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Multipole expansions and Fock symmetry of the hydrogen atom

A V Meremianin[1,2] **and J-M Rost**[1]

[1] Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187, Dresden, Germany
[2] REC-010, Voronezh State University, 394006, Voronezh, Russia

E-mail: avm@pks.mpg.de and rost@pks.mpg.de

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Abstract

The main difficulty in utilizing the $O(4)$ symmetry of the hydrogen atom in practical calculations is the dependence of the Fock stereographic projection on energy. This is due to the fact that the wavefunctions of the states with different energies are proportional to the hyperspherical harmonics (HSH) corresponding to different points on the hypersphere. Thus, the calculation of the matrix elements reduces to the problem of re-expanding HSH in terms of HSH depending on different points on the hypersphere. We solve this problem by applying the technique of multipole expansions for four-dimensional HSH. As a result, we obtain the multipole expansions whose coefficients are the matrix elements of the boost operator taken between hydrogen wavefunctions (i.e., hydrogen form factors). The explicit expressions for those coefficients are derived. It is shown that the hydrogen matrix elements can be presented as derivatives of an elementary function. Such an operator representation is convenient for the derivation of recurrence relations connecting matrix elements between states corresponding to different values of the quantum numbers n and l.

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1. Introduction

About 70 years ago, Fock in his paper [1] demonstrated that the wavefunctions of the hydrogen atom in momentum representation are proportional to the four-dimensional hyperspherical harmonics (HSH). From the point of view of the group theory, it means that the hydrogen wavefunctions possess the $O(4)$ symmetry. The source of this remarkable property of the quantum two-body Coulomb problem lies in the presence of an additional conserving vector quantity—the Laplace–Runge–Lenz operator.

The applications of the Fock's method to various problems of quantum mechanics are very extensive. Lieber used it to calculate the Lamb shift in the hydrogen atom [2]. Group-theoretical properties of $O(4)$ symmetry of the hydrogen atom have been analysed in [3]. Schwinger [4] showed that the hydrogen Green function can be presented in a simple form as the series of four-dimensional hyperspherical harmonics. Fock's method has been used for the calculation of the retardation effects in two-photon bound–bound transitions [5]. The four-dimensional HSH can be chosen as a Sturmian basis set in the many-centre Coulomb problem [6–18]. Recently, the Fock's projection method has been applied to the theory of anisotropic excitons, see [19].

As was pointed by Lieber [2], the main difficulty in applying Fock's symmetry to the specific problems is the dependence of the arguments of HSH on the energy. This prohibits the direct application of the Wigner–Eckart theorem to the calculation of matrix elements between different states of the two-body Coulomb system. Often, this problem can be avoided by using the above-mentioned set of Sturmian functions. Those functions (denoted sometimes as 'Sturmians') have the same form as the bound-state wavefunctions of the hydrogen atom whose arguments are chosen to be equal. Thus, it is possible to apply the technique of the angular momentum theory to the calculation of integrals involving Sturmian functions which belong to the same set [8, 20].

If one needs to calculate integrals between Sturmians from different sets, there appears the same problem as in the calculation of integrals involving hydrogen wavefunctions with different energies. Namely, the Wigner–Eckart theorem can be applied only for integrals containing HSH whose arguments correspond to the same point on the hypersphere. However, hydrogen wavefunctions with *different* energies (or Sturmians from different sets) correspond to *different* points on the hypersphere. In this paper, we show that this problem can be solved using the multipole expansion theorems for four-dimensional HSH. Mathematically, we have derived the connection between sets of HSH corresponding to different stereographic projections. That is, HSH depending on some point of the hypersphere can be presented as a series of HSH depending on some other point which corresponds to the different stereographic projection of the three-dimensional space onto the four-dimensional hypersphere. The coefficients in those expansions are, in fact, the form-factors of the hydrogen atom.

The form-factor integrals are also known as 'generalized oscillator strengths' (GOS). GOS play an important role in the theory of collisions of fast particles with atoms and molecules. Starting from the pioneering work by Bethe [21], there is a large number of papers addressing the properties of GOS of the hydrogen atom (see review [22]). In the book [23], the compact expressions for GOS corresponding to the transitions from 1s and 2s to n, l states are given. The hydrogenic form factors for transitions between arbitrary bound states were presented in [24] in terms of combinations of hypergeometric functions of two variables. The integrals between the hydrogen wavefunctions and the operator of the electromagnetic interaction have been calculated in [25] using the set of parabolic coordinates. The expressions for the bound-free matrix elements for the hydrogen atom may be found, e.g. in [26, 27]. In all above works, the calculations have been performed by means of straightforward evaluation of the three-dimensional integrals in spherical or parabolic coordinates.

Below we demonstrate that the hydrogen form-factor integrals can be explicitly calculated *without* evaluating any integrals. Our approach is based solely on the addition theorems for four-dimensional HSH which have been derived using the differential technique [28]. As a result, we can write the hydrogen form-factor integrals as a combination of multipole terms (they are equivalent to the radial integrals). Each multipole term can be presented in a compact closed form containing derivatives of some elementary function. This differential representation is very convenient for analysing various properties of the integrals such as their

asymptotic behaviour. Moreover, using the differential representations we have derived a number of recursion relations connecting radial integrals corresponding to different values of their indices.

The paper is organized as follows. In section 2, we consider the connection between matrix elements in coordinate and momentum representations as well as the general properties of the stereographic projection. The expression for the matrix element of the boost operator in terms of HSH is derived in section 2.1. We demonstrate that the calculation of the form-factor integral reduces to the problem of the derivation of a certain multipole expansion for the product of HSH with some scalar function. Then, in section 2.2, we use Fock's method of stereographic projections in order to analyse the properties of the function whose multipole expansion has to be derived.

In section 3, we calculate such multipole expansion. First, in section 3.1, the multipole expansion is derived in the tensor form, i.e. as a tensor product of HSH. Next, in section 3.2, we calculate the multipole coefficients explicitly. In section 4, the properties of the matrix elements are considered regarding the expressions for the multipole coefficients. In section 4.2, the dipole limit of the matrix elements is analysed in detail. Some concluding remarks are given in section 5. Appendix A contains the calculation of summations arising in the course of computation of the multipole coefficients. In appendix B, we derive explicit expressions for the multipole coefficients. Recurrence relations for the multipole coefficients are considered in appendix D.

Below we use bold font letters such as $\mathbf{p}, \mathbf{k}$ to denote vectors in four-dimensional space. For unit vectors in that space the hat is used, e.g. $\hat{\mathbf{x}}, \hat{\mathbf{y}}$. Three-dimensional vectors are denoted as $\vec{p}, \vec{k}$, etc.

2. Stereographic projections and matrix elements

In this section, we present the relation between hydrogen wavefunction in coordinate and momentum representations. This is done in section 2.1 where the expression for the matrix element of the boost operator in terms of HSH is also derived. Next, in section 2.2, we discuss the general properties of the Fock's stereographic mappings corresponding to HSH entering the form-factor integral.

2.1. The matrix elements in the momentum space

The hydrogen wavefunction in momentum representation $\psi_{nlm}(\vec{p})$ is defined as the Fourier transform of the wavefunction in coordinate representation,

$$\begin{aligned}\psi_{nlm}(\vec{p}) &= \frac{1}{(2\pi)^{3/2}}\int \mathrm{e}^{-\mathrm{i}\vec{p}\cdot\vec{r}}\,\psi_{nlm}(\vec{r})\,\mathrm{d}\vec{r},\\ \psi_{nlm}(\vec{r}) &= \frac{1}{(2\pi)^{3/2}}\int \mathrm{e}^{\mathrm{i}\vec{p}\cdot\vec{r}}\,\psi_{nlm}(\vec{p})\,\mathrm{d}\vec{p},\end{aligned} \tag{1}$$

where n is the principal quantum number, l, m are the angular momentum quantum numbers, $l = 0, 1, \ldots, n-1$ and $m = -l, -l+1, \ldots, l$. The explicit expression for the wavefunction in momentum space has the form [1]

$$\psi_{nlm}(\vec{p}) = \frac{4\beta^{5/2}}{(\beta^2 + (\vec{p})^2)^2} Y_{n-1lm}(\hat{\mathbf{y}}), \qquad \beta = Z/n. \tag{2}$$

Here, $Y_{n-1lm}(\hat{\mathbf{y}})$ is the four-dimensional HSH and $\hat{\mathbf{y}}$ is the unit 4-vector whose components are defined by

$$\hat{\mathbf{y}} = \left(\frac{2\beta\vec{p}}{\beta^2 + (\vec{p})^2}, \frac{\beta^2 - (\vec{p})^2}{\beta^2 + (\vec{p})^2} \right). \tag{3}$$

Functions Y_{nlm} are normalized to the unity:

$$\int Y^*_{nlm}(\hat{\mathbf{y}}) Y_{n'l'm'}(\hat{\mathbf{y}})\, \mathrm{d}\Omega_{\mathbf{y}} = \delta_{n,n'}\delta_{l,l'}\delta_{m,m'}. \tag{4}$$

Here, it is supposed that the parameters β entering the definition of $\hat{\mathbf{y}}$ do not depend on indices n, n'. The connection of the surface element of the four-dimensional hypersphere $\mathrm{d}\Omega$ with the three-dimensional volume element $\mathrm{d}\vec{p}$ has the form

$$\mathrm{d}\Omega_{\mathbf{y}} = \left(\frac{2\beta}{\beta^2 + (\vec{p})^2} \right)^3 \mathrm{d}\vec{p}. \tag{5}$$

Note that, in the case of hydrogen, the vector $\hat{\mathbf{y}}$ depends on the rank n of HSH (see definition (2) of the parameter β). The dependence of β on the principal quantum number n explains why the orthogonality relations cannot be directly applied to the calculation of matrix elements.

