Angular Fock coefficients: Refinement and further development

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The angular coefficients $\psi_{k,p}(\alpha,\theta)$ of the Fock expansion characterizing the S-state wave function of the two-electron atomic system are calculated in hyperspherical angular coordinates α and θ. To solve the problem the Fock recurrence relations separated into the independent individual equations associated with definite power j of the nucleus charge Z are applied. The "pure" j components of the angular Fock coefficients, orthogonal to the hyperspherical harmonics Y_{kl}, are found for even values of k. To this end, the specific coupling equation is proposed and applied. Effective techniques for solving the individual equations with the simplest nonseparable and separable right-hand sides are proposed. Some mistakes or misprints made earlier in representations of $\psi_{2,0}$, are noted and corrected. All j components of $\psi_{4,1}$ and the majority of components and subcomponents of $\psi_{3,0}$ are calculated and presented. All calculations are carried out with the help of Wolfram *Mathematica*.

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I. INTRODUCTION

The helium isoelectronic sequence presenting a two-electron atomic system contains the main features of a many-body system with Coulomb interaction. As such, it can serve as a simple basis for testing new quantum theories. The state of a three-body system when all the particles are in the same space point is known as the triple coalescence point (TCP). A long time ago, Bartlett *et al.* [1] showed that the ^1S helium wave function Ψ could not be expanded near the TCP as an analytic series in the interparticle coordinates r_1, r_2, and r_{12}. Later Bartlett [2] and Fock [3] proposed the following expansion containing logarithmic functions:

$$\Psi(r,\alpha,\theta) = \sum_{k=0}^{\infty} r^k \sum_{p=0}^{[k/2]} \psi_{k,p}(\alpha,\theta)(\ln r)^p, \tag{1}$$

where

$$\alpha = 2\arctan(r_2/r_1), \quad \theta = \arccos\left[\left(r_1^2 + r_2^2 - r_{12}^2\right)/2r_1 r_2\right] \tag{2}$$

are the hyperspherical angles and $r = \sqrt{r_1^2 + r_2^2}$ is the hyperspherical radius. The convergence of expansion (1) was rigorously studied in Refs. [4,5]. The method applied by Fock [3] to investigate the ^1S helium wave functions was generalized [6,7] for arbitrary systems of charged particles and for states of any symmetry. The Fock expansion was used to treat the two-hydrogen-atom system as the basic one for all subsequent calculations in the theory of dispersion forces [8]. The work of Fock was extended by expansion $\psi_{2,0}$ into hyperspherical harmonics (HH) [9,10]. The Fock expansion was somewhat generalized [11] to be applicable to any S state and its first two terms were determined. The first numerical solution of the equations for the Fock coefficients was presented in Ref. [12]. The most comprehensive investigation of the methods of derivation and calculation of the angular Fock coefficients was presented in the works of Abbott, Gottschalk and Maslen [13–15]. Methods for simplifying the recurrence relations generated by the Fock expansion (1) were used [13] to determine the highest-power logarithmic terms to sixth order. The wave function for S states was given to second order in r as single and double infinite sums [13]. The results of Ref. [14] hint at the existence of a closed-form wave function for the few-body system. The closed form of the heliumlike wave function including terms up to second order in r for ^1S states and up to fourth order for ^3S states was derived in [15].

In this paper we build on the work in [13] and therefore we try to adhere to the terminology used in that article. We correct some substantial errors or misprints made in the final formulas for $\psi_{2,0}$, which is the basis for derivation of the representations for $\psi_{k,p}$ with $k > 2$. We apply different techniques to calculate the angular Fock coefficients (AFCs) and to reduce some of them to the form of the one-dimensional series with fast convergence. This technique is close to that used in [15]. We separate the AFCs into the components associated with definite powers of the nucleus charge and present all components of $\psi_{4,1}$ and the majority of the components of $\psi_{3,0}$.

We extensively use all the tools of the Wolfram *Mathematica* program [16]. Its most recent version, *Mathematica 10*, will be referred as *Mathematica*. To ensure the correctness of our analytical results, all of them have been subjected to numerical verification.

II. GENERAL APPROACH

The Schrödinger equation for a system of two electrons, in the field of an infinitely massive nucleus, is

$$\left(-\tfrac{1}{2}\Delta + \boldsymbol{V}\right)\Psi = E\Psi, \tag{3}$$

where E is the energy and $\boldsymbol{V}$ is the Coulomb interaction. For a system with nuclear charge Z, it is useful to define the dimensionless potential $V \equiv \boldsymbol{V}r$ or

$$V = \frac{1}{\sqrt{1 - \sin\alpha\cos\theta}} - Z[\csc(\alpha/2) + \sec(\alpha/2)]. \tag{4}$$

The first term on the right-hand side (rhs) of Eq. (4) represents the electron-electron interaction and the second one the electron-nucleus interaction. The Laplacian is

$$\Delta = \frac{1}{r^5}\frac{\partial}{\partial r} r^5 \frac{\partial}{\partial r} - \frac{1}{r^2}\Lambda^2,$$

where the hyperspherical angular momentum (HAM) operator, projected on S states, is

$$\Lambda^2 = -\frac{4}{\sin^2\alpha}\left(\frac{\partial}{\partial\alpha}\sin^2\alpha\frac{\partial}{\partial\alpha} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right). \quad (5)$$

By substituting the Fock expansion (1) into the Schrödinger equation (3), one obtains the Fock recurrence relation (FRR) [13]

$$[\Lambda^2 - k(k+4)]\psi_{k,p} = h_{k,p}, \quad (6a)$$

$$h_{k,p} = 2(k+2)(p+1)\psi_{k,p+1} + (p+1)(p+2)\psi_{k,p+2} - 2V\psi_{k-1,p} + 2E\psi_{k-2,p}. \quad (6b)$$

Atomic units are used throughout the paper. It is important to note that $\psi_{k,p} \equiv 0$ for $k<0$ or $p>[k/2]$ (see, e.g., [13]).

We now solve the FRR (6) to find the angular Fock coefficients $\psi_{k,p}$. It is well known that the FRR can be solved by expanding the AFC in HH of the form (see, e.g., [13])

$$Y_{kl}(\alpha,\theta) = N_{kl}\sin^l\alpha\, C_{k/2-l}^{(l+1)}(\cos\alpha)P_l(\cos\theta),$$
$$k = 0,2,4,\ldots; \quad l = 0,1,2,\ldots,k/2, \quad (7)$$

where $C_n^\nu(x)$ and $P_l(z)$ are Gegenbauer and Legendre polynomials, respectively. The normalization constant is

$$N_{kl} = 2^l l!\sqrt{\frac{(2l+1)(k+2)(k/2-l)!}{2\pi^3(k/2+l+1)!}}, \quad (8)$$

so that

$$\int Y_{kl}(\alpha,\theta)Y_{k'l'}(\alpha,\theta)d\Omega = \delta_{kk'}\delta_{ll'}, \quad (9)$$

where δ_{mn} is the Kronecker delta and the appropriate volume element is

$$d\Omega = \pi^2\sin^2\alpha d\alpha\sin\theta d\theta, \quad \alpha\in[0,\pi], \theta\in[0,\pi]. \quad (10)$$

The HH (7) are the eigenfunctions of the operator Λ^2, with eigenvalues given by $k(k+4)$. They form a complete set of basis functions in $\{\alpha,\theta\}$.

Notice that any general function of α and θ can be expanded in hyperspherical harmonics as

$$\mathcal{F}(\alpha,\theta) = \sum_{n=0}^{\infty}\sum_{l=0}^{n/2}\mathcal{F}_{n,l}Y_{nl}(\alpha,\theta), \quad (11)$$

where the expansion coefficients are

$$\mathcal{F}_{n,l} = \int \mathcal{F}(\alpha,\theta)Y_{nl}(\alpha,\theta)d\Omega. \quad (12)$$

Note that the limits of summation in Eq. (11), as well as in all of the HH expansions throughout the paper, are defined by Eq. (7), which means that the step of summation over the first index of the HH equals 2.

Two important properties of the AFC must be emphasized.

(i) Any AFC $\psi_{k,p}$ can be separated into the independent parts (components)

$$\psi_{k,p}(\alpha,\theta) = \sum_{j=p}^{k-p}\psi_{k,p}^{(j)}(\alpha,\theta)Z^j \quad (13)$$

associated with a definite power of Z, according to the separation of the rhs (6b)

$$h_{k,p}(\alpha,\theta) = \sum_{j=p}^{k-p}h_{k,p}^{(j)}(\alpha,\theta)Z^j \quad (14)$$

of the FRR (6a). Hence, each of the FRRs (6) can be separated into the individual equations (IFRRs) for each component

$$[\Lambda^2 - k(k+4)]\psi_{k,p}^{(j)}(\alpha,\theta) = h_{k,p}^{(j)}(\alpha,\theta). \quad (15)$$

(ii) Any component of the angular Fock coefficient must be finite at each point of the two-dimensional angular space described by the hyperspherical angles $\alpha\in[0,\pi]$ and $\theta\in[0,\pi]$.

It is well known that the general solution of the inhomogeneous equation can be expressed as the sum of the general solution of the associated homogeneous (complementary) equation and the particular solution of the inhomogeneous equation. Note that the linear combination of HH Y_{kl} represents the general solution of the homogeneous equation associated with the inhomogeneous equation (15). It must be emphasized that the HH are defined by Eq. (7) only for even values of k. However, it may be verified that (a) the functions Y_{kl} defined by Eq. (7), but with odd values of k, also are solutions of the homogeneous equation for Eq. (15) and (b) the point $\alpha=\pi$ is a singular one for $Y_{kl}(\alpha,\theta)$ with odd k. It should be emphasized that this point is a pole of the order $l+1$, hence no linear combination of Y_{kl} with different l (for given odd k) can cancel this singularity. The important conclusion is that for odd k the finite particular solution of Eq. (15) represents the physical solution we are looking for. The exception is the case of the particular solution, which is singular at the point $\alpha=\pi$. This singularity can be removed by subtracting the homogeneous solution with equivalent behavior.

For even k, the solution $\sum_l a_{kl}Y_{kl}$ of the homogeneous equation associated with the FRR (6) must be included in the general solution. The coefficients a_{kl} for bound states are determined by ensuring that the wave function is normalizable as $r\to\infty$ (see, e.g., [15]). Hence, these coefficients cannot be determined by analysis of the behavior of the wave function (1) near the triple coalescence point. The exception is the case of $k=2p$, when $h_{2p,p}\equiv 0$ (see, e.g., [13]). Moreover, it was found [17] that a_{20} is identically zero (at least) for the ^1S state by the required exchange symmetry of the spatial part of the wave function. Otherwise, the particular solution of the inhomogeneous equation (15) for the IFRR can contain (in the general case) an admixture of some particular solution of the associated homogeneous equation. The examples for $\psi_{2,0}^{(1)}$ and $\widetilde{\psi}_{2,0}^{(1)}$ obtained in Ref. [15] will be presented in Sec. VI. In light of the foregoing, the physical solutions of the inhomogeneous equation (15), containing an admixture of the solution of the associated homogeneous equation, can be considered as multivalued. Accordingly, the physical solution of Eq. (15), containing no admixture of the solution of the associated homogeneous equation, can be considered as single valued. We present here single-valued solutions, which can be produced by orthogonalization of the obtained component $\psi_{k,p}^{(j)}$ to each of the Y_{kl}. The resulting solutions can be called "pure" because their HH expansions do not contain Y_{kl} for any possible l.

III. PREVIOUS RESULTS

In [13], the angular Fock coefficients were derived for the general Coulomb potential. For the case of the helium isoelectronic sequence the following AFCs become

$$\psi_{1,0}(\alpha,\theta) = -Z\varsigma + \tfrac{1}{2}\xi, \tag{16}$$

$$\psi_{2,1}(\alpha,\theta) = -Z\left(\frac{\pi-2}{3\pi}\right)\sin\alpha\cos\theta, \tag{17}$$

$$\psi_{3,1}(\alpha,\theta) = \frac{Z(\pi-2)}{36\pi}[6Z\varsigma\sin\alpha\cos\theta - \xi(6-5\xi^2)], \tag{18}$$

$$\psi_{4,2}(\alpha,\theta) = \frac{(\pi-2)(5\pi-14)}{180\pi^2}Z^2(1-2\sin^2\alpha\sin^2\theta), \tag{19}$$

where

$$\xi_1 \equiv \frac{r_1}{r} = \cos\left(\frac{\alpha}{2}\right), \quad \xi_2 \equiv \frac{r_2}{r} = \sin\left(\frac{\alpha}{2}\right), \quad \varsigma = \xi_1+\xi_2, \tag{20}$$

$$\xi \equiv \frac{r_{12}}{r} = \sqrt{1-\sin\alpha\cos\theta}. \tag{21}$$

Using *Mathematiaca*, we have verified that the AFCs presented above satisfy the FRR (6).

The derivation of the AFCs $\psi_{k,0}$ presents the most complicated problem. For $k=2$ this problem was successively solved in the works [13–15], where the S states of different symmetry were presented in the natural $\{r_1,r_2,r_{12}\}$ coordinates for the general Coulomb potential. The expression for $\psi_{2,0}$ in the so-called Pluvinage coordinates $\{\zeta,\eta\}$ was presented in Ref. [18]. In Ref. [19] the $\{\zeta,\eta\}$ representation from [18] was transformed into the $\{r_1,r_2,r_{12}\}$ coordinates. Here we present the closed form of the AFC $\psi_{2,0}$ expressed in the hyperspherical angular coordinates $\{\alpha,\theta\}$. The condensed form of this AFC obtained from the results of [15] and adapted to the helium isoelectronic sequence reads

$$\begin{aligned}\psi_{2,0} = \frac{1}{12}(1-2E) + \frac{Z}{6\pi}\bigg\{ & -2\pi y\cos\theta\ln(\varsigma+\xi) \\ & + \pi x\ln\left[\frac{(x+\varsigma\xi)^2}{\varsigma^2(\gamma+x)}\right] + \gamma(2\beta+\pi) \\ & + \pi(y-4\varsigma\xi) + x\beta\left[\ln\left(\frac{\gamma-x}{\gamma+x}\right) + \mathrm{i}(2\alpha-\pi)\right] \\ & + x\alpha\ln\left(\frac{1+\cos\theta}{1-\cos\theta}\right) + \mathrm{i}x\mathcal{L}\bigg\} + Z^2\left(\frac{1}{2}y+\frac{1}{3}\right),\end{aligned} \tag{22}$$

where

$$x = \cos\alpha, \quad y = \sin\alpha, \tag{23}$$

$$\beta = \arcsin(\sin\alpha\cos\theta), \quad \gamma = \xi\sqrt{2-\xi^2}, \tag{24}$$

$$\begin{aligned}\mathcal{L} = {} & \mathrm{Li}_2[e^{\mathrm{i}(\alpha-\beta)}] + \mathrm{Li}_2[-e^{-\mathrm{i}(\alpha-\beta)}] - \mathrm{Li}_2[-e^{-\mathrm{i}(\alpha+\beta)}] \\ & - \mathrm{Li}_2[e^{\mathrm{i}(\alpha+\beta)}].\end{aligned} \tag{25}$$

Here Li_2 is the dilogarithm function and $\mathrm{i} = \sqrt{-1}$. We used the most convenient representation

$$L(\phi) = \frac{\mathrm{i}}{2}[\mathrm{Li}_2(e^{2\mathrm{i}\phi}) - \mathrm{Li}_2(1) - \phi(\phi-\pi)]$$

for the Lobachevsky function $L(\phi)$, which is valid for $0 \leqslant \phi \leqslant \pi$ [20,21].

