sin\alpha\,e^{i\left[K\rho-\eta(\mathcal{C})\log(2K\rho)+\sigma_C(\ell,\mathcal{C})-\ell\frac{\pi}{2}\right]}. \tag{6.56b}$$

This model problem, although apparently simple, contains some of the difficulties of the real problem. The Coulombic potential $\frac{\mathcal{C}}{\rho}$ is simple in hyperspherical coordinates but does couple the r_1 and r_2 spherical coordinates. The driven term also couples the hyperspherical coordinates. In reference [83] the authors gave analytical expression for the solution of the model problem and of the scattering amplitude $\mathcal{A}_\alpha$

In order to test the efficiency of Quasi-Sturmian functions, we propose here to solve this problem by considering two alternative representations of the hyperradial part of the scattering solution. First, we take the Hulthén Sturmian functions $S^{(+)}_{n,0}$ introduced in **Section 3.2**. As a second approach, we use the functions $Q^{(+)}_{m,n}(\ell_m,\beta;\rho)$ presented in **Section 6.3.B**. In both cases the angular part is dealt with functions H_m.

Hulthén Sturmian functions

Starting with the Hulthén Sturmian functions $S_{n,0}^{(+)}$, we express

$$\Phi_{sc}^{S\,(+)}(\rho,\alpha) = \sum_{m,n} a_{m,n}^{S}\, S_{n,0}^{(+)}(\rho)\, H_m(\alpha). \tag{6.57}$$

Applying $[\mathbf{H}_{\rho,\alpha} - E]$ to one of the elements $S_{n,0}^{(+)}(\rho)\, H_m(\alpha)$, we use (3.8a) to obtain

$$\begin{aligned} &[\mathbf{H}_{\rho,\alpha} - E] S_{n,0}^{(+)}(\rho)\, H_m(\alpha) \\ &\qquad = \left[-\lambda_{n,0} \mathrm{v}_0 \frac{e^{-\frac{\rho}{a}}}{1-e^{-\frac{\rho}{a}}} + \frac{\upsilon_m(\upsilon_m+1)}{2\mu\rho^2} + \frac{\mathcal{C}}{\rho} \right] S_{n,0}^{(+)}(\rho)\, H_m(\alpha), \end{aligned} \tag{6.58}$$

where we set, for convenience, $\upsilon_m = 2m + \dfrac{3}{2}$. The parameters v_0 and a are the ones included in the Hulthén potential (3.6), and $\lambda_{n,0}$ is the eigenvalue (3.15) associated to $S_{n,0}^{(+)}$.

To seize the orthogonality property of the Sturmian functions we should take $\widetilde{\varphi}_{p,q}(\rho,\alpha) = S_{q,0}^{(+)}(\rho) H_p(\alpha)$ and $w \equiv 1$. We prefer, however, to use Laguerre-type functions for the radial part of $\widetilde{\varphi}_{p,q}$, a choice that allows us to analytically solve the three integrals involved in the Hamiltonian matrix elements (integrals performed in **Section 3.3**). Thus, we take

$$w(\rho,\alpha) = 1, \quad \widetilde{\varphi}_{p,q}(\rho,\alpha) = \phi_q^L(\ell,\beta;\rho) H_p(\alpha),$$

and we name

$$\begin{aligned} I_1 &= \int_0^\infty \phi_q^L(\ell,\beta;\rho)\, \frac{e^{-\frac{\rho}{a}}}{1-e^{-\frac{\rho}{a}}}\, S_{n,0}^{(+)}(\rho)\, d\rho \\ &\overset{(3.27)}{=} \frac{N_n^S}{N_{q,\ell}^L} \frac{1}{2\beta} \frac{\Gamma(\ell+2)}{\Gamma(2\ell+2)} \sum_{j=0}^{n} \frac{(-n)_j\, (n-2ika)_j}{(1-2ika)_j\, j!} \sum_s \left(\frac{2\beta a}{a(\beta-ik)+j+s+1} \right)^{\ell+2} \\ &\quad \times {}_2F_1\left(-q, \ell+2, 2\ell+2; \frac{2\beta a}{a(\beta-ik)+j+s+1} \right), \\ I_2 &= \int_0^\infty \phi_q^L(\ell,\beta;\rho)\, \frac{1}{\rho^2}\, S_{n,0}^{(+)}(\rho)\, d\rho \\ &\overset{(3.25)}{=} \frac{N_n^S}{N_{q,\ell}^L} \frac{\Gamma(\ell)}{\Gamma(2\ell+2)} (2\beta) \sum_{j=0}^{n} \frac{(-n)_j\, (n-2ika)_j}{(1-2ika)_j\, j!} \left(\frac{2\beta a}{a(\beta-ik)+j} \right)^{\ell} \\ &\quad \times {}_2F_1\left(-q, \ell, 2\ell+2; \frac{2\beta a}{a(\beta-ik)+j} \right), \end{aligned}$$

and

$$\begin{aligned} I_3 &= \int_0^\infty \phi_q^L(\ell,\beta;\rho)\frac{1}{\rho}S_{n,0}^{(+)}(\rho)\,d\rho \\ &\overset{(3.25)}{=} \frac{N_n^S}{N_{q,\ell}^L}\frac{\Gamma(\ell+1)}{\Gamma(2\ell+2)}\sum_{j=0}^{n}\frac{(-n)_j\,(n-2ika)_j}{(1-2ika)_j\,j!}\left(\frac{2\beta a}{a(\beta-ik)+j}\right)^{\ell+1} \\ &\quad\times {}_2F_1\left(-q,\ell+1,2\ell+2;\frac{2\beta a}{a(\beta-ik)+j}\right). \end{aligned}$$

Taking into account the orthogonality property (6.31b) satisfied by H_m, we obtain the matrix elements for the linear system (6.29)

$$O_{p,q;m,n} = \left(-\lambda_{n,0}\mathrm{v}_0\,I_1 + \frac{\upsilon_m(\upsilon_m+1)}{2\mu}\,I_2 + \mathcal{C}\,I_3\right)\delta_{p,m}. \tag{6.59}$$

The components of the vector $\mathbf{b}$ have also closed form. Using the series expansion (6.54) for the driven term, and the orthogonality property (6.31b), we find

$$\begin{aligned} b_{p,q} &= \int_0^{\frac{\pi}{2}}\int_0^\infty \phi_q(\ell,\beta;\rho)\,H_p(\alpha)\,f(\rho,\alpha)\,\rho^{5/2}\,\cos\alpha\,\sin\alpha\,d\rho\,d\alpha \\ &\overset{(B.23)}{=} \frac{\sqrt{\pi}\,[(-1)^p+1]}{8\,(p+1)\,(2p+1)!}\,\frac{1}{N_{q,\ell}\,\Gamma(2\ell+2)}\,\frac{(2\beta)^{\ell+1}}{(s+\beta)^{2p+t+\ell+\frac{9}{2}}}\,\Gamma\left(2p+t+\ell+\frac{9}{2}\right) \\ &\quad\times {}_2F_1\left(-q,2p+t+\ell+\frac{9}{2},2\ell+2;\frac{2\beta}{s+\beta}\right). \end{aligned} \tag{6.60}$$

The coefficients $a^S_{m,n}$ in (6.57) result from numerically solving the system $\mathbf{O}\cdot\mathbf{a^S}=\mathbf{b}$.

Laguerre Quasi-Sturmian functions

Now we propose the alternative representation

$$\Phi_{sc}^{Q\,(+)}(\rho,\alpha) = \sum_{m,n} a^Q_{m,n}Q^{L(+)}_{m,n}(\ell_m,\beta;\rho)\,H_m(\alpha) \tag{6.61}$$

using the functions introduced in **Section 6.3.B**, with $\ell_m = \upsilon_m = 2m + \dfrac{3}{2}$. We choose the charge of the Quasi-Sturmian functions as the charge of the model problem, $Z_{QS} = \mathcal{C}$, so that

$$[\mathbf{H}_{\rho,\alpha} - E]Q^{L(+)}_{m,n}(\ell_m,\beta;\rho)\,H_m(\alpha) = \frac{1}{\rho}\,H_m(\alpha)\phi_n^L(\ell_m,\beta;\rho). \tag{6.62}$$

Taking

$$w(\rho,\alpha)=1, \quad \widetilde{\varphi}_{p,q}(\rho,\alpha) = \phi_q^L(\ell_p,\beta;\rho)H_p(\alpha)$$

the matrix **O**, whose elements are given by (6.29b), is the identity matrix as a consequence of the orthogonality property satisfied by functions H_m and ϕ_n^L. Then the coefficients $a^Q_{m,n}$ coincide with the components of the vector **b** given by formula (6.60). Replacing $\ell_p = 2p + \frac{3}{2}$, the coefficients simplify

$$a^Q_{p,q} = \frac{\sqrt{\pi}\,[(-1)^p + 1]}{8\,(p+1)\,(2p+1)!} \frac{1}{N_{q,\ell_p}\,\Gamma(4p+5)} \frac{(2\beta)^{2p+\frac{5}{2}}}{(s+\beta)^{4p+6+t}} \Gamma\,(4p+6+t) \times {}_2F_1\left(-q, 4p+6+t, 4p+5; \frac{2\beta}{s+\beta}\right). \tag{6.63}$$

Taking the particular value $\beta = s$, the hypergeometric function simplifies

$${}_2F_1\,(-q, 4p+t+6, 4p+5; 1) \overset{(1.15)}{=} \frac{(-t-1)_q}{(4p+5)_q},$$

and this expression vanishes for $q > t+1$. As a consequence, for $\beta = s$, the first $t+2$ Quasi-Sturmian functions exactly solve the radial part of the equation. In this case the coefficients read

$$a^Q_{p,q} = \frac{\sqrt{\pi}\,[(-1)^p + 1]}{8\,(p+1)\,(2p+1)!} \frac{N_{q,\ell_p}\,\Gamma(4p+t+6)}{q!} \frac{(-t-1)_q}{(2s)^{2p+t+\frac{7}{2}}}. \tag{6.64}$$

Taking into account the asymptotic behavior of $Q^{(+)}_{m,n}$, given in (6.40c), we obtain

$$\Phi^{Q\,(+)}_{sc}(\rho,\alpha) \overset{\rho\to\infty}{\sim} \left\{\sum_{m,n} a^Q_{m,n}\,\mathcal{Q}^{L\ as}_{m,n}\,H_m(\alpha)\right\} e^{i\left[K\rho - \eta(\mathcal{C})\ln(2K\rho) + \sigma_C(\ell_m,\mathcal{C}) - \ell_m\,\frac{\pi}{2}\right]}. \tag{6.65}$$

The expression between braces is the expected amplitude $\mathcal{A}_\alpha$ of the scattering solution's asymptotic behavior (6.56b).

