ALTERNATIVE IMPLEMENTATION OF ATOMIC FORM FACTORS*

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Using a new result on the integral involving the product of Bessel functions and associated Laguerre polynomials, published in the mathematical literature some time ago, we present an alternative method for calculating discrete–discrete transition form factors for hydrogen-like atoms. An overview of two other commonly used methods is also given in the aim of comparison.

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1. Introduction

A bound state of muon and anti-muon (true muonium or dimuonium), although predicted long ago [1–4], has never been observed experimentally. Many mechanisms for the production of dimuonium have been proposed in the literature. Dimuonium can be formed in fixed-target experiments [5–9], in electron–positron collisions [1, 10–12], elementary particle decays [13–19], a quark–gluon plasma [20, 21], relativistic heavy-ion collisions [21–23], an astrophysical context [24], or in experiments with ultra-slow muon beams [25, 26].

As part of the first stage of the expensive and long-term super charm-tau factory project, the Budker Institute of Nuclear Physics (Novosibirsk) is currently developing plans to build an inexpensive, low-energy $\mu\mu$-tron machine [27]. Apart from purely accelerator studies, the $\mu\mu$-tron will make it possible to produce and investigate dimuonium experimentally. Studying the interactions of dimuonium with ordinary atoms as it passes through the foil is an integral part of the planned experiments.

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Elementary atoms, such as dimuonium, when passing through the foil interact with ordinary atoms predominantly via the Coulomb potential [28–30]. Such an interaction is treated in terms of atomic form factors, and a comprehensive review of atomic form factor calculations can be found in [31].

General analytical formulas for calculating the form factor of a hydrogen-like atom were obtained in [32] by group-theoretical methods. However, these formulas have a somewhat complicated form, requiring time-consuming calculations for each value of a transfer momentum [33].

A more convenient set of formulas was developed in [33, 34] and implemented as a Fortran program in [35]. Based on the mathematical results obtained in [36], in this article we present an alternative method for calculating the form factor, which in some sense complements the method presented in [33, 34].

As a byproduct of this research, some trigonometric identities involving Chebyshev polynomials of the second kind were obtained in [37].

Throughout the paper, we use dimuonium atomic units, in which $c = \hbar = 1$, the unit of mass is $\frac{1}{2}m_\mu$ (reduced mass in the dimuonium atom), and the unit of length is the radius of the first Bohr orbit in dimuonium: $a_{\rm B} = 2\,\frac{m_e}{m_\mu}\,a_0 \approx 512$ fm, where $a_0 \approx 5.29\times 10^{-11}$ m is the usual Bohr radius.

Although the motivation for the article was the Novosibirsk dimuonium program, we emphasize that the results obtained are in fact of much broader interest, mainly in atomic physics, see Devangan's review article [31].

2. Cross sections of dimuonium interactions with an external field

The differential cross section for the scattering of a particle with mass $m_{\rm i}$ and initial momentum $p_{\rm i} = |\vec{p}_{\rm i}|$ on the potential corresponding to the interaction Hamiltonian $H_{\rm int}$ is given by the expression [38]

$$\frac{{\rm d}\sigma}{{\rm d}\Omega} = (2\pi)^4 \frac{m_{\rm i} m_{\rm f} p_{\rm f}}{p_{\rm i}} |T_{\rm fi}|^2 \,, \tag{1}$$

where $m_{\rm f}$, $p_{\rm f} = |\vec{p}_{\rm f}|$ are the mass and momentum of the particle after scattering, and in the Born approximation

$$T_{\rm fi} = \langle \Psi_{\rm f} | H_{\rm int} | \Psi_{\rm i} \rangle \,. \tag{2}$$

Let us apply these relations in the case of scattering of dimuonium in the Coulomb field of the target atomic nucleus. If $\vec{r}_1$ is the radius vector of a muon in a dimuonium atom and $\vec{r}_2$ is the radius vector of an anti-muon, then the wave function of dimuonium with momentum $\vec{P}$ and the center-of-mass radius vector $\vec{R} = (m_1\vec{r}_1 + m_2\vec{r}_2)/(m_1+m_2)$ is given by

$$\Psi(\vec{r}_1, \vec{r}_2) = (2\pi)^{-3/2} {\rm e}^{i\vec{P}\cdot\vec{R}} \varphi(\vec{r}\,) \,, \tag{3}$$

where $m_1 = m_2 = m_\mu$, $\vec{r} = \vec{r}_1 - \vec{r}_2$, and $\varphi(\vec{r})$ is the Coulomb wave function of the relative motions of muon and anti-muon in the dimuonium atom. If $U(\vec{r})$ is the (screened) Coulomb field of the target nucleus, then

$$T_{\rm fi} = \int {\rm d}\vec{r}_1\, {\rm d}\vec{r}_2\, \Psi_{\rm f}^*(\vec{r}_1, \vec{r}_2) \left[eU(\vec{r}_1) - eU(\vec{r}_2)\right] \Psi_{\rm i}(\vec{r}_1, \vec{r}_2)\,, \tag{4}$$

where e is the muon charge.

It can be checked that changing of variables from $\vec{r}_1$, $\vec{r}_2$ to $\vec{R}$, $\vec{r}$ in the multiple integral (4) has a unit Jacobian. Using (3) and

$$U(\vec{r}) = \frac{1}{(2\pi)^3} \int {\rm d}\vec{q}\, {\rm e}^{i\vec{q}\cdot\vec{r}}\, \tilde{U}(\vec{q})\,, \qquad \vec{r}_1 = \vec{R} + \frac{1}{2}\,\vec{r}\,, \qquad \vec{r}_2 = \vec{R} - \frac{1}{2}\,\vec{r} \tag{5}$$

in (4), we get, after a simple integration in ${\rm d}\vec{R}$ (which produces $\delta(\vec{q}+\vec{P}_{\rm i}-\vec{P}_{\rm f})$ δ-function),

$$T_{\rm fi} = \frac{e\,\tilde{U}(\vec{q})}{(2\pi)^3} \left[F_{\rm fi}\left(\frac{\vec{q}}{2}\right) - F_{\rm fi}\left(-\frac{\vec{q}}{2}\right)\right]\,, \tag{6}$$

where

$$F_{\rm fi}(\vec{q}) = \int {\rm d}\vec{r}\, \varphi_{\rm f}^*(\vec{r})\, {\rm e}^{i\vec{q}\cdot\vec{r}}\, \varphi_{\rm i}(\vec{r})\,, \tag{7}$$

and $\vec{q} = \vec{P}_{\rm f} - \vec{P}_{\rm i}$. Therefore, according to (1),

$$\frac{{\rm d}\sigma}{{\rm d}\Omega} = \frac{1}{(2\pi)^2}\, \frac{M^2 P_{\rm f}}{P_{\rm i}}\, e^2 \left|\tilde{U}(\vec{q})\right|^2 \left|F_{\rm fi}\left(\frac{\vec{q}}{2}\right) - F_{\rm fi}\left(-\frac{\vec{q}}{2}\right)\right|^2\,, \tag{8}$$

where $M \approx 2m_\mu$ is the dimuonium mass.