We remark that the method of Sturmian functions has found wide use in various problems of the quantum chemistry and the theory of interaction of photons with atoms and molecules. In contrast to the set of the bound-state wavefunctions of the hydrogen atom, the set of Sturmian functions is complete. Sturmians in momentum representation are defined by equation (2) in which β must be a fixed number independent of n. Thus, the parameter β is the same for every function from the same Sturmian set.

In many problems of the collision theory it is necessary to calculate the form-factor integral,

$$F(\vec{k}) = \int \psi^*_{n_f}(\vec{r})\, \mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{r}} \psi_{n_i}(\vec{r})\, \mathrm{d}\vec{r}, \tag{6}$$

where, for the sake of shortness, we have omitted the angular momentum indices which are $l'm'$ and lm for the final and initial states n_f and n_i, respectively. Using equations (1), the matrix element $F(\vec{k})$ can be expressed in terms of momentum space functions $\psi(\vec{p})$ as

$$F(\vec{k}) = \frac{1}{(2\pi)^3} \int \mathrm{d}\vec{r} \int \mathrm{d}\vec{p}_1 \int \mathrm{d}\vec{p}_2 \psi^*_{n_f}(\vec{p}_1)\, \mathrm{e}^{-\mathrm{i}\vec{p}_1\cdot\vec{r}}\, \mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{r}} \psi_{n_i}(\vec{p}_2)\, \mathrm{e}^{\mathrm{i}\vec{p}_2\cdot\vec{r}}. \tag{7}$$

Using the definition of the three-dimensional Dirac δ-function, one can evaluate integrals over $\vec{p}_2$ and $\vec{r}$ in closed form which yields

$$F(\vec{k}) = \int \psi^*_{n_f}(\vec{p}) \psi_{n_i}(\vec{p} - \vec{k})\, \mathrm{d}\vec{p}. \tag{8}$$

Using explicit expressions (2) and (5) for the wavefunctions and introducing the indices $n = n_i - 1$ and $n' = n_f - 1$, the form factor becomes

$$F(\vec{k}) \equiv F_{n'l',nl} = \frac{2\alpha^{5/2}}{\beta^{1/2}} \int Y^*_{n'l'm'}(\hat{\mathbf{y}}) \frac{\beta^2 + (\vec{p})^2}{(\alpha^2 + (\vec{p} - \vec{k})^2)^2} Y_{nlm}(\hat{\mathbf{x}})\, \mathrm{d}\Omega_{\mathbf{y}}, \tag{9}$$

where the parameters α and β have the form

$$\alpha = \frac{Z}{n_i} = \frac{Z}{n+1}, \qquad \beta = \frac{Z}{n_f} = \frac{Z}{n'+1}, \tag{10}$$

and the components of the unit vector $\hat{\mathbf{x}}$ are defined by

$$\hat{\mathbf{x}} = \left(\frac{2\alpha(\vec{p} - \vec{k})}{\alpha^2 + (\vec{p} - \vec{k})^2}, \frac{\alpha^2 - (\vec{p} - \vec{k})^2}{\alpha^2 + (\vec{p} - \vec{k})^2} \right). \tag{11}$$

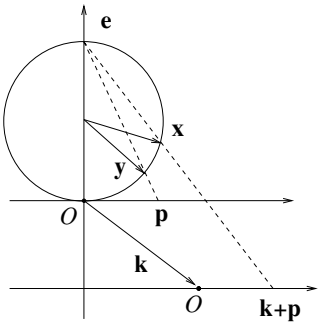

Figure 1. The cut through the four-dimensional hypersphere. The three-dimensional $\vec{p}$-space corresponds to the horizontal axes. The vertical z_0-axis (the energy axis) is denoted as **e**, the point O corresponds to the origin, $\vec{p} = 0$. The point $\hat{\mathbf{x}}$ on the hypersphere is the stereographic projection of the point **p** shifted by the vector **k**.

2.2. The properties of the stereographic projection

The geometrical meaning of the unit vectors $\hat{\mathbf{y}}$ and $\hat{\mathbf{x}}$ in equation (9) and their connection to the three-dimensional vectors $\vec{p}$ and $\vec{k}$ is demonstrated in figure 1. It is seen that there is a one-to-one correspondence between the three-dimensional space of vectors $\vec{p}$ and the unit four-dimensional hypersphere. Namely, every point $\hat{\mathbf{x}}$ on the hypersphere corresponds to only one vector $\vec{p}$ and vice versa. This $\hat{\mathbf{x}} \leftrightarrow \vec{p}$ mapping is called stereographic projection of the hyperplane (which is, in fact, the whole three-dimensional space) on the hypersphere of unit radius.

As follows from equation (9), in order to calculate the form-factor integral one has to expand the product

$$\frac{\beta^2 + (\vec{p})^2}{(\alpha^2 + (\vec{p} - \vec{k})^2)^2} Y_{nlm}(\hat{\mathbf{x}}) \tag{12}$$

in terms of HSH depending on the vector $\hat{\mathbf{y}}$. When done so, the integral $F(\vec{k})$ calculates trivially using the orthogonality property of HSH.

As a preliminary, we note that vectors $\hat{\mathbf{y}}$ and $\hat{\mathbf{x}}$ can be re-written in the compact form as

$$\hat{\mathbf{x}} = -\mathbf{e} + 2\alpha \frac{\mathbf{q}}{q^2}, \qquad \hat{\mathbf{y}} = -\mathbf{e} + 2\beta \frac{\mathbf{p}}{p^2}, \qquad \mathbf{q} = \mathbf{p} - \mathbf{k} \tag{13}$$

where **e** is the unit vector with components $\mathbf{e} = (0, 0, 0, 1)$ and 4-vectors **p** and **k** are defined by

$$\mathbf{p} = (\vec{p}, \beta), \qquad \mathbf{k} = (\vec{k}, \beta - \alpha). \tag{14}$$

With new notation, expression (9) for the form-factor integral assumes the form

$$F_{n'l',nl} = \frac{2\alpha^{5/2}}{\beta^{1/2}} \int Y^*_{n'l'm'}(\hat{\mathbf{y}}) \frac{p^2}{q^4} Y_{nlm}(\hat{\mathbf{x}})\, \mathrm{d}\Omega_{\mathbf{y}}. \tag{15}$$

Below, for simpler presentation, we will use the renormalized HSH $C_n(\hat{\mathbf{y}})$ connected to the normalized HSH by $C_{nlm}(\hat{\mathbf{y}}) = (-1)^{n-l}\sqrt{2\pi^2/(n+1)}Y_{nlm}(\hat{\mathbf{y}})$. We will also omit the projection indices l, m in the notation of HSH C_n, as far this will not lead to misunderstandings.

The possibility of the efficient use of the multipole expansion technique for the calculation of integrals stems from the surprising fact that both the products $p^{-2}C_n(\hat{\mathbf{y}})$ and $|\mathbf{p}-\mathbf{k}|^{-2}C_n(\hat{\mathbf{x}})$ satisfy the four-dimensional Laplace equation with respect to the vector $\mathbf{p}$. Namely,

$$\Delta_{\mathbf{p}}\frac{1}{p^2}C_n(\hat{\mathbf{y}}) = \left(\Delta_{\vec{p}} + \frac{\partial^2}{\partial p_0^2}\right)\frac{1}{p^2}C_n(\hat{\mathbf{y}}) = 0, \qquad \Delta_{\mathbf{p}}\frac{1}{|\mathbf{p}-\mathbf{k}|^2}C_n(\hat{\mathbf{x}}) = 0, \tag{16}$$

where the vector $\mathbf{p}$ has the components $\mathbf{p} = (\vec{p}, p_0)$ and the unit vectors $\hat{\mathbf{y}}$ and $\hat{\mathbf{x}}$ are defined by equations (13) in which β and α are constants. Note that equations (16) are valid for arbitrary values of $\mathbf{k}$.

Equations (16) can be proved using the multipole expansions formula derived in [28]:

$$\frac{1}{p^2}C_n(\hat{\mathbf{y}}) = \frac{2^{n/2}}{p^2}\left\{-\mathbf{e} + 2\beta\frac{\mathbf{p}}{p^2}\right\}_n = \frac{1}{p^2}\sum_{n_1=0}^{n}\binom{n}{n_1}(-1)^{n-n_1}\left(\frac{2\beta}{p}\right)^{n_1}\{C_{n-n_1}(\mathbf{e})\otimes C_{n_1}(\hat{\mathbf{p}})\}_n. \tag{17}$$

Here, the curly brackets mean the four-dimensional tensor products of the rank n which is the generalization of the conventional three-dimensional tensor product [29, 30]. The product $p^{-n_1-2}C_{n_1}(\hat{\mathbf{p}})$ which occurs on the rhs of equation (17) is the irregular solution of the Laplace equation. Therefore, the action of the Laplace operator $\Delta_{\mathbf{p}}$ on equation (17) gives zero:

$$\Delta_{\mathbf{p}}\frac{1}{p^{n_1+2}}C_{n_1}(\hat{\mathbf{p}}) = 0. \tag{18}$$

This completes the proof of the first equation in (16). The second equation can be proved analogously noting that

$$\Delta_{\mathbf{p}}F(\mathbf{p}-\mathbf{k}) = \Delta_{\mathbf{q}}F(\mathbf{q}),$$

where F is an arbitrary function and $\mathbf{q} = \mathbf{p} - \mathbf{k}$.

