Analytic calculation of the edge components of the angular Fock coefficients

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The present paper constitutes a development of our previous work devoted to calculations of the angular Fock coefficients $\psi_{k,p}(\alpha,\theta)$. Explicit analytic representations for the edge components $\psi_{k,0}^{(0)}$ and $\psi_{k,0}^{(k)}$ with $k \leqslant 8$ are derived. The methods developed enable such a calculation for arbitrary k. The single-series representation for subcomponent $\psi_{3,0}^{(2e)}$ missed in the author's previous paper is developed. It is also shown how to express some of the complicated subcomponents through hypergeometric and elementary functions. Using the operator FindSequenceFunction of Wolfram's *Mathematica*, simple explicit representations for some complicated mathematical expressions under consideration have been obtained.

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I. INTRODUCTION

As far back as the 1935s Bartlett *et al.* [1] showed that no ascending power series in the interparticle coordinates r_1, r_2, and r_{12} can be a formal solution of the Schrödinger equation for the ^1S-state of helium. Later Bartlett [2] argued the existence of the helium ground state expansion included $\ln(r_1^2+r_2^2)$. Finally, Fock [3] proposed the expansion

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

where $r=\sqrt{r_1^2+r_2^2}$ denotes the hyperspherical radius, and the hyperspherical angles α and θ are defined as

$$\alpha = 2\arctan{(r_2/r_1)},\ \ \theta=\arccos\left[\left(r_1^2+r_2^2-r_{12}^2\right)/(2r_1r_2)\right]. \qquad (2)$$

The convergence of expansion (1) for the ground state of helium was rigorously studied in Refs. [4,5]. The method proposed by Fock [3] for investigating 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 generalized [8] to be applicable to any S state, and its first two terms were determined. The most comprehensive investigation of the methods of derivation and calculation of the angular Fock coefficients (AFC) $\psi_{k,p}(\alpha,\theta)$ was presented in the works of Abbott, Gottschalk, and Maslen [9–11]. In Ref. [12] a further development of the methods of calculation of the AFC was presented. Separation of the AFC by the components, associated with definite powers of the nucleus charge Z, was introduced. Some of the AFC, or their components that were not calculated previously, were derived [12].

A number of variational methods were developed for calculation of the electronic structure of the helium isoelectronic sequence. It was mentioned in the classic paper of Fock [3] that the success in application of any variational method is substantially dependent upon the choice of basis functions, and that the technique proposed in [3] could be helpful to make such a choice. However, one should emphasize that this is the "next step" which was nevertheless realized (used for beginning the first terms of the Fock expansion), e.g, in the papers [6,7,13,14]. It is generally accepted that derivations of the angular functions (Fock coefficients) describing the Fock expansion constitute an independent problem of great complexity.

The present paper improves and develops methods and extends the results obtained in the previous work [12]. We derive exact expressions for the edge components of the most complicated AFC $\psi_{k,0}(\alpha,\theta)$. We calculate the subcomponent $\psi_{3,0}^{(2e)}$ missed in [12]. We show how to express some of the complicated subcomponents through elementary functions. Using the operator FindSequenceFunction of the Wolfram *Mathematica*, we obtain simple explicit representations for some complicated mathematical objects under consideration.

To solve the problems, we introduce some mathematical concepts that can serve as a basis for further consideration. It has been proven that the AFC satisfy (see, e.g., [9] or [12]) the Fock recurrence relation (FRR)

$$[\Lambda^2-k(k+4)]\psi_{k,p}=h_{k,p}, \qquad (3a)$$

$$h_{k,p}=2(k+2)(p+1)\psi_{k,p+1}+(p+1)(p+2)\psi_{k,p+2} -2V\psi_{k-1,p}+2E\psi_{k-2,p}, \qquad (3b)$$

where E is the energy and $V=V_0+ZV_1$ is the dimensionless Coulomb interaction for the two-electron atom and/or ions. The electron-electron V_0 and the electron-proton V_1 interactions are defined as follows

$$V_0=1/\xi, \qquad V_1=-[\csc(\alpha/2)+\sec(\alpha/2)], \qquad (4)$$

where the variable

$$\xi=\sqrt{1-\sin\alpha\cos\theta}. \qquad (5)$$

The hyperspherical angular momentum operator, projected on S states, is

$$\Lambda^2=-\frac{4}{\sin^2\alpha}\left(\frac{\partial}{\partial\alpha}\sin^2\alpha\frac{\partial}{\partial\alpha}+\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right), \qquad (6)$$

and its eigenfunctions are the hyperspherical harmonics (HH)

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

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

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

so that

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

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

$$d\Omega = \pi^2 \sin^2\alpha d\alpha \sin\theta d\theta, \qquad \alpha \in [0,\pi], \theta \in [0,\pi]. \tag{10}$$

It was shown [12] that any AFC $\psi_{k,p}$ can be separated into the independent parts (components)

$$\psi_{k,p}(\alpha,\theta) = \sum_{j=p}^{k-p} \psi_{k,p}^{(j)}(\alpha,\theta)Z^j \tag{11}$$

associated with a definite power of Z, according to the separation of the right-hand side (rhs) (3b)

$$h_{k,p}(\alpha,\theta) = \sum_{j=p}^{k-p} h_{k,p}^{(j)}(\alpha,\theta)Z^j \tag{12}$$

of the FRR. Accordingly, each of the FRR (3) can be separated into the individual equations (IFRR) for each component:

$$[\Lambda^2 - k(k+4)]\psi_{k,p}^{(j)}(\alpha,\theta) = h_{k,p}^{(j)}(\alpha,\theta). \tag{13}$$

II. THE EDGE COMPONENTS OF THE MOST COMPLICATED AFC

It is well-known that calculations of the logarithmless AFC $\psi_{k,0}(\alpha,\theta)$ with $k = 1,2,3,\ldots$ are the most complicated ones. However, it is easy to show that the edge components $\psi_{k,0}^{(0)}$ and $\psi_{k,0}^{(k)}$ of those AFC can be calculated without any problems. Indeed, for $p = 0$, Eq. (3b) reduces to the form

$$h_{k,0} = 2(k+2)\psi_{k,1} + 2\psi_{k,2} - 2V\psi_{k-1,0} + 2E\psi_{k-2,0}. \tag{14}$$

Substitution of Eqs. (11) and (12) for the coefficients of powers of Z into Eq. (14) yields for the right-hand sides of the IFFR (13) with the mentioned edge components

$$h_{k,0}^{(0)} = -2V_0\psi_{k-1,0}^{(0)} + 2E\psi_{k-2,0}^{(0)}, \tag{15}$$

$$h_{k,0}^{(k)} = -2V_1\psi_{k-1,0}^{(k-1)}, \tag{16}$$

where the angular dependent potentials V_0 and V_1 are defined by Eq. (4). It is seen that the rhs (15) and (16) of the order k are represented by the corresponding edge components of the order $k-1$ and $k-2$ (if exists). Moreover, taking into account that $\psi_{1,0}^{(1)}$ is a function of α {see Eq. (49) [12]}and $\psi_{1,0}^{(0)}$ is a function of ξ {see Eq. (36) [12]}, one can conclude that any component $\psi_{k,0}^{(k)}$ (for $k \geqslant 1$) must be a function of a single angle α, whereas $\psi_{k,0}^{(0)}$ (for $k \geqslant 1$) must be a function of a single variable ξ defined by Eq. (5). Representation (4) for the potentials was used to draw the above conclusions.

There is a specific difference between derivations of the edge components $\psi_{k,0}^{(0)}$ and $\psi_{k,0}^{(k)}$ for even and odd k. Therefore, we shall present such calculations in detail for $k = 4$ and $k = 5$, whereas for $k = 6,7,8$ the corresponding results will be presented without derivations.