If θ is dimuonium scattering angle, then $q^2 = P_{\rm f}^2 + P_{\rm i}^2 - 2P_{\rm f}P_{\rm i}\cos\theta$ and $q{\rm d}q = P_{\rm f}P_{\rm i}\sin\theta{\rm d}\theta$, which implies

$${\rm d}\Omega = 2\pi\sin\theta{\rm d}\theta = 2\pi\,\frac{q{\rm d}q}{P_{\rm i}P_{\rm f}}\,. \tag{9}$$

Besides, if the initial $\varphi_{\rm i}$ and final $\varphi_{\rm f}$ quantum states have definite angular momenta l and l', then

$$\begin{aligned} F_{\rm fi}(-\vec{q}) &= \int {\rm d}\vec{r}\, \varphi_{\rm f}^*(\vec{r})\, {\rm e}^{-i\vec{q}\cdot\vec{r}}\, \varphi_{\rm i}(\vec{r}) \\ &= \int {\rm d}\vec{r}\, \varphi_{\rm f}^*(-\vec{r})\, {\rm e}^{i\vec{q}\cdot\vec{r}}\, \varphi_{\rm i}(-\vec{r}) = (-1)^{l+l'} F_{\rm fi}(\vec{q})\,. \end{aligned} \tag{10}$$

In light of (8), (9) and (10), we can write the $(n,l,m) \to (n',l',m')$ discrete–discrete transition cross section in the scattering of dimuonium by the target nucleus' electric field U in the form of

$$\mathrm{d}\sigma_{nlm}^{n'l'm'}=\frac{e^2\left(1-(-1)^{l-l'}\right)}{\pi V^2}\left|\tilde{U}(\vec{q})\right|^2\left|F_{nlm}^{n'l'm'}\left(\frac{\vec{q}}{2}\right)\right|^2 q\mathrm{d}q\,, \tag{11}$$

where $V=P_{\mathrm{i}}/M$ is the initial velocity of dimuonium, and we used the fact that $(-1)^{l+l'}=(-1)^{l-l'+2l'}=(-1)^{l-l'}$, and, therefore $\left(1-(-1)^{l+l'}\right)^2=1-2(-1)^{l-l'}+(-1)^{2(l-l')}=2\left(1-(-1)^{l-l'}\right)$.

Summation over the complete set of final states gives the following sum rule:

$$\sum_f\left|F_{\mathrm{fi}}\left(\frac{\vec{q}}{2}\right)-F_{\mathrm{fi}}\left(-\frac{\vec{q}}{2}\right)\right|^2=2\left(1-F_{\mathrm{ii}}(\vec{q})\right)\,. \tag{12}$$

Indeed, using $\sum\limits_f|f\rangle\langle f|=1$, we get

$$\begin{aligned}&\sum_f\left|F_{\mathrm{fi}}\left(\frac{\vec{q}}{2}\right)-F_{\mathrm{fi}}\left(-\frac{\vec{q}}{2}\right)\right|^2=\sum_f\left\langle i\left|\left(\mathrm{e}^{-i\frac{\vec{q}\cdot\vec{r}}{2}}-\mathrm{e}^{i\frac{\vec{q}\cdot\vec{r}}{2}}\right)\right|f\right\rangle\\&\times\left\langle f\left|\left(\mathrm{e}^{i\frac{\vec{q}\cdot\vec{r}}{2}}-\mathrm{e}^{-i\frac{\vec{q}\cdot\vec{r}}{2}}\right)\right|i\right\rangle=\left\langle i\left|\left(\mathrm{e}^{-i\frac{\vec{q}\cdot\vec{r}}{2}}-\mathrm{e}^{i\frac{\vec{q}\cdot\vec{r}}{2}}\right)\left(\mathrm{e}^{i\frac{\vec{q}\cdot\vec{r}}{2}}-\mathrm{e}^{-i\frac{\vec{q}\cdot\vec{r}}{2}}\right)\right|i\right\rangle\\&=2\langle i|i\rangle-\langle i|(\mathrm{e}^{i\vec{q}\cdot\vec{r}}+\mathrm{e}^{-i\vec{q}\cdot\vec{r}})|i\rangle=2\left(1-\mathrm{Re}\,F_{\mathrm{ii}}(\vec{q})\right)\,.\end{aligned} \tag{13}$$

However, if the initial φ_{i} quantum state has a definite angular momentum l, then (7) and (10) show that $F_{\mathrm{ii}}(\vec{q})$ is real

$$F_{\mathrm{ii}}^*(\vec{q})=F_{\mathrm{ii}}(-\vec{q})=(-1)^{2l}F_{\mathrm{ii}}(\vec{q})=F_{\mathrm{ii}}(\vec{q})\,, \tag{14}$$

and (12) does follow.

With the help of the sum rule (12), we can calculate the total cross section of dimuonium transitions from the initial (n,l,m) quantum state to some final states (discrete or continuum) in the following way:

$$\mathrm{d}\sigma_{nlm}^{\mathrm{tot}}=\frac{e^2}{\pi V^2}\left|\tilde{U}(\vec{q})\right|^2\left[1-F_{nlm}^{nlm}(\vec{q})\right]q\mathrm{d}q\,. \tag{15}$$

The main results of this section, equations (11) and (15), were obtained long ago in [28]. Here, we present their derivations for the sake of reference and to establish the notation.

3. Master formula for form factor calculation

As equations (11) and (15) show, the central object in the study of interactions of dimuonium with matter is the hydrogen-like discrete–discrete atomic form factor (which is just the Fourier transform of $\varphi_{\rm f}^*(\vec r\,)\,\varphi_{\rm i}(\vec r\,)$ with respect to the transferred momentum $\vec q$ [31])

$$F_{n_1l_1m_1}^{n_2l_2m_2}(\vec q\,) = \int {\rm d}\vec r\,\varphi_{n_2l_2m_2}^*(\vec r\,)\,{\rm e}^{i\vec q\cdot\vec r}\,\varphi_{n_1l_1m_1}(\vec r\,)\,, \quad \varphi_{nlm}(\vec r\,) = R_{nl}(r)Y_{lm}(\Omega)\,, \tag{16}$$

where Y_{lm} are usual spherical functions and the hydrogen-like radial wave functions $R_{nl}(r)$ has the form of

$$R_{nl}(r) = \frac{2}{n^2}\sqrt{\frac{(n-l-1)!}{(n+l)!}}\,{\rm e}^{-r/n}\left(\frac{2r}{n}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2r}{n}\right)\,, \tag{17}$$

with L_n^m as the associated Laguerre polynomials.

Some words of caution might be appropriate here: unfortunately, the definitions of neither the ordinary nor the associated Laguerre polynomials that are used in the literature are universal [39]. In the mathematical literature, two standard definitions of the associated Laguerre polynomials are used: the definition of Arfken and Weber [40] and the definition of Spiegel [41]. We use the first one, so

$$L_n^m(x) = (n+m)!\sum_{k=0}^{n}\frac{(-1)^k}{k!(n-k)!(k+m)!}\,x^k\,. \tag{18}$$

In old physics literature, often some variant of Spiegel's definition is used. For example, the associated Laguerre polynomials $\tilde L_n^m$ used by Landau and Lifshitz in [42] are $\tilde L_n^m(x) = (-1)^m n!\,L_{n-m}^m(x)$ and they differ from Spiegel's definition by the factor $n!$.