As is seen from equation (16), it is convenient to work with the product $q^{-2}C_n(\hat{\mathbf{x}})$ rather than with $q^{-4}C_n(\hat{\mathbf{x}})$. In order to establish the connection between these two combinations, we employ the auxiliary identity

$$\frac{1}{q^4} = \frac{1+(\hat{\mathbf{x}}\cdot\mathbf{e})}{2\alpha^2}\frac{1}{q^2}$$

which can be proved by taking the square of the second equation in (13) and noting that $\mathbf{e}^2 = \hat{\mathbf{x}}^2 = 1$. Applying the Clebsch–Gordan expansion technique one can prove the relation

$$\begin{aligned}(\hat{\mathbf{x}}\cdot\mathbf{e})C_{nlm}(\hat{\mathbf{x}}) &= \tfrac{1}{\sqrt{2}}C_{100}(\hat{\mathbf{x}})C_{nlm}(\hat{\mathbf{x}}) \\ &= \tfrac{1}{\sqrt{2}}C^{(n-1)lm}_{100;nlm}C_{(n-1)lm}(\hat{\mathbf{x}}) + \tfrac{1}{\sqrt{2}}C^{(n+1)lm}_{100;nlm}C_{(n+1)lm}(\hat{\mathbf{x}}),\end{aligned} \tag{19}$$

where $C^{(n\pm1)lm}_{100;nlm}$ is the four-dimensional Clebsch–Gordan coefficient. At such particular values of parameters, the explicit expressions for those coefficients are given in [28]. As a result, the product $q^{-4}C_n(\hat{\mathbf{x}})$ can be written as

$$\begin{aligned}\frac{1}{q^4}C_{nlm}(\hat{\mathbf{x}}) = \frac{1}{2\alpha^2q^2}\Bigg(&C_{nlm}(\hat{\mathbf{x}}) + \frac{\sqrt{(n-l+1)(n+l+2)}}{2(n+1)}C_{(n+1)lm}(\hat{\mathbf{x}}) \\ &+ \frac{\sqrt{(n-l)(n+l+1)}}{2(n+1)}C_{(n-1)lm}(\hat{\mathbf{x}})\Bigg).\end{aligned} \tag{20}$$

Thus, the problem reduces to the calculation of the multipole decomposition of the function $q^{-2}C_n(\hat{\mathbf{x}})$. Once such a decomposition is known, the expression for the function $q^{-4}C_n(\hat{\mathbf{x}})$ can be derived using equation (20).

3. The multipole expansion of translated harmonics

In this section, we derive the expansion of the function $q^{-2}C_n(\hat{\mathbf{x}})$ in terms of HSH depending on the unit vector $\hat{\mathbf{y}}$. In section 3.1, the tensor form of the multipole expansion is derived by consequent application of the multipole series given in [28]. In section 3.2, the coefficients of that expansion are calculated in an explicit form.

3.1. The multipole expansion in terms of tensor products

As was noted above, it is sufficient to calculate the expansion of the product $q^{-2}C_n(\hat{\mathbf{x}})$. The calculations are performed in three steps. First, we expand the product $q^{-4}C_n(\hat{\mathbf{x}})$ in terms of HSH depending on the hyper-angles of the vector $\mathbf{q}$. Second, the resulting HSH is expanded in terms of HSH whose arguments are the hyper-angles of the four-dimensional momentum vector $\mathbf{p}$. The final, third, step is to expand HSH depending on $\mathbf{p}$ in terms of the HSH depending on the unit vector $\hat{\mathbf{y}}$. Clearly, at each step the series of irreducible tensor products of HSH will occur. However, as we will see below, only one of the three series is infinite. Further, the Clebsch–Gordan coefficients inherent to the irreducible tensor products arising during the computations have simple structure and can be written in a closed form.

We begin the calculations by using the expansion similar to equation (17),

$$\frac{1}{q^2}C_n(\hat{\mathbf{x}}) = \frac{1}{q^2}\sum_{n_1=0}^{n}\binom{n}{n_1}(-1)^{n-n_1}\left(\frac{2\alpha}{q}\right)^{n_1}\{C_{n-n_1}(\mathbf{e})\otimes C_{n_1}(\hat{\mathbf{q}})\}_n. \tag{21}$$

Now, we have to re-expand the function $q^{-n_1-2}C_{n_1}(\hat{\mathbf{q}})$ in terms of HSH depending on the vector $\mathbf{p}$. The use of the multipole expansion formula (equation (65) of [28]) yields

$$\frac{1}{q^{n_1+2}}C_{n_1}(\hat{\mathbf{q}}) = \sum_{n_2=0}^{\infty}\frac{k^{n_2}}{p^{n_1+n_2+2}}\binom{n_1+n_2+1}{n_2}\{C_{n_2}(\hat{\mathbf{k}})\otimes C_{n_1+n_2}(\hat{\mathbf{p}})\}_{n_1}. \tag{22}$$

Third, we have to go back from vectors $\mathbf{p}$ to vectors $\hat{\mathbf{y}}$. In order to do that we note that the terms containing vector $\mathbf{p}$ can be re-written as

$$\frac{1}{p^{n_1+n_2}}C_{n_1+n_2}(\hat{\mathbf{p}}) = \frac{2^{(n_1+n_2)/2}}{p^{2n_1+2n_2}}\{\mathbf{p}\}_{n_1+n_2} = 2^{(n_1+n_2)/2}\left\{\frac{\mathbf{p}}{p^2}\right\}_{n_1+n_2}. \tag{23}$$

The connection (13) between vectors $\mathbf{p}$ and $\hat{\mathbf{y}}$ leads to the chain of equations

$$\begin{aligned}2^{(n_1+n_2)/2}\left\{\frac{\mathbf{p}}{p^2}\right\}_{n_1+n_2} &= \frac{1}{(\sqrt{2}\beta)^{n_1+n_2}}\{\mathbf{e}+\hat{\mathbf{y}}\}_{n_1+n_2}\\ &= \frac{1}{(2\beta)^{n_1+n_2}}\sum_{n_3=0}^{n_1+n_2}\binom{n_1+n_2}{n_3}\{C_{n_1+n_2-n_3}(\mathbf{e})\otimes C_{n_3}(\hat{\mathbf{y}})\}_{n_1+n_2}.\end{aligned} \tag{24}$$

Finally, we have to substitute equations (22)–(24) into equation (21). As a result, we arrive at the identity

$$\begin{aligned}\frac{1}{q^2}C_{nlm}(\hat{\mathbf{x}}) = \frac{(-1)^n}{p^2}\sum_{n_1=0}^{n}\binom{n}{n_1}(-u)^{n_1}\sum_{n_2=0}^{\infty}v^{n_2}\binom{n_1+n_2+1}{n_2}\sum_{n_3=0}^{n_1+n_2}\binom{n_1+n_2}{n_3}\\ \times\{C_{n-n_1}(\mathbf{e})\otimes\{C_{n_2}(\hat{\mathbf{k}})\otimes\{C_{n_1+n_2-n_3}(\mathbf{e})\otimes C_{n_3}(\hat{\mathbf{y}})\}_{n_1+n_2}\}_{n_1}\}_{nlm},\end{aligned} \tag{25}$$

where the short-hand notation have been introduced:

$$u = \frac{\alpha}{\beta}, \qquad v = \frac{k}{2\beta} = \frac{\sqrt{(\beta-\alpha)^2+\vec{k}^2}}{2\beta}. \tag{26}$$

Equation (25) gives the connection between the hyperspherical harmonics $C_n(\hat{\mathbf{x}})$ and $C_{n_3}(\hat{\mathbf{y}})$. As is seen, among three summations only one (over the index n_2) is infinite. Expansion (25) is the farthest point one can reach using the angular momentum technique.

If we substitute expansion (25) into integral (15), then, due to the orthogonality of HSH, only the terms with $n_3 = n$ will remain. Thus, the matrix element will be defined by the two summations one of which is infinite. Below we demonstrate that the infinite summation can be evaluated in closed form as the derivatives of some elementary function.

3.2. Explicit expressions for the coefficients of the multipole expansion

The tensor product in expansion (25) has a remarkable property. Namely, the internal, as well as external, tensor products are 'minimal', i.e. the rank of the product is equal to the sum of ranks of HSH entering the product. The intermediate product having the rank n_1 contains tensor multipliers with the ranks n_2 and $n_1 + n_2$. Such a tensor product can be considered as 'maximal' since its rank is equal to the difference of the ranks of the constituent tensors. It turns out that the four-dimensional Clebsch–Gordan coefficients corresponding to the minimal or maximal tensor products can be evaluated in the closed form, see [28]. As a consequence, the tensor construction in equation (25) can be significantly simplified.

The calculation of the three-fold tensor product in equation (25) simplifies also by the fact that the hyperspherical harmonics of the unit basis vector $\mathbf{e}$ reduces to a constant number [28]:

$$C_{nlm}(\mathbf{e}) = \sqrt{n+1}\,\delta_{l,0}\delta_{m,0}. \tag{27}$$

Using this equation and the definition of the tensor product of HSH [28], we can write the tensor product from the right-hand side of equation (25) as

$$\begin{aligned} T^{(n_1n_2n_3)}_{nlm} &\equiv \{C_{n-n_1}(\mathbf{e}) \otimes \{C_{n_2}(\hat{\mathbf{k}}) \otimes \{C_{n_1+n_2-n_3}(\mathbf{e}) \otimes C_{n_3}(\hat{\mathbf{y}})\}_{n_1+n_2}\}_{n_1}\}_{nlm} \\ &= \sum_{l_2,l_3} \sum_{m_2,m_3} C^{nlm}_{(n-n_1)00;n_1lm} C^{n_1lm}_{n_2l_2m_2;(n_1+n_2)l_3m_3} C^{(n_1+n_2)l_3m_3}_{(n_1+n_2-n_3)00;n_3l_3m_3} \\ &\quad \times \sqrt{(n-n_1+1)(n_1+n_2-n_3+1)}\, C_{n_2l_2m_2}(\hat{\mathbf{k}}) C_{n_3l_3m_3}(\hat{\mathbf{y}}), \end{aligned} \tag{28}$$

where $C^{nlm}_{n'l'm';n''l''m''}$ denotes the Clebsch–Gordan coefficients of the $O(4)$ group (see equations (A2) and (A6) of [28]).