Illustration

To perform the following calculations, we fix $\mu = 1$, $\mathcal{C} = -1$, $E = 0.5$, $s = 2$, and $t = 0$, which are the values chosen by the authors in reference [83]. And we set

$$\overline{\Psi}_{sc}^{S\,(+)}(\rho,\alpha) = \rho^{5/2}\,\Psi_{sc}^{S\,(+)}(\rho,\alpha) = \frac{1}{\cos\alpha\,\sin\alpha}\,\Phi_{sc}^{S\,(+)}(\rho,\alpha), \tag{6.66a}$$

$$\overline{\Psi}_{sc}^{Q(+)}(\rho,\alpha) = \rho^{5/2}\,\Psi_{sc}^{Q\,(+)}(\rho,\alpha) = \frac{1}{\cos\alpha\,\sin\alpha}\,\Phi_{sc}^{Q\,(+)}(\rho,\alpha) \tag{6.66b}$$

where $\Phi_{sc}^{S\,(+)}$ and $\Phi_{sc}^{Q\,(+)}$ are given by (6.57) and (6.61), respectively.

As mentioned, for $\beta = s = 2$, only $t + 2 = 2$ Quasi-Sturmian functions ($n = 0, 1$) are necessary to exactly express the radial part of the solution,

$$\Phi_{sc}^{Q\,(+)}(\rho,\alpha) = \sum_m \frac{\sqrt{\pi}\,[(-1)^m+1]}{(m+1)\,(2m+1)!}\frac{\sqrt{\Gamma(4m+6)}}{2^{4m+10}} \times \left[\sqrt{4m+5}\;Q_{m,0}^{L(+)}(\ell_m,\beta;\rho) - Q_{m,1}^{L(+)}(\ell_m,\beta;\rho)\right] H_m(\alpha). \tag{6.67}$$

Taking the limit $\rho \to \infty$ we obtain

$$\Phi_{sc}^{Q\,(+)}(\rho,\alpha) \overset{\rho\to\infty}{\sim} \left\{\sum_m \frac{\sqrt{\pi}\,[(-1)^m+1]}{(m+1)\,(2m+1)!}\frac{\sqrt{\Gamma(4m+6)}}{2^{4m+10}}\left[\sqrt{4m+5}\;\mathcal{Q}_{m,0}^{L\;as} - \mathcal{Q}_{m,1}^{L\;as}\right] H_m(\alpha)\right\} \times\, e^{i\left[K\rho - \eta(\mathcal{C})\ln(2K\rho) + \sigma_C(\ell_m,\mathcal{C}) - \ell_m\,\frac{\pi}{2}\right]} \tag{6.68}$$

and the expression between braces is the amplitude $\mathcal{A}_\alpha$ of the asymptotic wave (6.56b). Let us define

$$\left|\mathcal{A}_\alpha^M\right|^2 = \left|\frac{1}{\cos\alpha\,\sin\alpha}\right| \times \left|\sum_{m=0}^{M} \frac{\sqrt{\pi}\,[(-1)^m+1]}{(m+1)\,(2m+1)!}\frac{\sqrt{\Gamma(4m+6)}}{2^{4m+10}}\left[\sqrt{4m+5}\;\mathcal{Q}_{m,0}^{L\;as} - \mathcal{Q}_{m,1}^{L\;as}\right] H_m(\alpha)\right|^2. \tag{6.69}$$

As a first illustration we present, in **Figure 6.4**, the real part (left panel) and the modulus (right panel) of $\overline{\Psi}_{sc}^{Q\,(+)}$ in spherical coordinates (r_1, r_2). We consider $\beta = s = 2$, and use expression (6.67) to evaluate the function, with four angular basis functions

$(m = 0, 2, 4, 6)$. The calculated scattering wave function matches perfectly the analytical solution found in reference [83].

In **Figure 6.5** we plot different angular sections of $|\overline{\Psi}_{sc}^{Q\,(+)}|^2$ evaluated from (6.67) for increasing values of the hyperradial variable: $\rho_0 = 60$ (line with dots) and $\rho_0 = 150$ (dashed line). We observe that, as expected, for increasing values of ρ, the different sections approach the asymptotic value $\left|\mathcal{A}_\alpha^M\right|^2$ given by (6.69) with $M = 6$ (full line).

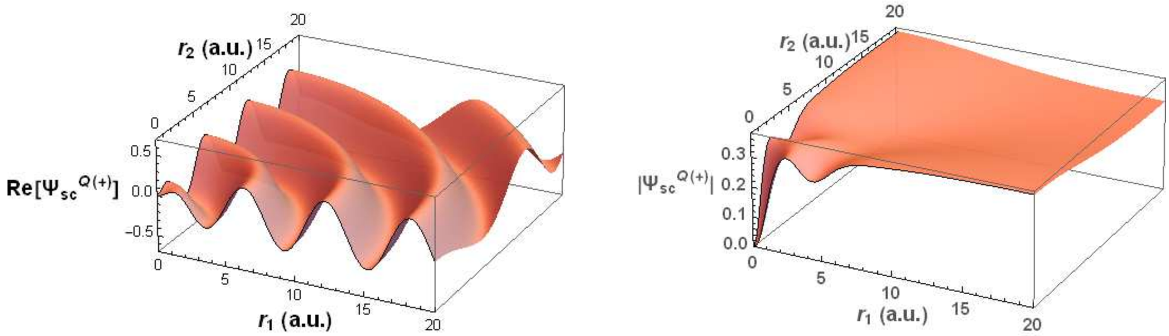

Figure 6.4: Real part (left panel) and modulus (right panel) of $\overline{\Psi}_{sc}^{Q(+)}$ as functions of (r_1, r_2) and taking $\beta = s = 2$. We fix $\mu = 1, \mathcal{C} = -1, E = 0.5, t = 0$.

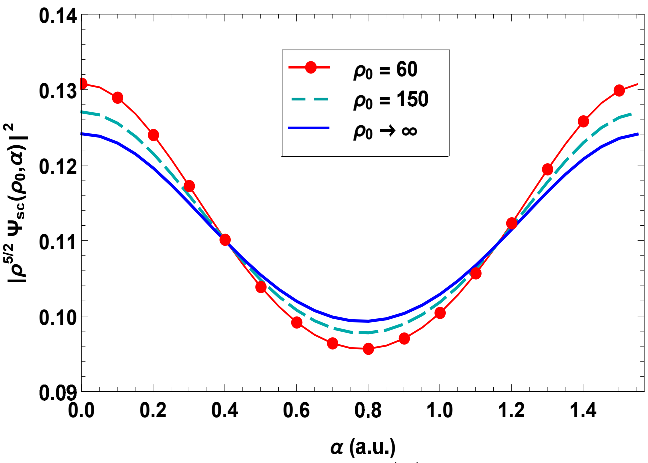

Figure 6.5: Different angular sections of $|\overline{\Psi}_{sc}^{Q(+)}|^2$ for $M = 6$, $\beta = s = 2$, $\mu = 1, Z_{QS} = \mathcal{C} = -1, E = 0.5, t = 0$. We fixed as values of the radial variable: $\rho_0 = 60$ (line with dots) and $\rho_0 = 150$ (dashed line). The full line correspond to $|\mathcal{A}_\alpha^M|^2$ given by (6.69).