Using plane-wave expansion [38]

$${\rm e}^{i\vec q\cdot\vec r} = 4\pi\sum_{l=0}^{\infty}\sum_{m=-l}^{l} i^l j_l(qr)Y_{lm}(\Omega_q)Y_{lm}^*(\Omega_r)\,, \tag{19}$$

in (16), we get

$$F_{n_1l_1m_1}^{n_2l_2m_2} = 4\pi\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\int_0^\infty r^2{\rm d}r\,R_{n_2l_2}^*(r)R_{n_1l_1}(r)i^l j_l(qr)Y_{lm}(\Omega_q)I_{l_1\ l_2\ l}^{m_1m_2m}\,, \tag{20}$$

where

$$I^{m_1 m_2 m}_{l_1\ l_2\ l} = \int \mathrm{d}\Omega\, Y^*_{l_2 m_2}(\Omega) Y^*_{lm}(\Omega) Y_{l_1 m_1}(\Omega) = (-1)^{m_2+m} \int \mathrm{d}\Omega\, Y_{l_2,-m_2}(\Omega) Y_{l,-m}(\Omega) Y_{l_1 m_1}(\Omega)\,. \quad (21)$$

The angular integral (21) can be expressed in terms of Wigner's $3j$-symbols [42]

$$I^{m_1 m_2 m}_{l_1\ l_2\ l} = (-1)^{m_2+m} \sqrt{\frac{(2l_1+1)(2l_2+1)(2l+1)}{4\pi}} \times \begin{pmatrix} l_1 & l_2 & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l \\ m_1 & -m_2 & -m \end{pmatrix}. \quad (22)$$

Energy conservation equation

$$\frac{\vec{P}_{\mathrm{i}}^2}{2M} + \epsilon_{\mathrm{i}} = \frac{\vec{P}_{\mathrm{f}}^2}{2M} + \epsilon_{\mathrm{f}}\,, \quad (23)$$

where ϵ_{i} and ϵ_{f} are dimuonium energy eigenvalues before and after scattering in the target nucleus' electric field, indicates that $\vec{P}_{\mathrm{f}}^2 \equiv (\vec{P}_{\mathrm{i}} + \vec{q})^2 = \vec{P}_{\mathrm{i}}^2 + 2M(\epsilon_{\mathrm{i}} - \epsilon_{\mathrm{f}}) \approx \vec{P}_{\mathrm{i}}^2$, and that $\vec{q}\cdot\vec{P}_{\mathrm{i}} \approx 0$ (note that $\vec{P}_{\mathrm{i}}^2 \gg -2M\epsilon_{\mathrm{i}}$ is the condition for the validity of the Born approximation [29]). Then, if the quantization axis (z-axis) is along the initial flow direction (*i.e.* in the direction of $\vec{P}_{\mathrm{i}}$), we will have $\cos\theta_q \approx 0$. However, $Y_{lm}(\theta,\varphi) \sim P_l^m(\cos\theta)$ and $P_l^m(-\cos\theta) = (-1)^{l+m} P_l^m(\cos\theta)$. Therefore, $Y_{lm}(\Omega_q)$ is nonzero only if $(-1)^{l+m} = 1$. On the other hand, $3j$-symbol $\begin{pmatrix} l_1 & l_2 & l \\ 0 & 0 & 0 \end{pmatrix}$ is nonzero only if $l + l_1 + l_2$ is an even integer [43], and $\begin{pmatrix} l_1 & l_2 & l \\ m_1 & -m_2 & -m \end{pmatrix}$ is nonzero only if $m = m_1 - m_2$ and $|l_1 - l_2| \le l \le l_1 + l_2$. Therefore, sum (20) is nonzero only if $(-1)^{l_1-m_1} = (-1)^{(l_1+l_2+l)-(l+m)-2l_2+l_2-m_2} = (-1)^{l_2-m_2}$. As we see, in discrete–discrete atomic transitions of dimuonium, the z-parity $P_z = (-1)^{l-m}$ is conserved [44].

Substituting (17) into (20), we get after some algebra

$$F^{n_2 l_2 m_2}_{n_1 l_1 m_1} = N \sum_{l=|l_1-l_2|}^{l_1+l_2} A_l\, I_l = N \sum_{s=0}^{\min(l_1,l_2)} A_{L-2s}\, I_{L-2s}\,, \quad (24)$$

where

$$N = \frac{(2a)^{l_1+1}\,(2b)^{l_2+1}}{n_1+n_2} \sqrt{(2l_1+1)(2l_2+1)\,\frac{(n_1-l_1-1)!\,(n_2-l_2-1)!}{(n_1+l_1)!\,(n_2+l_2)!}}\,, \quad (25)$$

$$A_l = i^l (-1)^{m_2+m} \sqrt{4\pi(2l+1)} \times \begin{pmatrix} l_1 & l_2 & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l \\ m_1 & -m_2 & -m \end{pmatrix} Y_{lm}(\Omega_q)\,, \tag{26}$$

$$I_l = \int_0^\infty x^{l_1+l_2+2}\, \mathrm{e}^{-x}\, j_l(\sigma x)\, L^{2l_1+1}_{n_1-l_1-1}(2ax)\, L^{2l_2+1}_{n_2-l_2-1}(2bx)\, \mathrm{d}x\,, \tag{27}$$

and we have introduced notations [35]

$$a = \frac{n_2}{n_1+n_2}\,, \qquad b = \frac{n_1}{n_1+n_2}\,, \qquad \sigma = \frac{n_1 n_2}{n_1+n_2}\, q\,,$$
$$x = \frac{r}{ab(n_1+n_2)}\,, \qquad s = \frac{1}{2}(L-l)\,, \qquad L = l_1 + l_2\,. \tag{28}$$

At last, if the quantization axis is parallel to the collision direction, we have [35]

$$Y_{lm}(\Omega_q) \approx Y_{lm}\left(\frac{\pi}{2}, \varphi\right) = (-1)^m 2^{-l} \mathrm{e}^{im\varphi} \cos\left(\frac{\pi}{2}(l+m)\right) \frac{\sqrt{(l+m)!\,(l-m)!}}{\Gamma\left(1+\frac{l+m}{2}\right)\, \Gamma\left(1+\frac{l-m}{2}\right)} \sqrt{\frac{2l+1}{4\pi}}\,, \tag{29}$$

since, as we have seen, the transferred momentum $\vec{q}$ is almost perpendicular to this axis (which is parallel to $\vec{P}_{\mathrm{i}}$).

A much simpler expression

$$Y_{lm}(\Omega_q) = Y_{lm}(0, \varphi) = \delta_{m0} \sqrt{\frac{2l+1}{4\pi}} \tag{30}$$

corresponds to the case when the direction of the transferred momentum $\vec{q}$ is taken as the direction of the quantization axis. However, the first choice is preferable when the initial momentum of the flying dimuonium is much larger than the transferred momentum, since in this case, the quantization axis will remain almost unchanged in successive collisions [35].