In the following sections we solve the IFFR (15) for the components $\psi_{k,p}^{(j)}$ of the AFC defined by Eq. (13). We propose special methods for solving Eq. (15) with different kinds of its right-hand sides defined by Eqs. (14) and (6b). First we show that these methods allow us to derive the correct expressions for the components of the AFCs (16)–(19) obtained previously and then we fix the incorrect representation for $\psi_{2,0}$ obtained in [13]. Finally, we derive the components of the AFCs $\psi_{4,1}$ and $\psi_{3,0}$ that were not obtained previously.

IV. TECHNIQUE FOR SOLVING THE IFRR WITH THE SIMPLEST NONSEPARABLE RHS

In this section we discuss the solution of Eq. (15) with the rhs $h_{k,p}^{(j)}$ represented by some polynomial in the variable $\xi \equiv \xi(\alpha,\theta)$ defined by Eq. (21). It follows from Eq. (6b) that $h_{1,0} = -2V$, hence $h_{1,0}^{(0)} = -2/\xi$ represents the simplest example of the rhs mentioned above. We will see that $h_{3,1}^{(1)}$, $h_{3,0}^{(0)}$, $h_{4,1}^{(1)}$, and many others are examples of the rhs of that kind. It is clear that a physical solution of the corresponding equation (15) reduces to a function $\Phi(\xi)$ of a single variable ξ. For example, it follows from Eq. (16) that $\psi_{1,0}^{(0)} = \xi/2$. It can be shown that the result of the direct action of the HAM (5) on a twice differentiable function $\Phi(\xi)$ is

$$\Lambda^2\Phi(\xi) = (\xi^2-2)\Phi''(\xi) + \frac{5\xi^2-4}{\xi}\Phi'(\xi). \tag{26}$$

Then Eq. (15) for $\psi_{k,p}^{(j)}(\alpha,\theta) \equiv \Phi_k(\xi)$ can be rewritten in the form

$$(\xi^2-2)\Phi_k''(\xi) + \frac{5\xi^2-4}{\xi}\Phi_k'(\xi) - k(k+4)\Phi_k(\xi) = \mathrm{h}(\xi), \tag{27}$$

where $h_{k,p}^{(j)}(\alpha,\theta) \equiv \mathrm{h}(\xi)$. The general solution of the homogeneous equation associated with Eq. (27) can be represented in the form

$$\Phi_k^{(h)}(\xi) = c_1\mathrm{u}_k(\xi) + c_2\mathrm{v}_k(\xi), \tag{28}$$

where the linearly independent solutions

$$\mathrm{u}_k(\xi) = \frac{P_{k+3/2}^{1/2}(\xi/\sqrt{2})}{\xi\sqrt[4]{2-\xi^2}}, \quad \mathrm{v}_k(\xi) = \frac{Q_{k+3/2}^{1/2}(\xi/\sqrt{2})}{\xi\sqrt[4]{2-\xi^2}} \tag{29}$$

are expressed via the associated Legendre functions $P_\nu^\mu(x)$ and $Q_\nu^\mu(x)$ of the first and second kinds, respectively. The particular solution of the inhomogeneous equation (27) can be found by the method of variation of parameters, which yields

$$\Phi_k^{(p)}(\xi) = \mathrm{v}_k(\xi)\int^{\xi}\frac{\mathrm{u}_k(\xi')\mathrm{h}(\xi')}{(\xi'^2-2)\mathcal{W}_k(\xi')}d\xi' - \mathrm{u}_k(\xi)\int^{\xi}\frac{\mathrm{v}_k(\xi')\mathrm{h}(\xi')}{(\xi'^2-2)\mathcal{W}_k(\xi')}d\xi', \qquad (30)$$

where the Wronskian has a simple form

$$\mathcal{W}_k(\xi) = \frac{\sqrt{2}(k+2)}{\xi^2(2-\xi^2)^{3/2}}. \qquad (31)$$

It was mentioned in Sec. II that the general solution of Eq. (27) presents a sum of solutions (28) and (30). The coefficients c_1 and c_2 in Eq. (28) must be chosen in such a way that the final solution becomes the physically acceptable one. It may be verified that $\mathrm{u}_k(\xi)$ is divergent, whereas $\mathrm{v}_k(\xi)$ is finite at the point $\xi = \sqrt{2}$ ($\alpha = \pi/2, \theta = \pi$) for all integral k. On the other hand, at the point $\xi = 0$ ($\alpha = \pi/2, \theta = 0$), $\mathrm{u}_k(\xi)$ is divergent for even values of k, whereas $\mathrm{v}_k(\xi)$ is divergent for odd k. This implies the following conclusions. For odd values of k, one should set $c_1 = c_2 = 0$ if the particular solution (30) satisfies the finiteness condition (ii); otherwise the coefficients c_1 and/or c_2 must be chosen in such a way as to remove the divergence. For even values of k, the additional condition of orthogonality of the final solution to $Y_{kl}(\alpha,\theta)$ enables us to obtain the pure solutions (see the end of Sec. II). In some complicated cases (see, e.g., Appendix C) the coupling equation (61) can be applied.

Equation (15), with all of the right-hand sides mentioned at the beginning of this section, can be solved by the method described above. However, for most of the right-hand sides, one can apply the simpler technique described below.

Substituting $\Phi(\xi) = B\xi^n$ into Eq. (26), one obtains the relation

$$\Lambda^2 B\xi^n = Bn\xi^n[n+4-2(n+1)\xi^{-2}],$$

where B is an arbitrary constant, from which one obtains

$$[\Lambda^2 - k(k+4)]B\xi^n = B\xi^n[(n-k)(n+k+4) - 2n(n+1)\xi^{-2}]. \qquad (32)$$

Given Eq. (32), the particular solution (satisfying the finiteness condition) of the corresponding equation

$$[\Lambda^2 - k(k+4)]\Phi_k(\xi) = \mathrm{h}(\xi) \qquad (33)$$

can be found in the form

$$\Phi_k(\xi) = \sum_{i=0}^{i_h-1} B_i\xi^{2i+i_0}, \qquad (34)$$

where $i_0 = 1$ for odd n, $i_0 = 0$ for even n, and i_h equals the number of terms in the polynomial representing $\mathrm{h}(\xi)$. The unknown coefficients B_i can be determined by substituting (34) into Eq. (33), using Eq. (32), and subsequently equating the coefficients of the same powers of ξ.

The FRR are solved in order of increasing k and decreasing p. We calculate the AFCs following this rule. Thus, setting $\psi_{0,0} = 1$, the FRR (6a) for $k = 1$ and $p = 0$ is separated into two

$$(\Lambda^2 - 5)\psi_{1,0}^{(j)} = h_{1,0}^{(j)} \quad (j = 0,1), \qquad (35)$$

where $h_{1,0}^{(0)} = -2/\xi$ (see the beginning of this section). The use of Eqs. (32)–(34) enables us to calculate the component of the AFC

$$\psi_{1,0}^{(0)} = \tfrac{1}{2}\xi. \qquad (36)$$

This result is certainly consistent with Eq. (16). Note that all solutions of Eq. (15) corresponding to the rhs $\mathrm{h}(\xi)$ (except $\psi_{3,0}^{(1c)}$, which is treated in Sec. VII) can be calculated by the simplified method presented by Eqs. (32)–(34).

V. TECHNIQUE FOR SOLVING THE IFRR WITH A SEPARABLE RHS

This section is devoted to the method of solving Eq. (15) with the rhs, represented by the product of functions, each of them depending on only one of the angle variables. According to Eq. (6b), the rhs of Eq. (35) with $j = 1$ has the form

$$h_{1,0}^{(1)} = 2[\csc(\alpha/2) + \sec(\alpha/2)]. \qquad (37)$$

Many components of the rhs, presented in Eq. (6b), have a form of the product

$$h_{k,p}^{(j)}(\alpha,\theta) = P_l(\cos\theta)(\sin\alpha)^l \mathrm{h}(\alpha), \qquad (38)$$

which for $l = 0$ reduces to a function of a single variable α, similar to Eq. (37). For convenience, we have introduced the notation $\mathrm{h}(\alpha) \equiv h_{k,p}^{(j)}(\alpha)$. To derive the corresponding component of the AFCs, we propose the technique described below.

It can be shown [15] that

$$\Lambda^2 P_l(\cos\theta)f(\alpha) = -4P_l(\cos\theta)\left[\frac{\partial^2}{\partial\alpha^2} + 2\cot\alpha\frac{\partial}{\partial\alpha} - \frac{l(l+1)}{\sin^2\alpha}\right]f(\alpha). \qquad (39)$$

Hence, the solution of Eq. (15) with $\psi_{k,p}^{(j)} = P_l(\cos\theta)f(\alpha)$ reduces to finding the function $f(\alpha)$ as a suitable solution of the equation

$$\left[4\frac{\partial^2}{\partial\alpha^2} + 8\cot\alpha\frac{\partial}{\partial\alpha} - \frac{4l(l+1)}{\sin^2\alpha} + k(k+4)\right]f(\alpha) = -(\sin\alpha)^l\mathrm{h}(\alpha). \qquad (40)$$

Setting $f(\alpha) = (\sin\alpha)^l \mathrm{g}(\alpha)$, one obtains

$$4\mathrm{g}''(\alpha) + 8(l+1)\cot\alpha\,\mathrm{g}'(\alpha) + (k-2l)(k+2l+4)\mathrm{g}(\alpha) = -\mathrm{h}(\alpha) \qquad (41)$$

for the function $\mathrm{g}(\alpha) \equiv g_{k,p}^{(j)}(\alpha)$. The required solution of Eq. (15) then becomes

$$\psi_{k,p}^{(j)}(\alpha,\theta) = P_l(\cos\theta)(\sin\alpha)^l\mathrm{g}(\alpha). \qquad (42)$$

To solve Eq. (41) it is convenient to make the change of variable

$$\rho = \tan(\alpha/2), \qquad (43)$$

which coincides with definition $\rho = (1-|x|)/y$ [given by (A11) [13]] for $0 \leqslant \alpha \leqslant \pi/2$, where x and y are defined by Eq. (23). Turning to the variable ρ, one obtains the following differential equation for the function $g(\rho) \equiv \mathrm{g}(\alpha)$, instead of Eq. (41):

$$(1+\rho^2)^2 g''(\rho) + 2\rho^{-1}[1+\rho^2 + l(1-\rho^4)]g'(\rho) + (k-2l)(k+2l+4)g(\rho) = -h(\rho), \tag{44}$$

where $h(\rho) \equiv \mathrm{h}(\alpha)$. Using the method of variation of parameters, one obtains the particular solution of Eq. (44) in the form

$$g(\rho) = v_{kl}(\rho)\int_{\rho_c}^{\rho} \frac{u_{kl}(\rho')h(\rho')}{(1+\rho'^2)^2 W_l(\rho')}d\rho' - u_{kl}(\rho) \times \int_0^{\rho} \frac{v_{kl}(\rho')h(\rho')}{(1+\rho'^2)^2 W_l(\rho')}d\rho', \tag{45}$$

where the linearly independent solutions of the homogeneous equation associated with Eq. (44) are

$$u_{kl}(\rho) = \rho^{-2l-1}(\rho^2+1)^{k/2+l+2} \times {}_2F_1\left(\frac{k+3}{2}, \frac{k}{2} - l + 1; \frac{1}{2} - l; -\rho^2\right), \tag{46a}$$

$$v_{kl}(\rho) = (\rho^2+1)^{k/2+l+2}\, {}_2F_1\left(\frac{k+3}{2}, \frac{k}{2} + l + 2; l + \frac{3}{2}; -\rho^2\right). \tag{46b}$$

Here ${}_2F_1$ is the Gauss hypergeometric function. It is important to note that (a) the corresponding Wronskian

$$W_l(\rho) = -\frac{2l+1}{\rho}\left(\frac{\rho^2+1}{\rho}\right)^{2l+1} \tag{47}$$

is independent of k and (b) for the case of $k = 2l$, the solution $v_{2l,l}(\rho) = 1$ follows directly from Eq. (44).

The lower limits of integration in Eq. (45) must be chosen in such a way as to remove singularities by subtracting the homogeneous solutions with equivalent behavior. This yields $\rho_c = 1$ for even k and $\rho_c = \infty$ for odd k.

One should emphasize that, in fact, the functions in Eq. (46) are represented by rather simple elementary functions. For the particular case of the rhs (37) corresponding to $k = 1$, $p = 0$, $l = 0$, $j = 1$, and $\rho_c = \infty$, one obtains

$$h(\rho) = \frac{2(1+\rho)\sqrt{1+\rho^2}}{\rho}, \quad u_{10}(\rho) = \frac{1-3\rho^2}{\rho\sqrt{1+\rho^2}}, \quad v_{10}(\rho) = \frac{3-\rho^2}{3\sqrt{1+\rho^2}}. \tag{48}$$

Application of the form (45) yields for this case

$$\psi_{1,0}^{(1)} = -\frac{1+\rho}{\sqrt{1+\rho^2}} = -[\sin(\alpha/2) + \cos(\alpha/2)], \tag{49}$$

which certainly corresponds to Eq. (16).

VI. EXPLICIT SOLUTION FOR $\psi_{2,p}$

For the case of $k = 2$ and $p = 1$, the AFC is represented by Eq. (17). Deriving the AFCs $\psi_{k,p}$ with $k = 2p$ is a very simple task. Its simple solution was described in Sec. 4.3 of Ref. [13].