The general IFRR (13) for $k = 4, p = 0, j = 0$ reduces to the form

$$(\Lambda^2 - 32)\psi_{4,0}^{(0)} = h_{4,0}^{(0)}, \tag{17}$$

where

$$\begin{aligned} h_{4,0}^{(0)} &\equiv -2V_0\psi_{3,0}^{(0)} + 2E\psi_{2,0}^{(0)} \\ &= -\frac{1}{36}[\xi^2(E-2) + 3(1-2E)^2] \end{aligned} \tag{18}$$

according to relation (15). The components $\psi_{3,0}^{(0)}$ and $\psi_{2,0}^{(0)}$ are presented in Table I and Eq. (55) of Ref. [12], respectively. It is seen that the rhs (18) of the IFRR (17) is a function of the single variable ξ. It was shown in Ref. [12] that in this case the solution of the IFRR (13) with the rhs $h_{k,p}^{(j)}(\alpha,\theta) \equiv \mathrm{h}(\xi)$ reduces to solving the differential equation

$$(\xi^2 - 2)\Phi_k''(\xi) + \frac{5\xi^2 - 4}{\xi}\Phi_k'(\xi) - k(k+4)\Phi_k(\xi) = \mathrm{h}(\xi), \tag{19}$$

where $\Phi_k(\xi) \equiv \psi_{k,p}^{(j)}(\alpha,\theta)$. A particular solution $\Phi_k^{(P)}$ of Eq. (19) can be found by the method of variation of parameters in the form

$$\begin{aligned} \Phi_k^{(P)}(\xi) = \frac{1}{(k+2)\sqrt{2}}\Bigg[&\mathrm{u}_k(\xi)\int \mathrm{v}_k(\xi)f(\xi)d\xi \\ &-\mathrm{v}_k(\xi)\int \mathrm{u}_k(\xi)f(\xi)d\xi\Bigg], \end{aligned} \tag{20}$$

where $f(\xi) = \mathrm{h}(\xi)\xi^2\sqrt{2-\xi^2}$. The linearly independent solutions of the homogeneous equation associated with Eq. (19) are defined by

$$\mathrm{u}_k(\xi) = \frac{P_{k+3/2}^{1/2}(\xi/\sqrt{2})}{\xi\sqrt[4]{2-\xi^2}}, \qquad \mathrm{v}_k(\xi) = \frac{Q_{k+3/2}^{1/2}(\xi/\sqrt{2})}{\xi\sqrt[4]{2-\xi^2}}, \tag{21}$$

where $P_\nu^\mu(x)$ and $Q_\nu^\mu(x)$ are the associated Legendre functions of the first and second kind, respectively. The general solution of the inhomogeneous equation (19) has the form

$$\Phi_k^{(P)}(\xi) + c_{1,k}\mathrm{u}_k(\xi) + c_{2,k}\mathrm{v}_k(\xi), \tag{22}$$

where the values of coefficients $c_{1,k}$ and $c_{2,k}$ are defined by requirements of the finiteness and "purity" of the final physical solution. The first requirement means that any component $\psi_{k,p}^{(j)}(\alpha,\theta)$ of the AFC must be finite at each point of the two-dimensional angular space described by the hyperspherical angles $\alpha \in [0,\pi]$ and $\theta \in [0,\pi]$. The second requirement is associated with only even values of k and concerns obtaining the single-valued solution containing no admixture of the HH $Y_{kl}(\alpha,\theta)$.

Turning to the component $\psi_{4,0}^{(0)}$, and simplifying the solutions (21) for $k = 4$, one obtains

$$\begin{aligned} \mathrm{u}_4(\xi) &= \frac{2^{3/4}[\xi^2(3-2\xi^2)^2 - 1]}{\xi\sqrt{\pi(2-\xi^2)}}, \\ \mathrm{v}_4(\xi) &= -\frac{\sqrt{\pi}}{2^{1/4}}(4\xi^4 - 8\xi^2 + 3). \end{aligned} \tag{23}$$

Substitution of the representations (18) and (23) into (20) yields

$$\Phi_4^{(P)}(\xi) = \frac{\xi^2}{1440}[10(2E-1)^2 - \xi^2(20E^2 - 21E + 7)]. \tag{24}$$

It is seen that the particular solution $\Phi_4^{(P)}$, as well as $v_4(\xi)$, are regular over the relevant angular space, whereas $u_4(\xi)$ is singular at the points $\xi = 0\,(\alpha = \pi/2, \theta = 0)$ and $\xi = \sqrt{2}\,(\alpha = \pi/2, \theta = \pi)$. Hence, first of all, one should set $c_{1,4} = 0$ in Eq. (22) to comply with the finiteness condition. It is clear that the requirement of "purity" reduces to the orthogonality condition

$$\int \psi_{4,0}^{(0)}(\alpha,\theta) Y_{4l}(\alpha,\theta) d\Omega = 0. \tag{25}$$

Given that $\psi_{4,0}^{(0)} = \Phi_4^{(P)}(\xi) + c_{2,4} v_4(\xi)$, one obtains for the coefficient

$$c_{2,4} = -\int \Phi_4^{(P)}(\xi) Y_{40}(\alpha,\theta) d\Omega \left[\int v_4(\xi) Y_{40}(\alpha,\theta) d\Omega\right]^{-1} = \frac{E(21-20E)-7}{2880\sqrt{\pi}\,2^{3/4}}. \tag{26}$$

Whence the final result for the "pure" component is

$$\psi_{4,0}^{(0)} = \frac{60E^2 - 63E + 21 + 8\xi^2(E-2)}{5760}. \tag{27}$$

Note that to derive Eq. (26) we put $l = 0$ in Eq. (25). However, putting $l = 2$ one obtains the same result, whereas for $l = 1$ one obtains identity.

The next step is deriving the solution of the IFRR (13) for $k = 4, p = 0, j = 4$, which becomes

$$(\Lambda^2 - 32)\psi_{4,0}^{(4)} = h_{4,0}^{(4)}. \tag{28}$$

Expression (16) yields for the rhs of Eq. (28)

$$h_{4,0}^{(4)} \equiv -2V_1 \psi_{3,0}^{(3)} = -\frac{1}{18}(2 + 5\sin\alpha)\left[\tan\left(\frac{\alpha}{2}\right) + \cot\left(\frac{\alpha}{2}\right) + 2\right], \tag{29}$$

where the component $\psi_{3,0}^{(3)}$ is presented in Table I of Ref. [12]. Transforming to the variable

$$\rho = \tan(\alpha/2), \tag{30}$$

one obtains

$$h(\rho) \equiv h_{4,0}^{(4)}(\alpha,\theta) = -\frac{(1+\rho)^2(1+5\rho+\rho^2)}{9\rho(1+\rho^2)}. \tag{31}$$

It was shown (see Sec. V in Ref. [12]) that in case the rhs $h_{k,p}^{(j)}$ of the IFRR (13) reduces to the function $h(\alpha) \equiv h(\rho)$ of a single variable α (or ρ), the solution of Eq. (13) represents a function $g(\rho) \equiv \psi_{k,p}^{(j)}(\alpha)$ satisfying the differential equation

$$(1+\rho^2)^2 g''(\rho) + 2\rho^{-1}(1+\rho^2) g'(\rho) + k(k+4) g(\rho) = -h(\rho). \tag{32}$$

The method of variation of parameters enables us to obtain the particular solution of Eq. (32) in the form

$$g(\rho) = u_k(\rho) \int \frac{v_k(\rho) h(\rho) \rho^2}{(\rho^2+1)^3} d\rho - v_k(\rho) \int \frac{u_k(\rho) h(\rho) \rho^2}{(\rho^2+1)^3} d\rho, \tag{33}$$

where the linearly independent solutions of the homogeneous equation associated with Eq. (32) are

$$u_k(\rho) = \frac{(1+\rho^2)^{k/2+2}}{\rho} {}_2F_1\left(\frac{k+3}{2}, \frac{k}{2}+1; \frac{1}{2}; -\rho^2\right), \tag{34}$$

$$v_k(\rho) = (1+\rho^2)^{k/2+2} {}_2F_1\left(\frac{k+3}{2}, \frac{k}{2}+2; \frac{3}{2}; -\rho^2\right). \tag{35}$$

The Gauss hypergeometric function ${}_2F_1$ was introduced in Eqs. (34) and (35). The general solution of the inhomogeneous equation (32) is defined as

$$g(\rho) + b_{1,k} u_k(\rho) + b_{2,k} v_k(\rho), \tag{36}$$

where the coefficients $b_{1,k}$ and $b_{2,k}$ can be determined by the requirements of finiteness and "purity", as explained earlier. Turning to the case of $k = 4$, one obtains for the independent solutions of the homogeneous equation:

$$u_4(\rho) = \frac{(1+\rho^2)^4}{\rho} {}_2F_1\left(\frac{7}{2}, 3; \frac{1}{2}; -\rho^2\right) = \frac{(1-\rho^2)(1-4\rho+\rho^2)(1+4\rho+\rho^2)}{\rho(1+\rho^2)^2}, \tag{37}$$

$$v_4(\rho) = (1+\rho^2)^4 {}_2F_1\left(\frac{7}{2}, 4; \frac{3}{2}; -\rho^2\right) = \frac{(\rho^2-3)(3\rho^2-1)}{3(1+\rho^2)^2}. \tag{38}$$

Substitution of the representations (37), (38), and (31) into the rhs of Eq. (33) yields for the particular solution

$$\psi_{4,0}^{(4)P} = \frac{\rho(3+7\rho+3\rho^2)}{54(1+\rho^2)^2} = \frac{1}{216}(6 + 7\sin\alpha)\sin\alpha. \tag{39}$$