4. Calculation of the radial integral I_l à la Dewangan

The most straightforward way to evaluate integral (27), outlined in [31], is to use expression (18) of the associated Laguerre polynomials. Applying (a variant) of the Cauchy product formula [45]

$$\sum_{m_1=0}^{M_1} \sum_{m_2=0}^{M_2} a_{m_1 m_2} = \sum_{k=0}^{M_1+M_2} \sum_{m_1=0}^{k} a_{m_1, k-m_1}\,, \tag{31}$$

we get

$$L^{2l_1+1}_{n_1-l_1-1}(2ax)\,L^{2l_2+1}_{n_2-l_2-1}(2bx)=\sum_{k=0}^{n_1+n_2-L-2}C_k\,x^k\,, \tag{32}$$

where

$$\begin{aligned}C_k &= \sum_{j=0}^{k}\frac{(-1)^k(n_1+l_1)!\,(n_2+l_2)!\,(2a)^j(2b)^{k-j}}{j!\,(k-j)!\,(2l_1+1+j)!\,(2l_2+1+k-j)!\,N_1!\,N_2!}\,,\\ N_1 &= n_1-l_1-1-j\,,\qquad N_2=n_2-l_2-1+j-k\,.\end{aligned} \tag{33}$$

Substitution of this result into (27) yields

$$I_l=\sum_{k=0}^{n_1+n_2-L-2}C_k\,\tilde{J}_k\,, \tag{34}$$

where

$$\tilde{J}_k=\int_0^\infty x^{L+k+2}\,\mathrm{e}^{-x}\,j_l(\sigma x)\,\mathrm{d}x=\sqrt{\frac{\pi}{2\sigma}}\int_0^\infty x^{L+k+\frac{3}{2}}\,\mathrm{e}^{-x}\,J_{l+\frac{1}{2}}(\sigma x)\,\mathrm{d}x\,. \tag{35}$$

But $L+k+\frac{3}{2}=2s+k+1+l+\frac{1}{2}$ and (35) can be rewritten as follows:

$$\tilde{J}_k=\sqrt{\frac{\pi}{2\sigma}}\left(-\frac{\partial}{\partial\alpha}\right)^{2s+k+1}\int_0^\infty x^{l+\frac{1}{2}}\,\mathrm{e}^{-\alpha x}\,J_{l+\frac{1}{2}}(\sigma x)\,\mathrm{d}x\Big|_{\alpha=1}\,. \tag{36}$$

The integral entering in this expression can be found in the classical table of integrals by Gradshteyn and Ryzhik [46] (entry 6.623.1. In [47], this integral is simply evaluated by using the heuristic method of brackets.)

$$\int_0^\infty \mathrm{e}^{-\alpha x}J_\nu(\beta x)\,x^\nu\,\mathrm{d}x=\frac{(2\beta)^\nu\Gamma\left(\nu+\frac{1}{2}\right)}{\sqrt{\pi}\,(\alpha^2+\beta^2)^{\nu+\frac{1}{2}}}\,. \tag{37}$$

Besides, we have [31]

$$\left(\frac{\partial}{\partial\alpha}\right)^s\frac{1}{[\alpha^2+\sigma^2]^{l+1}}=\sum_{p=0}^{[s/2]}\frac{(-1)^{s+p}\,s!\,(l+s-p)!\,(2\alpha)^{s-2p}}{(s-2p)!\,p!\,l!\,[\alpha^2+\sigma^2]^{l+1+s-p}}\,, \tag{38}$$

where $[s/2]$ denotes the integer part of $s/2$ (the largest integer $\leq s/2$). In light of (37) and (38), we finally get

$$\tilde{J}_k = (2\sigma)^{L-2s} \sum_{p=0}^{s+\left[\frac{k+1}{2}\right]} \frac{(-1)^p (2s+k+1)!\,(L-p+k+1)!\,2^{2(s-p)+k+1}}{[2(s-p)+k+1]!\,p!\,(1+\sigma^2)^{L-p+k+2}}\,. \tag{39}$$

Equations (24), (33), (34) and (39) determine the atomic form factor $F^{n_2 l_2 m_2}_{n_1 l_1 m_1}$ as a four-fold finite series of rational functions of q.

5. Calculation of the radial integral I_l à la Afanasyev and Tarasov

Now we outline the calculation of I_l as given in [34]. The starting point will be a Clebsch–Gordan-type linearisation relation for the product of two associated Laguerre polynomials obtained in [48] (valid for $a+b=1$)

$$L_n^{\alpha}(ax)\,L_m^{\beta}(bx) = \sum_{k=0}^{n+m} C_{nm}^{\alpha\beta}(a,b) L_k^{\alpha+\beta}(x)\,, \tag{40}$$

where

$$\begin{aligned} C_{nm}^{\alpha\beta}(a,b) \;&=\; \frac{k!\,(n+m-k)!}{n!\,m!}\,a^{k-m}\,b^{k-n} \\ &\quad \times P_{n+m-k}^{(k-m,\,k-n)}(b-a)\,P_{n+m-k}^{(\alpha+k-m,\,\beta+k-n)}(b-a)\,, \end{aligned} \tag{41}$$

and $P_n^{(\alpha,\beta)}(x)$ are Jacobi polynomials. Therefore,

$$L_{n_1-l_1-1}^{2l_1+1}(2ax)\,L_{n_2-l_2-1}^{2l_2+1}(2bx) = \sum_{k=0}^{n_1+n_2-L-2} H_k\,L_k^{2(L+1)}(2x)\,, \tag{42}$$

with

$$H_k = C^{2l_1+1,\,2l_2+1}_{n_1-l_1-1,\,n_2-l_2-1}(a,b)\,. \tag{43}$$

Note that Afanasyev and Tarasov do not cite [48] and provide their own derivation of (42) in [34] with a seemingly different result for H_k. However, it can be shown that their result is equivalent to (43) since

$$P_n^{(-m,\,-k)}(x) = \left(\frac{x-1}{2}\right)^m \left(\frac{x+1}{2}\right)^k P_{n-m-k}^{(m,k)}(x)\,. \tag{44}$$

This last identity can be proved by using the relation

$$P_n^{(-m,\beta)}(x) = \frac{\Gamma(n+\beta+1)}{\Gamma(n+\beta+1-m)}\,\frac{(n-m)!}{n!}\left(\frac{x-1}{2}\right)^m P_{n-m}^{(m,\beta)}(x)\,, \tag{45}$$

which can be found in the book [49] (formula 4.22.2), in combination with the symmetry relation

$$P_n^{(\alpha,\beta)}(x) = (-1)^n \, P_n^{(\beta,\alpha)}(-x)\,. \tag{46}$$

Next, using the formula [50]

$$\sum_{k=0}^{n} \frac{(-1)^k}{(n-k)!} \binom{m-n}{k} \left(\frac{2}{z}\right)^k J_{m-k}(z) = \frac{(-1)^n}{n!} J_{m-2n}(z)\,, \quad m>n\,, \tag{47}$$

analytically continued for a non-integer $m = L + \frac{1}{2}$, and rewritten in terms of spherical Bessel functions $j_n(z) = \sqrt{\frac{\pi}{2z}}\, J_{n+1/2}(z)$, Afanasyev and Tarasov expand

$$j_{L-2s}(\sigma x) = \sum_{p=0}^{s} B_{ps} \left(\frac{2}{\sigma x}\right)^p j_{L-p}(\sigma x)\,, \tag{48}$$

with

$$B_{ps} = (-1)^{s-p}\, \Gamma(p+1) \binom{s}{p} \binom{L-s+1/2}{p}\,. \tag{49}$$