According to (6), the FRR for $k = 2$ and $p = 0$ is

$$(\Lambda^2 - 12)\psi_{2,0} = 8\psi_{2,1} - 2V\psi_{1,0} + 2E. \tag{50}$$

Using Eqs. (4), (16), and (17), one can express Eq. (50) in components

$$(\Lambda^2 - 12)\psi_{2,0}^{(j)} = h_{2,0}^{(j)} \quad (j = 0,1,2), \tag{51}$$

where

$$h_{2,0}^{(0)} = 2E - 1, \tag{52a}$$

$$h_{2,0}^{(1)} = h_{2,0}^{(1a)} + h_{2,0}^{(1b)}, \tag{52b}$$

$$h_{2,0}^{(2)} = -4(1 + \csc\alpha); \tag{52c}$$

$$h_{2,0}^{(1a)} = \frac{2[\sin(\alpha/2) + \cos(\alpha/2)](2\csc\alpha - 3\cos\theta + 3)}{3\sqrt{1 - \sin\alpha\cos\theta}}, \tag{53a}$$

$$h_{2,0}^{(1b)} = \frac{\csc(\alpha/2) + \sec(\alpha/2)}{3\sqrt{1 - \sin\alpha\cos\theta}} - \frac{8(\pi - 2)\sin\alpha\cos\theta}{3\pi}. \tag{53b}$$

Using the technique presented in Sec. V, one obtains

$$u_{20}(\rho) = \frac{1}{\rho} + \rho - \frac{8\rho}{1+\rho^2}, \quad v_{20}(\rho) = \frac{1-\rho^2}{1+\rho^2}. \tag{54}$$

Application of the form (45) for $k = 2$, $p = 0$, $l = 0$, $j = 0$, and $\rho_c = 1$ yields

$$h(\rho) = 2E - 1, \quad \psi_{2,0}^{(0)} = \tfrac{1}{12}(1 - 2E). \tag{55}$$

Similarly, for $k = 2$, $p = 0$, $l = 0$, $j = 2$, and $\rho_c = 1$ one obtains

$$h(\rho) = -\frac{2(1+\rho)^2}{\rho}, \quad \psi_{2,0}^{(2)} = \frac{1}{3} + \frac{\rho}{1+\rho^2} = \frac{1}{3} + \frac{1}{2}\sin\alpha. \tag{56}$$

Specific solution for $\psi_{2,0}^{(1)}$

In Sec. III we presented (without derivation) the closed form of $\psi_{2,0}$ obtained from the results of the work [15]. This form defined by Eq. (22) is very convenient for expressing $\psi_{2,0}$ itself. However, it includes functions (e.g., dilogarithm function with its argument in the form of the exponential function) that are too complex for further mathematical processing required for derivation of the higher-order angular Fock coefficients. For example, according to Eq. (6b), the rhs $h_{3,0}$ of the FRR (6a) for the AFCs $\psi_{3,0}$ contains the term $-2V\psi_{2,0}$. To obtain the particular solution of the corresponding FRR, one needs to apply the integral formula (45) with integrands containing $h_{3,0}$. It is clear that the reduction of the required integration to the analytic form is impossible, whereas the representation of $\psi_{2,0}$ in the form of an infinite single or double series enables us to provide this integration. Such series were presented in [13]. The problem is that, unfortunately, there are too many errors or misprints in the important final formulas and the methods to obtain them have been described rather superficially or not at all. In this paper we rederive these formulas, while describing in detail our method, which differs from that of [13].

It is shown in Appendix A that the following representation is valid:

$$\psi_{2,0}^{(1)} = -\tfrac{1}{3}[\sin(\alpha/2)+\cos(\alpha/2)]\sqrt{1-\sin\alpha\cos\theta}+\chi_{20}(\alpha,\theta), \tag{57}$$

where the HH expansion for the function χ_{20} reads

$$\chi_{20}(\alpha,\theta) = \frac{2}{3}\sum_{nl}{}' \frac{D_{nl}}{(n-2)(n+6)}Y_{nl}(\alpha,\theta), \tag{58}$$

with D_{nl} defined by Eq. (A21). The limits of this summation are defined by Eq. (7) (replacing k by n, of course). The prime indicates that $n=2$ must be omitted from the summation. Note that (58) requires a double summation (over n and l), which converges slowly.

In [13] the following single series representation was proposed:

$$\chi_{20}(\alpha,\theta) = \sum_{l=0}^{\infty} P_l(\cos\theta)(\sin\alpha)^l\sigma_l(\alpha). \tag{59}$$

The problem is that the technique used to derive the functions σ_l is complex and ambiguous and the final formulas [(A19), (A22), and (A24) from [13]] were presented with errors or misprints. We present here an alternative method to derive σ_l.

Suppose that a regular function, having the unnormalized HH expansion (11), can be represented in the form of an infinite single series

$$\mathcal{F}(\alpha,\theta) = \sum_{l=0}^{\infty} P_l(\cos\theta)Q_l(\alpha). \tag{60}$$

Multiplication of the right-hand sides of Eqs. (11) and (60) by $Y_{2l'l'}(\alpha,\theta) \equiv (\sin\alpha)^{l'}P_{l'}(\cos\theta)$ and subsequent integration over the angular space (10) enables one to obtain

$$\mathcal{F}_{2l,l} = \frac{(l+1)!}{\sqrt{\pi}\Gamma(l+3/2)}\int_0^{\pi} Q_l(\alpha)(\sin\alpha)^{l+2}d\alpha \tag{61}$$

for the coefficients defined in Eq. (12). We used Eq. (8), the orthogonality equation (9) for HHs, and the well-known formula of orthogonality for the Legendre polynomials. Setting $Q_l(\alpha)=(\sin\alpha)^l\sigma_l(\alpha)$, where $\sigma_l(\alpha)$ is included in Eq. (59), using the expansion (58) and representation (A21), and simplifying, one obtains instead of the relation (61)

$$\begin{aligned}3(l-1)(l+1)(l+3)\int_0^{\pi}(\sin\alpha)^{2l+2}\sigma_l(\alpha)d\alpha - 1\\ = \frac{\sqrt{\pi}\Gamma(l+3/2)}{2^{l+2}l!}\,{}_3F_2\left(\frac{l+1}{2},\frac{l}{2}+1,l+\frac{3}{2};l+2,l+2;1\right).\end{aligned} \tag{62}$$

Note that the case of $l=1$ cannot be used in Eq. (62), because the term with Y_{21} is excluded from the HH expansion (58). It is clear that for $l=1$ the integral on the left-hand side (lhs) of Eq. (62) just equals zero.

Application of the relations (40)–(44) and (62) enables us (details can be found in Appendix B) to derive the following representations, which are valid in the range $\alpha \in [0,\pi/2]$:

$$\sigma_0 = \frac{1}{12}\left\{\left(2y-\frac{1}{y}\right)\alpha + x[1+2\ln(x+1)] - y - 2\right\}, \tag{63}$$

$$\begin{aligned}\sigma_1 = &\frac{1}{24\pi}\left[\left(\frac{1}{\rho^3}+\frac{9}{\rho}-9\rho-\rho^3\right)\arctan\rho\right.\\ &\left.-\frac{1}{\rho^2}-\rho^2-\pi-\frac{8}{3}+16G\right]\\ &-\frac{\rho(\rho^2-6\rho+3)}{72}+\frac{1}{6}\ln\left(\frac{1+\rho^2}{4}\right),\end{aligned} \tag{64}$$

$$\begin{aligned}\sigma_l = &-\frac{2^{-l-1}}{3}\left\{(1+\rho^2)^{l-1}\left[\frac{l\rho^3}{(l+1)(l+2)}-\frac{\rho^2}{l}\right.\right.\\ &\left.+\frac{\rho}{l+1}-\frac{l+1}{l(l-1)}\right]+\frac{(l-2)!\Gamma((l+1)/2)}{\Gamma(l+1/2)\Gamma(l/2+1)}\\ &\left.\times\,{}_2F_1\left(\frac{l-1}{2},\frac{l+3}{2};l+\frac{3}{2};y^2\right)\right\}\quad (l\geqslant 2),\end{aligned} \tag{65}$$

where $G \simeq 0.915\,965\,6$ is Catalan's constant and x,y and ρ are defined by Eqs. (23) and (48), respectively. For $\pi/2<\alpha\leqslant\pi$, one needs to replace α by $\pi-\alpha$, x by $-x$, and ρ by $1/\rho$. One can optionally set $\rho=(1-|x|)/y$, which is valid for the whole range $\alpha\in[0,\pi]$. Note that the factor 1/4 was missing in the corresponding expression (A24) from [13]. Moreover, we should emphasize that the representation (A22) from [13] for σ_1 is not correct, because it does not satisfy the inhomogeneous differential equation (B8) and does not agree with the definition (66) presented below.

Using series rearrangement (see [13,22]) of the double summation in Eq. (58), we obtain another representation

$$\sigma_l = \frac{1}{6}\sum_{m=\delta_{l1}}^{\infty}\frac{D_{4m+2l,l}}{(2m+l-1)(2m+l+3)}C_{2m}^{(l+1)}(x), \tag{66}$$

which is valid for any $l\geqslant 0$. The convergence of expansion (66) is very slow, however, it can be used to verify the correctness of Eqs. (63)–(65).

The component $\psi_{2,0}^{(1)}$ is represented by Eqs. (57) and (58). In contrast, using definition (13), one can separate the component $\widetilde{\psi}_{2,0}^{(1)}$ out of the AFCs $\psi_{2,0}$ defined by Eq. (22). We have intentionally put a tilde over ψ because the components obtained by these two different methods do not coincide at any point of the angular space $\{\alpha,\theta\}$, since both representations mentioned above are not the pure solutions (see the end of Sec. II) of Eq. (51). In other words, the HH expansions of both components include some admixture of the homogeneous solutions $Y_{2,l}$ $(l=0,1)$ of Eq. (51). It is clear that χ_{20} cannot contain such an admixture by definition (58). Thus, using definitions (57) and (12), one obtains the coefficient

$$\begin{aligned}C_{21}^{(p)} = &N_{21}^2\int Y_{21}(\alpha,\theta)\{-\tfrac{1}{3}[\sin(\alpha/2)+\cos(\alpha/2)]\\ &\times\sqrt{1-\sin\alpha\cos\theta}\}d\Omega = \frac{\pi+4}{9\pi}\end{aligned}$$

for the unnormalized HH, $Y_{21}(\alpha,\theta)=\sin\alpha\cos\theta$ in the HH expansion of $\psi_{2,0}^{(1)}$. It can be verified that $C_{20}^{(p)}=0$. Thus, one obtains the pure component in the form $\psi_{2,0}^{(1p)}=\psi_{2,0}^{(1)}-C_{21}^{(p)}\sin\alpha\cos\theta$. It is clear that another way to obtain the pure component $\psi_{2,0}^{(1p)}$ is to subtract $C_{21}^{(p)}$ from $\sigma_1(\alpha)$ defined by Eq. (64). The same method can be used to obtain the pure component $\widetilde{\psi}_{2,0}^{(1p)}=\widetilde{\psi}_{2,0}^{(1)}-\widetilde{C}_{21}^{(p)}\sin\alpha\cos\theta$ based on the analytic expression (22). Numerical integration yields the following value of the coefficient:

$$\widetilde{C}_{21}^{(p)} = N_{21}^2 \int Y_{21}(\alpha,\theta)\widetilde{\psi}_{2,0}^{(1p)}(\alpha,\theta)d\Omega = 0.315\,837\,352,$$

whereas $\widetilde{C}_{20}^{(p)} = 0$. The pure components $\psi_{2,0}^{(1p)}$ and $\widetilde{\psi}_{2,0}^{(1p)}$ certainly coincide for any angular point under consideration.

VII. SOLUTIONS FOR AFCs WITH $k > 2$

For $k = 3$ and $p = 1$, the FRR (6) reduces to

$$[\Lambda^2 - 21]\psi_{3,1} = -2V\psi_{2,1}, \tag{67}$$

where V and $\psi_{2,1}$ are defined by Eqs. (4) and (17), respectively. According to Eqs. (13)–(15), Eq. (67) can be represented in components as

$$[\Lambda^2 - 21]\psi_{3,1}^{(j)} = h_{3,1}^{(j)} \quad (j = 1,2), \tag{68}$$

where

$$h_{3,1}^{(1)} = 2B\left(\frac{1}{\xi} - \xi\right), \tag{69a}$$

$$h_{3,1}^{(2)} = -4B\cos\theta[\sin(\alpha/2) + \cos(\alpha/2)], \tag{69b}$$

with the constant $B = (\pi - 2)/3\pi$ and ξ defined by Eq. (21). Using the technique described in Sec. IV, one easily find the component

$$\psi_{3,1}^{(1)} = B\xi\left(\tfrac{5}{12}\xi^2 - \tfrac{1}{2}\right). \tag{70}$$

To solve Eq. (68) with $j = 2$, one can apply the technique described in Sec. V. Thus, for the case of $k = 3$, $p = 1$, $l = 1$, and $\rho_c = \infty$, one obtains

$$h(\rho) = -2B\frac{(\rho+1)\sqrt{\rho^2+1}}{\rho}, \quad u_{3,1}(\rho) = \frac{1 + 14\rho^2 - 35\rho^4}{\rho^3\sqrt{1+\rho^2}},$$
$$v_{3,1} = \frac{35 - 14\rho^2 - \rho^4}{35\sqrt{1+\rho^2}}. \tag{71}$$

Application of the formula (45) then yields

$$g(\rho) = \frac{B(1+\rho)}{2\sqrt{1+\rho^2}},$$
$$\psi_{3,1}^{(2)} = g\sin\alpha\cos\theta = \frac{B}{2}\left[\sin\left(\frac{\alpha}{2}\right) + \cos\left(\frac{\alpha}{2}\right)\right]\sin\alpha\cos\theta. \tag{72}$$

The components represented by Eqs. (70) and (72) are certainly consistent with the AFC $\psi_{3,1}$ presented by Eq. (18).