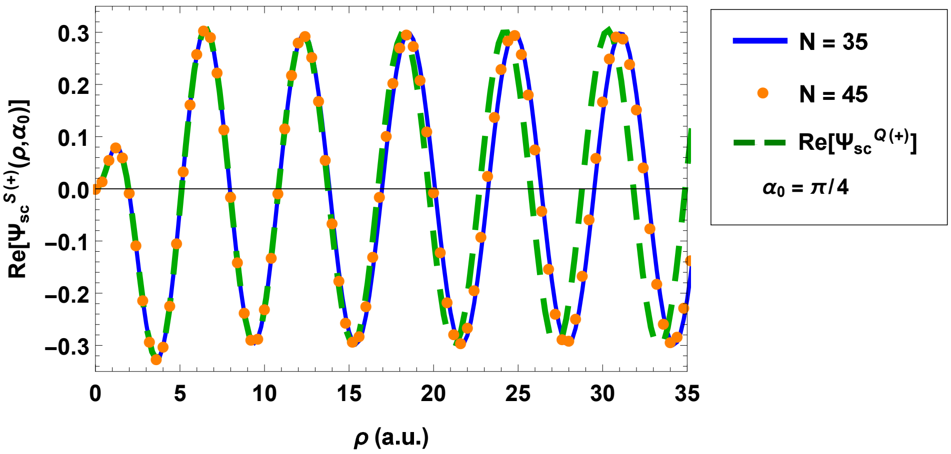

Figure 6.6: Real part of $\overline{\Psi}_{sc}^{S(+)}$*, for a fixed* $\alpha_0 = \frac{\pi}{4}$*, using four angular basis functions and different numbers* N *of radial terms. We take* $\beta = 8$*,* $\mu = 1, \mathcal{C} = -1, E = 0.5, t = 0, s = 2, a = 2, \mathrm{v}_0 = -1$*. The dashed line corresponds to the real part of* $\overline{\Psi}_{sc}^{Q(+)}$ *for* $\beta = 2$*.*

We also tested the approximated solution $\overline{\Psi}_{sc}^{Q\,(+)}$ taking $\beta = 1.2$ (arbitrary value) to show that even in this case Quasi-Sturmian functions are better than Sturmian functions. We needed only seven radial Quasi-Sturmian functions in (6.61) and four angular basis functions ($M = 6$) to find convergence in the series.

Using Hulthén Sturmian functions, we can not approach the scattering solution for values of ρ greater than $R = 10$ because of the asymptotic behavior of $S_{n,0}^{(+)}$, as explained in **Remark 3.1.1**. Not only these basis functions do not possess the appropriate behavior to describe the scattering solution in the asymptotic region, but also all Hulthén Sturmian functions reach their asymptotic behavior (the same behavior for all of them) at the same value $\rho = R$ determined by the generating potential. Thus, they do not represent the scattering wave function in the region $\rho > R$. This can be observed in **Figure 6.6**, where we plot a radial section of $\overline{\Psi}_{sc}^{S(+)}$, fixing $\alpha_0 = \frac{\pi}{4}$. We consider the first 35 (full line, noted $N = 35$) and 45 (line with dots, noted $N = 45$) radial terms. The full line corresponds to the same section calculated with $\overline{\Psi}_{sc}^{Q(+)}$ taking $\beta = s = 2$, i.e. using formula (6.67).

6.5 Chapter summary

We have presented the general form of three-body scattering problems using hyperspherical coordinates. In particular, we focused on the s-wave approach and described the procedure to approximate its solution.

Three different combinations of Laguerre Quasi-Sturmian functions (for the hyperradial part) and Jacobi polynomials (for the angular part) were proposed to represent the solution. In the first two cases we proposed purely radial Quasi-Sturmian functions, and we were able to give the matrix elements in closed form. The third option involved a set of Quasi-Sturmian functions which include the angular variable as a parameter, so that they are not purely radial functions. This coupling of the variables produces the desired asymptotic behavior for three-body scattering problems in hyperspherical coordinates. In this case, however, we could not solve analytically all integrals appearing in the matrix elements.

To illustrate the efficiency of these functions we have solved the analytically solvable model problem proposed in references [83] and [84].

Conclusions and perspectives

Throughout this work we have studied the mathematical properties of different functions that appear when describing scattering processes. We have proposed a novel set of radial or hyperradial functions, named Quasi-Sturmian functions, which may be considered an interesting alternative to expand the scattering solution. Their advantages are illustrated through their implementation in solving some particular two- and three-body scattering problems.

In the first part of this work we have introduced and developed the mathematical tools to be used in the second part dedicated to the study of scattering processes.

We started by presenting some basic functions (Slater-type orbitals, Laguerre-type functions, Coulomb wave functions and Coulomb Green's function) and their important properties needed in the rest of the work. In particular we have focused on their Laguerre expansion. As an extension of the known result for sine-like Coulomb wave functions, we have presented in closed form the coefficients of the other solutions of the radial Coulomb equation. Going further in the investigation of these coefficients, we have established that, when considering the charge as a variable, the coefficients of the sine-like Coulomb wave function are related to the Meixner-Pollaczek polynomials. Thus, all known properties of these polynomials can be extended to them, as we have shown by deducing an orthogonality and closure relation.

We have also studied two-variable hypergeometric functions. Specifically, we have extended to these functions a known strategy used to obtain the derivatives of one-variable hypergeometric functions with respect to their parameters. We have provided analytical expressions for the derivatives of the four Appell functions F_1, F_2, F_3, F_4 with respect to their parameters, explaining how to generalize the results to other two-variable hypergeometric series.

Generalized Sturmian functions were also presented, with a particular analysis of Hulthén Sturmian functions. We took advantage of the analyticity of the latter to derive various expressions which complement those given in standard collision theory and mathematical physics books.

As one of the main contributions of this work, we have presented a set of functions useful to approximate scattering solutions: the Quasi-Sturmian functions. They can be considered as an alternative to Generalized Sturmian functions, and also a generalization of the J-matrix solutions. Indeed, only the case of an $n = 0$ Laguerre-type function as driven term is presented in the literature; here, we have given the solution for any n and also for Slater-type orbitals as driven term.

Two remarkable features of these functions are their asymptotic behavior, which is proportional to the expected behavior of the scattered wave, and the fact that they can be expressed in closed form. Furthermore, their link with Laguerre-type functions (through the differential equation they satisfy) allowed us to establish very interesting relations and properties; in some cases, when the deduction of a formula was not quite rigorous, the obtained mathematical expressions were numerically validated. Moreover, since Laguerre-type functions can be used to expand any general function, a scattering solution may be approximated by a combination of the proposed Quasi-Sturmian functions. The analyticity of these functions and their properties resulted very helpful to perform analytically different integrals (matrix elements) appearing in scattering problems.

In the second part of this work we have employed the Hulthén Sturmian functions and Quasi-Sturmian functions to solve two- and three-body scattering problems.

For the two-body case we have presented the general formulation of the problem in spherical coordinates and the strategy to find an approximation of the scattering solution in terms of our proposed functions.

To illustrate the efficiency of Generalized Sturmian functions, we have applied them to describe the scattering produced by a Hulthén and a Yukawa potential. For the Hulthén case we obtained in closed form the approximated solution and the corresponding transition amplitude. Analytical results were verified numerically with an independent numerical procedure. For the scattering by a Yukawa potential, our numerical application achieved a more than fair agreement, using a relatively low number of basis elements, with the solution obtained with another numerical method. The efficiency is related to the built-in correct asymptotic behavior of each basis element and to the appropriate choice of the generating potential range.

We have also solved the scattering of a particle under the influence of a combined potential (Coulomb + Yukawa). When expressing the solution with Laguerre Quasi-Sturmian functions we found that with 15 terms the scattering solution was already converged, while it took 30 Generalized Sturmian functions (numerically constructed) to achieve the same accuracy. This illustrates the great efficiency of Quasi-Sturmian functions in two-body scattering problems, an efficiency inherent to the way they are constructed.

To describe three-body scattering processes we have proposed the use of hyperspherical coordinates since, in such coordinate system, the asymptotic form of the scattered wave takes a simpler expression. We have analysed a Temkin-Poet model for which only the hyperradial and one angular variables survive. We have proposed different variants of Laguerre Quasi-Sturmian functions to describe the hyperradial part of the scattering solution, while the angular part was dealt with Jacobi polynomials. One of the options, however, includes the angular variable in a parametric form in the Quasi-Sturmian function; these two variable functions include a coupling of its variables, a coupling that also occurs in the Schrödinger equation. We have presented, in close form, most of the integrals appearing in the matrix system. To test the efficiency of the proposed Quasi-Sturmian functions we have solved a Coulomb three-body model problem, finding that with a few terms a good approximation of the scattering wave function is obtained.

The next step in this direction is to use the proposed two-variable Quasi-Sturmian functions to solve a ionization Temkin-Poet model problem and corroborate that the asymptotic behavior these functions present is an advantage compared to other basis functions. Moreover, it is planned to extend the study of Quasi-Sturmian functions to include the dependence on the five angular hyperspherical variables. The knowledge of their properties may allow us to develop a strategy to implement such functions in solving three-body scattering problem with the full Coulomb potential.

Another subject to explore is the possibility of constructing angular Quasi-Sturmian functions from the linear or bilinear generating functions for Jacobi polynomials, many of which are Appell functions F_4.

Appendix A

Whittaker functions

The Whittaker functions $M_{\chi,\frac{\mu}{2}}(z)$, $W_{\chi,\frac{\mu}{2}}(z)$ are defined [42, 45]

$$M_{\chi,\frac{\mu}{2}}(z) = e^{-\frac{z}{2}} z^{\frac{1+\mu}{2}}\, {}_1F_1\left(\frac{1+\mu}{2} - \chi, 1+\mu; z\right), \tag{A.1a}$$

$$W_{\chi,\frac{\mu}{2}}(z) = e^{-\frac{z}{2}} z^{\frac{1+\mu}{2}}\, U\left(\frac{1+\mu}{2} - \chi, 1+\mu; z\right). \tag{A.1b}$$

where ${}_1F_1$ and U are Confluent hypergeometric functions of first and second kind respectively.