In light of (42) and (48), (27) takes the form of

$$I_l = \sum_{p=0}^{s} \sum_{k=0}^{n_1+n+2-L-2} B_{ps}\, H_k \left(\frac{2}{\sigma}\right)^p I_k^{(L,p)}(\sigma)\,, \tag{50}$$

where

$$I_k^{(L,p)}(\sigma) = \int\limits_0^\infty x^{L-p+2} \mathrm{e}^{-x} j_{L-p}(\sigma x)\, L_k^{2L+2}(2x)\, \mathrm{d}x\,. \tag{51}$$

Generating function for associated Laguerre polynomials [40]

$$\frac{\mathrm{e}^{-tx/(1-t)}}{(1-t)^{m+1}} = \sum_{n=0}^{\infty} L_n^m(x)\, t^n \tag{52}$$

indicates that

$$L_n^m(x) = \frac{1}{n!} \frac{\partial^n}{\partial t^n} \frac{\mathrm{e}^{-tx/(1-t)}}{(1-t)^{m+1}} \Bigg|_{t=0}\,. \tag{53}$$

Therefore, we can rewrite (51) in the following form:

$$I_k^{(L,p)}(\sigma) = \frac{1}{k!} \frac{\partial^k}{\partial t^k} \left(\frac{1}{(1-t)^{2L+3}} \int\limits_0^\infty x^{L-p+2}\, \mathrm{e}^{-\frac{1+t}{1-t}\,x}\, j_{L-p}(\sigma x)\, \mathrm{d}x \right) \Bigg|_{t=0}\,. \tag{54}$$

Now it is clear why expansion (48) was needed: it simplifies the calculation of the integral in (54) through (37). Indeed, with $\alpha = \frac{1+t}{1-t}$, we have

$$\int_0^\infty x^{L-p+2}\, \mathrm{e}^{-\alpha x}\, j_{L-p}(\sigma x)\, \mathrm{d}x = \sqrt{\frac{\pi}{2\sigma}} \int_0^\infty x^{L-p+\frac{3}{2}}\, \mathrm{e}^{-\alpha x}\, J_{L-p+\frac{1}{2}}(\sigma x)\, \mathrm{d}x$$

$$= \sqrt{\frac{\pi}{2\sigma}} \left(-\frac{\partial}{\partial \alpha}\right) \int_0^\infty x^{L-p+\frac{1}{2}}\, \mathrm{e}^{-\alpha x}\, J_{L-p+\frac{1}{2}}(\sigma x)\, \mathrm{d}x$$

$$= \frac{2\alpha\, (2\sigma)^{L-p}\, (L-p+1)!}{(\alpha^2+\sigma^2)^{L-p+2}}\,, \tag{55}$$

where at the last step, we used (37). Therefore, after some elementary algebra, we get

$$I_k^{(L,p)}(\sigma) = \frac{2\,(2\sigma)^{L-p}\,(L-p+1)!}{(1+\sigma^2)^{L-p+2}} \times \frac{1}{k!}\frac{\partial^k}{\partial t^k}\left(\frac{1+t}{(1-t)^{2p}\left(1+t^2-2\,\frac{\sigma^2-1}{\sigma^2+1}\,t\right)^{L-p+2}}\right)\Bigg|_{t=0}. \tag{56}$$

If $k \geq 1$, using Leibnitz's formula for the k^{th} derivative of the product of two functions, we get

$$\frac{1}{k!}\frac{\partial^k}{\partial t^k}\left(t\, f(t)\right)\Big|_{t=0} = \frac{1}{(k-1)!}\frac{\partial^{k-1}}{\partial t^{k-1}}\left(f(t)\right)\Big|_{t=0}\,, \tag{57}$$

and finally

$$I_k^{(L,p)}(\sigma) = \frac{2\,(2\sigma)^{L-p}\,(L-p+1)!}{(1+\sigma^2)^{L-p+2}} \times\left[C_k^{(L+2,p)}\left(\frac{\sigma^2-1}{\sigma^2+1}\right) + C_{k-1}^{(L+2,p)}\left(\frac{\sigma^2-1}{\sigma^2+1}\right)\right], \tag{58}$$

where

$$C_k^{(\lambda,p)}(x) = \frac{1}{k!}\frac{\partial^k}{\partial t^k}\left(\frac{1}{(1-t)^{2p}(1+t^2-2tx)^{\lambda-p}}\right)\Bigg|_{t=0}. \tag{59}$$

It is clear from (56) that (58) will be valid even for $k = 0$ if we take $C_{-1}^{(\lambda,p)}(x) = 0$.

Using

$$\frac{1}{(1-t)^{2p}}=\sum_{n=0}^{\infty}\binom{n+2p-1}{n}t^n\,,\qquad \frac{1}{(1+t^2-2tx)^{\lambda-p}}=\sum_{n=0}^{\infty}C_n^{\lambda-p}(x)\,t^n\,, \tag{60}$$

where $C_n^{(\alpha)}(x)$ are Gegenbauer (ultraspherical) polynomials [40], and the Cauchy product formula [45], we get

$$f(t)=\frac{1}{(1-t)^{2p}(1+t^2-2tx)^{\lambda-p}}=\sum_{k=0}^{\infty}\left[\sum_{l=0}^{k}\binom{l+2p-1}{l}C_{k-l}^{(\lambda-p)}(x)\right]t^k\,. \tag{61}$$

Therefore,

$$C_k^{(\lambda,\,p)}(x)=\sum_{l=0}^{k}\binom{l+2p-1}{l}C_{k-l}^{(\lambda-p)}(x) \tag{62}$$

can be considered as the generalized Gegenbauer polynomials. It is convenient to calculate them by using the recurrence relation, which we will now derive.

