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The generalized parabolic Coulomb wavefunction in spherical coordinates

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Abstract

In this work we present a detailed study of the recently introduced $\Delta_{m,n}$ basis for three Coulomb particles. We show that the scattering and generalized Coulomb problems as well as a Φ_2 approach can be viewed as particular cases of this basis. We derive a partial wave expansion for $\Delta_{m,n}$ functions and analyse the reduction to some of the precedent cases.

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1. Introduction

In the last years there has been intense activity in the study of the three-body Coulomb problem (3BCP). Different kinds of approximation have been proposed to deal with both the continuum and discrete spectra of the Hamiltonian for three charged particles. Based on the so-called C3 model [1, 2], some authors presented different approximated wavefunctions [3–5]. In the C3 model, the dynamics of the system is described by the product of three two-body Coulomb problem solutions, that is to say, a product of three Kummer hypergeometric functions. This function is an approximate separable solution of the 3BCP wave equation and hence some terms that include the three-body dynamic are lost in the C3 model. However, the computation of cross sections with this model shows a very good agreement for a variety of processes, such as ion–atom ionization, (e, 2e) collisions and photoionization. One way to include the dynamical correlation in the wavefunction is to introduce modifications to the relative momenta between the particles and the Sommerfeld parameters. Alt and co-workers changed the C3 model by including a coordinate-dependent relative momentum between the particles, and in this way they obtain a wavefunction with the correct behaviour in all the asymptotic regions [3]. On the other hand, Berakdar and Briggs introduced modifications in the Sommerfeld parameters by replacing the charges of the particles by momenta and coordinate-dependent charges respectively [4, 5].

We have tackled the problem from another point of view, proposing a correlated wavefunction called Φ_2 [6, 7], based on physically sound approximations to the neglected terms of the Hamiltonian in the C3 model. This approach was initially derived for two heavy and one light particles and generalized to a system of two light and one heavy particles [8]. For the first case, the motion of the system of the heavy particles is described by a two-body Coulomb wavefunction. The dynamic of the light particle in the field of the heavy ones is taken into account by a non-separable Appell degenerate hypergeometric function of two variables labeled Φ_2 [7, 9].

The application to the calculation of different cross section for heavy-ion–atom collisions shows that the correlation introduced by the Φ_2 wavefunction is in some aspects improved in comparison with other models based in the C3 one [10]. However, in the description of collision processes where the target has an internal structure, the Φ_2 model with an eikonal initial state underestimates the electron emission region known as soft electrons. In this description the effect of the passive electrons of the target is modelled by a simple Coulomb potential with effective charge giving rise to the non-orthogonality between the initial and final target states. The internal structure of the target has been taken into account by different approaches, and requires a partial wave decomposition of the wavefunction [11, 12].

Recently, Gasaneo and Miraglia and co-workers [6, 13] have shown that the Φ_2 function is a particular function of a more general basis. In this work we study the partial wave expansion for this basis. In section 2 we state the problem and define the basis to be studied and some limiting cases that can be obtained. In section 3 the general partial wave expansion is given, while in section 3 we study the reduction of the general problem to some well known particular cases. We draw some conclusions in section 4 and give a brief outlook. We have included in the appendix some useful algebraic formulae.

2. The generalized Coulombian basis

The wavefunction C3 treats all Coulomb interactions on equal footing, and, as we said before, can be written as a product of three two-body Coulomb functions. In the case of the continuum spectra and incoming boundary conditions, we have

$$\Psi_{C3} = \Phi_{PW} \prod_{j=1}^{3} F\begin{bmatrix} \mathrm{i}\alpha_j \\ 1 \end{bmatrix}, -\mathrm{i}k_j\xi_j\Bigg] \tag{1}$$

where the function $F\left[\begin{matrix} a \\ b \end{matrix}, x\right]$ is the Kummer function [15]. Here, Φ_{PW} are the plane waves representing the asymptotically free motion of the particles without interactions. α_j ($j = 1, 2, 3$) are the Sommerfeld parameters and k_j (r_j) is the relative momentum (position) between particles i and k, $i \neq j \neq k$. For brevity we have omitted the normalization factors of each Coulomb wave. The function Ψ_{C3}, equation (1), is written in the set of six parabolic coordinates [16]

$$\begin{aligned} \xi_j &= r_j + \hat{\boldsymbol{k}}_j \cdot \boldsymbol{r}_j \\ \eta_j &= r_j - \hat{\boldsymbol{k}}_j \cdot \boldsymbol{r}_j \qquad j = 1, 2, 3. \end{aligned} \tag{2}$$

In equation (1) the η_j coordinates are included in the plane wave:

$$\Phi_{PW} = \exp\left(\mathrm{i}\frac{\mu_1}{m_1}k_1\frac{(\xi_1 - \eta_1)}{2} + \mathrm{i}\frac{\mu_2}{m_2}k_2\frac{(\xi_2 - \eta_2)}{2} + \mathrm{i}\frac{\mu_3}{m_3}k_3\frac{(\xi_3 - \eta_3)}{2}\right) \tag{3}$$

the symbols m_i and μ_i ($i = 1, 2, 3$) are the masses and the reduced masses of the particles respectively.