Whittaker functions appear as solutions of the Coulomb problem. In this context we have the following relation between χ, μ, z and the parameters and variable describing the Coulomb problem, i.e. the Sommerfeld parameter η defined in (1.23a), the angular momentum ℓ, the momentum k and the radial variable r:

$$\chi = \pm i\,\eta(Z), \qquad \frac{\mu}{2} = \frac{2\ell+1}{2}, \qquad z = \pm 2ikr.$$

With these Coulomb parameters, $W_{\chi,\frac{\mu}{2}}$ takes the form [equation (18a), Section 2, of [45]]

$$W_{\pm i\eta(Z),\frac{2\ell+1}{2}}(\pm 2ikr) = \frac{\pi}{\sin[\pi(2\ell+1)]}\left\{-\frac{\mathcal{M}_{\pm i\eta(Z),\frac{2\ell+1}{2}}(\pm 2ikr)}{\Gamma(-\ell \mp i\eta(Z))} + \frac{\mathcal{M}_{\pm i\eta(Z),-\frac{2\ell+1}{2}}(\pm 2ikr)}{\Gamma(\ell+1 \mp i\eta(Z))}\right\} \tag{A.2}$$

where

$$\mathcal{M}_{\chi,\frac{\mu}{2}}(z) = \frac{1}{\Gamma(1+\mu)} M_{\chi,\frac{\mu}{2}}(z).$$

These expressions for $\mathcal{M}_{\pm i\eta(Z),\pm\frac{2\ell+1}{2}}$ and $W_{\pm i\eta(Z),\frac{2\ell+1}{2}}$ are not correct if $2\ell+1 \in \mathbb{N} \cup \{0\}$.

Nevertheless the limit for $2\ell+1$ approaching a non-negative integer number exists. Thus, to obtain the explicit form of $W_{\pm i\eta(Z),\frac{2\ell+1}{2}}$ when $2\ell+1 \in \mathbb{N}\cup\{0\}$ a limit must be performed

$$W_{\pm i\eta(Z),\frac{2\ell+1}{2}}(\pm 2ikr) := \lim_{\epsilon\to 0} W_{\pm i\eta(Z),\frac{2(\ell+\epsilon)+1}{2}}(\pm 2ikr). \tag{A.3}$$

Buchholz [45] solved the limit applying l'Hôpital's rule.

In order to find the coefficients $h_n^{(\pm)}$ of the series expansion of the Coulomb wave $H_n^{(\pm)}$ in terms of Laguerre-type functions, in **Chapter 1** we need to perform

$$I_W^{(\pm)}(\ell) = \int_0^\infty \phi_n(\ell,\beta;r)\,\frac{1}{r}\,W_{\mp i\,\eta(Z),\ell+\frac{1}{2}}(\mp 2ikr)\,dr. \tag{A.4}$$

The rest of this appendix is dedicated to $I_W^{(+)}$.

For the case $2\ell+1 \notin \mathbb{N}\cup\{0\}$, the definitions of the Laguerre-type function $\phi_n(\ell,\beta;r)$ (1.2) and of the Whittaker function (A.2), give

$$\begin{aligned}
I_W^{(+)}(\ell) = {} & \frac{(2\beta)^{\ell+1}}{N_{n,\ell}\,\Gamma(2\ell+2)}\,\frac{\pi}{\sin[\pi(2\ell+1)]} \\
& \times\Bigg\{-\frac{(-2ik)^{\ell+1}}{\Gamma(-\ell+i\eta(Z))\,\Gamma(2\ell+2)} \\
& \qquad \times\int_0^\infty e^{-(\beta-ik)r}r^{2\ell+1}\,{}_1F_1(-n,2\ell+2;2\beta r)\,{}_1F_1(\ell+1+i\eta(Z),2\ell+2;-2ikr)\,dr \\
& \quad +\frac{(-2ik)^{-\ell}}{\Gamma(\ell+1+i\eta(Z))\,\Gamma(-2\ell)} \\
& \qquad \times\int_0^\infty e^{-(\beta-ik)r}\,{}_1F_1(-n,2\ell+2;2\beta r)\,{}_1F_1(-\ell+i\eta(Z),-2\ell;-2ikr)\,dr\Bigg\} \\
\overset{(B.7)}{=} {} & \frac{(2\beta)^{\ell+1}}{N_{n,\ell}\,\Gamma(2\ell+2)}\,\frac{\pi}{\sin[\pi(2\ell+1)]} \\
& \times\Bigg\{-\frac{(-2ik)^{\ell+1}}{\Gamma(-\ell+i\eta(Z))\,(\beta-ik)^{2\ell+2}}\,F_2\left(2\ell+2,-n,\ell+1+i\eta(Z),2\ell+2,2\ell+2;x,y\right) \\
& \quad +\frac{(-2ik)^{-\ell}}{\Gamma(\ell+1+i\eta(Z))\,\Gamma(-2\ell)\,(\beta-ik)}F_2\left(1,-n,-\ell+i\eta(Z),2\ell+2,-2\ell;x,y\right)\Bigg\}
\end{aligned}$$

where we have introduced

$$x = \frac{2\beta}{\beta-ik}, \qquad y = -\frac{2ik}{\beta-ik}.$$

Alternative expressions can be obtained if we apply (B.6) to the first Appell's F_2 function or use the series representation (2.4) of F_2 in terms of Gauss's hypergeometric functions. For example, we find a formulation involving the coefficients s_n given in (1.30)

$$
\begin{aligned}
I_W^{(+)}(\ell) = {} & \frac{1}{\Gamma(\ell+1+i\eta(Z))}\,\frac{\pi}{\sin[\pi(2\ell+1)]} \\
& \times \left\{ \frac{2i\,\widetilde{N}_C^{(+)}(\ell)}{\Gamma(-\ell+i\eta(Z))}\, s_n \right. \\
& \left. + \frac{2\beta}{N_{n,\ell}\,\Gamma(2\ell+2)\,\Gamma(-2\ell)(\beta-ik)} \left(-\frac{\beta}{ik}\right)^{\ell} F_2\left(1,-n,-\ell+i\eta(Z),2\ell+2,-2\ell;x,y\right) \right\}
\end{aligned}
\tag{A.5}
$$

where $\widetilde{N}_C^{(+)}(\ell)$ is defined in (1.23d).

For the case $2\ell+1 \in \mathbb{N}\cup\{0\}$ we should calculate

$$
\int_0^\infty \phi_n(\ell,\beta;r)\,\frac{1}{r}\,\lim_{\epsilon\to 0} W_{-i\,\eta(Z),\ell+\epsilon+\frac{1}{2}}(-2ikr)\,dr,
\tag{A.6a}
$$

but we solve instead

$$
\begin{aligned}
I_W^{(+)}(\ell) &:= \lim_{\epsilon\to 0} I_W(\ell+\epsilon) \\
&= \lim_{\epsilon\to 0}\int_0^\infty \phi_n(\ell,\beta;r)\,\frac{1}{r}\,W_{-i\,\eta(Z),\ell+\epsilon+\frac{1}{2}}(-2ikr)\,dr.
\end{aligned}
\tag{A.6b}
$$

It is convenient to use the equivalent form (A.5) for $I_W(\ell)$,

$$
\begin{aligned}
I_W^{(+)}(\ell) = {} & \frac{(2\beta)^{\ell+1}}{N_{n,\ell}\,\Gamma(2\ell+2)}\,\frac{\pi}{\sin[\pi(2\ell+1)]}\,\frac{(-2ik)^{-\ell}}{(\beta-ik)\,\Gamma(\ell+1+i\eta(Z))\,\Gamma(-\ell+i\eta(Z))} \\
& \times \left\{ -(1-x)^n y^{2\ell+1} \sum_q \Gamma(\ell+1+i\eta(Z)+q)\frac{y^q}{q!}\ {}_2F_1\left(-n,-q,2\ell+2;\frac{x}{x-1}\right) \right. \\
& \left. + \sum_q (1)_q\,\frac{\Gamma(-\ell+i\eta(Z)+q)}{\Gamma(-2\ell+q)}\,\frac{y^q}{q!}\ {}_2F_1\left(-n,1+q,2\ell+2;x\right) \right\}
\end{aligned}
\tag{A.7}
$$

thus we must perform

$$
\begin{aligned}
I_W^{(+)}(\ell) &:= \frac{(2\beta)^{\ell+1}}{N_{n,\ell}\,\Gamma(2\ell+2)} \\
&\times \lim_{\epsilon\to 0} \frac{\pi}{\sin[\pi(2(\ell+\epsilon)+1)]} \frac{(-2ik)^{-(\ell+\epsilon)}}{(\beta-ik)\,\Gamma(\ell+\epsilon+1+i\eta(Z))\,\Gamma(-(\ell+\epsilon)+i\eta(Z))} \\
&\times \Bigg\{ -(1-x)^n y^{2(\ell+\epsilon)+1} \sum_{q=0}^{\infty} \Gamma(\ell+\epsilon+1+i\eta(Z)+q)\frac{y^q}{q!}\ {}_2F_1\left(-n,-q,2(\ell+\epsilon)+2;\frac{x}{x-1}\right) \\
&+ \sum_{q=0}^{\infty} (1)_q \frac{\Gamma(-(\ell+\epsilon)+i\eta(Z)+q)}{\Gamma(-2(\ell+\epsilon)+q)} \frac{y^q}{q!}\ {}_2F_1\left(-n,1+q,2(\ell+\epsilon)+2;x\right) \Bigg\}. \qquad \text{(A.8)}
\end{aligned}
$$

The following artifices are needed.