Note that

$$\begin{aligned}\frac{\frac{\partial}{\partial t}f(t)}{f(t)} &= \frac{\partial}{\partial t}\ln f(t)=\frac{2p}{1-t}+\frac{2(\lambda-p)(x-t)}{1+t^2-2tx}\\ &= \frac{2\left[\lambda t^2+(p(1-x)-\lambda(1+x))\,t+p(1-x)+\lambda x\right]}{-t^3+(1+2x)t^2-(1+2x)t+1}\equiv\frac{g_1(t)}{g_2(t)}\,.\end{aligned} \tag{63}$$

On the other hand, since

$$g_1(0)=2[p(1-x)+\lambda x]\,,\quad \left.\frac{\partial g_1}{\partial t}\right|_{t=0}=2[p(1-x)-\lambda(1+x)]\,,\quad \left.\frac{\partial^2 g_1}{\partial t^2}\right|_{t=0}=4\lambda\,, \tag{64}$$

and

$$g_2(0)=1\,,\quad \left.\frac{\partial g_2}{\partial t}\right|_{t=0}=-(1+2x)\,,\quad \left.\frac{\partial^2 g_2}{\partial t^2}\right|_{t=0}=2(1+2x)\,,\quad \left.\frac{\partial^3 g_2}{\partial t^3}\right|_{t=0}=-6\,, \tag{65}$$

we get

$$\begin{aligned}&\frac{1}{(k+1)!}\frac{\partial^{k+1}}{\partial t^{k+1}}\left(g_2(t)\frac{\partial f(t)}{\partial t}\right)\Bigg|_{t=0}\\ &=\sum_{n=0}^{k+1}\binom{k+1}{n}\frac{\partial^n g_2(t)}{\partial t^n}\,\frac{1}{(k+1)!}\,\frac{\partial^{k+2-n}f(t)}{\partial t^{k+2-n}}\Bigg|_{t=0}\\ &=(k+2)C_{k+2}^{(\lambda,\,p)}(x)-(k+1)(1+2x)C_{k+1}^{(\lambda,\,p)}(x)\\ &+k(1+2x)C_k^{(\lambda,\,p)}(x)-(k-1)C_{k-1}^{(\lambda,\,p)}(x)\,,\end{aligned} \tag{66}$$

and

$$\frac{1}{(k+1)!}\frac{\partial^{k+1}}{\partial t^{k+1}}\left(g_1(t)f(t)\right)\Big|_{t=0}$$
$$=\sum_{n=0}^{k+1}\binom{k+1}{n}\frac{\partial^n g_1(t)}{\partial t^n}\frac{1}{(k+1)!}\frac{\partial^{k+1-n}f(t)}{\partial t^{k+1-n}}\Big|_{t=0}=2[p(1-x)+\lambda x]$$
$$\times C_{k+1}^{(\lambda,p)}(x)+2[p(1-x)-\lambda(1+x)]C_k^{(\lambda,p)}(x)+2\lambda C_{k-1}^{(\lambda,p)}(x)\,. \qquad (67)$$

Since according to (63) $g_2(t)\frac{\partial f(t)}{\partial t}=g_1(t)f(t)$, these two expressions must be equal, and we obtain the following recurrence relation [34]:

$$(k+2)C_{k+2}^{(\lambda,p)}(x)=[k+1+2p+2x(k+\lambda-p+1)]\,C_{k+1}^{(\lambda,p)}(x)$$
$$-\,[k+2\lambda-2p+2x(k+\lambda+p)]\,C_k^{(\lambda,p)}(x)+(k+2\lambda-1)C_{k-1}^{(\lambda,p)}(x)\,. \quad (68)$$

Futher, by using $C_0^{(\alpha)}(x)=1$, $C_1^{(\alpha)}(x)=2\alpha x$, $C_2^{(\alpha)}(x)=-\alpha+2\alpha(1+\alpha)x^2$, we get from (62)

$$\begin{aligned} C_0^{(\lambda,p)}(x) &= 1\,, \qquad C_1^{(\lambda,p)}(x)=2\left[p+(\lambda-p)x\right]\,,\\ C_2^{(\lambda,p)}(x) &= 2(\lambda-p)(1+\lambda-p)x^2+4p(\lambda-p)x+2p(1+p)-\lambda\,. \end{aligned} \quad (69)$$

This gives the initial values for the recurrence relation (68).

Expressions (50) and (58) allow to calculate the radial integral I_l and hence the atomic form factor in a numerically more efficient way compared to the method of the previous section.

6. An alternative method for calculating the radial integral I_l

The following mathematical result [36]:

$$\int_0^\infty \mathrm{e}^{-\delta x}J_\nu(\mu x)x^\gamma L_n^\alpha(\beta x)\mathrm{d}x$$
$$=\sum_{k=0}^{n}\frac{(-\beta)^k\mu^\nu\Gamma(n+\alpha+1)\Gamma(\nu+\gamma+k+1)}{k!\Gamma(n-k+1)\Gamma(\alpha+k+1)2^\nu\Gamma(\nu+1)\delta^{\nu+\gamma+k+1}}$$
$$\times{}_2F_1\left(\frac{\nu+\gamma+k+1}{2},\frac{\nu+\gamma+k+2}{2};1+\nu;-\frac{\mu^2}{\delta^2}\right) \qquad (70)$$

can be used to envisage an alternative way for calculating the radial integral I_l. Note that this result was not available to the authors of [34], since [36] was published much later.

According to (18),

$$L^{2l_2+1}_{n_2-l_2-1}(2bx) = (n_2+l_2)! \sum_{k=0}^{n_2-l_2-1} \frac{(-1)^k (2bx)^k}{k!\,(n_2-l_2-1-k)!\,(2l_2+1+k)!}\,. \quad (71)$$

Therefore, (27) can be rewritten as follows:

$$I_l = (n_2+l_2)! \sum_{m_2=0}^{n_2-l_2-1} \frac{(-1)^{m_2}(2b)^{m_2}}{m_2!\,(n_2-l_2-1-m_2)!\,(2l_2+1+m_2)!} J_{l,m_2}\,, \quad (72)$$

where

$$\begin{aligned} J_{l,m_2} &= \int_0^\infty x^{l_1+l_2+2+m_2}\,\mathrm{e}^{-x}\,j_l(\sigma x)\,L^{2l_1+1}_{n_1-l_1-1}(2ax)\,\mathrm{d}x \\ &= \sqrt{\frac{\pi}{2\sigma}} \int_0^\infty x^{l_1+l_2+m_2+\frac{3}{2}}\,\mathrm{e}^{-x}\,J_{l+\frac{1}{2}}(\sigma x)\,L^{2l_1+1}_{n_1-l_1-1}(2ax)\,\mathrm{d}x\,. \end{aligned} \quad (73)$$

The integral is of the type of (70), and we get, after using $\Gamma(l+3/2) = (2l+1)!\,\sqrt{\pi}/(2^{2l+1}l!)$,

$$\begin{aligned} J_{l,m_2} &= \frac{4^l l!}{(2l+1)!} \sum_{m_1=0}^{n_1-l_1-1} \frac{(-2a)^{m_1}(n_1+l_1)!\,(l+l_1+l_2+m_1+m_2+2)!\,\sigma^l}{m_1!\,(n_1-l_1-1-m_1)!\,(2l_1+1+m_1)!\,2^l} \\ &\times {}_2F_1\left(\frac{N_1+1}{2}, \frac{N_1+2}{2}; l+\frac{3}{2}; -\sigma^2\right)\,, \qquad N_1 = l+l_1+l_2+m_1+m_2+2\,. \end{aligned} \quad (74)$$