AFCs that were not calculated previously

Let us consider the FRR for the following two cases: (i) $k = 3$ and $p = 0$ and (ii) $k = 4$ and $p = 1$. According to (6) one obtains

$$(\Lambda^2 - 21)\psi_{3,0} = 10\psi_{3,1} - 2V\psi_{2,0} + 2E\psi_{1,0}, \tag{73}$$

$$(\Lambda^2 - 32)\psi_{4,1} = 24\psi_{4,2} - 2V\psi_{3,1} + 2E\psi_{2,1}. \tag{74}$$

Using Eqs. (13)–(15) and the AFCs previously determined, one can represent the FRRs (73) and (74) in components as follows:

$$(\Lambda^2 - 21)\psi_{3,0}^{(j)} = h_{3,0}^{(j)} \quad (j = 0,1,2,3), \tag{75}$$

$$(\Lambda^2 - 32)\psi_{4,1}^{(j)} = h_{4,1}^{(j)} \quad (j = 1,2,3), \tag{76}$$

where

$$h_{3,0}^{(0)} = 2E\psi_{1,0}^{(0)} - 2V_0\psi_{2,0}^{(0)} = E\xi + \frac{2E-1}{6\xi}, \tag{77}$$

$$h_{3,0}^{(1)} = 2E\psi_{1,0}^{(1)} + 2V_1\psi_{2,0}^{(0)} - 2V_0\psi_{2,0}^{(1)} + 10\psi_{3,1}^{(1)} = -\frac{2}{\xi}\chi_{20}(\alpha,\theta) + \frac{5(\pi-2)(5\xi^3 - 6\xi)}{18\pi} + \left(\frac{1-2E}{3}\right) \times \frac{\varsigma}{\sin\alpha} + 2\left(\frac{1}{3} - E\right)\varsigma, \tag{78}$$

$$h_{3,0}^{(2)} = 2V_1\psi_{2,0}^{(1)} - 2V_0\psi_{2,0}^{(2)} + 10\psi_{3,1}^{(2)} = \frac{4\varsigma}{\sin\alpha}\chi_{20}(\alpha,\theta) - \frac{2}{3}\left(2\xi + \frac{1}{\xi}\right) - \frac{4\xi}{3\sin\alpha} - \frac{\sin\alpha}{\xi} + \frac{5(\pi-2)}{3\pi}\varsigma\sin\alpha\cos\theta, \tag{79}$$

$$h_{3,0}^{(3)} = 2V_1\psi_{2,0}^{(2)} = \frac{2}{3}\left(\frac{2}{\sin\alpha} + 3\right)\varsigma, \tag{80}$$

$$h_{4,1}^{(1)} = 2E\psi_{2,1}^{(1)} - 2V_0\psi_{3,1}^{(1)} = \frac{\pi-2}{18\pi}[6(1-2E) + (12E-5)\xi^2], \tag{81}$$

$$h_{4,1}^{(2)} = 2V_1\psi_{3,1}^{(1)} - 2V_0\psi_{3,1}^{(2)} + 24\psi_{4,2}^{(2)} = \frac{\pi-2}{15\pi^2} \times \left\{2(5\pi - 14)\left[1 - \frac{4}{3}\sin^2\alpha + \frac{4}{3}\sin^2\alpha P_2(\cos\theta)\right] + 5\pi\varsigma\left[\frac{5}{3\sin\alpha}\xi^3 + \left(1 - \frac{2}{\sin\alpha}\right)\xi - \frac{1}{\xi}\right]\right\}, \tag{82}$$

$$h_{4,1}^{(3)} = 2V_1\psi_{3,1}^{(2)} = \frac{\pi-2}{3\pi}\left[2 + \tan\left(\frac{\alpha}{2}\right) + \cot\left(\frac{\alpha}{2}\right)\right]\sin\alpha\cos\theta. \tag{83}$$

Here V_0 and V_1 are defined by the relation $V = V_0 - ZV_1$ and Eq. (4), whereas ς, ξ, and χ_{20} are defined by Eqs. (20), (21), and Eq. (59), respectively.

The right-hand sides $h_{3,0}^{(0)}$ and $h_{4,1}^{(1)}$ involve functions of only ξ, so that the corresponding components $\psi_{3,0}^{(0)}$ and $\psi_{4,1}^{(1)}$ can be derived by the simplified method described in Sec. IV [see Eqs. (32)–(34)]. The results are presented in Table I. The components $\psi_{3,0}^{(3)}$ and $\psi_{4,1}^{(3)}$, obtained by the technique described in Sec. V, are presented in Table I as well.

Extending the separation presented in Sec. II, one can obtain the solutions to the majority of subcomponents of the

TABLE I. Simplest subcomponents of the solutions and the corresponding right-hand sides of the FRRs.

k	p	j	$h_{k,p}^{(j)}$	$\psi_{k,p}^{(j)}$
1	0	0	$-2/\xi$	$\xi/2$
3	1	1	$\frac{2(\pi-2)}{3\pi}(\xi^{-1}-\xi)$	$\frac{\pi-2}{36\pi}(5\xi^2-6)\xi$
3	0	0	$E\xi+\frac{2E-1}{6}\xi^{-1}$	$\xi[\frac{1-2E}{24}+\frac{E-2}{72}\xi^2]$
3	0	$1a$	$-\frac{5(\pi-2)}{3\pi}\xi$	$\frac{5(\pi-2)}{72\pi}\xi^3$
3	0	$2a$	$-\frac{2}{3}(2\xi+\xi^{-1})$	$\frac{1}{6}\xi(1-\frac{1}{3}\xi^2)$
4	1	1	$\frac{\pi-2}{18\pi}[6(1-2E)+(12E-5)\xi^2]$	$\frac{\pi-2}{2880\pi}[3(32E-15)-8(12E-5)\xi^2]$
3	0	$1b$	$\frac{1}{3}\varsigma[\frac{1-2E}{\sin\alpha}+2(1-3E)]$	$\frac{1}{36}\varsigma[4E-1+(E-1)\sin\alpha]$
3	0	3	$\frac{2}{3}(\frac{2}{\sin\alpha}+3)\varsigma$	$-\frac{1}{36}(2+5\sin\alpha)\varsigma$
4	1	$2b$	$\frac{2(\pi-2)(5\pi-14)}{45\pi^2}(3-4\sin^2\alpha)$	$\frac{(\pi-2)(5\pi-14)}{540\pi^2}\csc\alpha[\alpha\cos(3\alpha)-\frac{1}{6}\sin(3\alpha)]$
4	1	3	$\frac{\pi-2}{3\pi}[2+\tan(\alpha/2)+\cot(\alpha/2)]\sin\alpha\cos\theta$	$-\frac{\pi-2}{120\pi}(4+5\sin\alpha)\sin\alpha\cos\theta$

remaining components represented by Eqs. (75) and (76). In particular, let us perform the additional separations

$$\psi_{3,0}^{(1)}=\psi_{3,0}^{(1a)}+\psi_{3,0}^{(1b)}+\psi_{3,0}^{(1c)}+\psi_{3,0}^{(1d)}, \tag{84}$$

$$\psi_{3,0}^{(2)}=\psi_{3,0}^{(2a)}+\psi_{3,0}^{(2b)}+\psi_{3,0}^{(2c)}+\psi_{3,0}^{(2d)}, \tag{85}$$

$$\psi_{4,1}^{(2)}=\psi_{4,1}^{(2b)}+\psi_{4,1}^{(2c)}+\psi_{4,1}^{(2d)}. \tag{86}$$

Subcomponents $\psi_{3,0}^{(1a)}$ and $\psi_{3,0}^{(2a)}$ are calculated using Eqs. (32)–(34) and are presented in Table I together with the corresponding right-hand sides. Subcomponents $\psi_{3,0}^{(1b)}$ and $\psi_{4,1}^{(2b)}$, obtained by the method described in Sec. V, are presented in Table I together with the corresponding right-hand sides. Note that the expression for $\psi_{4,1}^{(2b)}$ presented in Table I is correct for $0\leqslant\alpha\leqslant\pi/2$, whereas for $\pi/2<\alpha\leqslant\pi$ one should replace α by $\pi-\alpha$. The remaining right-hand sides are

$$h_{3,0}^{(1c)}=\frac{25(\pi-2)}{18\pi}\xi^3,\quad h_{3,0}^{(1d)}=-\frac{2}{\xi}\chi_{20}(\alpha,\theta), \tag{87}$$

$$h_{3,0}^{(2b)}=\frac{5(\pi-2)}{3\pi}\varsigma\sin\alpha\cos\theta,\quad h_{3,0}^{(2c)}=-\frac{4\xi}{3\sin\alpha},$$
$$h_{3,0}^{(2d)}=\frac{4\varsigma}{\sin\alpha}\chi_{20}(\alpha,\theta), \tag{88}$$

$$h_{4,1}^{(2c)}=\frac{8(\pi-2)(5\pi-14)}{45\pi^2}\sin^2\alpha\,P_2(\cos\theta), \tag{89a}$$

$$h_{4,1}^{(2d)}=\frac{\pi-2}{3\pi}\left[\sin\left(\frac{\alpha}{2}\right)+\cos\left(\frac{\alpha}{2}\right)\right]\times\left[\frac{5}{3\sin\alpha}\xi^3+\left(1-\frac{2}{\sin\alpha}\right)\xi-\frac{1}{\xi}\right]. \tag{89b}$$

To calculate the subcomponent $\psi_{3,0}^{(1c)}$, one can use the particular solution presented in Sec. IV. Setting $k=3$ and $\mathrm{h}(\xi)=\xi^3$ in Eq. (30), one obtains

$$\Phi_3^{(p)}(\xi)=\frac{1}{8}\left[\frac{\xi(3-5\xi^2)}{6}-\frac{(4\xi^4-10\xi^2+5)\arcsin(\xi/\sqrt{2})}{5\sqrt{2-\xi^2}}\right].$$

The problem is that $\Phi_3^{(p)}(\xi)$ is singular at the point $\xi=\sqrt{2}$ ($\alpha=\pi/2,\theta=\pi$). This singularity can be eliminated with the help of the function $\mathrm{u}_3(\xi)$ [see Eq. (29)] representing a solution of the associated homogeneous equation and having the same kind of singularity. Thus, given that

$$x_1=\lim_{\xi\to\sqrt{2}}\Phi_3^{(p)}(\xi)\sqrt{\xi-\sqrt{2}}=\frac{\mathrm{i}\pi}{80\times 2^{3/4}},$$

$$x_2=\lim_{\xi\to\sqrt{2}}\mathrm{u}_3(\xi)\sqrt{\xi-\sqrt{2}}=-\frac{\mathrm{i}}{\sqrt{2\pi}},$$

one obtains finally

$$\psi_{3,0}^{(1c)}(\alpha,\theta)=\frac{25(\pi-2)}{18\pi}\left[\Phi_3^{(p)}(\xi)-\frac{x_1}{x_2}\mathrm{u}_3(\xi)\right]=\frac{25(\pi-2)}{144\pi}\left[\frac{\xi(3-5\xi^2)}{6}+\frac{(4\xi^4-10\xi^2+5)\arccos(\xi/\sqrt{2})}{5\sqrt{2-\xi^2}}\right]. \tag{90}$$

Using the technique presented in Sec. V, one obtains for subcomponents with the right-hand sides $h_{3,0}^{(2b)}$ and $h_{4,1}^{(2c)}$ defined by Eqs. (88) and (89a), respectively,

$$\psi_{3,0}^{(2b)}=\frac{(\pi-2)(1+\rho^2)^{-3/2}}{288\pi\rho^2}[\alpha-2\rho+14\alpha\rho^2-35\rho^3(\pi-\alpha+2)-35\rho^4(\alpha+2)+(14\rho^5+\rho^7)(\pi-\alpha)-2\rho^6]\cos\theta, \tag{91}$$

$$\psi_{4,1}^{(2c)}=-\frac{(\pi-2)(5\pi-14)}{8640\pi^2}\sin^2\alpha\,P_2(\cos\theta)\left\{\frac{187}{15}+\frac{1}{4\rho^5}\times[\alpha(\rho^2-1)(3\rho^8+28\rho^6+178\rho^4+28\rho^2+3)+6\rho(\rho^8+8\rho^6+8\rho^2+1)]\right\}, \tag{92}$$

where ρ is defined by Eq. (43). Representations (91) and (92) are correct, as previously, for $\alpha\in[0,\pi/2]$. For $\pi/2<\alpha\leqslant\pi$ one should replace ρ by $1/\rho$, and α by $\pi-\alpha$. At first sight it may seem that the rhs of Eq. (91) diverges as $\alpha\to 0$. However,

TABLE II. Numerical coefficients $\mu_{ln}^{(1)}$ (columns 2–6) and λ_l included in Eq. (C14).

l \ n	0	1	2	3	4	λ_l
3	−522720	−1051985	255552	−90435	227872	495
4	−3953664	−8398510	3727360	−419475	3335168	2002
5	−30351360	−97464675	44154880	−6969375	39739392	6552
6	−2882764800	−9137296644	5778063360	−189629055	5234966528	235620
7	−270052392960	−1196759060145	696562155520	−65054175615	635252473856	7759752
8	−2853364039680	−12357527011830	9051962343424	−67609913085	8305992794112	27387360
9	−5615652962304	−31944952238815	21219319480320	−1350136582575	19579564720128	17341632
10	−132056403148800	−733168078648720	580357875302400	1595198130669	538208290996224	127481640

it may be verified that it is finite and moreover $\psi_{3,0}^{(2b)}$ tends to zero as $\alpha \to 0$.

For subcomponent $\psi_{4,1}^{(2d)}$ corresponding to the rhs (89b) we use the representation

$$\psi_{4,1}^{(2d)}(\alpha,\theta) = \sum_{l=0}^{\infty} P_l(\cos\theta)(\sin\alpha)^l \mathrm{t}_l(\alpha), \tag{93}$$

which is similar to Eq. (59). The function $\tau_l(\rho) \equiv \mathrm{t}_l(\alpha)$ can be represented (details can be found in Appendix C) in the form

$$\tau_0(\rho) = \frac{\pi-2}{108\pi(\rho^2+1)^2}\left\{\frac{1}{15}(19\rho^5+75\rho^4-60\rho^3+30\rho^2 +45\rho-45)+\left(\rho^5-15\rho^3+15\rho-\frac{1}{\rho}\right)\arctan\rho +(3\rho^4-10\rho^2+3)\left[\frac{247}{75\pi}-\frac{4G}{\pi}-\ln\left(\frac{\rho^2+1}{4}\right)\right]\right\}, \tag{94}$$

$$\tau_1(\rho) = -\frac{\pi-2}{302400\pi\rho^2(\rho^2+1)}\left\{1268\rho^7-2505\rho^6+1960\rho^5 +32\,263\rho^4+18900\rho^3+18\,305\rho^2-735 +735\left[\left(\rho^7+20\rho^5-90\rho^3+20\rho+\frac{1}{\rho}\right)\arctan\rho -32\rho^2(\rho^2-1)\ln\left(\frac{\rho^2+1}{2}\right)\right]\right\}, \tag{95}$$

$$\tau_2(\rho) = \frac{\pi-2}{14\,175\pi\rho^4}\left\{\frac{14}{\pi}\left(41-150G+\frac{3765\pi}{128}\right)\rho^4 +\frac{5}{128}(672\rho^9-465\rho^8+760\rho^7-6720\rho^6 -5880\rho^5+2520\rho^2+315) +525\left[\frac{(\rho^2-1)}{128}\left(3\rho^7+28\rho^5+178\rho^3+28\rho+\frac{3}{\rho}\right) \times\arctan\rho-\rho^4\ln\left(\frac{\rho^2+1}{4}\right)\right]\right\}, \tag{96}$$

$$\tau_l(\rho) = \frac{(\pi-2)(\rho^2+1)^{l-2}}{135\pi\, 2^{3(l+1)}\lambda_l\rho^{2l+1}}\left[\rho^{2l+2}\sum_{n=0}^{4}\mu_{ln}^{(1)}\rho^n+\rho\sum_{n=0}^{l}\mu_{ln}^{(2)}\rho^{2n} -\mu_{l0}^{(2)}(\rho^2+1)^6\arctan\rho\sum_{n=0}^{l-3}\mu_{ln}^{(3)}\rho^{2n}\right]+A_2(l)v_{4l}(\rho), \quad (l\geqslant 3), \tag{97}$$

where G is Catalan's constant and the function $v_{4l}(\rho)$ is defined by Eq. (46b) for $k=4$. The $A_2(l)$ factors are presented in Eqs. (C29)–(C31) and the coefficients $\mu_{nl}^{(i)}$ $(i=1,2,3)$ and λ_l can be found in Tables II and III. It is important that the $A_2(l)$ are equal to zero for odd l. Note that for $l=1$ we have obtained the admixture coefficient $\mathcal{F}_{41}=0$ (see Appendix C). This means that for all odd l in expansion (93), the solution of the form (45) just gives the correct results for τ_l satisfying the coupling equation (61) or the equivalent equation (C15).