1. A split of the second series with a transformation on one of the ${}_2F_1$ function

$$
\begin{aligned}
&\sum_{q=0}^{\infty} (1)_q \frac{\Gamma(-\ell-\epsilon+i\eta(Z)+q)}{\Gamma(-2\ell-2\epsilon+q)} \frac{y^q}{q!}\ {}_2F_1\left(-n,1+q,2\ell+2\epsilon+2;x\right) \\
&\quad= \sum_{q=0}^{2\ell} (1)_q \frac{\Gamma(-\ell-\epsilon+i\eta(Z)+q)}{\Gamma(-2\ell-2\epsilon+q)} \frac{y^q}{q!}\ {}_2F_1\left(-n,1+q,2\ell+2\epsilon+2;x\right) \\
&\qquad+ \sum_{q=2\ell+1}^{\infty} (1)_q \frac{\Gamma(-\ell-\epsilon+i\eta(Z)+q)}{\Gamma(-2\ell-2\epsilon+q)} \frac{y^q}{q!}\ {}_2F_1\left(-n,1+q,2\ell+2\epsilon+2;x\right) \\
&\quad\overset{Q=q-2\ell-1}{=} \sum_{q=0}^{2\ell} (1)_q \frac{\Gamma(-\ell-\epsilon+i\eta(Z)+q)}{\Gamma(-2\ell-2\epsilon+q)} \frac{y^q}{q!}\ {}_2F_1\left(-n,1+q,2\ell+2\epsilon+2;x\right) \\
&\qquad+(1-x)^n\, y^{2\ell+1} \sum_{Q=0}^{\infty} \frac{\Gamma(\ell-\epsilon+1+i\eta(Z)+Q)\,\Gamma(Q+1)}{\Gamma(Q+1-2\epsilon)} \frac{y^Q}{Q!} \\
&\qquad\qquad \times\ {}_2F_1\left(-n,2\epsilon-Q,2\ell+2\epsilon+2;\frac{x}{x-1}\right).
\end{aligned}
$$

2. From $\Gamma(1-z)\Gamma(z) = \dfrac{\pi}{\sin(\pi z)}$ and $\sin[\pi(\alpha+1)] = -\sin(\pi\alpha)$ we obtain

$$
\frac{\pi}{\sin[\pi(2\ell+2\epsilon+1)]} = -\Gamma(1-2\ell-2\epsilon)\Gamma(2\ell+2\epsilon) \qquad \text{(A.9)}
$$

and then

$$
\begin{aligned}
&\lim_{\epsilon\to 0} \frac{\pi}{\sin[\pi(2\ell+2\epsilon+1)]} \sum_{q=0}^{2\ell} (1)_q \frac{\Gamma(-\ell-\epsilon+i\eta(Z)+q)}{\Gamma(-2\ell-2\epsilon+q)} \frac{y^q}{q!}\ {}_2F_1\left(-n,1+q,2\ell+2\epsilon+2;x\right) \\
&\quad= \Gamma(2\ell+1)\Gamma(-\ell+i\eta(Z)) \sum_{q=0}^{2\ell} \frac{(1)_q\,(-\ell+i\eta(Z))_q}{(-2\ell)_q} \frac{y^q}{q!}\ {}_2F_1\left(-n,1+q,2\ell+2;x\right).
\end{aligned}
$$

Collecting these two results, the limit (A.8) becomes

$$
\begin{aligned}
I_W^{(+)}(\ell) = {} & \frac{(2\beta)^{\ell+1}}{N_{n,\ell}\,\Gamma(2\ell+2)}\,\frac{(-2ik)^{-\ell}}{\beta-ik}\,\frac{\Gamma(2\ell+1)}{\Gamma(\ell+1+i\eta(Z))} \\
& \times \sum_{q=0}^{2\ell} \frac{(1)_q\,(-\ell+i\eta(Z))_q}{(-2\ell)_q}\,\frac{y^q}{q!}\;{}_2F_1\left(-n,1+q,2\ell+2;x\right) \\
& + \frac{(2\beta)^{\ell+1}}{N_{n,\ell}\,\Gamma(2\ell+2)}\,\frac{(-2ik)^{-\ell}}{\beta-ik}\,(1-x)^n\;y^{2\ell+1} \\
& \times \lim_{\epsilon\to 0}\; -\frac{\pi}{\sin[\pi(2\ell+2\epsilon)]}\,\frac{1}{\Gamma(\ell+\epsilon+1+i\eta(Z))\,\Gamma(-\ell-\epsilon+i\eta(Z))} \\
& \times \left\{ -y^{2\epsilon}\sum_{q=0}^{\infty}\Gamma(\ell+\epsilon+1+i\eta(Z)+q)\,\frac{y^q}{q!}\;{}_2F_1\left(-n,-q,2\ell+2\epsilon+2;\frac{x}{x-1}\right)\right. \\
& \left. + \sum_{q=0}^{\infty}\frac{\Gamma(\ell-\epsilon+1+i\eta(Z)+q)\,\Gamma(q+1)}{\Gamma(q+1-2\epsilon)}\,\frac{y^q}{q!}\;{}_2F_1\left(-n,2\epsilon-q,2\ell+2\epsilon+2;\frac{x}{x-1}\right)\right\}.
\end{aligned}
$$

The next step consists in performing the Taylor series (about $\epsilon = 0$). For hypergeometric functions ${}_2F_1$ we use the results presented in [31] so that the two variable hypergeometric function ${}_2\Theta_1^{(1)}$ appears (see **Chapter 2**). The calculations are rather simple and will be omitted here. The closed form obtained for the integral in the case of a non-negative integer value of $2\ell+1$ is finally

$$
\begin{aligned}
I_W^{(+)}(\ell) = {} & \frac{1}{N_{n,\ell}\,\Gamma(2\ell+2)}\left(\frac{\beta}{k}i\right)^{\ell} x \\
& \times \left[\frac{\Gamma(2\ell+1)}{\Gamma(\ell+1+i\eta)}\sum_{q=0}^{2\ell}\frac{(-\ell+i\eta)_q}{(-2\ell)_q}\,y^q\,{}_2F_1(-n,q+1,2\ell+2;x) \right. \\
& - \frac{y^{2\ell+1}}{\Gamma(-\ell+i\eta)}\sum_{q=0}^{\infty}(\ell+1+i\eta)_q\frac{y^q}{q!} \\
& \times \Bigg\{ {}_2F_1(-n,2\ell+2+q,2\ell+2;x)\,[\psi(q+1)-\mathrm{Log}\,(y)-\psi(\ell+1+q+i\eta)] \\
& + \frac{n\,x}{4(\ell+1)^2}\left[-q(1-x)^{n-1}\;{}_2\Theta_1^{(1)}\left(\begin{array}{c} 1,1\,|\,2\ell+2,-n+1,-q+1 \\ 2\ell+3\,|\,2,2\ell+3 \end{array}\middle|\; ;x^*,x^*\right)\right. \\
& \left.\left. \left. + (2\ell+2+q)\;\;{}_2\Theta_1^{(1)}\left(\begin{array}{c} 1,1\,|\,2\ell+2,-n+1,2\ell+3+q \\ 2\ell+3\,|\,2,2\ell+3 \end{array}\middle|\; ;x,x\right)\right]\right\}\right]
\end{aligned}
\qquad \text{(A.10)}
$$

where ψ is the digamma function.

Remark A.0.1. In the deduction of the previous expression we have made an interchange between an integral an a limit process without looking at the conditions for this to be valid [equations (A.6)]. To show that it can be done, we compare the value obtained with a numerical calculation of the integral (A.6a) with that found using the analytical expression (A.10).

For $\ell = 1$ we use expression (A.10) to evaluate $I_W^{(+)}(\ell)$, formula (A.5) to calculate $I_W^{(+)}(\ell + \epsilon)$, and define a relative error

$$\mathcal{RE}(\epsilon) = \left| \frac{I_W^{(+)}(\ell) - I_W^{(+)}(\ell + \epsilon)}{I_W^{(+)}(\ell)} \right| .$$

In **Table A.1** we give the values obtained for $I_W^{(+)}(\ell+\epsilon)$ and the relative error with respect to $I_W^{(+)}(\ell)$. As expected, the error decreases for decreasing values of ϵ.

ϵ	$I_W(\ell + \epsilon)$	$\mathcal{RE}(\epsilon)$
0.1	$4.13629 - 0.331863i$	0.290127
0.01	$3.28478 - 0.324967i$	0.0255764
0.001	$3.21059 - 0.324081i$	0.0025261
0.0001	$3.20327 - 0.32399i$	0.000252297

Table A.1: Different values of $I_W^{(+)}(\ell + \epsilon)$ given by formula (A.5) for ϵ approaching 0 and the relative error with respect to the value of $I_W^{(+)}(\ell)$ calculated using (A.10). Parameters: $Z = -1$, $\mu = 1$, $k = 1.2$, $\beta = 3.8$, $\ell = 1$, $n = 6$.

Appendix B

Formulas and Integrals

In the first section of this appendix we present the formulas and integrals we use repeatedly throughout the six chapters of this thesis and the second part of this appendix. Most of them can be found in the book of I. S. Gradshteyn and I. M. Ryzhik [92], and the last two are given in a paper of N. Saad and R. Hall [91].