Therefore,

$$\begin{aligned} I_l &= \frac{2^l l!}{(2l+1)!} \\ &\times \sum_{m_1=0}^{n_1-l_1-1} \sum_{m_2=0}^{n_2-l_2-1} \frac{(-1)^{m_1+m_2}(2a)^{m_1}(2b)^{m_2}(n_1+l_1)!\,(n_2+l_2)!\,N_1!\,\sigma^l}{m_1!\,m_2!\,N_2!\,N_3!\,(2l_1+1+m_1)!\,(2l_2+1+m_2)!} \\ &\times {}_2F_1\left(\frac{N_1+1}{2}, \frac{N_1+2}{2}; l+\frac{3}{2}; -\sigma^2\right)\,, \\ N_1 &= l+l_1+l_2+m_1+m_2+2\,, \\ N_2 &= n_1-l_1-1-m_1\,, \qquad N_3 = n_2-l_2-1-m_2\,. \end{aligned} \quad (75)$$

The Gauss hypergeometric function ${}_2F_1$ in this formula can be expressed in terms of Jacobi polynomials. In particular,

$$
\begin{aligned}
&{}_2F_1\left(\frac{N_1+1}{2},\, \frac{N_1+2}{2};\, l+\frac{3}{2};\, -\sigma^2\right) \\
&= \begin{cases}
(\cos\phi)^{2(l+M+2)}\ \dfrac{P_M^{\left(l+\frac{1}{2},\,\frac{1}{2}\right)}(\cos 2\phi)}{P_M^{\left(l+\frac{1}{2},\,\frac{1}{2}\right)}(1)}, & \text{if } N_1-2(l+1)=2M\,, \\
(\cos\phi)^{2(l+M+2)}\ \dfrac{P_{M+1}^{\left(l+\frac{1}{2},\,-\frac{1}{2}\right)}(\cos 2\phi)}{P_{M+1}^{\left(l+\frac{1}{2},\,-\frac{1}{2}\right)}(1)}, & \text{if } N_1-2(l+1)=2M+1\,,
\end{cases}
\end{aligned}
\tag{76}
$$

where M is an integer, and the angle ϕ is defined by $\tan\phi=\sigma$.

To prove (76), first consider the case $l_1+l_2+m_1+m_2-l=2M+1$. Using the Pfaff transformation [51]

$$
{}_2F_1(a,b;c;x) = (1-x)^{-a}\ {}_2F_1\left(a, c-b; c; \frac{x}{x-1}\right)\,, \tag{77}
$$

we get

$$
\begin{aligned}
&{}_2F_1\left(l+M+2, l+M+\frac{5}{2}; l+\frac{3}{2}; -\tan^2\phi\right) \\
&= (\cos\phi)^{2(l+M+2)}\ {}_2F_1\left(l+M+2, -(M+1); l+\frac{3}{2}; \sin^2\phi\right),
\end{aligned}
\tag{78}
$$

and the second expression of (76) follows taking into account the relation between Jacobi polynomials and the hypergeometric function [51]

$$
\begin{aligned}
P_n^{(\alpha,\beta)}(x) &= \binom{n+\alpha}{n}\ {}_2F_1\left(-n, n+\alpha+\beta+1; \alpha+1; \frac{1-x}{2}\right) \\
&= P_n^{(\alpha,\beta)}(1)\ {}_2F_1\left(-n, n+\alpha+\beta+1; \alpha+1; \frac{1-x}{2}\right)\,,
\end{aligned}
\tag{79}
$$

and the symmetry property of the hypergeometric function ${}_2F_1(a,b;c;x) = {}_2F_1(b,a;c;x)$.

If $l_1+l_2+m_1+m_2-l=2M$, we can write the hypergeometric function in (76) in the form of

$$
\begin{aligned}
&{}_2F_1\left(l+M+2, l+\frac{3}{2}+M; l+\frac{3}{2}; -\tan^2\phi\right) \\
&= (\cos\phi)^{2(l+M+2)}\ {}_2F_1\left(l+M+2, -M; l+\frac{3}{2}; \sin^2\phi\right)\,,
\end{aligned}
\tag{80}
$$

and from (79), the first expression of (76) follows.

Jacobi polynomials are convenient in that they can be calculated using the three-term recurrence relation

$$\begin{aligned} P_{n+1}^{(\alpha,\,\beta)}(x) \;=\; & \left(\frac{(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)}{2(n+1)(n+\alpha+\beta+1)}\, x \right. \\ & \left. + \frac{(\alpha^2-\beta^2)(2n+\alpha+\beta+1)}{2(n+1)(n+\alpha+\beta+1)(2n+\alpha+\beta)} \right) P_n^{(\alpha,\,\beta)}(x) \\ & - \frac{(n+\alpha)(n+\beta)(2n+\alpha+\beta+2)}{(n+1)(n+\alpha+\beta+1)(2n+\alpha+\beta)}\, P_{n-1}^{(\alpha,\,\beta)}(x)\,, \end{aligned} \tag{81}$$

with

$$P_0^{(\alpha,\,\beta)}(x) = 1\,, \qquad P_1^{(\alpha,\,\beta)}(x) = \frac{1}{2}\left[(\alpha+\beta+2)x+\alpha-\beta\right] \tag{82}$$

as the initial values.

A much simpler expression can be obtained for the diagonal form factor F^{nlm}_{nlm}, which according to (15) is required in the total cross-section calculations, in the case when it is averaged over the magnetic quantum number [52]

$$F_{nl}(q) = \frac{1}{2l+1} \sum_{m=-l}^{l} F^{nlm}_{nlm}(q)\,. \tag{83}$$

Using Unsöld identity [53]

$$\sum_{m=-l}^{l} Y^*_{lm}(\theta,\varphi)\, Y_{lm}(\theta,\varphi) = \frac{2l+1}{4\pi}\,, \tag{84}$$

we get from (21)

$$\sum_{m=-l}^{l} I^{m\,m\,M}_{l\;l\;L} = \frac{2l+1}{\sqrt{4\pi}}\, \delta_{L0}\, \delta_{M0}\,, \tag{85}$$

and then (20) and (83) indicate that

$$F_{nl} = \int\limits_0^\infty r^2 \mathrm{d}r\, R^*_{nl}(r) R_{nl}(r) j_0(qr) = \frac{1}{2n}\, \frac{(n-l-1)!}{(n+l)!}\, I_0\,, \tag{86}$$

where

$$I_0 = \int\limits_0^\infty x^{2l+2}\, \mathrm{e}^{-x}\, j_0(\sigma x)\, \left[L^{2l+1}_{n-l-1}(x)\right]^2 \mathrm{d}x\,, \qquad \sigma = \frac{qn}{2}\,, \qquad x = \frac{2r}{n}\,. \tag{87}$$

Since

$$j_0(\sigma x) = \frac{\sin \sigma x}{\sigma x} = \frac{1}{2i\,\sigma x}\left(\mathrm{e}^{i\sigma x} - \mathrm{e}^{-i\sigma x}\right)\,, \tag{88}$$

the integral is of the type of (see [46], entry 7.414.4)

$$\int_0^\infty \mathrm{e}^{-\beta x} x^\alpha L_n^\alpha(\lambda x) L_m^\alpha(\mu x)\mathrm{d}x = \frac{\Gamma(m+n+\alpha+1)}{\Gamma(m+1)\Gamma(n+1)}\frac{(\beta-\lambda)^n(\beta-\mu)^m}{\beta^{n+m+\alpha+1}}$$
$$\times {}_2F_1\left(-m,-n;-m-n-\alpha;\frac{\beta(\beta-\lambda-\mu)}{(\beta-\mu)(\beta-\lambda)}\right). \tag{89}$$