We have to calculate the summation over the index n_2 in (25). First, we note the explicit expression for HSH $C_{n_2l_2m_2}(\hat{\mathbf{k}})$,

$$C_{n_2l_2m_2}(\hat{\mathbf{k}}) = (-\mathrm{i})^{l_2} \sqrt{\frac{2l_2+1}{n_2+1}}\, \chi^{n_2/2}_{l_2}(2\theta_0) C_{l_2m_2}(\theta,\phi), \tag{29}$$

where $C_{l_2m_2}(\theta,\phi)$ are the conventional spherical harmonics depending on the spherical angles θ, ϕ of the vector $\vec{k}$. The hyper-angle θ_0 is defined by

$$\cos\theta_0 = \frac{\beta-\alpha}{k} = \frac{\beta-\alpha}{\sqrt{(\beta-\alpha)^2+\vec{k}^2}}, \qquad \sin\theta_0 = \frac{|\vec{k}|}{\sqrt{(\beta-\alpha)^2+\vec{k}^2}}. \tag{30}$$

The functions $\chi^{n_2/2}_{l_2}$ in equation (29) are the generalized characters of the $O(3)$ rotation group which are connected to the Gegenbauer polynomials [31]. Thus, the explicit expression for HSH $C_{n_2l_2m_2}$ has the form

$$C_{n_2l_2m_2}(\hat{\mathbf{k}}) = (-\mathrm{i})^{l_2}(2l_2)!! \sqrt{\frac{(2l_2+1)(n_2-l_2)!}{(n_2+l_2+1)!}} (\sin\theta_0)^{l_2} C^{l_2+1}_{n_2-l_2}(\cos\theta_0) C_{l_2m_2}(\theta,\phi), \tag{31}$$

where $C^{l_2+1}_{n_2-l_2}$ is the Gegenbauer polynomial. Substituting this equation and equation (28) into equation (25), we arrive at the multipole expansion

$$\frac{1}{q^2}C_{nlm}(\hat{\mathbf{x}}) = \frac{(-1)^n}{p^2}\sum_{n_3=0}^{\infty}\sum_{l_3=0}^{n_3}\sum_{l_2}A^{(l_2)}_{n,l;n_3,l_3}C^{l_30}_{l0l_20}\sum_{m_2,m_3}C^{lm}_{l_2m_2l_3m_3}C_{l_2m_2}(\theta,\phi)C_{n_3l_3m_3}(\hat{\mathbf{y}}), \tag{32}$$

where $C^{lm}_{l_2m_2l_3m_3}$ is the three-dimensional Clebsch–Gordan coefficient, and the index l_2 runs from $|l-l_3|$ to $l+l_3$ so that the sum $l+l_2+l_3$ is an even number. This is due to the fact that the coefficients $C^{l_30}_{l0l_20}$ vanish at odd values of the sum $l+l_2+l_3$. The coefficients A in the above equation are defined by

$$A^{(l_2)}_{n,l;n_3,l_3} = (2\mathrm{i}\sin\theta_0)^{l_2}l_2!(2l_2+1)\sqrt{\frac{(n+l+1)!}{(n-l)!(n_3+l_3+1)!(n_3-l_3)!}}\sum_{n_1}\binom{n-l}{n-n_1}$$
$$\times\frac{(-u)^{n_1}}{(n_1+l+1)!}\sum_{n_2}v^{n_2}C^{l_2+1}_{n_2-l_2}(\cos\theta_0)\frac{(n_1+n_2+l_3+1)!(n_1+n_2-l_3)!}{(n_2+l_2+1)!(n_1+n_2-n_3)!}, \tag{33}$$

where the summations are performed over all non-negative values of indices n_1 and n_2 so that all binomial coefficients and factorials remain finite. As is seen, the summation over n_1 is finite while the summation over n_2 is infinite. These summations are calculated in appendix A. The sum over l_2 in (32) has simple physical meaning. It is the multipole expansion with respect to the 'momentum transfer' vector $\vec{k}$.

As was pointed above, the multipole expansion for the product $q^{-4}C_n(\hat{\mathbf{x}})$ can be derived from the expansion for the function $q^{-2}C_n(\hat{\mathbf{x}})$ by applying equation (20). Omitting the details of some routine transformations, we present the final result,

$$\frac{1}{q^4}C_{nlm}(\hat{\mathbf{x}}) = \frac{(-1)^n}{2\alpha^2p^2}\sum_{n_3=0}^{\infty}\sum_{l_3=0}^{n_3}\sum_{l_2}(-1)^{n_3}(-\mathrm{i})^{l_2}B^{(l_2)}_{n,l;n_3,l_3}C^{l_30}_{l0l_20}$$
$$\times\sum_{m_2,m_3}C^{lm}_{l_2m_2l_3m_3}C_{l_2m_2}(\theta,\phi)C_{n_3l_3m_3}(\hat{\mathbf{y}}), \tag{34}$$

where the coefficients $B^{(l_2)}_{n,l;n_3,l_3}(\theta_0)$ are

$$B^{(l_2)}_{n,l;n_3,l_3} = -\left(\frac{|\vec{k}|}{\beta}\right)^{l_2}\frac{l_2!(2l_2+1)}{2(n+1)}\sqrt{\frac{(n+l+1)!(n_3+l_3+1)!}{(n-l)!(n_3-l_3)!}}P^{(l_2)}_{n,l;n_3,l_3}, \tag{35}$$

and the functions $P^{(l_2)}_{n,l;n_3,l_3}$ are defined by equation (A.9).

At zero 'momentum transfer' (i.e., at $\vec{k}=0$), the properties of the three-dimensional Clebsch–Gordan coefficients in expansion (34) lead to the vanishing of all terms with $l_2>0$ and $l\neq l_3$. Thus, expansion (34) reduces to

$$\frac{1}{q^4}C_{nlm}(\hat{\mathbf{x}}) = \frac{1}{2\alpha^2p^2}\sum_{n_3=l}^{\infty}(-1)^{n+n_3}B^{(0)}_{n,l;n_3,l}C_{n_3lm}(\hat{\mathbf{y}}), \tag{36}$$

where the parameter $B^{(0)}_{n,0;n_3,0}(\vec{k}=0)$ is calculated in appendix B.

For the sake of completeness, we note that the multipole expansion (25) can also be written as the series containing the four-dimensional solid harmonics, $\mathcal{C}_{n_2l_2m_2}(\mathbf{k}) = k^{n_2}C_{n_2l_2m_2}(\hat{\mathbf{k}})$,

$$\frac{1}{q^2}C_{nlm}(\hat{\mathbf{x}}) = \frac{(-1)^n}{p^2}\sum_{n_2,n_3,l_2,l_3}C^{l_30}_{l0l_20}C^{lm}_{l_2m_2l_3m_3}C_{n_3l_3m_3}(\hat{\mathbf{y}})\mathcal{C}_{n_2l_2m_2}(\mathbf{k})D_{n_2n_3,ll_3}(\alpha,\beta), \tag{37}$$

where the coefficients $D_{n_2 n_3, l, l_3}(\alpha, \beta)$ are defined by

$$D_{n_2 n_3, l l_3}(\alpha, \beta) = D \sum_{n_1} \frac{(n_1 + n_2 + l_3 + 1)!(n_1 + n_2 - l_3)!}{(n - n_1)!(n_1 + n_2 - n_3)!(n_1 + l + 1)!(n_1 - l)!} (\alpha/\beta)^{n_1},$$
$$D = (-1)^{l_2} (2\beta)^{-n_2} \sqrt{\frac{(n + l + 1)!(n - l)!(2l_2 + 1)}{(n_3 + l_3 + 1)!(n_3 - l_3)!(n_2 + l_2 + 1)!(n_2 - l_2)!}}. \tag{38}$$

The summation over n_1 in equation (38) can be calculated in closed form which yields the hypergeometric function ${}_3F_2$, see [32]. Thus, the expression for the coefficients $D_{n_2 n_3, l l_3}$ becomes

$$D_{n_2 n_3, l l_3}(\alpha, \beta) = D \frac{(n_2 + l + l_3 + 1)!(n_2 + l - l_3)!}{(n_2 - n_3 + l)!(n - l)!(2l + 1)!} \times \left(\frac{\alpha}{\beta}\right)^{l} {}_3F_2 \left(\begin{matrix} l - n, & n_2 + l - l_3 + 1, & n_2 + l + l_3 + 2; \\ & n_2 - n_3 + l + 1, & 2l + 2 \end{matrix} \; -\tfrac{\alpha}{\beta} \right). \tag{39}$$

The analysis of the series (37) shows that the region of convergence with respect to the index n_2 is defined by the two conditions, $|\alpha| < |\beta|$ and $|(\alpha - \beta)^2 + \vec{k}^2| < 2|\beta|$. The series in (37) diverges when one of parameters α, β is purely imaginary and another one is real.