In the second section we perform a number of integrals appearing in the different chapters of this work.

B.1 Useful formulas and integrals

From I. S. Gradshteyn and I. M. Ryzhik [92]

2.539.4

$$\int \frac{\cos 2nx}{\sin x}\, dx = 2\sum_{k=1}^{n} \frac{\cos[(2k-1)x]}{2k-1} + \ln\left[\tan\left(\frac{x}{2}\right)\right] \tag{B.1}$$

2.539.8

$$\int \frac{\cos 2nx}{\cos x}\, dx = 2\sum_{k=1}^{n} (-1)^{n-k}\, \frac{\sin[(2k-1)x]}{2k-1} + (-1)^n \ln\left[\tan\left(\frac{\pi}{4} + \frac{x}{2}\right)\right] \tag{B.2}$$

3.385 For $\operatorname{Re}\lambda > 0$, $\operatorname{Re}\nu > 0$ and $|\arg(1-\beta)| < \pi$,

$$\int_0^1 x^{\nu-1}(1-x)^{\lambda-1}(1-\beta x)^{-\varrho} e^{-\mu x}\, dx = B(\nu,\lambda)\Phi_1(\nu,\varrho,\lambda+\nu;\beta,-\mu) \tag{B.3}$$

where B is the Beta function [42] and Φ_1 is one of the Horn's hypergeometric series [see (2.18a) and [52]].

Remark B.1.1. This formula has been modified form the one appearing in reference [92] to coincide with the definition of Φ_1 given in (2.18a).

■

7.414.7 For $\mathrm{Re}(\beta) > -1$, $\mathrm{Re}(s) > 0$,

$$\int_0^\infty e^{-st}\, t^\beta L_n^\alpha(t)\, dt = \frac{\Gamma(\beta+1)\,\Gamma(\alpha+n+1)}{n!\,\Gamma(\alpha+1)}\, s^{-\beta-1}\; {}_2F_1(-n, \beta+1, \alpha+1; s^{-1}) \tag{B.4}$$

7.512.2 For $n = 0, 1, 2, \ldots$, $\mathrm{Re}(\rho) > 0$, and $\mathrm{Re}(\beta-\gamma) > n-1$,

$$\int_0^1 x^{\rho-1}(1-x)^{\beta-\gamma-n}\; {}_2F_1(-n, \beta, \gamma; x)\, dx = \frac{\Gamma(\gamma)\,\Gamma(\rho)\,\Gamma(\beta-\gamma+1)\,\Gamma(\gamma-\rho+n)}{\Gamma(\gamma+n)\,\Gamma(\gamma-\rho)\,\Gamma(\beta-\gamma+\rho+1)} \tag{B.5}$$

From N. Saad and R. Hall [91]

◇ An identity for Appel F_2

$$F_2(d, a, a', d, d; x, y) = \frac{1}{(1-x)^a(1-y)^{a'}}\; {}_2F_1\left(a, a', d; \frac{x\,y}{(1-x)(1-y)}\right) \tag{B.6}$$

◇ For $\mathrm{Re}(d) > 0$ and $|k| + |k'| < |h|$,

$$\int_0^\infty dr\, r^{d-1}\, e^{-hr}\; {}_1F_1(a, b; k\,r)\; {}_1F_1(a', b'; k'r) = \frac{\Gamma(d)}{h^d}\, F_2\left(d, a, a', b, b'; \frac{k}{h}, \frac{k'}{h}\right) \tag{B.7}$$

B.2 Integrals related to scattering problems

1. The following two integrals appear when solving the scattering of a particle under the influence of a combined Coulomb plus Yukawa potential [see **Section 5.3.1**]:

$$
\begin{aligned}
&\int_0^\infty dr\, \phi_n^L(\ell,\beta;r)\, \frac{e^{-ar}}{r}\; F^{(s)}(\ell,k;r) \\
&\quad = \frac{1}{N_{n,\ell}\,\Gamma(2\ell+2)}\, N_C(\ell)\,(2\beta)^{\ell+1} \\
&\quad\quad \times \int_0^\infty dr\, e^{-(a+\beta-ik)r}\, r^{2\ell+1}\, {}_1F_1(-n,2\ell+2;2\beta r)\, {}_1F_1(\ell+1+i\eta,2\ell+2;-2ikr) \\
&\quad \overset{(B.7)}{=} \frac{1}{N_{n,\ell}\,\Gamma(2\ell+2)}\, N_C(\ell)\,(2\beta)^{\ell+1}\, \frac{\Gamma(2\ell+2)}{(a+\beta-ik)^{2\ell+2}} \\
&\quad\quad \times F_2\left(2\ell+2,-n,\ell+1+i\eta,2\ell+2,2\ell+2;\frac{2\beta}{a+\beta-ik},-\frac{2ik}{a+\beta-ik}\right) \\
&\quad \overset{(B.6)}{=} \frac{N_C(\ell)}{N_{n,\ell}}\, \frac{(2\beta)^{\ell+1}}{(a+\beta-ik)^{2\ell+2}} \left(\frac{a-\beta-ik}{a+\beta-ik}\right)^n \left(\frac{a+\beta+ik}{a+\beta-ik}\right)^{-\ell-1-i\eta} \\
&\quad\quad \times\ {}_2F_1\left(-n,\ell+1+i\eta,2\ell+2;-\frac{4\beta ki}{a^2-(\beta+ik)^2}\right) \\
&\quad = \frac{N_C(\ell)}{N_{n,\ell}} \left(\frac{2\beta}{(a+\beta)^2+k^2}\right)^{\ell+1} \left(\frac{a-\beta-ik}{a+\beta-ik}\right)^n \left(\frac{a+\beta-ik}{a+\beta+ik}\right)^{i\eta} \\
&\quad\quad \times\ {}_2F_1\left(-n,\ell+1+i\eta,2\ell+2;-\frac{4\beta ki}{a^2-(\beta+ik)^2}\right),
\end{aligned} \tag{B.8}
$$

and

$$
\begin{aligned}
&\int_0^\infty dr\, \phi_q^L(\ell,\beta;r)\, \frac{e^{-ar}}{r}\, \phi_j^L(\ell,\beta;r) \\
&\quad = \frac{(2\beta)^{2\ell+2}}{N_{q,\ell}\, N_{j,\ell}\, [\Gamma(2\ell+2)]^2} \\
&\quad\quad \times \int_0^\infty dr\, e^{-(a+2\beta)r} r^{2\ell+1}\, {}_1F_1(-q,2\ell+2;2\beta r)\, {}_1F_1(-j,2\ell+2;2\beta r) \\
&\quad \overset{(B.7)}{=} \frac{1}{N_{q,\ell}\, N_{j,\ell}\, [\Gamma(2\ell+2)]^2}\, (2\beta)^{2\ell+2} \frac{\Gamma(2\ell+2)}{(a+2\beta)^{2\ell+2}} \\
&\quad\quad \times F_2\left(2\ell+2,-q,-j,2\ell+2,2\ell+2;\frac{2\beta}{a+2\beta},\frac{2\beta}{a+2\beta}\right) \\
&\quad \overset{(B.6)}{=} \frac{1}{N_{q,\ell}\, N_{j,\ell}\, \Gamma(2\ell+2)} \left(\frac{2\beta}{a+2\beta}\right)^{2\ell+2} \left(\frac{a}{a+2\beta}\right)^{q+j} \\
&\quad\quad \times\ {}_2F_1\left(-q,\ -j;\ 2\ell+2;\ \left(\frac{2\beta}{a}\right)^2\right).
\end{aligned} \tag{B.9}
$$

2. The integral

$$\int_0^{\frac{\pi}{2}} C(\alpha)\, H_p(\alpha)\, H_m(\alpha)\, d\alpha$$

appears in the matrix elements of a three-body problem if we consider the basis functions as a product of one radial and one angular function [formula (6.37c)]. Here $C(\alpha)$ and $H_m(\alpha)$ are given by formulas (6.7b) and (6.30), respectively.

To perform the integral we first express

$$\begin{aligned} H_p(\alpha)H_m(\alpha) =& \frac{4}{\pi}\,\sin[2(p+1)\alpha]\,\sin[2(m+1)\alpha] \\ =& \frac{2}{\pi}\,\{\cos[2(p-m)\alpha]-\cos[2(p+m+2)\alpha]\}\,. \end{aligned}$$

Now observing that

$$C\left(\frac{\pi}{2}-\alpha\right)=C(\alpha), \qquad \text{and} \qquad H_p\left(\frac{\pi}{2}-\alpha\right)=(-1)^p H_p(\alpha),$$

we conclude that if m and p have different parity the integral vanishes, while if they have the same parity

$$\begin{aligned} &\int_0^{\frac{\pi}{2}} C(\alpha)\,H_p(\alpha)\,H_m(\alpha)\,d\alpha \\ &\quad = 2\int_0^{\frac{\pi}{4}} C(\alpha)\,H_p(\alpha)\,H_m(\alpha)\,d\alpha \\ &\quad = \frac{4}{\pi}\int_0^{\frac{\pi}{4}}\left\{-\frac{Z-1}{\cos\alpha}-\frac{Z}{\sin\alpha}\right\}\Big\{\cos[2(p-m)\alpha]-\cos[2(p+m+2)\alpha]\Big\}\,d\alpha\,. \end{aligned} \tag{B.10}$$