The function Ψ_{Φ_2} can be considered as an extension of the Ψ_{C3} for the case of dealing with a three-body system given by two heavy ions and one light particle. For instance, if 1 and 2 are ions, we can write for incoming boundary conditions

$$\Psi_{\Phi_2} = \Phi_{PW} F \begin{bmatrix} \mathrm{i}\alpha_3 \\ 1 \end{bmatrix}, -\mathrm{i}k_3\xi_3 \Bigg] \Phi_2 \begin{bmatrix} \mathrm{i}\alpha_1, \mathrm{i}\alpha_2 \\ 1 \end{bmatrix}, -\mathrm{i}k_1\xi_1, -\mathrm{i}k_2\xi_2 \Bigg]. \tag{4}$$

The hypergeometric function Φ_2 has been extensively studied by Erdelyi [9]. For our purpose, the most useful way to write it is as an expansion in terms of Kummer functions [14]:

$$\Phi_2 \left[\begin{matrix} a, a' \\ b \end{matrix}, x, y \right] = \sum_{m=0}^{\infty} A_m x^m y^m F \left[\begin{matrix} a+m \\ b+2m \end{matrix}, x \right] F \left[\begin{matrix} a'+m \\ b+2m \end{matrix}, y \right] \tag{5}$$

where

$$A_m = \frac{(a)_m \left(a'\right)_m}{(b+m-1)_m \, (m)_m \, m!} \tag{6}$$

and $(a)_n$ are the Pochhammer symbols.

Based on this expansion, Gasaneo [6] and Miraglia *et al* [13] introduced a general wavefunction with the form

$$\Phi = \Phi_{PW} \sum_{\boldsymbol{m},\boldsymbol{n}=0}^{\infty} A_{\boldsymbol{m},\boldsymbol{n}} \prod\nolimits_{j=1}^{3} \Delta_{m_j,n_j} \left(a_j, b_j, \mathrm{i}k_j\xi_j, -\mathrm{i}k_j\eta_j\right) \tag{7}$$

where

$$\Delta_{m,n}\,(a_i, b_i, x, y) = x^m F \left[\begin{matrix} \mathrm{i}\alpha_i + m \\ a_i \end{matrix}, x \right] y^n F \left[\begin{matrix} n \\ b_i \end{matrix}, y \right] \tag{8}$$

$\boldsymbol{m} = \{m_1, m_2, m_3\}$ and $\boldsymbol{n} = \{n_1, n_2, n_3\}$. The coefficients $A_{\boldsymbol{m},\boldsymbol{n}}$ and a_i, b_i are determined by constraining Φ to satisfy different physical requirements such as Redmond 's asymptotic behaviour and Kato's cusp conditions [13]. They have shown that in some cases the coefficients a, b have the form, for example, $a_1 = 1 + 2m$ and $b_1 = 1 + 2n$, that observed by the Φ_2 model [6, 7]. For these cases, the function $\Delta_{m,n}\,(a_i, b_i, x, y)$ can be associated with the two-body Coulomb wavefunction where the magnetic number is different from zero.

Even when the function Φ is a good proposal for the three-body Coulomb problem, the information about the dynamic of dressed charged centres can be considered only as effective charges since this expansion still relies on the coulombic form of the interaction potentials. The common way to deal with this problem is to obtain a partial wave expansion for the base function $\Delta_{m,n}\,(a_i, b_i, x, y)$. Once we have performed the transformation, it may be possible to compare the basis function with that obtained as a solution of the static potential proposed by Erskine [17]. In terms of a partial wave expansion for the Φ, alternative ways to fix the coefficients $A_{\boldsymbol{m},\boldsymbol{n}}$ can be implemented.

It is easy to see that each of the functions $\Delta_{m,n}\,(a_i, b_i, \xi, \eta)$ can be considered a particular case of the following general wave:

$$\begin{aligned} \Delta_{m_1,m_2}\,(\alpha, \beta) = {} & \mathrm{e}^{\mathrm{i}\frac{k}{2}\xi} \mathrm{e}^{\mathrm{i}\left(\frac{m_1+m_2}{2}\right)\phi} \left(-\mathrm{i}k\xi\right)^{\frac{m_1}{2}} F \left[\begin{matrix} \mathrm{i}\alpha + \frac{m_1}{2} \\ 1+m_1 \end{matrix}, -\mathrm{i}k\xi \right] \\ & \times \mathrm{e}^{-\mathrm{i}\frac{k}{2}\eta} \left(\mathrm{i}k\eta\right)^{\frac{m_2}{2}} F \left[\begin{matrix} \mathrm{i}\beta + \frac{m_2}{2} \\ 1+m_2 \end{matrix}, \mathrm{i}k\eta \right] \end{aligned} \tag{9}$$

$$-\alpha + \beta = \frac{Z\mu}{k}. \tag{10}$$

This function is an extension of the generalized Coulomb wavefunction. This means that the coefficients α, β, m_1 and m_2 can be fixed in such a way as to lead us to different wavefunctions:

(I) The scattering Coulomb wavefunction: $m_1 = m_2 = 0$

$$\psi_{\rm s}^{\pm} = {\rm e}^{{\rm i}\frac{k}{2}(\xi-\eta)} F\left[\begin{matrix}{\rm i}\alpha\\ 1\end{matrix}, -{\rm i}k\xi\right] F\left[\begin{matrix}{\rm i}\beta\\ 1\end{matrix}, {\rm i}k\eta\right]. \tag{11}$$

The incoming (outgoing) asymptotic behaviour results when $\beta = 0$ ($\alpha = 0$) taking into account the condition (10).