The convergence of expansions (34) and (37) with respect to the index n_3 of HSH is practically not important because these expansions in n_3 will always be truncated after the integration over the hyper-angles of the unit vector $\hat{\mathbf{y}}$.

4. Properties of the matrix elements

In this section, we derive the explicit expressions for the matrix element in equation (15) in terms of the coefficients $B^{(l_2)}_{n,l;n_3,l_3}$ and $P^{(l_2)}_{n,l;n_3,l_3}$ introduced in the previous section. In section 4.1, the general formulae are given and few examples are considered. In section 4.2, we analyse the long-wave (i.e., dipole) limit of the matrix elements.

4.1. Matrix elements in general case

In order to derive an expression for the form-factor matrix element, we replace in the decomposition (34) HSH C_{nlm} with the normalized HSH Y_{nlm} and insert the resulting expression into (15). This leads to

$$F_{n'l',nl} = \sum_{n_3,l_3,l_2} \mathrm{i}^{l_2} \sqrt{\frac{\alpha(n+1)}{\beta(n_3+1)}} B^{(l_2)}_{n,l;n_3,l_3} C^{l_3 0}_{l 0 l_2 0} \times \sum_{m_2,m_3} C^{lm}_{l_2 m_2 l_3 m_3} C_{l_2 m_2}(\theta, \phi) \int Y^*_{n'l'm'}(\hat{\mathbf{y}}) Y_{n_3 l_3 m_3}(\hat{\mathbf{y}}) \, \mathrm{d}\Omega_{\mathbf{y}}. \tag{40}$$

Since HSH are orthonormal, the integral over the hypersphere is equal to unity for $n_3 l_3 m_3 = n' l' m'$ and is zero otherwise. As a consequence, we obtain

$$F_{n'l',nl} = \sqrt{\frac{\alpha(n+1)}{\beta(n'+1)}} \sum_{l_2=|l-l'|}^{l+l'} \mathrm{i}^{l_2} C^{l'0}_{l 0 l_2 0} C^{lm}_{l_2 m_2 l' m'} C_{l_2 m_2}(\theta, \phi) B^{(l_2)}_{n,l;n',l'}. \tag{41}$$

If the transitions between the states of the hydrogen atom are considered then the factor under the square root reduces to unity as follows from the definition (10) of parameters α and β.

The above formula for the form factors $F_{n'l',nl}$ can be re-written in terms of radial integrals. Using explicit expressions for the radial hydrogen wavefunctions and decomposing the plane

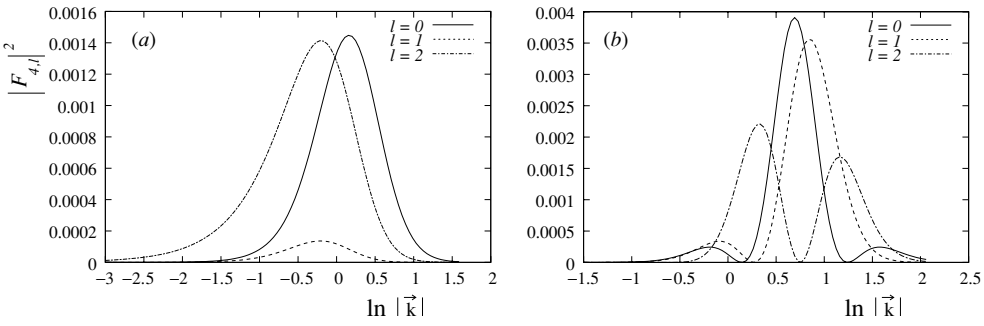

Figure 2. The parameters $|F_{4,l}|^2$. (*a*) The matrix elements for the hydrogen atom: $\alpha = 1$, $\beta = 1/5$. (*b*) The matrix elements for Sturmians: $\alpha = \beta = 1$.

wave in equation (6) over the three-dimensional spherical functions, equation (41) can be brought to the form

$$\int_0^\infty r^{l+l'+2}\,\mathrm{e}^{-(\alpha+\beta)r}\,j_{l_2}(|\vec{k}|r)\Phi(l'-n',2l'+2;2\beta r)\Phi(l-n,2l+2;2\alpha r)\,\mathrm{d}r$$
$$= (-1)^{l+l_2+l'+1}\frac{l_2!(2l+1)!(2l'+1)!}{(2\alpha)^{l+1}(2\beta)^{l'+2}}\left(\frac{|\vec{k}|}{\beta}\right)^{l_2}P^{(l_2)}_{n,l;n',l'}(u,w), \tag{42}$$

where the parameter w is defined by equation (A.10), $\Phi(l-n,2l+2;2\alpha r)$ is the confluent hypergeometric function and j_{l_2} is the spherical Bessel function. The definition (A.9) of functions $P^{(l_2)}_{n,l;n',l'}$ implies the following limitations on the indices in equation (42):

$$l \leqslant n, \qquad l' \leqslant n', \qquad l - l_2 + l' + 1 \geqslant 0. \tag{43}$$

(The requirement for the combination $l + l_2 + l'$ to be an even number is not necessary in equation (42).) Thus, we have shown that the integrals of the kind (42) can be written as a three-fold derivative of an elementary function (cf equations (42) and (A.9)). It turns out that for small values of indices n and l (or n' and l') the functions $P^{(l_2)}_{n,l;n',l'}$ can be written in a compact form as a combination of Gegenbauer polynomials.

For example, the matrix elements for the transitions from the ground state $n = l = 0$ can be written as

$$F_{n,l} = \int_0^\infty R_{0,0}(\alpha,r)\,j_l(kr)R_{n,l}(\beta,r)r^2\,\mathrm{d}r = -\frac{l!}{2}\left(\frac{k}{\beta}\right)^l\sqrt{\frac{\alpha(n+l+1)!}{\beta(n+1)(n-l)!}}\,P^{(l)}_{0,0;n,l}, \tag{44}$$

where $R_{n,l}$ are the normalized radial wavefunctions and the function $P^{(l)}_{0,0;n,l}$ is the combination of two Gegenbauer polynomials (see equation (C.6)). We recall that the index n above is equal to the principal quantum number minus unity. For hydrogen matrix elements one has $\alpha = 1$ and $\beta = 1/(n+1)$ while for Sturmian matrix elements the parameters α and β can be arbitrary numbers. As an example, in figure 2 the parameters $|F_{n,l}|^2$ corresponding to transition 1s $\to$ 5l are plotted as functions of $\ln|\vec{k}|$. (The reason for such a choice of abscissa variable is explained in [22, 33].) As is seen, the hydrogen matrix elements have strong maxima at some values of $|\vec{k}|$. The Sturmian matrix elements behave in less regular manner, e.g. they can have several peaks at different values of the momentum $|\vec{k}|$.

4.2. The dipole limit

In the dipole limit we have that $\vec{k} \to 0$ and, hence, it is necessary to retain only the terms of zeroth and first order with respect to $|\vec{k}|$. Such terms correspond to the two values of the multipole index, $l_2 = 0$ and $l_2 = 1$. The derivation of the parameters $P^{(l_2)}_{n,l;n',l'}$ for such values of l_2 is considered in appendix C.

According to equation (C.12), the parameters with $l_2 = 0$ can be written in closed form in terms of Gauss hypergeometric function:

$$P^{(0)}_{n,l;n',l}(u) = \frac{4(-1)^{n'}}{(2l+1)!}\left(\frac{-4u}{(1-u)^2}\right)^{l+1}\left(\frac{1-u}{1+u}\right)^{n+n'+1}\frac{n'+1-(n+1)u}{(1+u)^2} \times {}_2F_1\left(l-n, l-n'; 2l+2; \frac{-4u}{(1-u)^2}\right). \tag{45}$$

The Gauss function in this equation is a polynomial whose order is $\min(n-l, n'-l)$. It is easy to see that at $u = (n'+1)/(n+1)$ (as well as at $u = 1$) the parameter $P^{(0)}_{n,l;n',l}$ is

$$P^{(0)}_{n,l;n',l} = -2(n+1)\frac{(n-l)!}{(n+l+1)!}\delta_{n,n'}, \tag{46}$$

and the form-factor matrix element becomes

$$F_{n'l',nl}|_{\vec{k}=0} = \delta_{n,n'}. \tag{47}$$

This reflects the orthogonality property of the hydrogen wavefunctions (or, at $u = 1$, Sturmian functions from the same set).

The parameter $P^{(1)}_{n,l;n',l-1}$ describes the dipole transitions and expressed as (see equation (C.13))

$$P^{(1)}_{n,l;n',l-1}(u) = \frac{2(-1)^{n'}}{3(2l+1)!}\left(\frac{-4u}{(1-u)^2}\right)^{l+1}\left(\frac{1-u}{1+u}\right)^{n+n'}\{(n'+l+1)(n'+l+2)f_0 + 2(n'+l+1)(n'-l+1)f_1 + (n'-l+1)(n'-l)f_2\}, \tag{48}$$

where the coefficients f_k are defined by

$$f_k = \left(\frac{1-u}{1+u}\right)^{2-k}\frac{(n+1)u - n' - 2 + k}{(1+u)^2}{}_2F_1\left(l-n, l-1-n'+k; 2l+2; \frac{-4u}{(1-u)^2}\right). \tag{49}$$

In the case of matrix elements between the hydrogen states, we have that $u = (n'+1)/(n+1)$ and the coefficient f_1 vanishes. Thus, the matrix element in this case is a combination of two Gauss hypergeometric functions in agreement with the well-known Gordon formula [34]. The expression for the coefficient $P^{(l_2)}_{n,l;n',l+1}$ can be derived from equation (48) using the symmetry property (A.11) which in the dipole case has the form

$$P^{(1)}_{n,l;n',l'}(u) = u^{n+n'+2l'+2}P^{(1)}_{n',l';n,l}(1/u). \tag{50}$$

5. Conclusion

In the present paper, we have applied the method of Fock's stereographic projections to the calculation of matrix elements involving the hydrogen-type wavefunctions. We have shown (section 2) that the problem of the calculation of matrix elements is equivalent to the derivation of a multipole expansion of the four-dimensional hyperspherical harmonics with their arguments defined by means of the shifted stereographic projection.