Remember that the general solution of the FRR (74) must contain the addition of the form $a_{40}Y_{40}+a_{41}Y_{41}+a_{42}Y_{42}$, where the coefficients a_{4l} can be determined only by analysis of the asymptotic behavior of the wave function (see the end of Sec. III). Using Eqs. (11) and (12), one can detect the presence of an admixture of the HH Y_{4l} in any component $\psi_{4,1}^{(j)}$ and then get rid of such an admixture, just as was done in Sec. VI for $\psi_{2,0}^{(1)}$. Therefore, only the pure components $\psi_{4,1}^{(j)}$ are presented in Eqs. (92)–(97) and Table I.

The last subcomponent we present here is $\psi_{3,0}^{(2c)}$. It is the physical solution of Eq. (75) with its rhs $h_{3,0}^{(2c)}$ defined by Eq. (88). To apply the technique described in Sec. V, we again use the single sum representation

$$\psi_{3,0}^{(2c)}(\alpha,\theta) = \sum_{l=0}^{\infty} P_l(\cos\theta)(\sin\alpha)^l\phi_l(\rho), \tag{98}$$

where ρ is defined by Eq. (43). The function $\phi_l(\rho)$ is obtained (details can be found in Appendix D) in the form

$$\phi_l(\rho) = \phi_l^{(p)}(\rho)+c_l v_{3l}(\rho), \tag{99}$$

where the reduction of the formula (46b) for $k=3$ and $0\leqslant\rho\leqslant 1$ yields

$$v_{3l}(\rho) = (\rho^2+1)^{l-3/2}\left[\frac{(2l-3)(2l-1)}{(2l+3)(2l+5)}\rho^4 +\frac{2(2l-3)}{2l+3}\rho^2+1\right]. \tag{100}$$

TABLE III. Numerical coefficients $\mu_{ln}^{(2)}$ and $\mu_{ln}^{(3)}$ included in Eq. (C14).

l \ μ	$\mu_{ln}^{(2)}$ $(n = 0,1,\ldots,l)$	$\mu_{ln}^{(3)}$ $(l = 0,\ldots,l-3)$
3	$\{-72765, -412335, -960498, -2625678\}$	$\{1\}$
4	$\{1273965, 5945170, 9597203, 3639900, -14747117\}$	$\{1, -1\}$
5	$\{-8513505, -34999965, -45846801, -10135125, 10135125, -146271983\}$	$\{1, -\frac{14}{9}, 1\}$
6	$\{1456717185, 5473725180, 6250641012, 983757060, -777756650,$ $983757060, -13174180236\}$	$\{1, -\frac{21}{11}, \frac{21}{11}, -1\}$
7	$\{-101948591745, -358127104335, -370912265724, -46034728740, 31617756170,$ $-31617756170, 46034728740, -1585784814084\}$	$\{1, -\frac{28}{13}, \frac{378}{143}, -\frac{28}{13}, 1\}$
8	$\{1804845357315, 6016151191050, 5790931172103, 602937350136, -374632125450,$ $328821494780, -374632125450, 602937350136, -16476813837561\}$	$\{1, -\frac{7}{3}, \frac{42}{13}, -\frac{42}{13}, \frac{7}{3}, -1\}$
9	$\{-2508790869585, -8018292387105, -7290251115147, -663280843995, 381499104294,$ $-306553004730, 306553004730, -381499104294, 663280843995, -39837938484597\}$	$\{1, -\frac{42}{17}, \frac{63}{17}, -\frac{924}{221},$ $\frac{63}{17}, -\frac{42}{17}, 1\}$
10	$\{95748321954285, 295643941472880, 256791268415682, 21004496987760,$ $-11353909326045, 8538680495904, -7845295711140, 8538680495904,$ $-11353909326045, 21004496987760, -931653655078718\}$	$\{1, -\frac{49}{19}, \frac{1323}{323}, -\frac{1617}{323},$ $\frac{1617}{323}, -\frac{1323}{323}, \frac{49}{19}, -1\}$

The particular solution $\phi_l^{(p)}$ of the corresponding differential equation in ρ [see Eq. (D4)] can be represented in the form

$$\phi_l^{(p)}(\rho) = \frac{2^{-l}(\rho^2+1)^{l-3/2}}{3(2l-3)(2l-1)(2l+3)(2l+5)} \times \left[2f_{1l}(\rho) + \frac{2f_{2l}(\rho)+f_{3l}(\rho)}{2l+1}\right], \tag{101}$$

where

$$f_{1l}(\rho) = [9-4l(l+2)]\rho + (13-4l^2)\rho^3, \tag{102}$$

$$f_{2l}(\rho) = [(2l-3)(2l-1)\rho^4 + 2(2l-3)(2l+5)\rho^2 + (2l+3)(2l+5)]\arctan(\rho), \tag{103}$$

$$f_{3l}(\rho) = -[(2l+3)(2l+5)\rho^4 + 2(2l-3)(2l+5)\rho^2 + (2l-3)(2l-1)]\frac{\rho}{l+1}\,{}_2F_1(1,l+1;l+2;-\rho^2). \tag{104}$$

Note that the hypergeometric function presented in Eq. (104) can be expressed through elementary functions [see Eq. (D8)]. The coefficient c_l is defined by Eqs. (D17)–(D25). It is clear that formulas (99)–(104) are valid for $0 \leqslant \alpha \leqslant \pi/2$. For $\pi/2 < \alpha \leqslant \pi$, one should replace ρ by $1/\rho$.

There are only two subcomponents $\psi_{3,0}^{(1d)}$ and $\psi_{3,0}^{(2d)}$ that were not determined in this research. The reason is that the right-hand sides $h_{3,0}^{(1d)}$ and $h_{3,0}^{(2d)}$ of the corresponding IFRRs [see Eqs. (87) and (88)] include the function χ_{20} presented in expansion (59), which complicates the calculations and dramatically increases the size of the final formulas.

VIII. CONCLUSION

Solutions of the Fock recurrence relations (6) were used to derive the angular coefficients $\psi_{k,p}(\alpha,\theta)$ of the Fock expansion (1) describing the S-state wave function of the two-electron atomic system. The hyperspherical coordinates with hyperspherical angles (2) were applied.

The FRRs were separated into the independent individual equations (15) associated with each definite power j $(p \leqslant j \leqslant k-p)$ of the nucleus charge Z. The appropriate solutions $\psi_{k,p}^{(j)}$ of Eq. (15) present the independent components (of the AFC) defined by Eqs. (13) and (14). The property of finiteness at the boundary points of the hyperspherical angular space was extensively used to derive each component. The pure components not containing the admixture of the HH Y_{kl} were found for even values of k.

A few methods for solving the individual FRRs were proposed. A simple technique for solving the IFRRs with the simplest nonseparable right-hand side (14) was described in Sec. IV; an effective method for solving the IFRRs with a separable right-hand side of a specific but frequent kind was presented in Sec. V.

Some mistakes or misprints made in Ref. [13] for the double and single infinite series representations of the component $\psi_{2,0}^{(1)}$ were noted and corrected.

The coupling equation (61) was proposed and applied in the case of a single series representation for the component of the AFC.

Using the techniques mentioned above, all the components of the AFC $\psi_{4,1}$ and the majority of components and subcomponents of $\psi_{3,0}$ were calculated and presented in Tables I–III and in the explicit formulas of Sec. VII. Details of all these calculations are in Appendixes A–D. All calculations (both analytical and numerical) were carried out with the help of the program *Mathematica*.

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APPENDIX A

For ease of comparison, let us express $\psi_{2,0}^{(1)}$ defined by Eqs. (51), (52b), and (53), in the form

$$\psi_{2,0}^{(1)} = \chi_{20}(\alpha,\theta) + \varphi(\alpha,\theta), \tag{A1}$$

where

$$\varphi(\alpha,\theta) = -\tfrac{1}{3}[\sin(\alpha/2) + \cos(\alpha/2)]\sqrt{1 - \sin\alpha\cos\theta}. \tag{A2}$$

By direct action of the HAM operator defined by Eq. (5), one obtains

$$(\Lambda^2 - 12)\varphi(\alpha,\theta) = h_{2,0}^{(1a)}, \tag{A3}$$

where the rhs of Eq. (A3) is defined by Eq. (53a). Hence,

$$(\Lambda^2 - 12)\chi_{20}(\alpha,\theta) = h_{2,0}^{(1b)}, \tag{A4}$$

where the rhs of Eq. (A4) is defined by Eq. (53b).

First, we need to solve Eq. (A4) by expanding χ_{20} in HH. To this end, following [13], let us consider the HH expansion of the function

$$f(\alpha,\theta) \equiv \frac{\cos(\alpha/2) + \sin(\alpha/2)}{\sin\alpha\sqrt{1 - \sin\alpha\cos\theta}} = \sum_{nl} D_{nl} Y_{nl}(\alpha,\theta), \tag{A5}$$

where the Y_{nl} are the unnormalized HH. It follows from (7), (11), and (12) that

$$D_{nl} = N_{nl}^2 \int f(\alpha,\theta) Y_{nl}(\alpha,\theta) d\Omega. \tag{A6}$$

According to Refs. [13,23], the following representation holds for $\nu > -2$:

$$\xi^{\nu} = \frac{\sqrt{\pi}}{\Gamma(-\nu/2)} \sum_{l=0}^{\infty} P_l(\cos\theta) \frac{\Gamma(l-\nu/2)}{\Gamma(l+1/2)} \left(\frac{\sin\alpha}{2}\right)^l F_{l,\nu}(\alpha), \tag{A7}$$

where

$$F_{l,\nu}(\alpha) = {}_2F_1\left(\frac{l}{2} - \frac{\nu}{4}, \frac{l}{2} - \frac{\nu}{4} + \frac{1}{2}; l + \frac{3}{2}; \sin^2\alpha\right) \tag{A8}$$

represents the Gauss hypergeometric function and ξ is defined by Eq. (21).

Inserting (7) (for unnormalized HH) and (A7) for $\nu = -1$ into (A6) and using the orthogonality of the Legendre polynomials, one obtains

$$D_{nl} = N_{nl}^2 \frac{\pi^2 2^{1-l}}{2l+1} \int_0^{\pi} (\sin\alpha)^{2l+1} C_{n/2-l}^{(l+1)}(\cos\alpha) f^{+}(\alpha) d\alpha, \tag{A9}$$

where

$$f^{+}(\alpha) = [\cos(\alpha/2) + \sin(\alpha/2)]\, {}_2F_1\left(\frac{l}{2} + \frac{1}{4}, \frac{l}{2} + \frac{3}{4}; l + \frac{3}{2}; \sin^2\alpha\right).$$

It is important to emphasize the following substantial property. It may be verified that the integral on the rhs of Eq. (A9) differs from zero only for even values of $n/2 - l$.

The following relation has been proved to be correct [see, e.g., Eq. (90) in [13]]:

$$f^{+}(\alpha) = {}_2F_1\left(\frac{l}{2}, \frac{l+1}{2}; l+1; \sin^2\alpha\right) + \frac{1}{2}\sin\alpha\, {}_2F_1\left(\frac{l+1}{2}, \frac{l}{2} + 1; l+2; \sin^2\alpha\right). \tag{A10}$$

Inserting (A10) into (A9), one obtains

$$D_{nl} = N_{nl}^2 \frac{\pi^2 2^{1-l}}{2l+1} \left(\mathcal{I}_1 + \frac{1}{2}\mathcal{I}_2\right), \tag{A11}$$

where

$$\mathcal{I}_1 = \int_{-1}^{1} y^{2l} C_{n/2-l}^{(l+1)}(x)\, {}_2F_1\left(\frac{l}{2}, \frac{l+1}{2}; l+1; y^2\right) dx, \tag{A12}$$

$$\mathcal{I}_2 = \int_{-1}^{1} y^{2l+1} C_{n/2-l}^{(l+1)}(x)\, {}_2F_1\left(\frac{l+1}{2}, \frac{l}{2} + 1; l+2; y^2\right) dx. \tag{A13}$$

We made the change of variable, corresponding to the notation in (23), that is, $x = \cos\alpha$ and $y = \sin\alpha$. Recall the well-known formula of orthogonality for the Gegenbauer polynomials (in terms of x and y)

$$\int_{-1}^{1} y^{2l+1} C_m^{(l+1)}(x) C_n^{(l+1)}(x) dx = \frac{\pi(n+2l+1)!}{2^{2l+1} n!(n+l+1)(l!)^2}\delta_{mn}, \tag{A14}$$

where δ_{mn} is the Kronecker delta. In order to apply Eq. (A14) to reduce the integral (A12), we propose to use expansion (A9) from [13] with $n = -1$ and $\nu = l+1$, which gives

$$y^{-1}\, {}_2F_1\left(\frac{l}{2},\frac{l+1}{2};l+1;y^2\right) = \frac{(l!)^2}{\pi}\sum_{m=0}^{\infty}\frac{(l+2m+1)\Gamma^2(m+1/2)}{\Gamma^2(l+m+3/2)} G_1(l,m) C_{2m}^{(l+1)}(x), \tag{A15}$$

where

$$G_1(l,m) = {}_3F_2\left(\frac{l}{2},\frac{l+1}{2},\frac{1}{2};\frac{1}{2}-m,l+m+\frac{3}{2};1\right) \tag{A16}$$

is the generalized hypergeometric function. Inserting (A15) into (A12) and using (A14), one easily obtains

$$\mathcal{I}_1 = \frac{\Gamma(m+1/2)(l+m)!}{m!\Gamma(l+m+3/2)} G_1(l,m), \tag{A17}$$

where $m = n/4 - l/2$.

In order to apply Eq. (A14) to the reduction of the integral (A13), we propose to use expansion (A6) from [13] with $\nu = l+1$, which gives

$${}_2F_1\left(\frac{l+1}{2},\frac{l}{2}+1;l+2;y^2\right) = \frac{(l+1)!}{\sqrt{\pi}}\sum_{m=0}^{\infty}\frac{(-1/4)^m\Gamma(m+1/2)}{(l+m+1)!} G_2(l,m) C_{2m}^{(l+1)}(x), \tag{A18}$$

where

$$G_2(l,m) = {}_3F_2\left(\frac{l}{2}+m+\frac{1}{2},\frac{l}{2}+m+1,l+m+\frac{3}{2};l+m+2,l+2m+2;1\right). \tag{A19}$$

Inserting (A19) into (A13) and using (A14), one obtains

$$\mathcal{I}_2 = \frac{\pi(l+1)(-1)^m(2l+2m+1)!}{2^{n+1} l! m!(l+2m+1)(l+m+1)!} G_2(l,m), \tag{A20}$$

where again $m = n/4 - l/2$. Substitution of Eqs. (A17), (A20), and (8) into (A11) yields finally

$$D_{nl} = \frac{2^l (l!)^2 (2m)!}{\sqrt{\pi} m!(2l+2m+1)!}\left[\frac{2(l+2m+1)\Gamma(m+1/2)(l+m)!}{\sqrt{\pi}\Gamma(l+m+3/2)} G_1(l,m) + \frac{(l+1)(-1)^m\Gamma(l+m+3/2)}{2^{2m} l!(l+m+1)} G_2(l,m)\right], \tag{A21}$$

where $m = n/4 - l/2$ is a non-negative integer. By direct numerical comparison with definition (A6), it is easy to verify that relation (A21) is correct, whereas formula (93) in [13] is not correct. Note that Eq. (A21) is not a single representation for D_{nl}. We have found at least two other representations.