It is seen that the particular solution $g(\rho)$ and the solution $v_4(\rho)$ of the homogeneous equation are regular over the relevant angular space, whereas $u_4(\rho)$ is singular at the point $\rho = 0\,(\alpha = 0)$. Hence, one should set $b_{1,4} = 0$ in Eq. (36) to comply with the finiteness condition. The requirement of "purity" can be expressed through the relation

$$\int \psi_{4,0}^{(4)}(\alpha,\theta) Y_{4l}(\alpha,\theta) d\Omega = 0. \tag{40}$$

Given that $\psi_{4,0}^{(4)} = g(\rho) + b_{2,4} v_4(\rho)$, one obtains for the coefficient

$$b_{2,4} = -\int g(\rho) Y_{40}(\alpha,\theta) d\Omega \left[\int v_4(\rho) Y_{40}(\alpha,\theta) d\Omega\right]^{-1} = \frac{7}{288} + \frac{2}{45\pi}. \tag{41}$$

Whence the final result for the "pure" component is

$$\psi_{4,0}^{(4)} = \frac{120\pi\sin\alpha + 128\cos(2\alpha) + 105\pi + 64}{4320\pi}. \tag{42}$$

Note that for $l = 1,2$ the orthogonality condition (40) is an identity.

Putting $k=5, p=0, j=0$ in Eq. (13), one obtains

$$(\Lambda^2-45)\psi_{5,0}^{(0)}=h_{5,0}^{(0)}, \tag{43}$$

where according to relation (15)

$$h_{5,0}^{(0)}\equiv -2V_0\psi_{4,0}^{(0)}+2E\psi_{3,0}^{(0)}=\frac{63E-21-60E^2+8(2+29E-60E^2)\xi^2+80E(E-2)\xi^4}{2880\xi}. \tag{44}$$

We used Eq. (27) for the representation of the component $\psi_{4,0}^{(0)}$.

The independent solutions (21) of the homogeneous equation associated with Eq. (19) for $k=5$ become

$$\mathrm{u}_5(\xi)=\frac{2^{1/4}(8\xi^6-28\xi^4+28\xi^2-7)}{\sqrt{\pi(2-\xi^2)}},$$
$$\mathrm{v}_5(\xi)=\frac{\sqrt{\pi}(1-12\xi^2+20\xi^4-8\xi^6)}{2^{3/4}\xi}. \tag{45}$$

Substitution of the representations (44) and (45) into the particular solution (20) of the inhomogeneous equation (19) for $k=5$ yields

$$\Phi_5^{(P)}=\frac{\xi}{172800}[45(7-21E+20E^2)-5(113-199E+60E^2)\xi^2+2(113-119E+20E^2)\xi^4]. \tag{46}$$

It is seen that the particular solution (46) is regular over the relevant angular space, whereas $\mathrm{u}_5(\xi)$ is singular at the point $\xi=\sqrt{2}$, and $\mathrm{v}_5(\xi)$ is singular at the point $\xi=0$. Hence, the physical solution of Eq. (43) coincides with the particular solution (46), that is,

$$\psi_{5,0}^{(0)}=\Phi_5^{(P)}. \tag{47}$$

The general IFRR (13) for $k=5$, $p=0$, $j=5$ reduces to the form

$$(\Lambda^2-45)\psi_{5,0}^{(5)}=h_{5,0}^{(5)}, \tag{48}$$

where according to Eq. (16)

$$h_{5,0}^{(5)}\equiv -2V_1\psi_{4,0}^{(4)}=\frac{(1+\rho)[64(3-10\rho^2+3\rho^4)+15\pi(1+\rho^2)(7+16\rho+7\rho^2)]}{2160\pi\rho(1+\rho^2)^{3/2}}, \tag{49}$$

is expressed through the variable ρ defined by Eq. (30). According to Eqs. (34) and (35) the linearly independent solutions of the homogeneous equation associated with Eq. (32) for $k=5$ can be simplified to the form

$$u_5(\rho)=\frac{(1+\rho^2)^{9/2}}{\rho}{}_2F_1\left(4,\frac{7}{2};\frac{1}{2};-\rho^2\right)=\frac{1-7\rho^2(3-5\rho^2+\rho^4)}{\rho(1+\rho^2)^{5/2}}, \tag{50}$$

$$v_5(\rho)=(1+\rho^2)^{9/2}{}_2F_1\left(4,\frac{9}{2};\frac{3}{2};-\rho^2\right)=\frac{7-35\rho^2+21\rho^4-\rho^6}{7(1+\rho^2)^{5/2}}. \tag{51}$$

Substituting representations (49)–(51) into the rhs of Eq. (33), one obtains for the particular solution of Eq. (32) with $k=5$

$$\psi_{5,0}^{(5)P}=-\frac{1}{453\,600\pi\rho(1+\rho^2)^{5/2}}[64(23+161\rho-168\rho^2-700\rho^3+105\rho^4+315\rho^5)$$
$$+15\pi(43+301\rho-168\rho^2-700\rho^3+805\rho^4+735\rho^5)]. \tag{52}$$

The physical solution $\psi_{5,0}^{(5)}$ of the IFRR (48) must be finite for all values of $0\leqslant\alpha\leqslant\pi$ and hence for $\rho\geqslant 0$. Therefore, let us consider the power series expansions of the particular solution $\psi_{5,0}^{(5)P}(\rho)$ and the individual solutions $u_5(\rho)$ and $v_5(\rho)$ of the corresponding homogeneous equation about $\rho=0$ and $\rho=\infty$. One obtains

$$\psi_{5,0}^{(5)P}(\rho)\underset{\rho\to 0}{=}-\frac{1}{\rho}\left(\frac{43}{30\,240}+\frac{46}{14\,175\pi}\right)-\left(\frac{43}{4320}+\frac{46}{2025\pi}\right)+O(\rho), \tag{53a}$$

$$\psi_{5,0}^{(5)P}(\rho)\underset{\rho\to\infty}{=}-\frac{1}{\rho}\left(\frac{7}{288}+\frac{2}{45\pi}\right)-\frac{1}{\rho^2}\left(\frac{23}{864}+\frac{2}{135\pi}\right)+O\left(\frac{1}{\rho^3}\right), \tag{53b}$$

$$u_5(\rho)\underset{\rho\to 0}{=}\frac{1}{\rho}-\frac{47\rho}{2}+O(\rho^3), \tag{54a}$$

$$u_5(\rho)\underset{\rho\to\infty}{=}-7+\frac{105}{2\rho^2}+O\left(\frac{1}{\rho^3}\right), \tag{54b}$$

$$v_5(\rho) \underset{\rho\to 0}{=} 1 - \frac{15\rho^2}{2} + O(\rho^3), \tag{55a}$$

$$v_5(\rho) \underset{\rho\to\infty}{=} -\frac{\rho}{7} + \frac{47}{14\rho} + O\left(\frac{1}{\rho^3}\right). \tag{55b}$$

It is seen that $v_5(\rho)$ is divergent as $\rho \to \infty$, whereas $u_5(\rho)$ and $\psi_{5,0}^{(5)P}(\rho)$ are singular at the point $\rho = 0$. Thus, in order to comply with the finiteness condition, one should set $b_{2,5} = 0$ and

$$b_{1,5} = \frac{43}{30\,240} + \frac{46}{14\,175\pi} \tag{56}$$

in the general solution

$$\psi_{5,0}^{(5)P}(\rho) + b_{1,5}u_5(\rho) + b_{2,5}v_5(\rho). \tag{57}$$

The final result expressed in terms of the hyperspherical angle α is

$$\psi_{5,0}^{(5)} = -\frac{\left[\cos\left(\frac{\alpha}{2}\right) + \sin\left(\frac{\alpha}{2}\right)\right][4(32+45\pi) + 3(448+155\pi)\cos(2\alpha) + (704+465\pi)\sin\alpha]}{64\,800\pi}. \tag{58}$$