There is a conceptual similarity between our approach and the work [35]. In that paper, the two-photon transitions between the states of the hydrogen atom have been considered using the representation of the Coulomb–Green function with two free parameters. Our multipole expansions of the hydrogen wavefunction in momentum space (see equations (32) and (34)) also contain free parameters β and $\vec{k}$. By 'tuning' the energy parameter β, we can move the argument of HSH to any desirable point on the hypersphere. Usually, the choice of the parameter β is fixed by demanding the orthogonality of HSH entering the integral. The same approach was used in [35]. The proper choice of free parameters can result in the significant simplification of expressions for the compound matrix elements or in the improving the accuracy of numerical computations. The method developed in the present paper can also be used to generalize the results of [35, 36] in order to account the non-dipole effects.

The expression for the form-factor matrix element in terms of the multipole functions $P^{(l_2)}_{n,l;n',l'}$ is given in section 4. We showed that the functions $P^{(l_2)}_{n,l;n',l'}$ are, in fact, integrals between the radial hydrogen wavefunctions and the spherical Bessel function arising from the multipole expansion of the boost operator $\exp(\mathrm{i}\vec{k}\cdot\vec{r})$.

It turns out that the closed expression for $P^{(l_2)}_{n,l;n',l'}$ in terms of special function of a single variable does not exist in the general case of arbitrary values of the indices n, l, n', l', l_2 and arguments α, β and $\vec{k}$. Only in some particular situations, e.g. in the long-wave (i.e., dipole) limit as well as for the transitions from the ground 1s state, the functions $P^{(l_2)}_{n,l;n',l'}$ can be written as a combination of Gauss hypergeometric functions[3]. Surprisingly, there exists a remarkably simple differential representation for coefficients $P^{(l_2)}_{n,l;n',l'}$. It is given by equation (A.9). This differential formula can serve as a source for many explicit expressions for functions $P^{(l_2)}_{n,l;n',l'}$. The differential representation can also be effectively used for the derivations of the recurrence relations for P-functions. A number of such relations are derived in appendix D. We also note that recursions involving radial hydrogen matrix elements of the powers r^k have been considered in [37].

The results of the present paper can also be generalized in the case of bound-free transitions. In general, this can be achieved by applying the replacements $n \to \pm\mathrm{i}/\sqrt{E}$, where $E > 0$ is the energy of the continuum state. At this stage, the differential operators in equation (A.9) become undefined. However, this problem can be avoided by using the contour representations for the derivatives.

The matrix elements of the operator of electromagnetic interaction $\vec{\epsilon}\exp(\mathrm{i}\vec{k}\cdot\vec{r})$ can also be derived using the formalism developed in this paper. In this case, one should replace q^{-4} with $(\boldsymbol{\epsilon}\cdot\hat{\mathbf{x}})q^{-4}$ in equation (15) where $\boldsymbol{\epsilon} = (0, \vec{\epsilon})$ is the four-dimensional photon polarization vector. Then, one can apply the Wigner–Eckart theorem to the ensuing integral. The corresponding results can be written again in terms of the functions $P^{(l_2)}_{n,l;n',l'}$.

One of the possible applications of the technique developed above could be the calculation of the two-centre Coulomb integrals. Namely, by applying the Fourier transform to the function $1/|\vec{r}_1 - \vec{r}_2|$ one arrives at the form-factor integrals for which the differential representations can be used. The work on this problem is in progress.

Acknowledgments

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[3] More precisely, as Jacobi or Gegenbauer polynomials, see appendix C.

Appendix A. The calculation of summations in equation (33)

In this appendix, we calculate the two summations in (33). We begin by calculating the sum over n_2 which we denote as S_{n_1},

$$S_{n_1} = \sum_{n_2=l_2}^{\infty} v^{n_2} C_{n_2-l_2}^{l_2+1}(\cos\theta_0) \frac{(n_1+n_2+l_3+1)!(n_1+n_2-l_3)!}{(n_1+n_2-n_3)!(n_2+l_2+1)!}. \tag{A.1}$$

Replacing the summation variable by $k = n_2 - l_2$, we obtain

$$S_{n_1} = v^{l_2} \sum_{k=0}^{\infty} v^k C_k^{l_2+1}(\cos\theta_0) \frac{(k+n_1+l_2+l_3+1)!(k+n_1+l_2-l_3)!}{(k+n_1-n_3+l_2)!(k+2l_2+1)!}. \tag{A.2}$$

Factorials in this identity can be removed by introducing the differential operators

$$\frac{(k+n_1+l_2+l_3+1)!(k+n_1+l_2-l_3)!}{(k+n_1-n_3+l_2)!(k+2l_2+1)!} = (-1)^{n_1+n_3+l_2} \partial_t^{n_3-l_3} t^{n_3+l_3+1} \partial_\tau^{n_1-l_2+l_3} (t+\tau)^{-(k+2l_2+2)}|_{t=1,\tau=0}, \tag{A.3}$$

where $\partial_t = \partial/\partial t$ and $\partial_\tau = \partial/\partial\tau$. Inserting equation (A.3) into (A.2) one arrives at the series, which can be evaluated using the generating function for Gegenbauer polynomials [38],

$$(t+\tau)^{-(2l_2+2)} \sum_{k=0}^{\infty} \left(\frac{v}{t+\tau}\right)^k C_k^{l_2+1}(\cos\theta_0) = (t+\tau)^{-(2l_2+2)} \left(1 - \frac{2v\cos\theta_0}{t+\tau} + \frac{v^2}{(t+\tau)^2}\right)^{-l_2-1}$$
$$= [v^2 - 2v\cos\theta_0(t+\tau) + (t+\tau)^2]^{-l_2-1}. \tag{A.4}$$

Thus, the parameter S_{n_1} can be written as

$$S_{n_1} = (-1)^{n_1+n_3+l_2} v^{l_2} \partial_t^{n_3-l_3} t^{n_3+l_3+1} \partial_\tau^{n_1-l_2+l_3} [v^2 - 2v\cos\theta_0(t+\tau) + (t+\tau)^2]^{-l_2-1}|_{t=1,\tau=0}. \tag{A.5}$$

Now we have to evaluate the sum over n_1 in equation (35):

$$S_n = \sum_{n_1=l}^{n} \binom{n-l}{n-n_1} \frac{(-u)^{n_1}}{(n_1+l+1)!} S_{n_1} = \sum_{n_1=0}^{n-l} \binom{n-l}{n_1} \frac{(-u)^{n_1+l}}{(n_1+2l+1)!} S_{n_1+l}. \tag{A.6}$$

Using equation (A.5) we write S_n in its full form:

$$S_n = (-1)^{n_3+l_2} v^{l_2} \partial_t^{n_3-l_3} t^{n_3+l_3+1} \sum_{n_1=0}^{n-l} \binom{n-l}{n_1} \frac{u^{n_1+l}}{(n_1+2l+1)!}$$
$$\times \partial_\tau^{n_1+l-l_2+l_3} [v^2 - 2v(t+\tau)\cos\theta_0 + (t+\tau)^2]^{-l_2-1}|_{t=1,\tau=0}. \tag{A.7}$$

After some rearrangements using the chain differentiation rule, this identity can be written in closed form:

$$S_n = (-1)^{n_3+l_2} \frac{v^{l_2} u^{-l-1}}{(n+l+1)!} \partial_t^{n_3-l_3} t^{n_3+l_3+1} \partial_\tau^{n-l} (u+\tau)^{n+l+1} \partial_\tau^{l-l_2+l_3}$$
$$\times [v^2 - 2v(t+\tau)\cos\theta_0 + (t+\tau)^2]^{-l_2-1}|_{t=1,\tau=0}. \tag{A.8}$$

As is seen, the two-fold summation in (33) reduces to the derivatives of an elementary function.

According to equation (20), in order to calculate the coefficients in expansion (34) of the function $q^{-4} C_n(\hat{\mathbf{x}})$, one has to evaluate the combination of three functions S_n. Omitting the

details of some routine transformations, we present the final result for the parameters $P^{(l_2)}_{n,l;n_3,l_3}$ in (35),

$$P^{(l_2)}_{n,l;n_3,l_3}(u,w) = \frac{u^{-l}}{(n+l+1)!(n_3+l_3+1)!}\partial_\tau^{n-l}(u+\tau)^{n+l+1}\partial_t^{n_3-l_3}(1+t)^{n_3+l_3+1} \times \partial_\tau^{l-l_2+l_3+1}[w^2+(1+u)(t+\tau)+(t+\tau)^2]^{-l_2-1}|_{t,\tau=0}, \tag{A.9}$$

where the short-hand notation have been introduced:

$$w = \sqrt{1-2v\cos\theta_0+v^2} = \frac{\sqrt{(\alpha+\beta)^2+\vec{k}^2}}{2\beta}. \tag{A.10}$$

We also note the following symmetry property of functions $P^{(l_2)}_{n,l;n_3,l_3}(u,w)$:

$$P^{(l_2)}_{n,l;n_3,l_3}(u,w) = u^{n+n_3+2l_3+2}P^{(l_2)}_{n_3,l_3;n,l}(1/u, w/u). \tag{A.11}$$

This equation can be proved by making the replacements $t \to u\tau$ and $\tau \to ut$ in the definition (A.9).