It should be emphasized that representation (A21) for D_{nl} is correct only for even $n/2 - l$; otherwise, $D_{nl} = 0$. In particular, $D_{20} = 0$. It follows from (A21) that $D_{21} = 4 - 8/\pi$, which means that using Eqs. (A5) and (53b), one can rewrite Eq. (A4) in the form

$$(\Lambda^2 - 12)\chi_{20}(\alpha,\theta) = \frac{2}{3}\sum_{nl}{}' D_{nl} Y_{nl}(\alpha,\theta), \tag{A22}$$

where the prime indicates that $n = 2$ is omitted from the summation. Taking into account that the eigenvalues of the Λ^2 operator are given by $n(n+4)$, one obtains for the HH expansion $\sum_{nl} X_{nl} Y_{nl}$ of the function χ_{20}

$$(\Lambda^2 - 12)\chi_{20}(\alpha,\theta) = \sum_{nl}{}' X_{nl}(n-2)(n+6) Y_{nl}(\alpha,\theta). \tag{A23}$$

Comparison of (A22) and (A23) yields

$$\chi_{20}(\alpha,\theta) = \frac{2}{3}\sum_{nl}{}' \frac{D_{nl}}{(n-2)(n+6)} Y_{nl}(\alpha,\theta). \tag{A24}$$

Recall that the contributions of the terms with $n = 2$ must be treated separately as the solutions of the associated homogeneous equation.

APPENDIX B

To obtain the analytical representations for σ_l, it is necessary to substitute expansion (59) and representation (A7) for $\nu = -1$ into the lhs and rhs of Eq. (A4), respectively. Subsequent application of the relations (40) and (41) for $k = 2$ yields

$$\sum_{l=0}^{\infty} P_l(\cos\theta)(\sin\alpha)^l[4\sigma_l''(\alpha) + 8(l+1)\cot\alpha\,\sigma_l'(\alpha) - 4(l-1)(l+3)\sigma_l(\alpha)]$$
$$= \frac{8(\pi-2)}{3\pi}\sin\alpha\cos\theta - \frac{1}{3}\left[\csc\left(\frac{\alpha}{2}\right) + \sec\left(\frac{\alpha}{2}\right)\right]\sum_{l=0}^{\infty} P_l(\cos\theta)\left(\frac{\sin\alpha}{2}\right)^l {}_2F_1\left(\frac{l}{2}+\frac{1}{4},\frac{l}{2}+\frac{3}{4};l+\frac{3}{2};\sin^2\alpha\right). \quad \text{(B1)}$$

Equating the expansion coefficients for the Legendre polynomials (in $\cos\theta$) of the same order, one obtains ordinary differential equations that must be solved using the boundary conditions (ii) and the coupling equation (62). We solve these equations using the variable ρ defined by Eq. (43). Given that

$$\sin\alpha = 2\rho/(\rho^2+1), \quad \csc(\alpha/2) + \sec(\alpha/2) = \rho^{-1}(\rho+1)\sqrt{\rho^2+1}, \quad \text{(B2)}$$

the following relationship will be useful for further consideration:

$${}_2F_1\left(\frac{l}{2}+\frac{1}{4},\frac{l}{2}+\frac{3}{4};l+\frac{3}{2};\frac{4\rho^2}{(\rho^2+1)^2}\right) = \begin{cases}(\rho^2+1)^{l+1/2}, & 0 \leqslant \rho \leqslant 1\\ (\rho^2+1)^{l+1/2}\rho^{-2l-1}, & \rho > 1.\end{cases} \quad \text{(B3)}$$

Special cases of $l = 0$, $l = 1$, and $l \geqslant 2$ will be considered.

1. Case $l = 0$

Equating coefficients for the Legendre polynomials of zeroth order ($l = 0$) on both sides of Eq. (B1) and turning to the variable ρ, one can employ Eq. (44) for $k = 2$ and $l = 0$. This yields

$$(\rho^2+1)^2 S_0''(\rho) + \frac{2(\rho^2+1)}{\rho}S_0'(\rho) + 12S_0(\rho) = -h(\rho), \quad \text{(B4)}$$

where the substitution $g(\rho) = S_0(\rho) \equiv \sigma_0(\alpha)$ was applied. Using Eqs. (B2) and (B3), one obtains for the rhs, in the range $\rho \in [0,1]$ $(0 \leqslant \alpha \leqslant \pi/2)$,

$$h(\rho) = \frac{(\rho+1)(\rho^2+1)}{3\rho}. \quad \text{(B5)}$$

For $l = 0$ one can employ formula (45) with $k = 2$ and $\rho_c = 1$, which gives the following solution of Eq. (B4) for $0 \leqslant \rho \leqslant 1$:

$$S_0(\rho) = \frac{\rho\{2(\rho^2-1)\ln[(\rho^2+1)/2] - \rho(3\rho+2) - 1\} - (\rho^4 - 6\rho^2 + 1)\arctan\rho}{12\rho(\rho^2+1)}. \quad \text{(B6)}$$

An alternative representation is

$$\sigma_0 = \frac{1}{12}\left\{\left(2y - \frac{1}{y}\right)\alpha + x[1 + 2\ln(x+1)] - y - 2\right\}, \quad 0 \leqslant \alpha \leqslant \pi/2, \quad \text{(B7)}$$

where x and y are defined by Eq. (23). It is clear that for $\pi/2 < \alpha \leqslant \pi$, one needs to replace ρ by $1/\rho$, x by $-x$, and α by $\pi - \alpha$. Representation (B7) is simpler than the corresponding one (A19) from [13], which also is correct only for $0 \leqslant \alpha \leqslant \pi/2$. It is easy to verify that σ_0 presented in Eq. (B7) corresponds to the pure component $\psi_{2,0}^{(1)}$ (see the end of Sec. II) because the HH expansion coefficient

$$\mathcal{F}_{2,0} \propto \int \sigma_0(\alpha)Y_{20}(\alpha,\theta)d\Omega$$

equals zero.

2. Case $l = 1$

In this case, equating coefficients for $P_1(\cos\theta) = \cos\theta$ on both sides of Eq. (B1), using (B2) and (B3), and simplifying, one obtains the equation

$$(1+\rho^2)^2 S_1''(\rho) + \frac{2(2-\rho^2)(1+\rho^2)}{\rho}S_1'(\rho) = \frac{8(\pi-2)}{3\pi} - \frac{(1+\rho)(1+\rho^2)^2}{6\rho}, \quad 0 \leqslant \rho \leqslant 1, \quad \text{(B8)}$$

where $S_1(\rho) \equiv \sigma_1(\alpha)$. Formula (45) with $k=2$, $l=1$, and $\rho_c=1$ yields the particular solution to Eq. (B8) in the form

$$S_1^{(p)}(\rho) = \frac{1}{24\pi}\left[\left(\frac{1}{\rho^3}+\frac{9}{\rho}-9\rho-\rho^3\right)\arctan\rho - \frac{1}{\rho^2}-\rho^2+2-\frac{2\pi}{3}\right] - \frac{\rho(\rho^2-6\rho+3)}{72}+\frac{1}{6}\ln\left(\frac{1+\rho^2}{2}\right). \tag{B9}$$

To obtain the pure (single-valued) solution to Eq. (B8), one needs to calculate the coefficient $\mathcal{F}_{2,1}$ of the unnormalized HH expansion of the solution (B9). Recall that representation (B9) is correct only for $0 \leqslant \rho \leqslant 1$ $(0 \leqslant \alpha \leqslant \pi/2)$. For $\rho > 1$ $(\pi/2 < \alpha \leqslant \pi)$, one should replace ρ by $1/\rho$ on the rhs of Eq. (B9). Thus, using Eqs. (11) and (12) for $n=2$ and $l=1$ one obtains

$$\begin{aligned}\mathcal{F}_{2,1} = N_{21}^2\int \sigma_1^{(p)}(\alpha)Y_{21}(\alpha,\vartheta)d\Omega &= 64N_{21}^2\pi^2\int_0^1\frac{S_1^{(p)}(\rho)\rho^4}{(1+\rho^2)^5}d\rho\int_0^\pi \sin\theta\cos^2\theta\, d\theta\\ &= \frac{14-48G+\pi(1+12\ln 2)}{72\pi},\end{aligned} \tag{B10}$$

where G is Catalan's constant and N_{21} is defined by Eq. (8). The final result is $\sigma_1 = S_1^{(p)}(\rho) - \mathcal{F}_{2,1}$.

The same result can be obtained using Eq. (62), which for $l=1$ reduces to

$$\int_0^{\pi/2} y^4\sigma_1(\alpha)d\alpha = 0, \tag{B11}$$

where $\sigma_1(\alpha)$ represents the general solution of Eq. (B8) satisfying the condition (ii) of finiteness.

3. Case $l \geqslant 2$

The required function σ_l $(l \geqslant 2)$ can certainly be obtained by means of application of the particular solution (45) and subsequent use of Eq. (62). However, in this case we apply the following simplified procedure.

Equating coefficients for $P_l(\cos\theta)$ on both sides of Eq. (B1) (for $l \geqslant 2$), using (B2) and (B3), and introducing the function $Q_l(\rho)$ by means of the relationship

$$\sigma_l(\alpha) \equiv S_l(\rho) = -\frac{2^{-l}}{3}(\rho^2+1)^{l-1}Q_l(\rho), \tag{B12}$$

one obtains the differential equation

$$\rho(\rho^2+1)Q_l''(\rho) + 2[(l-2)\rho^2+l+1]Q_l'(\varrho) - 6(l-1)\rho Q_l(\rho) = (\rho+1)(\rho^2+1), \tag{B13}$$

which is correct only for $0 \leqslant \rho \leqslant 1$ $(0 \leqslant \alpha \leqslant \pi/2)$. *Mathematica* gives the following general solution to the homogeneous equation associated with the inhomogeneous equation (B13):

$$Q_l^{(h)}(\rho) = C_1\,{}_2F_1\left(-\tfrac{3}{2}, l-1; l+\tfrac{3}{2}; -\rho^2\right) + C_2\rho^{-2l-1}\,{}_2F_1\left(-\tfrac{3}{2}, -l-2; \tfrac{1}{2}-l; -\rho^2\right). \tag{B14}$$

Assuming that a particular solution has the form $a+b\rho+c\rho^2+d\rho^3$ and substituting the latter one into the lhs of Eq. (B13), one easily finds this particular solution in the form

$$Q_l^{(p)}(\rho) = \frac{1}{2}\left[\frac{l\rho^3}{(l+1)(l+2)} - \frac{\rho^2}{l} + \frac{\rho}{l+1} - \frac{l+1}{l(l-1)}\right]. \tag{B15}$$

One should set $C_2 = 0$ to satisfy the condition (ii) of finiteness. Thus, using (B12), (B14), and (B15) we obtain

$$S_l(\rho) = -\frac{2^{-l-1}}{3}\left\{(1+\rho^2)^{l-1}\left[\frac{l\rho^3}{(l+1)(l+2)} - \frac{\rho^2}{l} + \frac{\rho}{l+1} - \frac{l+1}{l(l-1)}\right] + 2C_1\,{}_2F_1\left(\frac{l-1}{2}, \frac{l+3}{2}; l+\frac{3}{2}; y^2\right)\right\}, \tag{B16}$$

where the relationship

$${}_2F_1\left(\frac{l-1}{2}, \frac{l+3}{2}; l+\frac{3}{2}; y^2\right) = (1+\rho^2)^{l-1}\,{}_2F_1\left(-\frac{3}{2}, l-1; l+\frac{3}{2}; -\rho^2\right)$$

was used (see 7.3.1.54 in [24]). Now we can apply the coupling equation (62) to find the constant $C_1 \equiv C_1(l)$. To this end, we first need to calculate explicitly the integral

$$\int_0^\pi y^{2l+2}\sigma_l(\alpha)d\alpha = \mathcal{K}_1(l) + C_1\mathcal{K}_2(l), \tag{B17}$$

where using Eq. (B16) one obtains

$$\mathcal{K}_1(l) = -\frac{2^{l+3}}{3}\int_0^1\frac{\rho^{2l+2}}{(\rho^2+1)^{l+4}}\left[\frac{l\rho^3}{(l+1)(l+2)} - \frac{\rho^2}{l} + \frac{\rho}{l+1} - \frac{l+1}{l(l-1)}\right]d\rho, \tag{B18}$$

$$\mathcal{K}_2(l) = -\frac{2^{-l}}{3}\int_{-1}^{1} y^{2l+1}\,{}_2F_1\left(\frac{l-1}{2},\frac{l+3}{2};l+\frac{3}{2};y^2\right)dx. \tag{B19}$$

Mathematica gives for the integral (B18)

$$\mathcal{K}_1(l) = \frac{1}{3l}\left[\frac{l+1}{(l-1)(2l+3)}\,{}_2F_1\left(-\frac{3}{2},1;l+\frac{5}{2};-1\right) + \frac{1}{2l+5}\,{}_2F_1\left(-\frac{1}{2},1;l+\frac{7}{2};-1\right) - \frac{l}{(l+1)(l+3)}\right]. \tag{B20}$$

To reduce the integral (B19) we applied the expansion (A9) from [13], which for parametrization $n = l$ and $\nu = 1/2$ becomes

$$y^{2l+1}\,{}_2F_1\left(\frac{l-1}{2},\frac{l+3}{2};l+\frac{3}{2};y^2\right) = \frac{1}{2}\Gamma^2\left(l+\frac{3}{2}\right)\sum_{m=0}^{\infty}\frac{(-1)^m(4m+1)\Gamma(m+1/2)}{m!(l+m+1)!\Gamma(l-m+3/2)}$$
$$\times{}_3F_2\left(\frac{l-1}{2},\frac{l+3}{2},l+\frac{3}{2};l+\frac{3}{2}-m,l+m+2;1\right)C_{2m}^{(1/2)}(x).$$

Substitution of this representation into Eq. (B19), and subsequent application of the formula of orthogonality for the Gegenbauer polynomials, finally yields

$$\mathcal{K}_2(l) = -\frac{2^{-l}\sqrt{\pi}\Gamma(l+3/2)}{3\Gamma((l+1)/2)\Gamma((l+5)/2)}. \tag{B21}$$