It is clear that using the technique described above, one can subsequently calculate the edge components of any given order k. Here we present such components up to $k = 8$. They are

$$\psi_{6,0}^{(0)} = \frac{1}{29\,030\,400}[3007 - 11\,361E + 16\,460E^2 - 10\,080E^3 - (4180E^2 - 12\,705E + 6215)\xi^2 + 24(113 - 119E + 20E^2)\xi^4], \tag{59}$$

$$\psi_{7,0}^{(0)} = \frac{\xi}{36\,578\,304\,000}[630(3007 - 11\,361E + 16\,460E^2 - 10\,080E^3) + 105(30\,240E^3 - 141\,700E^2 + 164\,283E - 60\,341)\xi^2 - 14(60\,480E^3 - 491\,860E^2 + 873\,789E - 430\,523)\xi^4 + 4(22\,680E^3 - 266\,950E^2 + 660\,219E - 430\,523)\xi^6], \tag{60}$$

$$\psi_{8,0}^{(0)} = \frac{1}{21\,069\,103\,104\,000}[5(30\,481\,920E^4 - 68\,266\,800E^3 + 72\,613\,544E^2 - 39\,544\,113E + 8\,871\,475) + 40(3\,250\,800E^3 - 13\,370\,360E^2 + 13\,273\,113E - 4\,324\,891)\xi^2 - 420(71\,280E^3 - 556\,120E^2 + 934\,809E - 430\,523)\xi^4 + 128(22\,680E^3 - 266\,950E^2 + 660\,219E - 430\,523)\xi^6], \tag{61}$$

$$\psi_{6,0}^{(6)} = \frac{1}{21\,772\,800\pi}[80(448+255\pi) + 144(448+155\pi)\cos(2\alpha) + 315(64+55\pi)\sin\alpha + 7(10\,816+4335\pi)\sin(3\alpha)], \tag{62}$$

$$\psi_{7,0}^{(7)} = -\frac{\left[\cos\left(\frac{\alpha}{2}\right) + \sin\left(\frac{\alpha}{2}\right)\right]}{609\,638\,400\pi}[3(585\pi - 10\,304)\sin\alpha + 3(58\,845\pi + 142\,016)\sin(3\alpha) + 8(4485\pi + 12\,992)\cos(2\alpha) + 97\,560\pi + 211\,456], \tag{63}$$

$$\psi_{8,0}^{(8)} = \frac{1}{1\,843\,546\,521\,600\pi^2}\{94\,502\,912 + 75\pi(1\,946\,944 + 626\,787\pi) + 2[94\,502\,912 + 3\pi(43\,273\,408 + 12\,251\,925\pi)]\cos(2\alpha) + 4096(46\,144 + 19\,275\pi)\cos(4\alpha) + 1008\pi[105(448+225\pi)\sin\alpha + (142\,016 + 58\,845\pi)\sin(3\alpha)]\}. \tag{64}$$

III. SINGLE-SERIES REPRESENTATION FOR THE SUBCOMPONENT $\psi_{3,0}^{(2e)}$

It was shown in Ref. [12] that the AFC component $\psi_{3,0}^{(2)}$ represents the sum of subcomponents $\psi_{3,0}^{(2x)}$ with $x = a,b,c,d$. Unfortunately, the extra subcomponent $\psi_{3,0}^{(2e)}$ corresponding to the rhs

$$h_{3,0}^{(2e)} = -\frac{\sin\alpha}{\xi}, \tag{65}$$

of the IFFR

$$(\Lambda^2 - 21)\psi_{3,0}^{(2e)} = h_{3,0}^{(2e)} \tag{66}$$

was missed in Ref. [12]. Using the technique described in Sec. V of Ref. [12], we have found the mentioned subcomponent (details can be found in Appendix A) in the form of the single-series representation

$$\psi_{3,0}^{(2e)} = \sum_{l=0}^{\infty} P_l(\cos\theta)(\sin\alpha)^l \lambda_l(\rho). \tag{67}$$

For $0 \leqslant \rho \leqslant 1$ the functions $\lambda_l(\rho)$ can be written in the form

$$\lambda_l(\rho) = \frac{1}{2l+1}\{u_{3,l}(\rho)\mathcal{V}_{3,l}(\rho) - v_{3,l}(\rho)[\mathcal{U}_{3,l}(\rho) - (2l+1)s_l]\}, \tag{68}$$

where

$$u_{3,l}(\rho) = \frac{(\rho^2+1)^{l-\frac{3}{2}}}{\rho^{2l+1}}\left[\frac{(2l+3)(2l+5)}{(2l-3)(2l-1)}\rho^4 + \frac{2(2l+5)}{2l-1}\rho^2 + 1\right], \tag{69}$$

$$v_{3,l}(\rho) = (\rho^2+1)^{l-\frac{3}{2}}\left[\frac{(2l-3)(2l-1)}{(2l+3)(2l+5)}\rho^4 + \frac{2(2l-3)}{2l+3}\rho^2 + 1\right], \tag{70}$$

$$\mathcal{U}_{3,l}(\rho) = -\frac{l(l+1)\left[(\rho^2+1)^4\arctan(\rho) + \rho^7 - \rho\right] + (l^2-7l-10)\rho^5 - (l^2+9l-2)\rho^3}{2^l(2l-3)(2l-1)(\rho^2+1)^4}, \tag{71}$$

$$\mathcal{V}_{3,l}(\rho) = -[(-2)^l(l-2)(l-1)(2l+3)(2l+5)]^{-1}\{12[B_{-\rho^2}(l+1,-3) - B_{-\rho^2}(l+1,-4)] + (2l-3)\rho^2[2l^2+l-7+(l-2)(2l-1)\rho^2][(3-l)B_{-\rho^2}(l+1,-3) - 4B_{-\rho^2}(l+1,-4)]\} \tag{72}$$

Here $B_z(a,b)$ is the Euler beta function. It is seen that expression (72) cannot be applied directly for $l = 1,2$. For these values of l, one obtains

$$\mathcal{V}_{3,1}(\rho) = \frac{1}{140}\left[\frac{3+10\rho^2+11\rho^4-20\rho^6}{(1+\rho^2)^4} + 2\ln(1+\rho^2)\right], \tag{73}$$

$$\mathcal{V}_{3,2}(\rho) = -\frac{1}{84}\left[\frac{5+14\rho^2+9\rho^4-6\rho^6+24\rho^8+6\rho^{10}}{6(1+\rho^2)^4} + \ln(1+\rho^2)\right]. \tag{74}$$

Using the *Mathematica* operator FindSequenceFunction we have found a simple representation (the details can be found in Appendix A) for the coefficient

$$s_l = \frac{2^{-l-3}}{(2l-3)(2l-1)(2l+1)}[2l(l+1)(H_{\frac{l+1}{2}} - H_{\frac{l}{2}} - \pi) + 2l + 3], \tag{75}$$

in expression (68) for $\lambda_l(\rho)$. The functions H_z denote the harmonic numbers with a primary definition of the form

$$H_z = \gamma + \psi(z+1),$$

where $\psi(\bar{z})$ is the digamma function, and γ is the Euler-Mascheroni constant. Remember that for $\rho > 1$ one should replace ρ with $1/\rho$ in Eqs. (68) to (74).

IV. ELABORATION OF SOME RESULTS OBTAINED PREVIOUSLY

In Ref. [12] the various components of the AFC were derived in the form of a one-dimensional series with fast convergence. In particular, the solution of the IFRR

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

with the rather complicated rhs,

$$h_{4,1}^{(2d)} = \frac{\pi-2}{3\pi}\left[\sin\left(\frac{\alpha}{2}\right) + \cos\left(\frac{\alpha}{2}\right)\right] \times\left[\frac{5}{3\sin\alpha}\xi^3 + \left(1 - \frac{2}{\sin\alpha}\right)\xi - \frac{1}{\xi}\right], \tag{77}$$

was represented by a single series of the form

$$\psi_{4,1}^{(2d)} = \sum_{l=0}^{\infty} P_l(\cos\theta)(\sin\alpha)^l \tau_l(\rho), \tag{78}$$

where the variables ξ and ρ are defined by Eqs. (5) and (30), respectively. It was shown that for $l > 2$ the function $\tau_l(\rho)$ can be expressed by the formula

$$\tau_l(\rho) = \tau_l^{(P)}(\rho) + A_2(l)v_{4,l}(\rho), \tag{79}$$

where

$$\tau_l^{(P)}(\rho) = \frac{1}{2l+1}[u_{4,l}(\rho)\mathcal{V}_{4,l}(\rho) - v_{4,l}(\rho)\mathcal{U}_{4,l}(\rho)], \tag{80}$$

$$u_{4,l}(\rho) = \rho^{-2l-1}(\rho^2+1)_2^{l+4}F_1\left(\frac{7}{2},3-l;\frac{1}{2}-l;-\rho^2\right), \tag{81a}$$

$$v_{4,l}(\rho) = (\rho^2+1)_2^{l+4}F_1\left(\frac{7}{2},4+l;l+\frac{3}{2};-\rho^2\right). \tag{81b}$$

However, the function $\tau_l^{(P)}(\rho)$ as well as the coefficient $A_2(l)$ were represented in the closed form (see Eq. (C14) of Ref. [12]) only for $l \leqslant 10$.