(II) The general Coulomb function: $m_1 = m_2 = m$

$$\psi_{\rm C}^{\pm} = {\rm e}^{{\rm i}\frac{k}{2}(\xi-\eta)}{\rm e}^{{\rm i}m\phi}\,(-{\rm i}k\xi)^{\frac{m}{2}}\, F\left[\begin{matrix}{\rm i}\alpha+\frac{m}{2}\\ 1+m\end{matrix}, -{\rm i}k\xi\right](\mathrm{i}k\eta)^{\frac{m}{2}}\, F\left[\begin{matrix}{\rm i}\beta+\frac{m}{2}\\ 1+m\end{matrix}, {\rm i}k\eta\right]. \tag{12}$$

The asymptotic behaviour of $\psi_{\rm C}^{\pm}$ is different from that given by $\psi_{\rm s}^{\pm}$. For $r \to \infty$ and for example $\beta = 0$, $\psi_{\rm C}^{-}$ leads to

$$\begin{aligned}\psi_{\rm C}^{-} \to {\rm e}^{{\rm i}m\phi}\Bigg[&\frac{\Gamma(1+m)\,\Gamma(1+m)}{\Gamma\left(1+\frac{m}{2}-{\rm i}\alpha\right)\Gamma\left(1+\frac{m}{2}\right)}{\rm e}^{{\rm i}\frac{k}{2}(\xi-\eta)}\,({\rm i}k\xi)^{-{\rm i}\alpha}\\ &+{\rm i}\frac{\Gamma(1+m)\,\Gamma(1+m)}{\Gamma\left({\rm i}\alpha+\frac{m}{2}\right)\Gamma\left(1+\frac{m}{2}\right)}\frac{{\rm e}^{-{\rm i}\frac{k}{2}(\xi+\eta)}}{k\xi}\,(-{\rm i}k\xi)^{{\rm i}\alpha}\\ &-{\rm i}\frac{\Gamma(1+m)\,\Gamma(1+m)}{\Gamma\left(1+\frac{m}{2}-{\rm i}\alpha\right)\Gamma\left(\frac{m}{2}\right)}\frac{{\rm e}^{{\rm i}\frac{k}{2}(\xi+\eta)}}{k\eta}\,({\rm i}k\xi)^{-{\rm i}\alpha}\Bigg].\end{aligned} \tag{13}$$

In this equation we can recognize a plane wave and incoming and outgoing spherical waves, all of them distorted by a logarithmic phase $({\rm i}k\xi)^{\pm{\rm i}\alpha}$ similar to that observed in the asymptotic form of $\psi_{\rm s}^{-}$. We can say that in this case, by similarity with the scattering Coulomb problem with $\beta = 0$, the wavefunction has an incoming asymptotic behaviour. The plane wave of equation (13) is similar to that of $\psi_{\rm s}^{-}$. Besides the 'outgoing' plane wave, the $\psi_{\rm s}^{-}$ presents an incoming spherical wave. Then, the $\psi_{\rm C}^{-}$ adds an outgoing spherical wave to the asymptotic $\psi_{\rm s}^{-}$. This means that the total outgoing probability flux is given by the contributions of the plane and spherical outgoing waves. Also, it changes in each of the planes associated with different values of the angle ϕ.

(III) The Φ_2 case: $\beta = m_2 = 0$ and $m_1 = 2m$.

$$\psi_{\Phi_2}^{-} = {\rm e}^{{\rm i}\frac{k}{2}(\xi-\eta)}{\rm e}^{{\rm i}m\phi}\,(-{\rm i}k\xi)^{m}\, F\left[\begin{matrix}{\rm i}\alpha+m\\ 1+2m\end{matrix}, -{\rm i}k\xi\right]. \tag{14}$$

A function with this form appear in each of the orders of the sum that defines the three-body Φ_2 wavefunction given by equation (4). The asymptotic behaviour of ψ_{Φ_2} is given by

$$\psi_{\Phi_2} \to {\rm e}^{{\rm i}m\phi}\left[\frac{\Gamma(1+2m)}{\Gamma(1+m-{\rm i}\alpha)}{\rm e}^{{\rm i}\frac{k}{2}(\xi-\eta)}\,({\rm i}k\xi)^{-{\rm i}\alpha} + \frac{\Gamma(1+2m)}{\Gamma({\rm i}\alpha+m)}{\rm e}^{-{\rm i}\frac{k}{2}(\xi+\eta)}\,(-{\rm i}k\xi)^{{\rm i}\alpha-1}\right]. \tag{15}$$

A comparative analysis between $\psi_{\Phi_2}^{-}$ and ψ_{s}^{-} shows that both functions have the same asymptotic form, but the normalization and the scattering transition amplitudes are different [18].

All these functions can be written in terms of the Coulomb spherical wavefunctions defined by

$$\langle \boldsymbol{r}|k, l, m\rangle = R_{k,l}^{-} Y_l^m \tag{16}$$

where the function $R^{-}_{k,l}$ represents the radial eigenfunction [19]:

$$R^{-}_{k,l} = \mathrm{e}^{-\mathrm{i}kr} (2kr)^{l} \; F \left[\begin{matrix} \mathrm{i}\alpha + l + 1 \\ 2l + 2 \end{matrix}, 2\mathrm{i}kr \right] \tag{17}$$

and Y^{m}_{l} is the spherical harmonic of θ and ϕ [19, 20]. The normalization constant of the function $R^{-}_{k,l}$ was not included in equation (17) and is given by

$$\mathcal{N}_{k,l} = \sqrt{\frac{2}{\pi}} \frac{k \left| \Gamma\left(l + 1 - \mathrm{i}\alpha\right)\right|}{(2l+2)!} \mathrm{e}^{\frac{\pi}{2}\alpha}. \tag{18}$$

A partial wave expansion of the general basis of equation (7) can be achieved by partial wave decomposition of each of the factors $\Delta_{m_j,n_j}\left(a_j, b_j, x_j, y_j\right)$. However, the function $\Delta_{m_1,m_2}(\alpha, \beta)$ is more general than the factors of the basis and then, in the next section we shall look for an expression of $\Delta_{m_1,m_2}(\alpha, \beta)$ in terms of the basis defined in equation (16).