Appendix B. The explicit expressions for the functions $P^{(l_2)}_{n,l;n_3,l_3}$

In order to calculate the functions $P^{(l_2)}_{n,l;n_3,l_3}$ in equation (A.9) in an explicit form, we use the generating function for the Gegenbauer polynomials:

$$[w^2-2\xi w(t+\tau)+(t+\tau)^2]^{-l_2-1} = \sum_{q=0}^{\infty} w^{-2l_2-2-q}(t+\tau)^q C_q^{l_2+1}\left(-\frac{u+1}{2w}\right). \tag{B.1}$$

Acting by the operator $\partial_\tau^{l-l_2+l_3+1}$ on this equation, one observes that the terms with $q < l-l_2+l_3+1$ vanish. Thus, the functions $P^{(l_2)}_{n,l;n_3,l_3}$ can be written as a combination of Gegenbauer polynomials:

$$P^{(l_2)}_{n,l;n_3,l_3}(u,w) = \frac{u^{l+1}}{w^{l+l_2+l_3+3}}\sum_{q=0}^{q_{max}} w^{-q}C_q(u)C^{l_2+1}_{l-l_2+l_3+q+1}\left(-\frac{u+1}{2w}\right), \tag{B.2}$$

where $q_{max} = n+n_3-l-l_3$ and parameters C_q are polynomials in u,

$$C_q(u) = \sum_{m=0}\binom{n-l}{m}\binom{n_3-l_3}{q-m}\frac{(l-l_2+l_3+q+1)!}{(2l+1+m)!(2l_3+q+1-m)!}u^m, \tag{B.3}$$

where the summation over m is taken over all non-negative integer values at which factorials remain finite. The parameters $C_q(u)$ can also be written in the following form:

$$C_q(u) = (-1)^q\frac{(n-l)!(n_3-l_3)!(l-l_2+l_3+q+1)!}{(n+l+1)!(n_3+l_3+1)!q!}\partial_t^q L^{(2l+1)}_{n-l}(ut)L^{(2l_3+1)}_{n_3-l_3}(t)\Big|_{t=0},$$

where $L^{(2l+1)}_{n-l}$ is the Laguerre polynomial [38]. This equation can be proved by straightforward calculations. Thus, the parameter $C_q(u)$ is proportional to the coefficient at the qth power of the product of two Laguerre polynomials.

One can obtain an explicit expression for $C_q(u)$ in terms of generalized hypergeometric function ${}_3F_2$. There are two cases which must be considered separately. For $q \leqslant n_3-l_3$, the index m in (B.3) runs from 0 to $\min(q, n-l)$. This leads to

$$C_q(u) = \binom{n_3-l_3}{q}\frac{(l-l_2+l_3+q+1)!}{(2l_3+q+1)!(2l+1)!}{}_3F_2\left(\begin{matrix}-q, & l-n, & -q-2l_3-1; \\ & 2l+2, & n_3-l_3-q+1\end{matrix}\;\; -u\right). \tag{B.4}$$

For $q > n_3 - l_3$ one has that $q - n_3 + l_3 \leqslant m \leqslant n - l$. In this case, the above formula is invalid and the correct expression has the form

$$C_q(u) = \binom{n-l}{q-n_3+l_3} \frac{(l-l_2+l_3+q+1)!}{(2l-n_3+l_3+q+1)!(n_3+l_3+1)!} u^{q-n_3+l_3} \times {}_3F_2\left(\begin{matrix} l+l_3-n-n_3+q, & l_3-n_3, & -l_3-n_3-1; \\ & 2l+2, & l_3-n_3+q+1 \end{matrix} \middle| -u \right). \tag{B.5}$$

Appendix C. Functions $P^{(l_2)}_{n,l;n_3,l_3}$ in particular cases

In this appendix, we analyse the situations when the functions $P^{(l_2)}_{n,l;n_3,l_3}$ can be written in closed form. Our consideration is based on the general differential relation

$$\partial_t^n (\alpha+\beta t)^{n+\gamma} f(t)|_{t=0} = \alpha^{2\gamma+n+1} \partial_t^n (\alpha-\beta t)^{-\gamma-1} f\left(\frac{\alpha t}{\alpha-\beta t}\right)\Big|_{t=0}. \tag{C.1}$$

Here, α, β, γ are the arbitrary numbers and $f(t)$ is an arbitrary function. This formula can be proved by expanding the function f into Taylor series and comparing coefficients at the expansion terms.

Let us consider the functions P corresponding to the transition from the ground 1s state. In this case we have $n = l = 0$ and, hence, $l_2 = l_3 \equiv l$. According to the definition, equation (A.9), we can write

$$P^{(l)}_{0,0;n,l} = \frac{u}{(n+l+1)!} \partial_t^{n-l} (1+t)^{n+l+1} \partial_t [w^2 + (u+1)t + t^2]^{-l-1}|_{t=0}. \tag{C.2}$$

In order to calculate the action of the differential operators we note the formula

$$(1+t)^{n+l+1} \partial_t = \partial_t (1+t)^{n+l+1} - (n+l+1)(1+t)^{n+l}. \tag{C.3}$$

Now the parameter $P^{(l)}_{0,0;n,l}$ can be re-written as

$$P^{(l)}_{0,0;n,l} = \frac{u}{(n+l+1)!} \left(\partial_t^{n-l+1}(1+t) - (n+l+1)\partial_t^{n-l}\right)(1+t)^{n+l} [w^2 + (u+1)t + t^2]^{-l-1}|_{t=0}. \tag{C.4}$$

By applying the differential transformation (C.1) to this equation, we arrive at

$$P^{(l)}_{0,0;n,l} = \frac{u}{(n+l+1)!} \left(\partial_t^{n-l+1} - (n+l+1)\partial_t^{n-l}\right)(1-t)[w^2 - 2at + (tv)^2]^{-l-1}|_{t=0}, \tag{C.5}$$

where $a = w^2 - (u+1)/2$ and the parameter v is defined in equation (26). The calculation of derivatives can be performed by expanding the term in square brackets similarly to equation (B.1). After some simple algebraic manipulations, we obtain

$$P^{(l)}_{0,0;n,l} = \frac{(n-l)!}{(n+l+1)!} \frac{u}{w^{2l+3}} \left(\frac{v}{w}\right)^{n-l} \left(-2(n+1)(w-xv) C^{l+1}_{n-l}(x) + (n+l+1)\frac{w^2-v^2}{v} C^{l+1}_{n-l-1}(x)\right), \tag{C.6}$$

where the argument of the Gegenbauer polynomial is

$$x = \frac{w^2 - (u+1)/2}{vw} = \frac{\alpha^2 - \beta^2 + \vec{k}^2}{4\beta^2 vw}. \tag{C.7}$$

Similarly, one can derive rather compact expressions for the P-coefficients for the transitions from 2s and 2p states. However, for the sake of shortness, we do not present here the corresponding equations.

C.1. The dipole limit

Now, let us consider the functions $P^{(l_2)}_{n,l;n_3,l_3}$ in the limit of small $|\vec{k}|$, i.e., the dipole limit. In this case, only the zeroth- and first-order terms (with respect to $|\vec{k}|$) should be taken into account. Thus, in the dipole limit one has that $w = (u+1)/2$ and it is necessary to retain only the terms with $l_2 = 0$ and $l_2 = 1$ in equation (A.9).

Let us first calculate the function $P^{(0)}_{n,l;n_3,l}$. Since $\vec{k} = 0$, the term in square brackets in equation (A.9) reduces to $[w+t+\tau]^{-2}$. This simplifies the calculations, so that equation (A.9) becomes

$$P^{(0)}_{n,l;n_3,l} = \frac{-u^{-l}(2l+2)!}{(n+l+1)!(n_3+l+1)!}\partial_\tau^{n-l}(u+\tau)^{n+l+1}\partial_t^{n_3-l}(1+t)^{n_3+l+1}(w+t+\tau)^{-2l-3}|_{t,\tau=0}. \tag{C.8}$$

It is convenient to present the last multiplicand in this equation as $(w+t+\tau)^{-2l-3} = -(1/(2l+2))\partial_w(w+t+\tau)^{-2l-2}$:

$$P^{(0)}_{n,l;n_3,l} = \frac{u^{-l}(2l+1)!}{(n+l+1)!(n_3+l+1)!}\partial_w\partial_\tau^{n-l}(u+\tau)^{n+l+1}\partial_t^{n_3-l}(1+t)^{n_3+l+1}(w+t+\tau)^{-2l-2}|_{t,\tau=0}. \tag{C.9}$$

Using the auxiliary identity (C.1) we can calculate the derivative over t in closed form:

$$\partial_t^{n_3-l}(w+\tau+t)^{-2l-2}(1+t)^{n_3+l+1}|_{t=0} = \frac{(n_3+l+1)!}{(2l+1)!}(w+\tau)^{-n_3-l-2}(w-1+\tau)^{n_3-l}. \tag{C.10}$$

By applying equation (C.1) to the calculation of the derivative over τ one arrives at the Gauss hypergeometric function,

$$P^{(0)}_{n,l;n_3,l} = \frac{u^{n+1}}{(2l+1)!}\partial_w w^{-n-n_3-2}(w-1)^{n_3-n}z^{l-n}{}_2F_1(l-n, l-n_3; 2l+2; z), \tag{C.11}$$

where $z = u/[(w-u)(w-1)]$.