Here, we present the functions mentioned above in a few general closed forms which are applicable for any $l \geqslant 3$. In particular, it is shown in Appendix B that the functions $\mathcal{U}_{4,l}$ and $\mathcal{V}_{4,l}$ included in the rhs of expression (80) can be represented in the form:

$$\mathcal{U}_{4,l}(\rho) = a_{0l}\frac{8(l-3)!}{15\sqrt{\pi}\Gamma(l+1/2)}\sum_{m=0}^{l-3}\frac{\Gamma(m+7/2)\Gamma(l-m+1/2)(-1)^m}{m!(l-m-3)!}\sum_{n=1}^{5}a_{nl}\left(\frac{\rho^{2m+n}-1}{2m+n}+\frac{\rho^{2m+n+1}-1}{2m+n+1}\right), \tag{82}$$

$$\begin{aligned}\mathcal{V}_{4,l}(\rho) = {}& \frac{4a_{0l}\Gamma(l+3/2)}{15\sqrt{\pi}}\rho^{2l+3}\sum_{m=0}^{2}\frac{m!}{(1+\rho^2)^{5-m}}\sum_{k=0}^{m}\frac{\Gamma(k+7/2)}{k!(m-k)!\Gamma(k+l+3/2)}\left(-\frac{\rho^2}{1+\rho^2}\right)^k\\ &\times\left[\frac{(k+l+3)!\Gamma(l+m+3/2)}{(l+3)!\Gamma(k+l+m+5/2)}b_{2m+1,l}\rho^{2m}{}_2F_1\left(l+m-1,m-\frac{3}{2};k+l+m+\frac{5}{2};-\rho^2\right)\right.\\ &\left.+\frac{b_{2(2-m),l}}{k+l-m+3}\rho^{3-2m}{}_2F_1\left(l-2,m-\frac{3}{2};k+l+\frac{3}{2};-\rho^2\right)\right],\end{aligned} \tag{83}$$

where

$$a_{0l} = -\frac{(\pi-2)2^{-l-1}}{3\pi(2l-1)(2l+3)}, \quad a_{1l} = \frac{15-4l(l+1)(4l+11)}{(2l-3)(2l+5)}, \quad a_{2l} = 4l(2l+3),$$
$$a_{3l} = 2, \quad a_{4l} = 4(l+1)(2l-1), \quad a_{5l} = \frac{(2l-1)(4l+5)}{2l+5}, \tag{84}$$

$$b_{0,l} = a_{1l}, \quad b_{5,l} = a_{5l}, \quad b_{s,l} = a_{sl} + a_{s+1l} \quad (s = 1,2,3,4). \tag{85}$$

Moreover, it is shown in Appendix B that all of the Gauss hypergeometric functions in Eqs. (81) and (83) can be expressed as elementary functions. A simple representation of the function $\mathcal{V}_{4,l}(\rho)$ through the generalized hypergeometric functions ${}_3F_2$ is also derived.

Making use of the *Mathematica* operator FindSequenceFunction, the following representation was derived (see the details in Appendix C) for the factor $A_2(l)$ in the rhs of Eq. (79):

$$A_2(l) = \frac{(2-\pi)\pi^{-3/2}}{360l(l-2)\Gamma(l+\frac{1}{2})}\left\{\frac{[l(l+1)(688l^4+1376l^3-2480l^2-3168l+465)+450]\Gamma\left(\frac{l-1}{2}\right)\Gamma\left(\frac{l+1}{2}\right)}{(2l-3)(2l-1)(2l+1)(2l+3)(2l+5)} - \frac{56}{l-1}\left(\frac{l}{2}!\right)^2\right\}. \tag{86}$$

Note that Eq. (86) is correct only for even $l > 2$, whereas $A_2(l) \equiv 0$ for odd values of l.

The last subcomponent derived in Ref. [12] in the form of a single-series representation was

$$\psi_{3,0}^{(2c)}(\alpha,\theta) = \sum_{l=0}^{\infty} P_l(\cos\theta)(\sin\alpha)^l\phi_l(\rho). \tag{87}$$

It is the physical solution of the IFFR

$$(\Lambda^2 - 21)\psi_{3,0}^{(2c)} = h_{3,0}^{(2c)}, \tag{88}$$

with the rhs

$$h_{3,0}^{(2c)} = -\frac{4\xi}{3\sin\alpha}. \tag{89}$$

The function $\phi_l(\rho)$ was obtained [12] in the form

$$\phi_l(\rho) = \phi_l^{(P)}(\rho) + c_l v_{3,l}(\rho), \tag{90}$$

where closed-form expressions for the functions $\phi_l^{(P)}(\rho)$ were derived in [12] (see also Appendix D), and the function $v_{3,l}(\rho)$ is defined by Eq. (70). The problem is that the coefficient c_l was obtained in a very complicated integral form. A simple form of this coefficient can be written as follows:

$$c_l = \frac{2(2l+1) - \pi - H_{\frac{l}{2}} + H_{\frac{l-1}{2}}}{6(2l-3)(2l-1)(2l+1)2^l}, \tag{91}$$

where H_z are the harmonic numbers. The details can be found in Appendix D.

V. CONCLUSIONS

The individual Fock recurrence relations introduced in [12] were used to derive explicit expressions for the components $\psi_{k,0}^{(0)}$ and $\psi_{k,0}^{(k)}$ of the AFC $\psi_{k,0}$. Using the methods described in [12], the above-mentioned edge components were calculated and presented for $4 \leqslant k \leqslant 8$. However, since the IFRR for the edge components of the order k contain only the edge components of the lower order, there is no problem to calculate the edge components with arbitrary k. Moreover, it was stated that the components $\psi_{k,0}^{(k)}$ for $k \geqslant 1$ are functions of the hyperspherical angle α only, whereas the components $\psi_{k,0}^{(0)}$ are functions of the single variable ξ defined by Eq. (5).

The single-series representation [see Eq. (67)] was derived for the subcomponent $\psi_{3,0}^{(2e)}$ missed in [12]. This subcomponent is the physical solution of the IFRR (66) with its rhs of the form (65). The specific coefficient s_l, which is a part of the mentioned representation, was found in a simple explicit form. This coefficient was derived by an application of the *Mathematica* operator FindSequenceFunction. The same method was applied to find simple expressions for the coefficients c_l and $A_2(l)$ in the single-series representations of the subcomponents

$\psi^{(2c)}_{3,0}$ and $\psi^{(2d)}_{4,1}$, respectively. For the latter subcomponent we also derived closed explicit representations in terms of hypergeometric functions and elementary functions.

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APPENDIX A

In this Appendix we describe the details of deriving the subcomponent $\psi^{(2e)}_{3,0}$ representing the solution of the IFRR (66) with its rhs of the form (65). The physical solution of Eq. (66) we shall seek in the form of the single-series (67). First, using the Sack representation for ξ^{-1} (see, e.g., [9] or [12]), let us represent the rhs of the IFRR (66) in the form

$$h^{(2e)}_{3,0} = \sum_{l=0}^{\infty} P_l(\cos\theta)(\sin\alpha)^l \mathrm{h}_l(\alpha), \tag{A1}$$

where

$$\mathrm{h}_l(\alpha) = -2^{-l}(\sin\alpha)\,{}_2F_1\left(\frac{l}{2}+\frac{1}{4},\frac{l}{2}+\frac{3}{4};l+\frac{3}{2};\sin^2\alpha\right) = -2^{-l}\sin\alpha \begin{cases}\sec^{2l+1}\left(\frac{\alpha}{2}\right), & 0\leqslant\alpha\leqslant\frac{\pi}{2}\\ \csc^{2l+1}\left(\frac{\alpha}{2}\right). & \frac{\pi}{2}\leqslant\alpha\leqslant\pi.\end{cases} \tag{A2}$$

For $0\leqslant\rho\leqslant 1$ [see definition (30)] Eq. (A2) reduces to {see Eq. (B3) in Ref. [12]}

$$h_l(\rho) \equiv \mathrm{h}_l(\alpha) = -2^{1-l}\rho(1+\rho^2)^{l-1/2}. \tag{A3}$$

To derive the function $\lambda_l(\rho)$ one needs to solve Eq. (44) of Ref. [12] for $k=3$, which is

$$(1+\rho^2)^2\lambda_l''(\rho) + 2\rho^{-1}[1+\rho^2+l(1-\rho^4)]\lambda_l'(\rho) + (3-2l)(2l+7)\lambda_l(\rho) = -h_l(\rho). \tag{A4}$$