3. The change of basis

The partial wave expansion of function $\Delta_{m_1,m_2}(\alpha, \beta)$, equation (9), will look like

$$\Delta_{m_1,m_2}(\alpha, \beta) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \mathcal{C}_{l,m} R_{l,m} Y^{m}_{l}(\Omega). \tag{19}$$

First, we replace the Kummer functions in $\Delta_{m_1,m_2}(\alpha, \beta)$ by its series expansion [15]. We also write the parabolic coordinates in terms of the spherical coordinates (see [19]). After some algebra we obtain

$$\begin{aligned} \Delta_{m_1,m_2}(\alpha, \beta) = (-1)^{\frac{m_1}{2}} \mathrm{e}^{-\mathrm{i}kr} (\mathrm{i}kr)^{\frac{m_1+m_2}{2}} \sum_{p,q=0}^{\infty} \frac{\left(1 - \mathrm{i}\alpha + \frac{m_1}{2}\right)_p \left(\mathrm{i}\beta + \frac{m_2}{2}\right)_q}{p!q!\,(1+m_1)_p\,(1+m_2)_q} (\mathrm{i}kr)^{p+q} \\ \times (1+\cos\theta)^{\frac{m_1}{2}+p} (1-\cos\theta)^{\frac{m_2}{2}+q} \mathrm{e}^{\mathrm{i}\left(\frac{m_1+m_2}{2}\right)\phi}. \end{aligned} \tag{20}$$

In this way we separate the angular part of the wavefunction. We can expand it in terms of spherical harmonics as follows:

$$(1+\cos\theta)^{\frac{m_1}{2}+p} (1-\cos\theta)^{\frac{m_2}{2}+q} \mathrm{e}^{\mathrm{i}\left(\frac{m_1+m_2}{2}\right)\phi} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \tilde{a}_{l,m,q,p} Y^{m}_{l} \tag{21}$$

where the coefficients $\tilde{a}_{l,m_1,m_2,q,p}$ are given by (see the appendix)

$$\tilde{a}_{l,m,q,p} = 2^{\frac{m_1+m_2}{2}+p+q} a_{l,m_1,m_2,q,p} \tag{22}$$

and $a_{l,m_1,m_2,q,p}$ can be written in terms of the hypergeometric function ${}_3F_2$ [22]:

$$\begin{aligned} a_{l,m_1,m_2,p,q} = 4\pi\,(-1)^{\frac{3(m_1+m_2)}{4}} N_{l,\frac{m_1+m_2}{2}} \frac{\Gamma\left(q+1+\frac{m_1+3m_2}{4}\right)\Gamma\left(p+1+\frac{3m_1+m_2}{4}\right)}{\Gamma\left(\frac{m_1+m_2}{2}+1\right)\Gamma\left(m_1+m_2+p+q+2\right)} \\ \times {}_3F_2 \left[\begin{matrix} q+1+\frac{m_1+3m_2}{4}, \frac{m_1+m_2}{2} - l, \frac{m_1+m_2}{2} + l + 1 \\ 1 + \frac{m_1+m_2}{2}, m_1+m_2+p+q+2 \end{matrix}, 1 \right] \end{aligned} \tag{23}$$

that resembles the expression of Clebsch–Gordan coefficients in terms of hypergeometric functions [23]. It is possible to find this equivalence; however, we have not found it useful for our purposes.

This expansion leads us to write $\Delta_{m_1,m_2}(\alpha, \beta)$ as a series in terms of angular momenta. The magnetic quantum number m is fixed by the index $\frac{m_1+m_2}{2}$ that appears in the exponential of the equation (9). In this way, all the angular part of the $\Delta_{m_1,m_2}(\alpha,\beta)$ is in the spherical harmonic functions and we can rewrite it as

$$\Delta_{m_1,m_2}(\alpha,\beta) = \sum_{l=0}^{\infty}\sum_{s=0}^{\infty} \mathcal{C}_{l,s,m_1,m_2}\mathcal{R}_{k,s} Y_l^{\frac{m_1+m_2}{2}}(\Omega) \tag{24}$$

$$\Delta_{m_1,m_2}(\alpha,\beta) = \sum_{l=0}^{\infty} \mathcal{R}_{l,m_1,m_2} Y_l^{\frac{m_1+m_2}{2}} \tag{25}$$

where the function $\mathcal{R}_{l,m_1,m_2}$

$$\mathcal{R}_{l,m_1,m_2} = (-1)^{\frac{m_1}{2}} \mathrm{e}^{-\mathrm{i}kr} (2\mathrm{i}kr)^{\frac{m_1+m_2}{2}} \sum_{p,q=0}^{\infty} \frac{\left(1-\mathrm{i}\alpha+\frac{m_1}{2}\right)_p \left(\mathrm{i}\beta+\frac{m_2}{2}\right)_q}{p!q!\,(1+m_1)_p\,(1+m_2)_q} (2\mathrm{i}kr)^{p+q} a_{l,m_1,m_2,p,q}$$

has all the dependence in the radial coordinate. The double series that appear in this equation can be rewritten in a different and more convenient way. Using the relation [21]

$$\sum_{p,q}^{\infty} c_{p,q} x^{p+q} = \sum_{q=0}^{\infty}\sum_{p=0}^{q} c_{q-p,p} x^q \tag{26}$$

one of the series can be re-summed to obtain

$$\mathcal{R}_{l,m_1,m_2} = \mathrm{e}^{-\mathrm{i}kr} (2\mathrm{i}kr)^{\frac{m_1+m_2}{2}} \sum_{p=0}^{\infty} \mathcal{A}_{l,m_1,m_2,p} (2\mathrm{i}kr)^p \tag{27}$$

where the coefficient $\mathcal{A}_{l,m_1,m_2,q}$ is given by

$$\mathcal{A}_{l,m_1,m_2,q} = (-1)^{\frac{m_1}{2}} \sum_{p=0}^{q} \frac{\left(1-\mathrm{i}\alpha+\frac{m_1}{2}\right)_{q-p} \left(\mathrm{i}\beta+\frac{m_2}{2}\right)_p}{(q-p)!p!\,(1+m_1)_{q-p}\,(1+m_2)_p} a_{l,m_1,m_2,q-p,p}. \tag{28}$$