Using Eqs. (62) and (B17), one obtains

$$C_1 = \frac{\mathcal{K}(l)}{3(l-1)(l+1)(l+3)\mathcal{K}_2(l)}, \tag{B22}$$

where

$$\mathcal{K}(l) = \mathcal{K}_3(l) + 1 - 3(l-1)(l+1)(l+3)\mathcal{K}_1(l), \tag{B23}$$

$$\mathcal{K}_3(l) = \frac{\sqrt{\pi}\Gamma(l+3/2)}{2^{l+2}l!}\,{}_3F_2\left(\frac{l+1}{2},\frac{l}{2}+1,l+\frac{3}{2};l+2,l+2;1\right). \tag{B24}$$

The simplest way to reduce $\mathcal{K}(l)$ is to calculate numerically the first entries of the sequence, that is, to calculate $\mathcal{K}(l)$ for $l = 2,3,4,5$. Using *Mathematica*, one obtains the required sequence $-5/2, -7/3, -9/4, -11/5$. It can be seen that $\mathcal{K}(l) = -(2l+1)/l$. Simplifying, we have finally

$$C_1 = \frac{(l-2)!\Gamma((l+1)/2)}{2\Gamma(l+1/2)\Gamma(l/2+1)}. \tag{B25}$$

APPENDIX C

The solution of the FRR (76) for the subcomponent with $j = 2d$ implies that we need to find a suitable solution to the equation

$$(\Lambda^2 - 32)\psi_{4,1}^{(2d)} = h_{4,1}^{(2d)}, \tag{C1}$$

where $h_{4,1}^{(2d)}$ and $\psi_{4,1}^{(2d)}$ are defined by Eq. (89b) and expansion (93), respectively. Inserting expansion (A7) for $\nu = -1,1,3$ into the rhs of Eq. (89b), one obtains the expansion

$$h_{4,1}^{(2d)}(\alpha,\theta) = \sum_{l=0}^{\infty} P_l(\cos\theta)(\sin\alpha)^l \mathrm{h}_l(\alpha) \tag{C2}$$

for the rhs of Eq. (C1), where

$$\mathrm{h}_l(\alpha) = \frac{\pi-2}{3\pi(2l-1)2^l}\left[\sin\left(\frac{\alpha}{2}\right)+\cos\left(\frac{\alpha}{2}\right)\right]\left[\frac{5}{(2l-3)\sin\alpha}F_{l,3}(\alpha) - \left(1-\frac{2}{\sin\alpha}\right)F_{l,1}(\alpha) - (2l-1)F_{l,-1}(\alpha)\right] \tag{C3}$$

and where the hypergeometric function $F_{l,\nu}$ is defined by Eq. (A8). Thus, according to Eq. (41), with $\mathrm{g}(\alpha) = \mathrm{t}_l(\alpha)$ and $k = 4$, and expansions (93) and (C2), one obtains the differential equation

$$4\mathrm{t}_l''(\alpha) + 8(l+1)\cot\alpha\;\mathrm{t}_l'(\alpha) + 4(2-l)(l+4)\mathrm{t}_l(\alpha) = -\mathrm{h}_l(\alpha) \tag{C4}$$

for the function $\mathrm{t}_l(\alpha)$ defined by Eq. (93). Transformation of Eq. (C4) to the variable $\rho = \tan(\alpha/2)$ yields [see Eq. (44)]

$$(1+\rho^2)^2\tau_l''(\rho) + 2\rho^{-1}[1+\rho^2+l(1-\rho^4)]\tau_l'(\rho) + 4(2-l)(l+4)\tau_l(\rho) = -h_l(\rho), \tag{C5}$$

where $h_l(\rho) \equiv \mathrm{h}_l(\alpha)$ and $\tau_l(\rho) \equiv \mathrm{t}_l(\alpha)$. Turning to the variable ρ in Eq. (C3) and simplifying, one obtains the following compact representation for the rhs of Eq. (C5):

$$h_l(\rho) = -\frac{(\pi-2)(\rho+1)(\rho^2+1)^{l-1}}{3\pi(2l-1)(2l+3)2^{l+1}}\left[\frac{15-4l(l+1)(4l+11)}{(2l-3)(2l+5)\rho}+4l(2l+3)+2\rho+4(l+1)(2l-1)\rho^2+\frac{(2l-1)(4l+5)\rho^3}{2l+5}\right], \tag{C6}$$

where $0 \leqslant \rho \leqslant 1$. One possible way to solve Eq. (C5) is to take into account that its rhs (C6) contains some linear combination of terms of the form

$$h_{n,l}(\rho) = \rho^n(\rho+1)(\rho^2+1)^{l-1}, \tag{C7}$$

with the integral $n > -2$. The particular solution $T_{n,l}(\rho)$ of Eq. (C5), with the exchange of $h_l(\rho)$ for $h_{n,l}(\rho)$ defined by Eq. (C7), reads

$$T_{n,l}(\rho) = \frac{(\rho^2+1)^{l+4}\rho^{n+2}}{2l+1}\left\{{}_2F_1\left(\frac{7}{2},3-l;\frac{1}{2}-l;-\rho^2\right)\left[\frac{{}_3F_2(7/2,l+4,l+(n+4)/2;l+3/2,l+(n+6)/2;-\rho^2)\rho}{2l+n+4}\right.\right.$$
$$\left.+\frac{{}_3F_2(7/2,l+4,l+(n+3)/2;l+3/2,l+(n+5)/2;-\rho^2)}{2l+n+3}\right] - {}_2F_1\left(\frac{7}{2},l+4;l+\frac{3}{2};-\rho^2\right)$$
$$\left.\times\left[\frac{{}_3F_2(7/2,3-l,(n+3)/2;1/2-l,(n+5)/2;-\rho^2)\rho}{n+3}+\frac{{}_3F_2(7/2,3-l,n/2+1;1/2-l,n/2+2;-\rho^2)}{n+2}\right]\right\}. \tag{C8}$$

This solution was derived by means of application of Eq. (45) with an exchange of definite integration for indefinite integration over ρ (that is, setting the antiderivatives for the lower limit equal to zero).

Here we present the particular solutions $\tau_l^{(p)}$ of Eq. (C5) obtained by the exact formula (45) with $k=4$. We consider the cases of $l=0,1,2$ (for $l_{\max}=k/2$) and $l \geqslant 3$, separately.

Application of Eqs. (45)–(47), with $h(\rho)=h_l(\rho)$ defined by Eq. (C6), and $\rho_c=1$ yields, for $l=0,1,2$,

$$\tau_0^{(p)}(\rho) = -\frac{\pi-2}{108\pi(\rho^2+1)^2}\left[\frac{1-\rho}{15}(19\rho^4+142\rho^3+82\rho^2-48\rho-3)-\left(\rho^5-15\rho^3+15\rho-\frac{1}{\rho}\right)\arctan\rho\right.$$
$$\left.+(3\rho^4-10\rho^2+3)\ln\left(\frac{\rho^2+1}{2}\right)\right], \tag{C9}$$

$$\tau_1^{(p)}(\rho) = \frac{\pi-2}{302\,400\pi\rho^2(\rho^2+1)}\left[1268\rho^7-2505\rho^6+1960\rho^5+32\,263\rho^4+18\,900\rho^3+18\,305\rho^2-735\right.$$
$$\left.+735\left(\rho^7+20\rho^5-90\rho^3+20\rho+\frac{1}{\rho}\right)\arctan\rho-23\,520\rho^2(\rho^2-1)\ln\left(\frac{\rho^2+1}{2}\right)\right], \tag{C10}$$

$$\tau_2^{(p)}(\rho) = \frac{\pi-2}{362\,880\pi\rho^4}\left[672\rho^9-465\rho^8+760\rho^7-6720\rho^6-5880\rho^5+8798\rho^4+2520\rho^2+315\right.$$
$$\left.+105(\rho^2-1)\left(3\rho^7+28\rho^5+178\rho^3+28\rho+\frac{3}{\rho}\right)\arctan\rho-13\,440\rho^4\ln\left(\frac{\rho^2+1}{2}\right)\right]. \tag{C11}$$

It was mentioned in Sec. II that in order to obtain the pure component $\psi_{4,1}^{(2d)}$ one needs to select and then to get rid of the admixture of the HH Y_{4l}. In other words, we need to orthogonalize $\psi_{4,1}^{(2d)}$ to each of the Y_{4l}. First, according to expansion (93) and Eqs. (11) and (12), we need to calculate the unnormalized HH expansion coefficients

$$\mathcal{F}_{4,l} = \pi^2 N_{4l}^2\left[\int_0^{\pi/2} d\alpha\,\tau_l^{(p)}(\rho)(\sin\alpha)^{l+2}\int_0^{\pi} Y_{4l}(\alpha,\theta)P_l(\cos\theta)\sin\theta\,d\theta\right.$$
$$\left.+\int_{\pi/2}^{\pi} d\alpha\,\tau_l^{(p)}(1/\rho)(\sin\alpha)^{l+2}\int_0^{\pi} Y_{4l}(\alpha,\theta)P_l(\cos\theta)\sin\theta\,d\theta\right], \tag{C12}$$

where the factor N_{4l} is defined by Eq. (8). Direct integration with the use of solutions (C9)–(C11) yields

$$\mathcal{F}_{4,0} = -\frac{(\pi-2)}{8100\pi^2}[5\pi(15\ln 2-16)+247-300G], \tag{C13a}$$

$$\mathcal{F}_{4,1} = 0, \tag{C13b}$$

$$\mathcal{F}_{4,2} = -\frac{(\pi-2)}{113\,400\pi^2}[5\pi(840\ln 2+109)+4592-16\,800G], \tag{C13c}$$

where G is Catalan's constant. Thus, to obtain the pure subcomponent $\psi_{4,1}^{(2d)}$, one needs to replace $\tau_0^{(p)}$ by $\tau_0 = \tau_0^{(p)} - \mathcal{F}_{4,0}(4\cos^2\alpha - 1)$ and $\tau_2^{(p)}$ by $\tau_2 = \tau_2^{(p)} - \mathcal{F}_{4,2}$ in expansion (93).

For $l \geqslant 3$, the particular solution of Eq. (C5) obtained by Eq. (45) can be represented in the form

$$\tau_l^{(p)}(\rho) = \frac{(\pi-2)(\rho^2+1)^{l-2}}{135\pi 2^{3(l+1)}\lambda_l \rho^{2l+1}}\left[\rho^{2l+2}\sum_{n=0}^{4}\mu_{ln}^{(1)}\rho^n + \rho\sum_{n=0}^{l}\mu_{ln}^{(2)}\rho^{2n} - \mu_{l0}^{(2)}(\rho^2+1)^6\arctan\rho\sum_{n=0}^{l-3}\mu_{ln}^{(3)}\rho^{2n}\right], \tag{C14}$$

where the coefficients λ_l and $\mu_{ln}^{(1)}$ are presented in Table II; $\mu_{ln}^{(2)}$ and $\mu_{ln}^{(3)}$ are presented in Table III in the form of lists. The number of coefficients is limited by $l \leqslant 10$.

It is clear that all the terms of expansion (93) with $l \geqslant 3$ are automatically orthogonal to the Y_{4l}. Therefore, in this case we use relation (61), which becomes

$$\mathcal{T}_{2l,l} = \frac{(l+1)!}{\sqrt{\pi}\Gamma(l+3/2)}\int_0^{\pi} \mathrm{t}_l(\alpha)(\sin\alpha)^{2l+2}d\alpha = \frac{2^{2(l+2)}(l+1)!}{\sqrt{\pi}\Gamma(l+3/2)}\int_0^1 \tau_l(\rho)\frac{\rho^{2l+2}}{(1+\rho^2)^{2l+3}}d\rho, \tag{C15}$$

where $\mathcal{T}_{n,l}$ are the unnormalized HH expansion coefficients for the considered subcomponent

$$\psi_{4,1}^{(2d)}(\alpha,\theta) = \sum_{nl}{}' \mathcal{T}_{n,l} Y_{nl}(\alpha,\theta). \tag{C16}$$

The prime indicates that $n = 4$ is omitted from the summation for the pure component.

The general solution of Eq. (C5) reads

$$\tau_l(\rho) = \tau_l^{(p)}(\rho) + A_1 u_{4l}(\rho) + A_2 v_{4l}(\rho), \tag{C17}$$

where the solutions u_{4l} and v_{4l} of the homogeneous equation associated with Eq. (C5) are defined by Eqs. (46) and the constants A_1 and A_2 are currently undetermined. It is clear that in order for $\psi_{4,1}^{(2d)}$ to satisfy the finiteness condition (ii), the function $(\sin\alpha)^l\tau_l(\rho)$ for each l must satisfy this condition, according to expansion (93). It is easy to verify that $(\sin\alpha)^l u_{4l}(\rho)$ is divergent at $\rho = 0$ ($\alpha \to 0$), whereas both functions $(\sin\alpha)^l v_{4l}(\rho)$ and $(\sin\alpha)^l \tau_l^{(p)}(\rho)$ are finite at this point. Hence, one should set $A_1 = 0$. Thus, Eq. (C15) can be rewritten in the form

$$\mathcal{T}_{2l,l} = \frac{2^{2(l+2)}(l+1)!}{\sqrt{\pi}\Gamma(l+3/2)}[\mathcal{P}_1(l) + A_2\mathcal{P}_2(l)], \tag{C18}$$

where

$$\mathcal{P}_1(l) = \int_0^1 \tau_l^{(p)}(\rho)\frac{\rho^{2l+2}}{(1+\rho^2)^{2l+3}}d\rho, \tag{C19}$$

$$\mathcal{P}_2(l) = \int_0^1 v_{4l}(\rho)\frac{\rho^{2l+2}}{(1+\rho^2)^{2l+3}}d\rho = \frac{\sqrt{\pi}2^{-2(l+2)}\Gamma(l+3/2)}{\Gamma(l/2+3)\Gamma(l/2)}. \tag{C20}$$

Note that for each value of $l \geqslant 3$ the integral (C19) can be calculated in the exact explicit form.