Using the method of variation of parameters, a particular solution of Eq. (A4) can be obtained in the form

$$\lambda_l^{(P)}(\rho) = \frac{1}{2l+1}[u_{3,l}(\rho)\mathcal{V}_{3,l}(\rho) - v_{3,l}(\rho)\mathcal{U}_{3,l}(\rho)], \tag{A5}$$

where the individual solutions $u_{3,l}(\rho)$ and $v_{3,l}(\rho)$ of the homogeneous equation associated with Eq. (A4) are represented by Eqs. (69) and (70) {see also Eqs. (D6) and (D7) of Ref. [12]}, whereas for the integral factors one obtains

$$\mathcal{U}_{3,l}(\rho) \equiv \int \frac{u_{3,l}(\rho)h_l(\rho)\rho^{2l+2}}{(\rho^2+1)^{2l+3}}d\rho = -\frac{l(l+1)[(\rho^2+1)^4\arctan(\rho)+\rho^7-\rho] + (l^2-7l-10)\rho^5 - (l^2+9l-2)\rho^3}{2^l(2l-3)(2l-1)(\rho^2+1)^4}, \tag{A6}$$

$$\begin{aligned}\mathcal{V}_{3,l}(\rho) \equiv \int \frac{v_{3,l}(\rho)h_l(\rho)\rho^{2l+2}}{(\rho^2+1)^{2l+3}}d\rho = &-[(-2)^l(l-2)(l-1)(2l+3)(2l+5)]^{-1}\{12[B_{-\rho^2}(l+1,-3) - B_{-\rho^2}(l+1,-4)]\\ &+(2l-3)\rho^2[2l^2+l-7+(l-2)(2l-1)\rho^2][(3-l)B_{-\rho^2}(l+1,-3) - 4B_{-\rho^2}(l+1,-4)]\}.\end{aligned} \tag{A7}$$

It is seen that expression (A7) cannot be applied directly for $l=1$ or 2. For these values of l, one easily obtains the expressions (73) and (74).

It can be verified that $u_{3,l}(\rho)$ is singular, whereas $v_{3,l}(\rho)$ and the particular solution $\lambda_l^{(P)}(\rho)$ are regular at the point $\rho=0\,(\alpha=0)$ for any $l\geqslant 0$. Hence, the physical solution is of the form

$$\lambda_l(\rho) = \lambda_l^{(P)}(\rho) + s_l v_{3,l}(\rho), \tag{A8}$$

where the coefficient s_l can be found by the coupling equation (61) of Ref. [12], which for this case becomes

$$\mathcal{Q}_{2l,l} = \frac{2^{2(l+2)}(l+1)!}{\sqrt{\pi}\,\Gamma\left(l+\frac{3}{2}\right)}\int_0^1 \left[\lambda_l^{(P)}(\rho) + s_l v_{3,l}(\rho)\right]\frac{\rho^{2l+2}}{(\rho^2+1)^{2l+3}}d\rho. \tag{A9}$$

Here, $\mathcal{Q}_{n,l}$ denotes the unnormalized HH expansion coefficients for subcomponent

$$\psi^{(2e)}_{3,0}(\alpha,\theta) = \sum_{nl}\mathcal{Q}_{n,l}Y_{nl}(\alpha,\theta). \tag{A10}$$

To derive the closed-form expression for $\mathcal{Q}_{n,l}$, we first obtain the unnormalized HH expansion

$$h^{(2e)}_{3,0}(\alpha,\theta) = \sum_{nl}\mathcal{H}_{n,l}Y_{nl}(\alpha,\theta) \tag{A11}$$

for the rhs of Eq. (66), where by definition

$$\mathcal{H}_{n,l} = N_{nl}^2\int h^{(2e)}_{3,0}(\alpha,\theta)Y_{nl}(\alpha,\theta)d\Omega \tag{A12}$$

with the normalization constant defined by Eq. (8). Inserting Eqs. (A1) and (A2) and the HH definition (7) into the rhs of Eq. (A12), one obtains

$$\mathcal{H}_{n,l} = -\frac{2^{l+2}N_{nl}^2\pi^2}{2l+1}\left[\int_0^{\pi/2}\sin^{2l+1}\left(\frac{\alpha}{2}\right)\sin^2\alpha C_{n/2-l}^{(l+1)}(\cos\alpha)d\alpha + \int_{\pi/2}^{\pi}\cos^{2l+1}\left(\frac{\alpha}{2}\right)\sin^2\alpha C_{n/2-l}^{(l+1)}(\cos\alpha)d\alpha\right], \quad \text{(A13)}$$

where the orthogonality of the Legendre polynomials was used. On the other hand, substitution of expansion (A10) into the left-hand side of Eq. (66) yields

$$(\Lambda^2 - 21)\psi_{3,0}^{(2e)} = \sum_{nl}\mathcal{Q}_{n,l}(n-3)(n+7)Y_{nl}(\alpha,\theta). \quad \text{(A14)}$$

According to Eq. (66), the right-hand sides of Eqs. (A14) and (A11) can be equated, which yields

$$\mathcal{Q}_{n,l} = \frac{\mathcal{H}_{n,l}}{(n-3)(n+7)}. \quad \text{(A15)}$$

Thus, making use of the relation (A13) for $n = 2l$, one obtains

$$\mathcal{Q}_{2l,l} \equiv \frac{\mathcal{H}_{2l,l}}{(2l-3)(2l+7)} = -\frac{2^{l+4}(l+1)!}{\sqrt{\pi}(2l-3)(2l+7)\Gamma(l+3/2)}B_{\frac{1}{2}}\left(l+2,\frac{3}{2}\right). \quad \text{(A16)}$$

Equating the rhs of Eqs. (A9) and (A16), we find the required coefficient in the form

$$s_l = [\mathcal{I}_1(l) - \mathcal{I}_2(l)]\mathcal{I}_3^{-1}(l), \quad \text{(A17)}$$

where

$$\mathcal{I}_1(l) = -\frac{2^{-l}}{(2l-3)(2l+7)}B_{\frac{1}{2}}\left(l+2,\frac{3}{2}\right), \quad \text{(A18)}$$

$$\mathcal{I}_2(l) = \int_0^1 \lambda_l^{(P)}(\rho)\frac{\rho^{2l+2}}{(\rho^2+1)^{2l+3}}d\rho, \quad \text{(A19)}$$

$$\mathcal{I}_3(l) = \int_0^1 v_{3,l}(\rho)\frac{\rho^{2l+2}}{(\rho^2+1)^{2l+3}}d\rho = \frac{2^{-l-3/2}(2l+1)}{(2l+3)(2l+7)}. \quad \text{(A20)}$$

It is seen that Eqs. (A17) to (A20) yield a very complicated expression for the coefficient s_l included [see Eq. (A8)] in representation (68) for $\lambda_l(\rho)$. The easiest method of finding the simplest representation for s_l is the use of the *Mathematica* operator FindSequenceFunction. In particular, using Eqs. (A17) to (A20) we have calculated the coefficient s_l for $3 \leqslant l \leqslant 30$, and found that it has the form

$$s_l = a_l + b_l\pi + c_l\ln 2, \quad \text{(A21)}$$

where a_l, b_l, and c_l are rational numbers. Making use of the calculated sequences for each of the coefficients a_l, b_l, and c_l, the *Mathematica* operator FindSequenceFunction enables us to find the general forms of these coefficients as functions of l. Notice that for a given sequence there is a minimal number of terms needed for *Mathematica* to find the formula for the general term. In particular, for the coefficients b_l and c_l, this minimal number is 8, whereas for a_l it is 22. Finally, one obtains

$$s_l = \frac{2^{-l-3}}{(2l-3)(2l-1)(2l+1)}[2l(l+1)(H_{\frac{l+1}{2}} - H_{\frac{l}{2}} - \pi) + 2l + 3], \quad \text{(A22)}$$

where H_z are the harmonic numbers.

APPENDIX B

To solve the IFRR (76) with the rhs of the form (77), we used the single-series representation (78) for the subcomponent $\psi_{4,1}^{(2d)}$. It was shown in Ref. [12] that the function $\tau_l(\rho)$ in Eq. (78) represents the physical solution of the equation

$$(1+\rho^2)^2\tau_l''(\rho) + 2\rho^{-1}[1+\rho^2+l(1-\rho^4)]\tau_l'(\rho) + 4(2-l)(l+4)\tau_l(\rho) = -h_l(\rho), \quad \text{(B1)}$$

where {see Eq. (C6) of Ref. [12]}

$$h_l(\rho) = -\frac{(\pi-2)(\rho+1)(\rho^2+1)^{l-1}}{3\pi(2l-1)(2l+3)2^{l+1}}\left[\frac{15-4l(l+1)(4l+11)}{(2l-3)(2l+5)\rho} + 4l(2l+3) + 2\rho + 4(l+1)(2l-1)\rho^2 + \frac{(2l-1)(4l+5)\rho^3}{2l+5}\right] \quad \text{(B2)}$$

for $0 \leqslant \rho \leqslant 1$. The method of variation of parameters enables us to obtain the particular solution of Eq. (B1) in the form (80), where

$$\mathcal{V}_{4,l}(\rho) = \int_0^\rho v_{4,l}(t)h_l(t)t^{2l+2}(1+t^2)^{-2l-3}dt, \tag{B3}$$

$$\mathcal{U}_{4,l}(\rho) = \int_1^\rho u_{4,l}(t)h_l(t)t^{2l+2}(1+t^2)^{-2l-3}dt, \tag{B4}$$

and the individual solutions $u_{4,l}$ and $v_{4,l}$ of the homogeneous equation associated with (B1) are defined by (81) according to formulas (46) of Ref. [12] for $k = 4$.