A careful inspection of equation (27) shows that the radial function $\mathcal{R}_{l,m_1,m_2}$ does not have the form of $R_{k,l}^-$, equation (17). The coefficients $\mathcal{A}_{l,m_1,m_2,q}$ have a quite complicated form, which cannot be easily related to the coefficient of the Kummer function of $R_{k,l}^-$. To obtain an expression of $\mathcal{R}_{l,m_1,m_2}$ in terms of the radial Coulomb functions $R_{k,l}^-$, we propose a series expansion for $\mathcal{R}_{l,m_1,m_2}$ in terms of $R_{k,l+s}^-$

$$\mathcal{R}_{l,m_1,m_2} = \sum_{s=0}^{\infty} \mathcal{C}_{l,m_1,m_2,s} R_{k,l+s}^- \tag{29}$$

and look for the coefficients $\mathcal{C}_{l,m_1,m_2,s}$. To relate both $\mathcal{C}_{l,m_1,m_2,s}$ and $\mathcal{A}_{l,m_1,m_2,q}$, we replace the series expansion for the Kummer function in equation (29) and we use the relation given by equation (26), which allows us to express $\mathcal{R}_{l,m_1,m_2}$ as a single series with the following form:

$$\sum_{s=0}^{\infty} \mathcal{C}_{l,m_1,m_2,s} R_{k,l+s}^- = \mathrm{e}^{-\mathrm{i}kr} (2\mathrm{i}kr)^l \sum_{s=0}^{\infty} \mathcal{B}_{l,m_1,m_2,s} (2\mathrm{i}kr)^s . \tag{30}$$

We have introduced the coefficient $\mathcal{B}_{l,m_1,m_2,s}$

$$\mathcal{B}_{l,m_1,m_2,s} = \sum_{q=0}^{s} \frac{(\mathrm{i}\alpha+l+q+1)_{s-q}}{(s-q)!\,(2(l+q)+2)_{s-q}} \mathcal{C}_{l,m_1,m_2,q} \tag{31}$$

to work with a shorter notation and make the procedure to obtain $\mathcal{C}_{l,m_1,m_2,s}$ clear enough.

Now, the coefficient $\mathcal{C}_{l,m_1,m_2,s}$ can be related to $\mathcal{A}_{l,m_1,m_2,p}$ by setting equal order to order the right-hand side of equations (27) and (30), i.e.

$$(2\mathrm{i}kr)^l \sum_{s=0}^{\infty} \mathcal{B}_{l,m_1,m_2,s} (2\mathrm{i}kr)^s = (2\mathrm{i}kr)^{\frac{m_1+m_2}{2}} \sum_{q=0}^{\infty} \mathcal{A}_{l,m_1,m_2,q} (2\mathrm{i}kr)^q \tag{32}$$

where we have factored the exponential e^{-ikr}. The equation (32) can be satisfied only if the following condition is fulfilled:

$$l + s = \frac{m_1 + m_2}{2} + q \tag{33}$$

and the coefficients $\mathcal{B}_{l,m_1,m_2,s}$ and $\mathcal{A}_{l,m_1,m_2,q}$ are related as follows:

$$\mathcal{B}_{l,m_1,m_2,s} \equiv \sum_{q=0}^{s} \frac{(i\alpha + l + q + 1)_{s-q}}{(s-q)!\,(2\,(l+q)+2)_{s-q}} \mathcal{C}_{l,m_1,m_2,q} = \mathcal{A}_{l,m_1,m_2,l-\frac{m_1+m_2}{2}+s}. \tag{34}$$

This equation defines $\mathcal{C}_{l,m_1,m_2,s}$ in terms of $\mathcal{A}_{l,m_1,m_2,q}$ for each s. To obtain $\mathcal{C}_{l,m_1,m_2,q}$ we have to invert the sum upon q in the last equation taking into account that equation (33) should be fulfilled. Using the relations

$$\sum_{q=0}^{s} d_{sq} C_q = A_s \qquad C_s = \frac{1}{d_{ss}} \left[A_s - \sum_{q=0}^{s-1} d_{sq} C_q \right] \qquad s \geqslant 1$$

the series which appear in the equation (34) can be inverted taking into account that $C_0 = A_0$.

Thus, $\mathcal{C}_{l,m_1,m_2,s}$ reads

$$\mathcal{C}_{l,m_1,m_2,s} = \mathcal{A}_{l,m_1,m_2,l-\frac{m_1+m_2}{2}+s} - \sum_{q=0}^{s-1} \frac{(i\alpha + l + q + 1)_{s-q}}{(s-q)!\,(2\,(l+q)+2)_{s-q}} \mathcal{C}_{l,m_1,m_2,q} \tag{35}$$

for $s \geqslant 1$.