The calculation of the derivative over w simplifies by the fact that $\partial_w z(w) = 0$ at the point $w = (u+1)/2$. Thus, the parameter $P^{(0)}_{n,l;n_3,l}$ assumes the form

$$P^{(0)}_{n,l;n_3,l} = \frac{u^{n+1}}{(2l+1)!}\frac{(w-1)^{n_3-n-1}}{w^{n+n_3+3}}[n_3-n+2(n+1)(1-w)] \times z^{l-n}{}_2F_1(l-n, l-n_3; 2l+2; z). \tag{C.12}$$

In the case of $l_2 = 1$ there are two possibilities. Since the combination $l + l_2 + l_3$ must be an even number, we have that $l_3 = l \pm 1$. Below we calculate the coefficient $P^{(1)}_{n,l;n_3,l-1}(u, w)$. (The coefficient $P^{(1)}_{n,l-1;n_3,l}$ can be derived using the symmetry relation (A.11).) The calculation procedure is similar to that considered above. As a result, we have

$$P^{(1)}_{n,l;n_3,l-1} = \frac{u^{n_3+2}}{6(2l+1)!}\partial_w w^{-n-n_3-3}(w-u)^{n-n_3-1}\partial_t^2 t^{n_3+l+2} \times z^{l-1-n_3}{}_2F_1(l-n, l-1-n_3; 2l+2; z)|_{t=1}, \tag{C.13}$$

where $z = ut/[(w-u)(w-t)]$. Omitting the details of somewhat lengthy calculations we only present the final result which is given by equation (48).

Appendix D. Recurrence relations for the functions $P^{(l_2)}_{n,l;n_3,l_3}$

The differential representation (A.9) can be used for the derivation of the recurrence relations for the functions $P^{(l_2)}_{n,l;n_3,l_3}$. Such relations can be derived using the properties of the differential operators. For example, we note the following operator identity:

$$(n_3-l_3)\partial_t^{n_3-1-l_3}(1+t)^{n_3+l_3}+\partial_t^{n_3-l_3}(1+wt)^{n_3+l_3} = (n_3+l_3+1)\partial_t^{n_3-l_3-1}(1+wt)^{n_3+l_3}+\partial_t^{n_3-l_3-1}(1+wt)^{n_3+l_3+1}\partial_t. \tag{D.1}$$

(It can be proved by straightforward calculations.) A similar identity can be written for the operators ∂_τ. These two identities result into a pair of recurrences for the functions $P^{(l_2)}_{n,l;n_3,l_3}$ with fixed multipole index l_2,

$$\begin{aligned}&(n_3+l_3+1)P_{n,l;n_3,l_3}-(n_3-l_3)P_{n,l;n_3-1,l_3}=P_{n,l;n_3,l_3-1}-P_{n,l;n_3-1,l_3-1},\\&(n+l+1)P_{n,l;n_3,l_3}-(n-l)P_{n-1,l;n_3,l_3}=P_{n,l-1;n_3,l_3}-P_{n-1,l-1;n_3,l_3},\end{aligned} \tag{D.2}$$

where we have omitted the superscript l_2 for the sake of shortness. The recursion connecting functions with different indices l_2 can be derived using the differential identity,

$$\partial_\tau^{l-l_2+l_3+2}R_{l_2}=2(l_2+1)\big[(\xi-t-\tau)\partial_\tau^{l-l_2+l_3+1}R_{l_2+1}-(l-l_2+l_3+1)\partial_\tau^{l-l_2+l_3}R_{l_2+1}\big], \tag{D.3}$$

where $R_{l_2}=[1-2\xi(t+\tau)+(t+\tau)^2]^{-l_2-1}$ and $\xi=-(1+u)/(2w)$. After some transformations, the above identity leads to the recursion connecting functions P with indices l_2, l_2+1,

$$\begin{aligned}(n+l+2)P^{(l_2)}_{n+1,n_3}+(n-l)P^{(l_2)}_{n-1,n_3}-2(n+1)P^{(l_2)}_{n,n_3} &= (l_2+1)\big((n+l+2)(1-u)P^{(l_2+1)}_{n+1,n_3}\\&+(n-l)(1+u)P^{(l_2+1)}_{n-1,n_3}+2[u(n_3+l_2+2)-n-1]P^{(l_2+1)}_{n,n_3}\\&-2(n_3+l_3+2)uP^{(l_2+1)}_{n,n_3+1}\big).\end{aligned} \tag{D.4}$$

where $P^{l_2}_{n,n_3}=P^{(l_2)}_{n,l;n_3,l_3}$, etc. The recursion connecting P-functions with fixed values of angular momentum indices l, l_2, l_3 can be derived using the fact that $\partial_\tau R_{l_2}=\partial_t R_{l_2}$. Omitting the detail of the routine transformations, we only present the final result,

$$\begin{aligned}(n_3+l_3+2)uP_{n,n_3+1}+(n_3-l_3)uP_{n,n_3-1}-(n+l+2)P_{n+1,n_3}-(n-l)P_{n-1,n_3}\\+2[n+1-u(n_3+1)]P_{n,n_3}=0,\end{aligned} \tag{D.5}$$

where $P_{n,n_3}\equiv P^{(l_2)}_{n,l;n_3,l_3}$.

Finally, we note that there are two other recurrence relations which connect functions P with different values of indices n, n_3. Both of those recursions contain eight terms and they form a complete set with respect to the indices n and n_3. It means that having ten 'neighbour' parameters one can recursively calculate the parameters P_{n,n_3} with arbitrary n and n_3. However, since these recursions have quite cumbersome form, we do not present them here.

References

[1] Fock W 1935 *Z. Phys.* **98** 145
[2] Lieber M 1968 *Phys. Rev.* **174** 2037
[3] Bander M and Itzykson C 1966 *Rev. Mod. Phys.* **38** 330
[4] Schwinger J 1964 *J. Math. Phys.* **5** 1606
[5] Maquet A 1977 *Phys. Rev.* A **15** 1088
[6] Shibuya T and Wulfman C E 1965 *Proc. R. Soc.* A **286** 376
[7] Avery J 2004 *Int. J. Quantum Chem.* **100** 121
[8] Avery J 2000 *Hyperspherical Harmonics and Generalized Sturmians* (*Progress in Theoretical Chemistry and Physics* vol 4) (Dordrecht: Kluwer)

[9] Aquilanti V, Cavalli S and Coletti C 1998 *Phys. Rev. Lett.* **80** 3209
[10] Aquilanti V, Caligiana A, Cavalli S and Coletti C 2003 *Int. J. Quantum Chem.* **92** 212
[11] Aquilanti V, Cavalli S, Coletti C, di Domenico D and Grossi G 2001 *Int. Rev. Phys. Chem.* **20** 673
[12] Aquilanti V, Cavalli S and Coletti C 1997 *Chem. Phys.* **214** 1
[13] Aquilanti V, Cavalli S, Coletti C and Grossi G 1996 *Chem. Phys.* **209** 405
[14] Avery J and Avery J 2004 *J. Phys. Chem.* A **108** 8848
[15] Avery J and Shim R 2001 *Int. J. Quantum Chem.* **83** 1
[16] Avery J 1997 *J. Math. Chem.* **21** 285
[17] Avery J and Hansen T B 1996 *Int. J. Quantum Chem.* **60** 201
[18] Avery J, Hansen T B, Wang M C and Antonsen F 1996 *Int. J. Quantum Chem.* **57** 401
[19] Muljarov E A, Yablonskii A L, Tikhodeev S G, Bulatov A E and Birman J L 2000 *J. Math. Phys.* **41** 6026
[20] Aquilanti V and Caligiana A 2002 *Chem. Phys. Lett.* **366** 157
[21] Bethe H 1930 *Ann. Phys.* **5** 325
[22] Inokuti M 1971 *Rev. Mod. Phys.* **43** 297
[23] Mott N F and Massey H S W 1965 *The Theory of Atomic Collisions* vol II (Oxford: Oxford University Press)
[24] Jetzke S and Broad J T 1986 *J. Phys. B: At. Mol. Phys.* **19** L199
[25] Parzyński R and Sobczak M 2003 *Opt. Commun.* **225**
[26] Holt A R 1969 *J. Phys. B: At. Mol. Phys.* **2** 1209
[27] Datta S 1985 *J. Phys. B: At. Mol. Phys.* **18** 853
[28] Meremianin A V 2006 *J. Phys. A: Math. Gen.* **39** 3099
[29] Manakov N L, Marmo S I and Meremianin A V 1996 *J. Phys. B: At. Mol. Opt. Phys.* **29** 2711
[30] Meremianin A V and Briggs J S 2003 *Phys. Rep.* **384** 121
[31] Varshalovich D A, Moskalev A N and Khersonskii V K 1988 *Quantum Theory of Angular Momentum* (Singapore: World Scientific)
[32] Erdelyi A, Magnus W, Oberhettinger F and Tricomi F G 1953 *Higher Transcendental Functions* vol I (New York: McGraw-Hill)
[33] Miller W F and Platzman R L 1957 *Proc. Phys. Soc.* A **70** 299
[34] Gordon W 1929 *Ann. Phys.* **2** 1031
[35] Krylovetsky A A, Manakov N L and Marmo S I 2001 *J. Exp. Theor. Phys.* **92** 37
[36] Manakov N L, Marmo S I and Pronin E A 2004 *J. Exp. Theor. Phys.* **98** 254
[37] Hey J D 2006 *J. Phys. B: At. Mol. Opt. Phys.* **39** 2641
[38] Erdelyi A, Magnus W, Oberhettinger F and Tricomi F G 1953 *Higher Transcendental Functions. Bateman Manuscript Project* vol II (New York: McGraw-Hill)