Our aim is to find closed-form representations for the integrals (B3) and (B4) through special and elementary functions. To this end, it would be useful, first of all, to express the solutions $u_{4,l}(\rho)$ and $v_{4,l}(\rho)$ through elementary functions. It is seen from Eq. (81a) that for $l \geqslant 3$, we can write

$$u_{4,l}(\rho) = \frac{8(l-3)!(1+\rho^2)^{l+4}}{15\sqrt{\pi}\Gamma(l+1/2)\rho^{2l+1}} \sum_{m=0}^{l-3} \frac{(-1)^m\Gamma(m+7/2)\Gamma(l-m+1/2)}{m!(l-m-3)!}\rho^{2m}. \tag{B5}$$

The well-known formula (7.3.1.140) of Ref. [15] was applied. Notice that the explicit expressions for the particular solutions $\tau_l^{(P)}(\rho)$ with $l = 0,1,2$ were presented in Eqs. (C9) to (C11) of Ref. [12].

The solution of the problem for $v_{4,l}(\rho)$, defined by Eq. (81b), is more complicated. The use of the relation (7.3.1.9) of Ref. [15] for $m = l - 3$ and subsequent application of the transformation (7.3.1.3) of Ref. [15] yield

$${}_2F_1\left(\frac{7}{2},l+4;l+\frac{3}{2};-\rho^2\right) = \frac{16\Gamma(l+3/2)}{105\sqrt{\pi}\rho^{2(l-3)}(1+\rho^2)^7} \sum_{p=0}^{l-3} \frac{(-1)^p}{p!(l-p-3)!}\,{}_2F_1\left(1,l-p+4;\frac{9}{2};\frac{\rho^2}{1+\rho^2}\right). \tag{B6}$$

The next step is the application of the relation (7.3.1.132) of Ref. [15] to the Gauss hypergeometric functions in the rhs of Eq. (B6). This gives

$$\begin{aligned}{}_2F_1\left(1,l-p+4;\frac{9}{2};\frac{\rho^2}{1+\rho^2}\right) = \frac{7\Gamma(l-p+1/2)}{2(l-p+3)!}\Bigg\{\frac{15(1+\rho^2)^{l-p+4}}{8\rho^8}\left[\frac{2\rho}{\sqrt{\pi}}\arctan(\rho) - \sum_{m=1}^{3}\frac{(m-1)!}{\Gamma(m+1/2)}\left(\frac{\rho^2}{1+\rho^2}\right)^m\right] \\ + \sum_{m=0}^{l-p-1}\frac{(l-p-m+2)!}{\Gamma(l-p-m+1/2)}(1+\rho^2)^{m+1}\Bigg\}.\end{aligned} \tag{B7}$$

Inserting Eqs. (B6) and (B7) into Eq. (81b), one obtains the following representation for the second solution of the homogeneous equation:

$$\begin{aligned}v_{4,l}(\rho) = \frac{\Gamma(l+3/2)}{\sqrt{\pi}}\left(\frac{1+\rho^2}{\rho^2}\right)^{l-3}\sum_{p=0}^{l-3}\frac{(-1)^p\Gamma(l-p+1/2)}{p!(l-p-3)!(l-p+3)!}\Bigg\{\frac{(1+\rho^2)^{l-p+4}}{\rho^8} \\ \times\left[\frac{2\rho}{\sqrt{\pi}}\arctan(\rho) - \sum_{m=1}^{3}\frac{(m-1)!}{\Gamma(m+1/2)}\left(\frac{\rho^2}{1+\rho^2}\right)^m\right] + \frac{8}{15}\sum_{m=0}^{l-p-1}\frac{(l-p-m+2)!}{\Gamma(l-p-m+1/2)}(1+\rho^2)^{m+1}\Bigg\}.\end{aligned} \tag{B8}$$

To find analytic representations for the integrals (B3) and (B4), it is convenient to represent the rhs of (B2) in the compact form

$$h_l(\rho) = a_{0l}(\rho+1)(\rho^2+1)^{l-1}\sum_{n=1}^{5}a_{nl}\rho^{n-2}, \tag{B9}$$

where the coefficients a_{nl} are defined by Eq. (84). Inserting representations (B5) and (B9) into the rhs of Eq. (B4), and performing the trivial integration, one obtains

$$\mathcal{U}_{4,l}(\rho) = a_{0l}\frac{8(l-3)!}{15\sqrt{\pi}\Gamma(l+1/2)}\sum_{m=0}^{l-3}\frac{\Gamma(m+7/2)\Gamma(l-m+1/2)(-1)^m}{m!(l-m-3)!}\sum_{n=1}^{5}a_{nl}\left(\frac{\rho^{2m+n}-1}{2m+n} + \frac{\rho^{2m+n+1}-1}{2m+n+1}\right). \tag{B10}$$

Using Eqs. (81b) and (B9) one can write Eq. (B3) in the form

$$\mathcal{V}_{4,l}(\rho) = a_{0l}\sum_{n=0}^{5}b_{n,l}\int_0^\rho t^{2l+n+1}{}_2F_1\left(\frac{7}{2},l+4;l+\frac{3}{2};-t^2\right)dt, \tag{B11}$$

where the coefficients $b_{n,l}$ are defined by Eq. (85). The use of the relation (1.16.1) of Ref. [15] yields

$$\mathcal{V}_{4,l}(\rho) = a_{0l} \sum_{n=0}^{5} \left(\frac{b_{n,l}}{2l+n+2} \right) \rho^{2l+n+2} {}_3F_2\left(\frac{7}{2}, l+4, l+1+\frac{n}{2}; l+\frac{3}{2}, l+2+\frac{n}{2}; -\rho^2 \right). \tag{B12}$$

This last relation gives the representation of the integral (B3) through generalized hypergeometric functions. To derive representation of the integral (B3) through the Gauss hypergeometric functions, one should first apply the relation (7.4.1.2) of Ref. [15]. A subsequent reorganization of summation along with application of the linear transformation (7.3.1.4) of Ref. [15] gives the required expression (83).

Now we shall show that the Gauss hypergeometric functions included into Eq. (83) can be expressed as elementary functions. The use of the relation (7.3.1.10) of Ref. [15] and subsequent application of the linear transformation (7.3.1.3) of Ref. [15] give

$$\begin{aligned} {}_2F_1\left(l-2, m-\frac{3}{2}; k+l+\frac{3}{2}; -\rho^2 \right) &= \frac{(-\rho^2)^{3-l}\left(k+\frac{9}{2}\right)_{l-3}}{1+\rho^2} \sum_{p=0}^{l-3} \frac{(-1)^p}{p!(l-p-3)!} \\ &\quad \times {}_2F_1\left(1, k+p+6-m; k+\frac{9}{2}; \frac{\rho^2}{1+\rho^2} \right). \end{aligned} \tag{B13}$$

In turn, using (7.3.1.10) of Ref. [15], and then applying (7.3.1.3) of Ref. [15], one obtains

$$\begin{aligned} {}_2F_1\left(l+m-1, m-\frac{3}{2}; k+l+m+\frac{5}{2}; -\rho^2 \right) &= \frac{\left(k+\frac{9}{2}\right)_{l+m-2}}{(1+\rho^2)\left(-\rho^2\right)^{l+m-2}} \sum_{p=0}^{l+m-2} \frac{(-1)^p}{p!(l+m-p-2)!} \\ &\quad \times {}_2F_1\left(1, k+p+6-m; k+\frac{9}{2}; \frac{\rho^2}{1+\rho^2} \right). \end{aligned} \tag{B14}$$

Finally, application of the relation (7.3.1.132) of Ref. [15] yields

$$\begin{aligned} {}_2F_1\left(1, k+p+6-m; k+\frac{9}{2}; \frac{\rho^2}{1+\rho^2} \right) &= \frac{\Gamma(k+9/2)\Gamma(p-m+5/2)(1+\rho^2)^{k-m+p+6}}{\pi(k-m+p+5)!\rho^{2(k+4)}} \\ &\quad \times \left[2\rho \arctan(\rho) - \sqrt{\pi} \sum_{s=1}^{k+3} \frac{(s-1)!}{\Gamma(s+1/2)} \left(\frac{\rho^2}{1+\rho^2} \right)^s \right] \\ &\quad + \frac{2k+7}{2(k-m+p+5)} \sum_{s=0}^{p-m+1} \frac{(-1)^s\left(m-p-\frac{3}{2}\right)_s (1+\rho^2)^{s+1}}{(k-m+p-s+5)_s}, \end{aligned} \tag{B15}$$

where $(a)_n$ is the Pochhammer symbol. Thus, Eqs. (B13) to (B15) together with Eq. (83) give a representation of the integral (B3) through rational functions and the arctangent of ρ. The latter result, together with Eqs. (B5), (B8), and (B10), gives the particular solution $\tau_l^{(P)}(\rho)$ in terms of elementary functions.