With the definition obtained for the coefficient $\mathcal{C}_{l,m_1,m_2,s}$, we can finally write $\Delta_{m_1,m_2}(\alpha,\beta)$ in the following form:

$$\Delta_{m_1,m_2}(\alpha,\beta) = \sum_{l=0}^{\infty}\sum_{s=0}^{\infty} \mathcal{C}_{l,m_1,m_2,s} e^{-ikr}(2kr)^{l+s}\ F\left[\begin{matrix} i\alpha + l + s + 1 \\ 2\,(l+s)+2 \end{matrix}, 2ikr\right] Y_l^{\frac{m_1+m_2}{2}}. \tag{36}$$

In this way, we have written $\Delta_{m_1,m_2}(\alpha,\beta)$ in terms of the spherical solution of the Coulomb problem. In the next section, we shall study the particular cases discussed in the previous section. To perform the analysis it will be convenient to introduce alternative expressions of $\Delta_{m_1,m_2}(\alpha,\beta)$ which result from using equation (26). Applying it to equation (36) we obtain

$$\Delta_{m_1,m_2}(\alpha,\beta) = \sum_{l=0}^{\infty} e^{-ikr}(2kr)^{l}\ F\left[\begin{matrix} i\alpha + l + 1 \\ 2l+2 \end{matrix}, 2ikr\right] \sum_{s=0}^{l} \mathcal{C}_{S,m_1,m_2,l-s} Y_S^{\frac{m_1+m_2}{2}} \tag{37}$$

or

$$\Delta_{m_1,m_2}(\alpha,\beta) = \sum_{s=0}^{\infty} e^{-ikr}(2kr)^{s}\ F\left[\begin{matrix} i\alpha + s + 1 \\ 2s+2 \end{matrix}, 2ikr\right] \sum_{l=0}^{s} \mathcal{C}_{s-l,m_1,m_2,l} Y_{s-l}^{\frac{m_1+m_2}{2}}. \tag{38}$$

4. The particular cases

In this section we show that the basis element $\Delta_{m_1,m_2}(\alpha,\beta)$ given by equation (36) reduces to the well known partial wave series expansion for the scattering Coulomb cases. We shall give expressions for the general Coulomb case and we shall also give some comments for the Φ_2 case mentioned in section 2.

4.1. The scattering Coulomb case

As we discussed before, the scattering Coulomb case results from $\Delta_{m_1,m_2}(\alpha,\beta)$ by choosing $m_1 = m_2 = \beta = 0$ (see equation (9)). Under this conditions the relation given by equation (33) reduces to $l + s = q$. The indices l and q run from zero to ∞, and then s must be given by $q - s$. Besides this condition, the coefficients $\mathcal{C}_{l,0,0,s}$ and $\mathcal{A}_{l,0,0,q}$ should satisfy normalization relations

$$\mathcal{C}_{l,0,0,0} = \mathcal{A}_{l,0,0,l} = \frac{4\pi N_{l,0}}{\Gamma(1-\mathrm{i}\alpha)} \frac{\Gamma(1-\mathrm{i}\alpha+l)}{\Gamma(1-\mathrm{i}\alpha)\,\Gamma(2l+2)} \tag{39}$$

and then

$$\mathcal{C}_{l,0,0,s} = \mathcal{A}_{l,0,0,l+s} - \sum_{q=0}^{s-1} \frac{(\mathrm{i}\alpha+l+q+1)_{s-q}}{(s-q)!\,(2(l+q)+2)_{s-q}} \mathcal{C}_{l,0,0,q}. \tag{40}$$

It is easy to see that the coefficients $\mathcal{C}_{l,0,0,s}$ contribute to the double series of equation (36) only when $s = 0$. For s different from zero, $\mathcal{C}_{l,0,0,s}$ is given by

$$\mathcal{C}_{l,0,0,s} = \mathcal{A}_{l,0,0,l+s} - \frac{(\mathrm{i}\alpha+l+1)_s}{s!\,(2l+2)_s} \mathcal{C}_{l,0,0,0}. \tag{41}$$

We can verify that both terms of the right-hand side of the last equation add to zero except for $s = 0$. The previous analysis allow us to write the following expression for the wavefunction $\Delta_{0,0}(\alpha, 0)$:

$$\begin{aligned}\Delta_{0,0}(\alpha,0) = {} & \frac{1}{\Gamma(1-\mathrm{i}\alpha)} \sum_{l=0}^{\infty} (2l+1) \frac{\Gamma(1-\mathrm{i}\alpha+l)}{\Gamma(2l+2)} \mathrm{e}^{-\mathrm{i}kr} (2kr)^l \\ & \times F\left[\begin{matrix}\mathrm{i}\alpha+l+1\\ 2l+2\end{matrix}, 2\mathrm{i}kr\right] P_l(\cos\theta)\end{aligned} \tag{42}$$

which is the well known partial wave expansion for the scattering Coulomb function, apart from a normalization factor.

4.2. The general Coulomb function

As we showed in section 2, the general Coulomb wavefunction results for $\beta = 0$ and $m_1 = m_2 = m$ (see equations (9) and (12)). The study of this case can be performed using the partial wave expansion of equation (37).

Note from equation (12) that the radial part of $\Delta_{m,m}(\alpha, 0)$ is given by $R^-_{k,l}$, equation (17), i.e. by the radial Coulomb eigenfunction. However, the angular part is given by the sum of different angular eigenfunctions Y^m_S. Nevertheless, this is just a consequence of the general character of the equations (36)–(38). After replacing the constraints $\beta = 0$ and $m_1 = m_2 = m$ in equation (37), and analysing the obtained result we can see that it simplifies considerably. A careful study of the coefficient $\mathcal{C}_{s,m,m,l-s}$ shows us that only for $s = l$ is it different from zero, and in this case it reduces to $\mathcal{C}_{l,m,m,0} = \mathcal{A}_{l,m,m,l-m}$. Then, the function $\Delta_{m,m}(\alpha, 0)$ becomes the partial wave series expansion as intuitively expected:

$$\Delta_{m,m}(\alpha,0) = \sum_{l=0}^{\infty} \mathcal{A}_{l,m,m,l-m}\, \mathrm{e}^{-\mathrm{i}kr} (2kr)^l\; F\left[\begin{matrix}\mathrm{i}\alpha+l+1\\ 2l+2\end{matrix}, 2\mathrm{i}kr\right] Y^m_l \tag{43}$$

that is, a series expansion over the whole spherical Coulomb base. $\Delta_{m,m}(\alpha, 0)$ results in a series over all the possible values of l for a fixed value of m, similar to that obtained for the scattering case.