We separately calculate

(A)

$$\begin{aligned} &\int_0^{\frac{\pi}{4}} \frac{\cos[2(p-m)\alpha]-\cos[2(p+m+2)\alpha]}{\cos\alpha}\,d\alpha \\ &\overset{(B.2)}{=} \left\{2\sum_{k=1}^{|p-m|}(-1)^{|p-m|-k}\,\frac{\sin[(2k-1)\alpha]}{2k-1}+(-1)^{|p-m|}\,\ln\left[\tan\left(\frac{\pi}{4}+\frac{\alpha}{2}\right)\right]\right\}\Bigg|_0^{\frac{\pi}{4}} \\ &\quad -\left\{2\sum_{k=1}^{p+m+2}(-1)^{p+m+2-k}\,\frac{\sin[(2k-1)\alpha]}{2k-1}+(-1)^{p+m+2}\,\ln\left[\tan\left(\frac{\pi}{4}+\frac{\alpha}{2}\right)\right]\right\}\Bigg|_0^{\frac{\pi}{4}}. \end{aligned}$$

Notice that for p, m having the same parity, $|p-m|$ and $p+m$ are even, and then the previous integral simplifies

$$\int_0^{\frac{\pi}{4}} \frac{\cos[2(p-m)\alpha]-\cos[2(p+m+2)\alpha]}{\cos\alpha}\,d\alpha = -2\sum_{k=|p-m|+1}^{p+m+2}(-1)^k\,\frac{\sin[\frac{(2k-1)\pi}{4}]}{2k-1}. \tag{B.11a}$$

(B)

$$\begin{aligned}
&\int_0^{\frac{\pi}{4}} \left\{\frac{\cos[2(p-m)\alpha]}{\sin\alpha} - \frac{\cos[2(p+m+2)\alpha]}{\sin\alpha}\right\} d\alpha \\
&\overset{(B.1)}{=} \left\{2\sum_{k=1}^{|p-m|} \frac{\cos[(2k-1)\alpha]}{2k-1} + \ln\left[\tan\left(\frac{\alpha}{2}\right)\right]\right\}\Bigg|_0^{\frac{\pi}{4}} \\
&\quad - \left\{2\sum_{k=1}^{p+m+2} \frac{\cos[(2k-1)\alpha]}{2k-1} + \ln\left[\tan\left(\frac{\alpha}{2}\right)\right]\right\}\Bigg|_0^{\frac{\pi}{4}} \\
&= -2\sum_{k=|p-m|+1}^{p+m+2} \frac{\cos[\frac{(2k-1)\pi}{4}]-1}{2k-1}.
\end{aligned} \tag{B.11b}$$

With (B.11a) and (B.11b), we get the result for (B.10): for m, p having the same parity we have

$$\begin{aligned}
&\int_0^{\frac{\pi}{2}} C(\alpha)\, H_p(\alpha)\, H_m(\alpha)\, d\alpha \\
&\quad = \frac{4}{\pi}\int_0^{\frac{\pi}{4}} \Big\{\cos[2(p-m)\alpha] - \cos[2(p+m+2)\alpha]\Big\}\left\{-\frac{Z-1}{\cos\alpha} - \frac{Z}{\sin\alpha}\right\} d\alpha \\
&\quad = \frac{8}{\pi}\left\{(Z-1)\sum_{k=|p-m|+1}^{p+m+2} (-1)^k \frac{\sin[\frac{(2k-1)\pi}{4}]}{2k-1} + Z\sum_{k=|p-m|+1}^{p+m+2} \frac{\cos[\frac{(2k-1)\pi}{4}]-1}{2k-1}\right\}
\end{aligned} \tag{B.12}$$

and otherwise this integral vanishes.

3. We now perform an integral related to the matrix elements of a three-body problem for which the basis functions couple the angular variable [formula (6.51)],

$$\int_0^{\frac{\pi}{2}} H_p(\alpha)\frac{\partial^2}{\partial\alpha^2}\left[g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\right] d\alpha. \tag{B.13}$$

Special care is required here because the function C, and thus the function $g_{q,n}^{(\pm)}$ given by (1.66) with Z replaced by C, is not defined at the endpoints of the interval $A = \left(0, \frac{\pi}{2}\right)$. Nevertheless the limit of the integrand at these two points exists, so integral (6.49) converges over A. In addition, the derivative of C is not defined at $\alpha = \dfrac{\pi}{4}$, then integral (6.50) must be calculated with a limit process,

$$\begin{aligned}
\int_0^{\frac{\pi}{2}} H_p(\alpha)\frac{\partial^2}{\partial\alpha^2}\left[g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\right] d\alpha &= \lim_{b\to\frac{\pi}{4}^-}\int_0^{b} H_p(\alpha)\frac{\partial^2}{\partial\alpha^2}\left[g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\right] d\alpha \\
&\quad + \lim_{b\to\frac{\pi}{4}^+}\int_b^{\frac{\pi}{2}} H_p(\alpha)\frac{\partial^2}{\partial\alpha^2}\left[g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\right] d\alpha.
\end{aligned} \tag{B.14}$$

With the technique of integration by parts we obtain a primitive for these integrals

$$
\begin{aligned}
\int H_p(\alpha)\frac{\partial^2}{\partial\alpha^2} & \left[g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\right] d\alpha \\
= \quad & H_p(\alpha)\frac{\partial}{\partial\alpha}\left[g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\right] - \int \frac{\partial}{\partial\alpha}H_p(\alpha)\ \frac{\partial}{\partial\alpha}\left[g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\right] d\alpha \\
= \quad & H_p(\alpha)\frac{\partial}{\partial\alpha}\left[g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\right] - g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\frac{\partial}{\partial\alpha}H_p(\alpha) \\
& + \int g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\frac{\partial^2}{\partial\alpha^2}H_p(\alpha)\ d\alpha \\
\overset{(6.31c)}{=} \quad & H_p(\alpha)\frac{\partial}{\partial\alpha}\left[g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\right] - g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\frac{\partial}{\partial\alpha}H_p(\alpha) \\
& -4(p+1)^2\int g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)H_p(\alpha)\ d\alpha
\end{aligned}
\tag{B.15}
$$

and then

$$
\begin{aligned}
\lim_{b\to\frac{\pi}{4}^-}\int_0^b H_p(\alpha) & \frac{\partial^2}{\partial\alpha^2}\left[g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\right] d\alpha \\
= \quad & \lim_{b\to\frac{\pi}{4}^-}\left\{H_p(\alpha)\frac{\partial}{\partial\alpha}\left[g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\right] - g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\frac{\partial}{\partial\alpha}H_p(\alpha)\right\}\Bigg|_0^b \\
& -4(p+1)^2\lim_{b\to\frac{\pi}{4}^-}\int_0^b g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)H_p(\alpha)\ d\alpha \\
\overset{(6.31a)}{=} \quad & \lim_{b\to\frac{\pi}{4}^-}\left\{H_p(b)\ \frac{\partial}{\partial\alpha}\left[g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\right]\Bigg|_{\alpha=b} - g_{q,n}^{(\pm)}(b)H_m(b)\ \frac{\partial}{\partial\alpha}H_p(\alpha)\Bigg|_{\alpha=b}\right\} \\
& -4(p+1)^2\int_0^{\frac{\pi}{4}} g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)H_p(\alpha)\ d\alpha.
\end{aligned}
$$

The derivative of $H_p(\alpha)$ is a continuous function in $\alpha = \dfrac{\pi}{4}$ then, changing the limit notation, we find

$$
\begin{aligned}
\lim_{b\to\frac{\pi}{4}^-}\int_0^b & H_p(\alpha)\frac{\partial^2}{\partial\alpha^2}\left[g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\right] d\alpha \\
&= - g_{q,n}^{(\pm)}\left(\frac{\pi}{4}\right)H_m\left(\frac{\pi}{4}\right)\ \frac{\partial}{\partial\alpha}H_p(\alpha)\Bigg|_{\alpha=\frac{\pi}{4}} + \lim_{\alpha\to\frac{\pi}{4}^-} H_p(\alpha)\frac{\partial}{\partial\alpha}\left[g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\right] \\
&\quad - 4(p+1)^2\int_0^{\frac{\pi}{4}} g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)H_p(\alpha)\ d\alpha.
\end{aligned}
\tag{B.16a}
$$

Repeating the same procedure for the integral over the interval $\left(b, \dfrac{\pi}{2}\right)$ we obtain

$$\begin{aligned}
\lim_{b\to\frac{\pi}{4}^+} \int_b^{\frac{\pi}{2}} H_p(\alpha)\frac{\partial^2}{\partial\alpha^2}\left[g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\right] d\alpha \\
&= g_{q,n}^{(\pm)}\left(\frac{\pi}{4}\right) H_m\left(\frac{\pi}{4}\right) \frac{\partial}{\partial\alpha}H_p(\alpha)\bigg|_{\alpha=\frac{\pi}{4}} - \lim_{\alpha\to\frac{\pi}{4}^+} H_p(\alpha)\frac{\partial}{\partial\alpha}\left[g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\right] \\
&\quad - 4(p+1)^2 \int_{\frac{\pi}{4}}^{\frac{\pi}{2}} g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)H_p(\alpha)\ d\alpha. \qquad \text{(B.16b)}
\end{aligned}$$