APPENDIX C

In Ref. [12] the coefficient $A_2(l)$ in the physical solution (79) was derived in a general but very complicated (integral) form. In particular (see Appendix C of Ref. [12]),

$$A_2(l) = \frac{1}{\mathcal{P}_2(l)} \left[\frac{(\pi-2)2^{-3(l+2)}}{3\pi(2l-1)(l-2)(l+4)} \mathcal{P}_3(l) - \mathcal{P}_1(l) \right], \tag{C1}$$

where

$$\mathcal{P}_1(l) = \int_0^1 \tau_l^{(P)}(\rho) \frac{\rho^{2l+2}}{(1+\rho^2)^{2l+3}} d\rho, \tag{C2}$$

$$\mathcal{P}_2(l) = \int_0^1 v_{4,l}(\rho) \frac{\rho^{2l+2}}{(1+\rho^2)^{2l+3}} d\rho = \frac{\sqrt{\pi} 2^{-2(l+2)} \Gamma(l+3/2)}{\Gamma(l/2+3)\Gamma(l/2)}, \tag{C3}$$

$$\begin{aligned} \mathcal{P}_3(l) = -\frac{2^{l+1}}{(l+3)(2l-3)(2l+3)(2l+5)} &\left\{ \frac{30}{l+1} - \frac{26}{l+2} + 13 - 4l[47 - 2l(2l(l+3)-9)] + 2^{l+1} \right. \\ &\left. \times \left[(l+1)[4l(l(4l+3)-17)+45] B_{\frac{1}{2}}\left(l+\frac{3}{2}, \frac{1}{2} \right) + 8l[l(l(4l(l+4)+3)-56)-62] B_{\frac{1}{2}}\left(l+\frac{3}{2}, \frac{3}{2} \right) \right] \right\}. \end{aligned} \tag{C4}$$

The *Mathematica* calculation of the coefficients $A_2(l)$ for any integer $l \geqslant 3$ shows that

(1) for odd values of l the coefficients $A_2(l)$ equal zero;

(2) for even values of l the coefficients $A_2(l)$ are reduced to the form

$$A_2(l) = \frac{2-\pi}{\pi^2}\mathcal{A}(l), \tag{C5}$$

with $\mathcal{A}(l) = (a_l + \pi b_l)$ where a_l and b_l are rational numbers. Using the effective *Mathematica* code, we have calculated the rational numbers a_l and b_l for $l = 4$ up to $l = 60$ (in steps of 2). Making use of the *Mathematica* operator FindSequenceFunction, it is possible to find a general simple form of the coefficients a_l and b_l. Remember that for a given sequence there is a minimal number of terms needed for *Mathematica* to find the formula for the general term. In particular, for the coefficients a_l and b_l these minimal numbers are 10 and 26, corresponding to $l = 4,6,8,\ldots,22$ and $l = 4,6,8,\ldots,54$, respectively. Thus, application of the *Mathematica* operator FindSequenceFunction to the sequences mentioned above yields

$$\mathcal{A}(l) = \frac{\sqrt{\pi}}{360l(l-2)\Gamma\left(l+\frac{1}{2}\right)}\left\{\frac{[l(l+1)(688l^4+1376l^3-2480l^2-3168l+465)+450]\Gamma\left(\frac{l-1}{2}\right)\Gamma\left(\frac{l+1}{2}\right)}{(2l-3)(2l-1)(2l+1)(2l+3)(2l+5)} - \frac{56}{l-1}\left(\frac{l}{2}!\right)^2\right\}. \tag{C6}$$

APPENDIX D

It was derived in Ref. [12] that the function $\phi_l(\rho)$ defined by Eq. (90) represents the physical solution of the inhomogeneous differential equation

$$(1+\rho^2)^2\phi_l''(\rho) + 2\rho^{-1}[1+\rho^2+l(1-\rho^4)]\phi_l'(\rho) + (3-2l)(7+2l)\phi_l(\rho) = -h_l(\rho), \tag{D1}$$

with

$$h_l(\rho) = \frac{2^{1-l}(\rho^2+1)^{l+\frac{1}{2}}[(1-2l)\rho^2+2l+3]}{3(2l-1)(2l+3)\rho}. \tag{D2}$$

The particular solution $\phi_l^{(P)}$ of the equation (D1) was represented in the form {see Eqs. (101) to (104) of Ref. [12]}

$$\phi_l^{(P)}(\rho) = \frac{2^{-l}(\rho^2+1)^{l-\frac{3}{2}}}{3(2l-3)(2l-1)(2l+3)(2l+5)}\left[2f_{1l}(\rho) + \frac{2f_{2l}(\rho)+f_{3l}(\rho)}{2l+1}\right], \tag{D3}$$

where

$$f_{1l}(\rho) = [9-4l(l+2)]\rho + (13-4l^2)\rho^3, \tag{D4}$$

$$f_{2l}(\rho) = [(2l-3)(2l-1)\rho^4 + 2(2l-3)(2l+5)\rho^2 + (2l+3)(2l+5)]\arctan(\rho), \tag{D5}$$

$$f_{3l}(\rho) = -[(2l+3)(2l+5)\rho^4 + 2(2l-3)(2l+5)\rho^2 + (2l-3)(2l-1)]\frac{\rho}{l+1}\,{}_2F_1(1,l+1;l+2;-\rho^2). \tag{D6}$$

It was shown that the coefficient c_l in solution (90) can be expressed as:

$$c_l = \frac{\mathcal{M}_1(l) - \mathcal{M}_2(l)}{\mathcal{M}_3(l)}, \tag{D7}$$

where

$$\mathcal{M}_1(l) = \frac{2^{-3l-2}l!\sqrt{\pi}}{3(2l-3)(2l-1)(2l+7)\Gamma(l+3/2)}\,{}_3F_2\left(\frac{2l-1}{4},\frac{2l+1}{4},l+1;l+\frac{3}{2},l+\frac{3}{2};1\right), \tag{D8}$$

$$\mathcal{M}_3(l) \equiv \int_0^1 v_{3,l}(\rho)\frac{\rho^{2l+2}}{(\rho^2+1)^{2l+3}}d\rho = \frac{2^{-l-\frac{3}{2}}(2l+1)}{(2l+3)(2l+7)}, \tag{D9}$$

$$\mathcal{M}_2(l) \equiv \int_0^1 \phi_l^{(P)}(\rho)\frac{\rho^{2l+2}}{(\rho^2+1)^{2l+3}}d\rho. \tag{D10}$$

It is seen that according to Eqs. (D3) to (D10) the coefficient c_l is represented by a very complicated function of l. However, *Mathematica* calculations with any given integer $l \geqslant 0$ show that the parameter c_l has the form $c_{0,l} + c_{1,l}\pi + c_{2,l}\ln 2$, where $c_{i,l}$ $(i = 0,1,2)$ are rational numbers. Using the *Mathematica* operator FindSequenceFunction, one obtains the following simple result

$$c_l = \frac{2l+1-(\pi/2)-\Phi(-1,1,l+1)}{3(2l-3)(2l-1)(2l+1)2^l}, \tag{D11}$$

where $\Phi(z,s,a)$ is the Lerch transcendent. Note that for the case under consideration we have

$$\Phi(-1,1,l+1) = \frac{1}{2}\left[\psi\left(\frac{l}{2}+1\right) - \psi\left(\frac{l}{2}+\frac{1}{2}\right)\right] = \frac{1}{2}\left(H_{\frac{l}{2}} - H_{\frac{l-1}{2}}\right), \tag{D12}$$

where $\psi(z)$ and H_z are the digamma function and harmonic numbers, respectively. The minimal lengths of sequences needed for *Mathematica* to find simple representations for $c_{0,l}$, $c_{1,l}$, and $c_{2,l}$ are 22, 6, and 6 (repeatedly), respectively.

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