The case of the Φ_2 function introduces a further complication. We recall that to reduce the $\Delta_{m_1,m_2}(\alpha, \beta)$ function to the Φ_2 case we should set $\beta = m_2 = 0$ and $m_1 = 2m$. This introduces an asymmetric behaviour in the m indexes and we have not obtained a simple enough expression for the partial wave expansion of the Φ_2 function.

5. Conclusions and outlook

The generalization of the two-body Coulomb wavefunction called $\Delta_{m_1,m_2}(\alpha, \beta)$ has been studied. The Coulomb scattering, the general Coulomb problem and the so-called Φ_2 approach were shown as limit cases of $\Delta_{m_1,m_2}(\alpha, \beta)$. This function can be considered as a generalized basis element for the expansion of three-body continuum wavefunctions.

We have proposed a partial wave expansion of these basis elements in terms of the spherical solutions of the two-body Coulomb problem. The obtained functions are regular in the whole coordinate space. We should note that the asymptotic behaviour described in section 2 is preserved after the partial wave expansion of $\Delta_{m_1,m_2}(\alpha, \beta)$.

We have also obtained some particular cases. When $m_1 = m_2 = 0$ and $\beta = 0$, the $\Delta_{m_1,m_2}(\alpha, \beta)$ base leads to the well known partial wave series expansion for the scattering Coulomb problem. Besides, by setting $m_1 = m_2 = m$ and $\beta = 0$, the $\Delta_{m,m}(\alpha, 0)$ function represents a partial wave expansion of the two-body Coulomb problem with the magnetic number different from zero. For this situation we have shown that only a series in the angular momentum remains and that this is upon the expected spherical harmonic angular eigenfunctions with the same magnetic number. The partial wave series expansion which results when $m_1 = 2m$ and $m_2 = \beta = 0$, which define the Φ_2 limit, could not be cast in a simple form.

The expansions obtained here can help us to understand the physical aspects of the wavefunctions such as the Φ_2 three-body wavefunction or the Φ one. The physical conditions such as the Kato´s ones and the united atom are fundamental in the calculation of cross sections for different atomic processes [25, 26]. A partial wave expansion can be useful to elucidate how these constraints effectively contribute to the cross sections.

On the other hand, these expansions would enable us go beyond the effective charge approximation in the computation of cross sections in atomic collisions. To this end we could replace the Coulomb interaction potentials of the Hamiltonian by some model approximations that take into account the effect of passive electrons in most of the atomic species. This kind of potential has spherical symmetry and then the angular part of its solutions remains unaltered. A partial wave expansion of the solution of these potentials is achieved simply by replacing the radial part of the partial wave expansion. Furthermore, a partial wave series expansion for the Φ, as described in the introduction, can be easily improved. The general solution of a static potential with the magnetic number different from zero can be used as a sort of $\Delta_{m_1,m_2}(\alpha, \beta)$ base. The radial solution of this two-body potential can be numerically solved in general and for some particular cases a closed-form solution can be found [27].

Appendix

In this appendix we shall obtain an expression for the coefficient $\tilde{a}_{l,m_1,m_2,q,p}$, equation (22), of the expansion given by equation (21). After projecting the left-hand side of equation (21) upon the Y_l^m basis and integrating over θ and ϕ we obtain

$$\tilde{a}_{l,m_1,m_2,q,p} = \int \mathrm{d}\Omega\ (1+\cos\theta)^{\frac{m_1}{2}+p}\,(1-\cos\theta)^{\frac{m_2}{2}+q}\,\mathrm{e}^{\mathrm{i}\left(\frac{m_1+m_2}{2}\right)\phi}\left(Y_l^m\right)^* \qquad (44)$$

that, after performing the integral in the angle ϕ and in terms of the associated Legendre functions results in

$$\tilde{a}_{l,m_1,m_2,q,p} = (-1)^{\frac{m_1+m_2}{2}} (2\pi)\, N_{l,\frac{m_1+m_2}{2}} \int_{-1}^{1} \mathrm{d}x\ (1+x)^{\frac{m_1}{2}+p} (1-x)^{\frac{m_2}{2}+q} P_l^{-\frac{m_1+m_2}{2}}(x) \tag{45}$$

where the change of variables $x = \cos\theta$ have been made. The constant $N_{l,\frac{m_1+m_2}{2}}$ is given by

$$N_{l,\frac{m_1+m_2}{2}} = (-1)^{\frac{m_1+m_2}{2}} \left[\frac{(2l+1)}{4\pi} \frac{\left(l-\frac{m_1+m_2}{2}\right)!}{\left(l+\frac{m_1+m_2}{2}\right)!} \right]^{\frac{1}{2}}. \tag{46}$$

Now, using the relation [22],

$$P_l^m(x) = \frac{\Gamma(l+m+1)}{\Gamma(l-m+1)} P_l^{-m}(x) \qquad m \in \text{integer} \tag{47}$$

we can rewrite $\tilde{a}_{l,m_1,m_2,q,p}$ as follows:

$$\tilde{a}_{l,m_1,m_2,q,p} = (-1)^{\frac{m_1+m_2}{2}} (2\pi)\, N_{l,\frac{m_1+m_2}{2}} \frac{\Gamma\left(l-\frac{m_1+m_2}{2}+1\right)}{\Gamma\left(l+\frac{m_1+m_2}{2}+1\right)} \times \int_{-1}^{1} \mathrm{d}x\, (1+x)^{\frac{m_1}{2}+p} (1-x)^{\frac{m_2}{2}+q} P_l^{\frac{m_1+m_2}{2}}(x). \tag{48}$$