To derive the closed expression for $\mathcal{T}_{n,l}$ according to definition (C16), let us first obtain the HH expansion for the rhs of Eq. (C1),

$$h_{4,1}^{(2d)} = \sum_{nl}\mathcal{H}_{n,l}^{(4)} Y_{nl}(\alpha,\theta), \tag{C21}$$

where, according to Eq. (12) for unnormalized HH,

$$\mathcal{H}_{n,l}^{(4)} = N_{nl}^2 \int h_{4,1}^{(2d)}(\alpha,\theta) Y_{nl}(\alpha,\theta) d\Omega \tag{C22}$$

and the normalization coefficient N_{nl} is defined by Eq. (8). Substitution of representations (C2) and (C3) into (C22) yields

$$\mathcal{H}_{n,l}^{(4)} = \frac{N_{nl}^2\pi(\pi-2)}{3(2l-1)(2l+1)2^{l-1}}\int_0^{\pi}(\sin\alpha)^{2l+2}\left[\cos\left(\frac{\alpha}{2}\right)+\sin\left(\frac{\alpha}{2}\right)\right]C_{n/2-l}^{(l+1)}(\cos\alpha)$$
$$\times\left[\frac{5}{(2l-3)\sin\alpha}F_{l,3}(\alpha) - \left(1-\frac{2}{\sin\alpha}\right)F_{l,1}(\alpha) - (2l-1)F_{l,-1}(\alpha)\right]d\alpha. \tag{C23}$$

The orthogonality of the Legendre polynomials was used to derive formula (C23). Inserting expansion (C16) into the lhs of Eq. (C1), one obtains

$$(\Lambda^2 - 32)\psi_{4,1}^{(2d)} = \sum_{nl}\mathcal{T}_{n,l}(n-4)(n+8)Y_{nl}(\alpha,\theta). \tag{C24}$$

According to Eq. (C1), the right-hand sides of Eqs. (C24) and (C21) can be equated, which yields

$$\mathcal{T}_{n,l} = \frac{\mathcal{H}^{(4)}_{n,l}}{(n-4)(n+8)}. \tag{C25}$$

Thus, for the required case of $n = 2l$ ($l > 2$), one obtains, using (C25) and (C23),

$$\mathcal{T}_{2l,l} = \frac{(\pi-2)2^{l-1}(l+1)(l!)^2}{3\pi^2(2l-1)(l-2)(l+4)(2l+1)!}\mathcal{P}_3(l), \tag{C26}$$

where

$$\mathcal{P}_3(l) = \int_0^\pi (\sin\alpha)^{2l+2}\left[\cos\left(\frac{\alpha}{2}\right)+\sin\left(\frac{\alpha}{2}\right)\right]\left[\frac{5}{(2l-3)\sin\alpha}F_{l,3}(\alpha) - \left(1-\frac{2}{\sin\alpha}\right)F_{l,1}(\alpha) - (2l-1)F_{l,-1}(\alpha)\right]d\alpha. \tag{C27}$$

The integral (C27) can be evaluated in explicit form. The result is

$$\mathcal{P}_3(l) = -\frac{2^{l+1}}{(l+3)(2l-3)(2l+3)(2l+5)}\left(\frac{30}{l+1} - \frac{26}{l+2} + 13 - 4l\{47 - 2l[2l(l+3)-9]\} + 2^{l+1}\right.$$
$$\left.\times\left[(l+1)\{4l[l(4l+3)-17]+45\}B_{1/2}\left(l+\frac{3}{2},\frac{1}{2}\right) + 8l(l\{l[4l(l+4)+3]-56\}-62)B_{1/2}\left(l+\frac{3}{2},\frac{3}{2}\right)\right]\right), \tag{C28}$$

where $B_z(a,b)$ is the incomplete Beta function. Equating the right-hand sides of Eqs. (C18) and (C26), one obtains the required coefficient in the form

$$A_2 \equiv A_2(l) = \frac{1}{\mathcal{P}_2(l)}\left[\frac{(\pi-2)2^{-3(l+2)}}{3\pi(2l-1)(l-2)(l+4)}\mathcal{P}_3(l) - \mathcal{P}_1(l)\right]. \tag{C29}$$

It may be verified that for odd values of l, the coefficients $A_2(l)$ equal zero. For even values of l, formula (C29) yields

$$A_2(l) = -\frac{(\pi-2)}{\pi^2}\mathcal{A}(l), \tag{C30}$$

where

$$\begin{aligned}
\mathcal{A}(4) &= \frac{5515\pi - 11\,648}{29\,48400},\\
\mathcal{A}(6) &= \frac{191\,095\pi - 396\,032}{1\,378\,377\,000},\\
\mathcal{A}(8) &= \frac{66\,779\,345\pi - 137\,592\,832}{4\,085\,509\,428\,000},\\
\mathcal{A}(10) &= \frac{59\,227\,659\pi - 121\,716\,736}{25\,014\,766\,104\,900}.
\end{aligned} \tag{C31}$$

APPENDIX D

The IFRR (75) for subcomponent $\psi^{(2c)}_{3,0}$ reads

$$(\Lambda^2 - 21)\psi^{(2c)}_{3,0} = h^{(2c)}_{3,0}, \tag{D1}$$

where the rhs $h^{(2c)}_{3,0}$ is defined by Eq. (88). To find a suitable solution in the form of expansion (98), let us express the rhs of Eq. (D1) in the form

$$h^{(2c)}_{3,0} \equiv -\frac{4\xi}{3\sin\alpha} = \sum_{l=0}^{\infty} P_l(\cos\theta)(\sin\alpha)^l \mathrm{h}_l(\alpha), \tag{D2}$$

where, using expansion (A7) for $\nu = 1$, one obtains

$$\mathrm{h}_l(\alpha) = \frac{2^{2-l}}{3(2l-1)\sin\alpha}\, {}_2F_1\left(\frac{l}{2}-\frac{1}{4},\frac{l}{2}+\frac{1}{4};l+\frac{3}{2};\sin^2\alpha\right). \tag{D3}$$

Inserting expansions (D2) and (98) into the IFFR (D1), equating the factors for the Legendre polynomials $P_l(\cos\theta)$ of the same order, and turning to the variable $\rho = \tan(\alpha/2)$, one obtains the inhomogeneous differential equation

$$(1+\rho^2)^2\phi_l''(\rho) + 2\rho^{-1}[1+\rho^2+l(1-\rho^4)]\phi_l'(\rho) + (3-2l)(7+2l)\phi_l(\rho) = -h_l(\rho), \tag{D4}$$

which represents Eq. (44) with $k=3$ and with an exchange of $h(\rho)$ for $h_l(\rho)\equiv \mathrm{h}_l(\alpha)$ and $g(\rho)$ for $\phi_l(\rho)$. Simplification of the rhs of Eq. (D4) yields, for $0\leqslant\rho\leqslant 1$,

$$h_l(\rho)=\frac{2^{1-l}(\rho^2+1)^{l+1/2}[(1-2l)\rho^2+2l+3]}{3(2l-1)(2l+3)\rho}. \tag{D5}$$

Simplifying the solutions (46) of the homogeneous equation associated with Eq. (D4), one obtains, for $k=3$,

$$u_{3l}(\rho)=\frac{(\rho^2+1)^{l-3/2}}{\rho^{2l+1}}\left[\frac{(2l+3)(2l+5)}{(2l-3)(2l-1)}\rho^4+\frac{2(2l+5)}{2l-1}\rho^2+1\right], \tag{D6}$$

$$v_{3l}(\rho)=(\rho^2+1)^{l-3/2}\left[\frac{(2l-3)(2l-1)}{(2l+3)(2l+5)}\rho^4+\frac{2(2l-3)}{2l+3}\rho^2+1\right]. \tag{D7}$$

The particular solution $\phi_l^{(p)}(\rho)$ of Eq. (D4) can be obtained by formula (45), but with an exchange of definite integration for indefinite integration (that is, setting the antiderivatives for the lower limits equal to zero). The result is presented in Eqs. (101)–(104). It is worth noting that the hypergeometric function included in Eq. (104) can be represented in the form (see Eq. 7.3.1.135 in [24])

$${}_2F_1(1,l+1;l+2;-\rho^2)=-\frac{l+1}{(-\rho^2)^{l+1}}\left[\ln(1+\rho^2)+\sum_{k=1}^{l}\frac{(-\rho^2)^k}{k}\right]. \tag{D8}$$

It can be easily shown that the homogeneous solution $u_{3l}(\rho)$ is singular and $v_{3l}(\rho)$ and the particular solution $\phi_l^{(p)}(\rho)$ are regular at the point $\rho=0$ ($\alpha=0$) for any $l\geqslant 0$. The conclusion is that the physical solution must be sought in the form (99). The problem is to find the coefficient c_l. To solve the problem we apply the coupling equation (61), which for this case becomes

$$\mathcal{O}_{2l,l}=\frac{(l+1)!2^{2(l+2)}}{\sqrt{\pi}\Gamma\left(l+\frac{3}{2}\right)}\int_0^1\left[\phi_l^{(p)}(\rho)+c_lv_{3l}(\rho)\right]\frac{\rho^{2l+2}}{(\rho^2+1)^{2l+3}}d\rho, \tag{D9}$$

where $\mathcal{O}_{n,l}$ represent the unnormalized HH expansion coefficients for subcomponent

$$\phi_{3,0}^{(2c)}(\alpha,\theta)=\sum_{nl}\mathcal{O}_{n,l}Y_{nl}(\alpha,\theta). \tag{D10}$$

For this case (odd value of $k=3$) the rhs of Eq. (D10) represents the physical solution we are looking for (see the end of Sec. II). To derive the closed expression for $\mathcal{O}_{n,l}$ we first obtain the unnormalized HH expansion

$$h_{3,0}^{(2c)}(\alpha,\theta)=\sum_{nl}\mathcal{H}_{n,l}^{(3)}Y_{nl}(\alpha,\theta) \tag{D11}$$

for the rhs of Eq. (D1), where by definition

$$\mathcal{H}_{n,l}^{(3)}=N_{nl}^2\int h_{3,0}^{(2c)}(\alpha,\theta)Y_{nl}(\alpha,\theta)d\Omega. \tag{D12}$$

Inserting expansions (D2) and (D3) into (D12), one obtains

$$\mathcal{H}_{n,l}^{(3)}=\frac{N_{nl}^2\pi^2 2^{3-l}}{3(2l-1)(2l+1)}\int_0^\pi {}_2F_1\left(\frac{l}{2}-\frac{1}{4},\frac{l}{2}+\frac{1}{4};l+\frac{3}{2};\sin^2\alpha\right)(\sin\alpha)^{2l+1}C_{n/2-l}^{(l+1)}(\cos\alpha)d\alpha, \tag{D13}$$

where the orthogonality of the Legendre polynomials was used. Substitution of expansion (D10) into the lhs of Eq. (D1) yields

$$(\Lambda^2-21)\psi_{3,0}^{(2c)}=\sum_{nl}\mathcal{O}_{n,l}(n-3)(n+7)Y_{nl}(\alpha,\theta). \tag{D14}$$

According to Eq. (D1), the right-hand sides of Eqs. (D11) and (D14) can be equated, which yields

$$\mathcal{O}_{n,l}=\frac{\mathcal{H}_{n,l}^{(3)}}{(n-3)(n+7)}. \tag{D15}$$

Thus, inserting (D13) into Eq. (D15) for $n=2l$ ($l\geqslant 0$), one obtains

$$\begin{aligned}\mathcal{O}_{2l,l}&=\frac{2^{l+4}l!(l+1)!}{3\pi(2l-3)(2l-1)(2l+7)(2l+1)!}\int_0^{\pi/2}{}_2F_1\left(\frac{l}{2}-\frac{1}{4},\frac{l}{2}+\frac{1}{4};l+\frac{3}{2};\sin^2\alpha\right)(\sin\alpha)^{2l+1}d\alpha\\&=\frac{2^{2-l}l!(l+1)!}{3(2l-3)(2l-1)(2l+7)\Gamma^2(l+3/2)}\,{}_3F_2\left(\frac{l}{2}-\frac{1}{4},\frac{l}{2}+\frac{1}{4},l+1;l+\frac{3}{2},l+\frac{3}{2};1\right).\end{aligned} \tag{D16}$$

Equating the right-hand sides of Eqs. (D9) and (D16), we find the required coefficient

$$c_l = \frac{\mathcal{M}_1(l) - \mathcal{M}_2(l)}{\mathcal{M}_3(l)}, \tag{D17}$$

where

$$\mathcal{M}_1(l) = \frac{2^{-3l-2} l! \sqrt{\pi}}{3(2l-3)(2l-1)(2l+7)\Gamma(l+3/2)}\, {}_3F_2\left(\frac{2l-1}{4}, \frac{2l+1}{4}, l+1; l+\frac{3}{2}, l+\frac{3}{2}; 1\right), \tag{D18}$$

$$\mathcal{M}_3(l) \equiv \int_0^1 v_{3l}(\rho) \frac{\rho^{2l+2}}{(\rho^2+1)^{2l+3}} d\rho = \frac{2^{-l-3/2}(2l+1)}{(2l+3)(2l+7)}. \tag{D19}$$

According to representations (101)–(104), the function $\mathcal{M}_2(l)$ can be represented in the form

$$\begin{aligned}\mathcal{M}_2(l) &\equiv \int_0^1 \phi_l^{(p)}(\rho) \frac{\rho^{2l+2}}{(\rho^2+1)^{2l+3}} d\rho \\ &= \frac{2^{-l}}{3(2l-3)(2l-1)(2l+3)(2l+5)}\left[2\mathcal{M}_{21}(l) + \frac{2\mathcal{M}_{22}(l) + \mathcal{M}_{23}(l)}{2l+1}\right],\end{aligned} \tag{D20}$$

where

$$\mathcal{M}_{21}(l) = -\frac{1}{6}\left[\frac{13-4l^2}{2^{l+5/2}} + \frac{8l^3+28l^2-2l-79}{l+2}\, {}_2F_1\left(l+2, l+\frac{9}{2}; l+3; -1\right)\right], \tag{D21}$$

$$\mathcal{M}_{22}(l) = \frac{(2l+1)(2l+5)}{(2l+3)(2l+7)^2}\left\{\frac{(2l+3)}{2^{l+7/2}}\left[\pi(2l+7) - \frac{4(4l^2+24l+23)}{(2l+1)(2l+5)}\right] - \frac{2\sqrt{\pi}(l+1)!}{\Gamma(l+1/2)} + 2^{3/2}(l+1)\, {}_2F_1\left(-\frac{1}{2}, -l; \frac{1}{2}; \frac{1}{2}\right)\right\}, \tag{D22}$$

$$\mathcal{M}_{23}(l) = (-1)^{l+1}\left[\mathcal{D}_l + \sum_{k=1}^{l} \frac{(-1)^k}{k} \mathcal{G}_{kl}\right]. \tag{D23}$$

In the function (D23) we have introduced the following notation:

$$\begin{aligned}\mathcal{D}_l = \frac{2^{-l-3/2}}{(2l+3)(2l+5)(2l+7)^2}\{&181 \times 2^{l+5/2} - 525 \ln 2 - 1046 + l[2^{l+11/2}(l+3)[11+2l(l+3)] \\ &- 8\{195 + 4l[31 + l(l+9)]\} - 2(985 + 4l\{303 + 2l[83 + l(21+2l)]\}) \ln 2]\},\end{aligned} \tag{D24}$$

$$\begin{aligned}\mathcal{G}_{kl} = &\frac{(2l-3)(2l-1)}{2(k+1)}\, {}_2F_1\left(k+1, l+\frac{9}{2}; k+2; -1\right) \\ &+ (2l+5)\left(\frac{2l-3}{k+2}\, {}_2F_1\left(k+2, l+\frac{9}{2}; k+3; -1\right) + \frac{2l+3}{2(k+3)}\, {}_2F_1\left(k+3, l+\frac{9}{2}; k+4; -1\right)\right).\end{aligned} \tag{D25}$$

To derive formulas (D23)–(D25), the representation (D8) was used.

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