Collecting results (B.16a) and (B.16b) in (B.14), we find

$$\begin{aligned}
\int_0^{\frac{\pi}{2}} H_p(\alpha)\frac{\partial^2}{\partial\alpha^2}\left[g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\right] d\alpha \\
&= \lim_{\alpha\to\frac{\pi}{4}^-} H_p(\alpha)\frac{\partial}{\partial\alpha}\left[g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\right] - 4(p+1)^2\int_0^{\frac{\pi}{4}} g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)H_p(\alpha)\ d\alpha \\
&\quad - \lim_{\alpha\to\frac{\pi}{4}^+} H_p(\alpha)\frac{\partial}{\partial\alpha}\left[g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\right] - 4(p+1)^2\int_{\frac{\pi}{4}}^{\frac{\pi}{2}} g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)H_p(\alpha)\ d\alpha \\
&= S_{p,q;m,n} - 4(p+1)^2\int_0^{\frac{\pi}{2}} g_{q,n}^{(\pm)}(\alpha)\, H_p(\alpha)\, H_m(\alpha)\, d\alpha, \qquad \text{(B.17)}
\end{aligned}$$

where we define the jump quantity $S_{p,q;m,n}$ as

$$S_{p,q;m,n} = \lim_{\alpha\to\frac{\pi}{4}^-} H_p(\alpha)\frac{\partial}{\partial\alpha}\left[g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\right] - \lim_{\alpha\to\frac{\pi}{4}^+} H_p(\alpha)\frac{\partial}{\partial\alpha}\left[g_{q,n}^{(\pm)}(\alpha)H_m(\alpha)\right]. \qquad \text{(B.18)}$$

Noticing that $H_m(\alpha)$ and $g_{q,n}^{(\pm)}(\alpha)$ are continuous functions at $\alpha = \dfrac{\pi}{4}$, and

$$\frac{\partial}{\partial\alpha}g_{q,n}^{(\pm)}(\alpha)$$

is not continuous at $\alpha = \dfrac{\pi}{4}$ but one-sided limits exist [see (6.10)], this jump can be written as

$$\begin{aligned}
S_{p,q;m,n} &= \lim_{\alpha\to\frac{\pi}{4}^-} H_p(\alpha)\left(\frac{\partial}{\partial\alpha}g_{q,n}^{(\pm)}(\alpha)\right)H_m(\alpha) + \lim_{\alpha\to\frac{\pi}{4}^-} H_p(\alpha)\ g_{q,n}^{(\pm)}(\alpha)\left(\frac{\partial}{\partial\alpha}H_m(\alpha)\right) \\
&\quad - \lim_{\alpha\to\frac{\pi}{4}^+} H_p(\alpha)\left(\frac{\partial}{\partial\alpha}g_{q,n}^{(\pm)}(\alpha)\right)H_m(\alpha) - \lim_{\alpha\to\frac{\pi}{4}^+} H_p(\alpha)g_{q,n}^{(\pm)}(\alpha)\left(\frac{\partial}{\partial\alpha}H_m(\alpha)\right) \\
&= H_p\left(\frac{\pi}{4}\right)H_m\left(\frac{\pi}{4}\right)\left[\lim_{\alpha\to\frac{\pi}{4}^-}\left(\frac{\partial}{\partial\alpha}g_{q,n}^{(\pm)}(\alpha)\right) - \lim_{\alpha\to\frac{\pi}{4}^+}\left(\frac{\partial}{\partial\alpha}g_{q,n}^{(\pm)}(\alpha)\right)\right].
\end{aligned}$$

Now, taking into account that

$$g^{(\pm)}_{q,n}\left(\frac{\pi}{4}-\alpha\right) = g^{(\pm)}_{q,n}(\alpha) \qquad \Longrightarrow \qquad \frac{\partial}{\partial\alpha} g^{(\pm)}_{q,n}(\alpha)\bigg|_{\alpha=\frac{\pi}{4}-\widetilde{\alpha}} = -\frac{\partial}{\partial\alpha} g^{(\pm)}_{q,n}(\alpha)\bigg|_{\alpha=\widetilde{\alpha}},$$

and

$$H_p\left(\frac{\pi}{4}\right) = \begin{cases} 0, & \text{if } p \text{ is odd,} \\ \dfrac{2}{\sqrt{\pi}}(-1)^{\frac{p}{2}}, & \text{if } p \text{ is even,} \end{cases}$$

we find a simplified expression for $S_{p,q;m,n}$

$$S_{p,q;m,n} = \begin{cases} \dfrac{8}{\pi}(-1)^{\frac{m+p}{2}} \lim\limits_{\alpha\to\frac{\pi}{4}^-} \dfrac{\partial}{\partial\alpha} g^{(\pm)}_{q,n}(\alpha), & \text{if } m,p \text{ are even,} \\ 0, & \text{otherwise.} \end{cases} \tag{B.19}$$

4. Another integral we need to solve corresponds to the Laguerre expansion of the driven term considered in the three-body model problem studied in **Section 6.4** [formula (6.60)],

$$\int_0^{\frac{\pi}{2}} \int_0^{\infty} \phi^L_q(\ell_p,\beta;\rho)\, H_p(\alpha)\, f(\rho,\alpha)\, \rho^{5/2} \cos\alpha\, \sin\alpha\, d\rho\, d\alpha$$

for H_p, ϕ^L_q and f defined in (6.30), (1.2) and (6.53) respectively. We use the series representation of f given in [83],

$$f(\rho,\alpha) = \sum_{n=0}^{\infty} b_n\, e^{-a\rho} \rho^{2n+t}\, \frac{H_n(\alpha)}{\cos\alpha\, \sin\alpha} \tag{B.20}$$

$$b_n = \frac{\sqrt{\pi}\, \left[(-1)^n + 1\right]}{8\,(n+1)\, 2^{2n} \left(\frac{3}{2}\right)_n n!}. \tag{B.21}$$

First we remark that, as a consequence of the property [42]

$$\Gamma\left(z+\frac{1}{2}\right)\Gamma(z) = 2^{1-2z}\, \sqrt{\pi}\, \Gamma(2z)$$

we find

$$2^{2n}\left(\frac{3}{2}\right)_n n! = 2^{2n}\, \frac{\Gamma\left(n+1+\frac{1}{2}\right)}{\Gamma\left(\frac{3}{2}\right)}\, \Gamma(n+1) = \Gamma(2n+2)$$

and thus the coefficients b_n have the alternative simpler expression

$$b_n = \frac{\sqrt{\pi}\,\left[(-1)^n + 1\right]}{8\,(n+1)\,(2n+1)!}. \tag{B.22}$$

Now, using the series expansion of f given in (B.20) the two-dimensional integral reduces to a sum of products of one-dimensional integrals,

$$\begin{aligned}\int_0^{\frac{\pi}{2}}\int_0^{\infty} \phi_q^L(\ell_p,\beta;\rho)\,H_p(\alpha)\,f(\rho,\alpha)\rho^{5/2}\cos\alpha\,\sin\alpha\,d\rho\,d\alpha \\ = \sum_{n=0}^{\infty} b_n\,\left(\int_0^{\frac{\pi}{2}} H_p(\alpha)\,H_n(\alpha)\,d\alpha\right)\left(\int_0^{\infty}\phi_q^L(\ell_p,\beta;\rho)\,e^{-a\rho}\rho^{2n+t+\frac{5}{2}}\,d\rho\right).\end{aligned}$$

The integral over α gives a Kronecker delta $\delta_{p,n}$ while the integral over ρ with $n = p$ reads

$$\begin{aligned}\int_0^{\infty}\phi_q^L(\ell_p,\beta;\rho)\quad & e^{-a\rho}\rho^{2p+t+\frac{5}{2}}\,d\rho \\ = \quad & \frac{N_{q,\ell_p}}{(2\beta)^{2p+t+\frac{5}{2}}}\int_0^{\infty} e^{-\frac{a+\beta}{2\beta}\,2\beta\rho}\,(2\beta\rho)^{\ell_p+2p+t+\frac{7}{2}}\,L_q^{2\ell_p+1}(2\beta\rho)\,d\rho \\ \overset{(B.4)}{=}\quad & N_{q,\ell_p}\,\frac{(2\ell_p+2)_q}{q!}\,\frac{(2\beta)^{\ell_p+1}}{(a+\beta)^{2p+t+\ell_p+\frac{9}{2}}}\,\Gamma\left(2p+t+\ell_p+\frac{9}{2}\right) \\ & \times {}_2F_1\left(-q, 2p+t+\ell_p+\frac{9}{2}, 2\ell_p+2; \frac{2\beta}{a+\beta}\right).\end{aligned}$$

Then, using (B.22) for the coefficients b_n we finally obtain

$$\begin{aligned}\int_0^{\frac{\pi}{2}}\int_0^{\infty} \phi_q^L(\ell_p,\beta;\rho)\,H_p(\alpha)\,f(\rho,\alpha)\rho^{5/2}\cos\alpha\,\sin\alpha\,d\rho\,d\alpha \\ = \frac{\sqrt{\pi}\,\left[(-1)^p+1\right]}{8\,(p+1)(2p+1)!}\,\frac{1}{N_{q,\ell_p}\,\Gamma(2\ell_p+2)}\,\frac{(2\beta)^{\ell_p+1}}{(a+\beta)^{2p+t+\ell_p+\frac{9}{2}}}\,\Gamma\left(2p+t+\ell_p+\frac{9}{2}\right) \\ \times\ {}_2F_1\left(-q, 2p+t+\ell_p+\frac{9}{2}, 2\ell_p+2; \frac{2\beta}{a+\beta}\right).\end{aligned} \tag{B.23}$$

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