The integral that appears in the last equation is of the kind

$$J = \int_{-1}^{1} (1+x)^{\alpha-1} (1-x)^{\beta-1} P_\nu^\mu(x)\, \mathrm{d}x. \tag{49}$$

The result of this integral is incorrectly quoted in [24]. However, it can be performed straightforwardly using the Gauss representation for the $P_\nu^\mu(x)$, valid for $\mu = 0, 1, 2 \ldots$:

$$P_\nu^\mu(x) = (-1)^{\frac{\mu}{2}} \frac{\Gamma(\nu+\mu+1)}{\mu!\Gamma(\nu-\mu+1)} 2^{-\mu} (1+x)^{\frac{\mu}{2}} (1-x)^{\frac{\mu}{2}} F\left[\begin{matrix} 1+\mu+\nu & \mu-\nu \\ & 1+\mu \end{matrix}, \frac{1-x}{2} \right] \tag{50}$$

where the function $F\left[\begin{matrix} a & b \\ & c \end{matrix}, z\right]$ represents the Gauss hypergeometric function. Replacing equation (50) in equation (49) we obtain

$$J = (-1)^{\frac{\mu}{2}} \frac{\Gamma(\nu+\mu+1)}{\mu!\Gamma(\nu-\mu+1)} 2^{-\mu} \times \int_{-1}^{1} (1+x)^{\alpha+\frac{\mu}{2}-1} (1-x)^{\beta+\frac{\mu}{2}-1} F\left[\begin{matrix} 1+\mu+\nu & \mu-\nu \\ & 1+\mu \end{matrix}, \frac{1-x}{2} \right] \mathrm{d}x. \tag{51}$$

Introducing the change of variable $u = \frac{(1-x)}{2}$, J results as

$$J = (-1)^{\frac{\mu}{2}} \frac{2^{\alpha+\beta-1}\Gamma(\nu+\mu+1)}{\Gamma(\mu+1)\Gamma(\nu-\mu+1)} \times \int_{0}^{1} (1-u)^{\alpha+\frac{\mu}{2}-1} u^{\beta+\frac{\mu}{2}-1} F\left[\begin{matrix} 1+\mu+\nu & \mu-\nu \\ & 1+\mu \end{matrix}, u \right] \mathrm{d}u. \tag{52}$$

The integral that appears in the last equation can be performed [24], and then we finally obtain

$$J = (-1)^{\frac{\mu}{2}} 2^{\alpha+\beta-1} \frac{\Gamma(\nu+\mu+1)\Gamma\left(\beta+\frac{\mu}{2}\right)\Gamma\left(\alpha+\frac{\mu}{2}\right)}{\Gamma(\mu+1)\Gamma(\nu-\mu+1)\Gamma(\alpha+\beta+\mu)} \times F\left[\begin{matrix} \beta+\frac{\mu}{2} & \mu-\nu & \mu+\nu+1 \\ & 1+\mu & \alpha+\beta+\mu \end{matrix}, 1 \right]. \tag{53}$$

The function $F\left[\begin{matrix} a & b & c \\ & d & f \end{matrix}, z\right]$ represents the generalized hypergeometric function [22].

With the obtained result for J we can finally write an expression for the integral of the equation (48); choosing

$$\alpha = \frac{m_1}{2} + p + 1 \qquad \beta = \frac{m_2}{2} + q + 1 \tag{54}$$

$$\nu = l \qquad \mu = \frac{m_1 + m_2}{2} \tag{55}$$

we obtain

$$\begin{aligned} J = {} & (-1)^{\frac{m_1+m_2}{4}} \, 2^{\frac{m_1+m_2}{2}+p+q+1} \\ & \times \frac{\Gamma\left(l + \frac{m_1+m_2}{2} + 1\right)\Gamma\left(\frac{m_2}{2} + q + 1 + \frac{m_1+m_2}{4}\right)\Gamma\left(\frac{m_1}{2} + p + 1 + \frac{m_1+m_2}{4}\right)}{\Gamma\left(\frac{m_1+m_2}{2} + 1\right)\Gamma\left(l - \frac{m_1+m_2}{2} + 1\right)\Gamma\left(m_1 + m_2 + p + q + 2\right)} \\ & \times F\left[\begin{matrix} \frac{m_2}{2} + q + 1 + \frac{\frac{m_1+m_2}{2}}{2} & \frac{m_1+m_2}{2} - l & \frac{m_1+m_2}{2} + l + 1 \\ 1 + \frac{m_1+m_2}{2} & \frac{m_1}{2} + p + 1 + \frac{m_2}{2} + q + 1 + \frac{m_1+m_2}{2} & \end{matrix}, 1\right]. \end{aligned} \tag{56}$$

Finally the coefficient $\tilde{a}_{l,m_1,m_2,q,p}$ can be written as

$$\begin{aligned} \tilde{a}_{l,m_1,m_2,q,p} = {} & \pi \, (-1)^{\frac{3(m_1+m_2)}{4}} \, 2^{\frac{m_1+m_2}{2}+p+q+2} N_{l,\frac{m_1+m_2}{2}} \\ & \times \frac{\Gamma\left(q + 1 + \frac{m_1+3m_2}{4}\right)\Gamma\left(p + 1 + \frac{3m_1+m_2}{4}\right)}{\Gamma\left(\frac{m_1+m_2}{2} + 1\right)\Gamma\left(m_1 + m_2 + p + q + 2\right)} \\ & \times F\left[\begin{matrix} q + 1 + \frac{m_1+3m_2}{4} & \frac{m_1+m_2}{2} - l & \frac{m_1+m_2}{2} + l + 1 \\ 1 + \frac{m_1+m_2}{2} & m_1 + m_2 + p + q + 2 & \end{matrix}, 1\right]. \end{aligned} \tag{57}$$

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