Introducing $\tan\phi = \sigma = \frac{nq}{2}$, $\beta = 1 - i\sigma$, and noting that

$$\frac{\beta(\beta-2)}{(\beta-1)^2} = \frac{\beta^*(\beta^*-2)}{(\beta^*-1)^2}\frac{1+\sigma^2}{\sigma^2} = \frac{1}{\sin^2\phi}\,, \tag{90}$$

we get

$$I_0 \;=\; \frac{1}{2i\sigma}\frac{(2n-1)!}{[(n-l-1)!]^2}\left[\frac{(\beta-1)^{2(n-l-1)}}{\beta^{2n}} - \frac{(\beta^*-1)^{2(n-l-1)}}{\beta^{*\,2n}}\right]$$
$$\times {}_2F_1\left(-(n-l-1),-(n-l-1);1-2n;\frac{1}{\sin^2\phi}\right). \tag{91}$$

But $\beta - 1 = -i\sigma$, $\beta^* - 1 = i\sigma$, $\beta = 1 - i\tan\phi = \frac{\mathrm{e}^{-i\phi}}{\cos\phi}$ and, therefore,

$$\frac{1}{2i\sigma}\left[\frac{(\beta-1)^{2(n-l-1)}}{\beta^{2n}} - \frac{(\beta^*-1)^{2(n-l-1)}}{\beta^{*\,2n}}\right]$$
$$= (-1)^{n-l-1}(\sin\phi)^{2(n-l)-3}(\cos\phi)^{2l+3}\sin(2n\phi)\,. \tag{92}$$

The hypergeometric function ${}_2F_1$ satisfies the following identity [54]:

$${}_2F_1(-n,b;c;z) = \frac{(b)_n}{(c)_n}(-z)^n\,{}_2F_1\left(-n,1-c-n;1-b-n;\frac{1}{z}\right), \tag{93}$$

where $(x)_n = \Gamma(x+n)/\Gamma(x)$ is Pochhammer's symbol with the property

$$(-x)_n = (-1)^n(x-n+1)_n\,, \tag{94}$$

which implies

$$\frac{(-(n-l-1))_{n-l-1}}{(-(2n-1))_{n-l-1}} = \frac{(1)_{n-l-1}}{(n+l+1)_{n-l-1}} = \frac{(n-l-1)!\,(n+l)!}{(2n-1)!}\,. \tag{95}$$

As a result, we get

$$ {}_2F_1\left(-(n-l-1),-(n-l-1);1-2n;\,\frac{1}{\sin^2\phi}\right)=\frac{(-1)^{n-l-1}}{(\sin\phi)^{2(n-l-1)}} \times\frac{(n-l-1)!\,(n+l)!}{(2n-1)!}\,{}_2F_1\left(-(n-l-1),n+l+1;1;\,\sin^2\phi\right)\,. \qquad (96) $$

Combining (86), (91), (92) and (96), we get

$$ F_{nl}=\frac{\sin\left(2n\phi\right)\,\left(\cos\phi\right)^{2l+4}}{n\,\sin 2\phi}\,{}_2F_1\left(-(n-l-1),n+l+1;1;\,\sin^2\phi\right)\,. \qquad (97) $$

This result was first obtained in [52]. In light of (96), F_{nl} can be expressed in terms of Jacobi polynomials

$$ \begin{aligned} F_{nl} &= \frac{\sin\left(2n\phi\right)\,\left(\cos\phi\right)^{2l+4}}{n\,\sin 2\phi}\,P^{(0,\,2l+1)}_{n-l-1}(\cos 2\phi) \\ &= \frac{\left(\cos\phi\right)^{2l+4}}{n}\,U_{n-1}(\cos 2\phi)\,P^{(0,\,2l+1)}_{n-l-1}(\cos 2\phi)\,. \end{aligned} \qquad (98) $$

Here, $U_n(\cos\phi)=\sin\left((n+1)\phi\right)/\sin\phi$ are Chebyshev polynomials of the second kind.

For $l=0$, (98) further simplifies. Jacobi polynomials satisfy the relation [46]

$$ P^{(\alpha,\,\beta+1)}_n(x)=\frac{2}{2n+\alpha+\beta+2}\,\frac{(n+\beta+1)\,P^{(\alpha,\,\beta)}_n(x)+(n+1)\,P^{(\alpha,\,\beta)}_{n+1}(x)}{1+x}\,. \qquad (99) $$

Therefore,

$$ P^{(0,\,1)}_{n-1}(\cos 2\phi)=\frac{1}{2\cos^2\phi}\left[P_{n-1}(\cos 2\phi)+P_n(\cos 2\phi)\right]\,, \qquad (100) $$

where $P_n(x)=P^{(0,\,0)}_n(x)$ are Legendre polynomials, and (98) for $l=0$ takes the form of (in agreement with [33])

$$ F^{n00}_{n00}=F_{n0}=\frac{\cos^2\phi}{2n}\,U_{n-1}(\cos 2\phi)\left[P_{n-1}(\cos 2\phi)+P_n(\cos 2\phi)\right]\,. \qquad (101) $$

Since

$$ \cos^2\phi=\frac{1}{1+\tan^2\phi}=\frac{4}{4+n^2q^2}\,, \qquad \cos 2\phi=2\cos^2\phi-1=\frac{4-n^2q^2}{4+n^2q^2}\,, \qquad (102) $$

equation (101) allows to simply compute the diagonal atomic form factor F^{n00}_{n00} as a rational function of q^2 using some computer algebra system. Examples are given in the appendix.

7. Concluding remarks

The study of the interactions of dimuonium with matter requires knowledge of atomic form factors. We have presented an overview of two commonly used methods for calculating discrete–discrete transition form factors for hydrogen-like atoms. An alternative method, described in the previous chapter, is based on the results of [36] on an integral involving the product of Bessel functions and associated Laguerre polynomials. This new method complements the methods presented in [31] and [34] in the sense that it combines the simplicity and straightforwardness of the first method with the computational efficiency of the second.

We have implemented all three methods described in the text in the Fortran program. As expected, for relatively large quantum numbers ($n \sim 10$), the first method results in significantly longer runtimes compared to the other two. The availability of various computational methods proved to be very useful at the stage of program development, as it made it possible to recognize and correct some subtle errors in the computer program.

The results of [36] have already been used in [55] for analytical evaluation of atomic form factors and applied to the Rayleigh scattering by neutral atoms. However, our presentation is more detailed and has very few, if any, overlaps with [55].

In conclusion, we note two important publications that offer other methods for evaluation of atomic form factors not discussed in this article. In [56], the parabolic quantum numbers and the corresponding wave functions were used. Calculation of the form factor in the parabolic basis is less complicated than in the spherical one. Moreover, if the atom is in a constant electric field, the parabolic basis is preferable. However, many applications require the knowledge of form factors in spherical basis and, correspondingly, the connection formula between the parabolic and spherical wave functions should be used to transform the Bersons–Kulsh analytical form factors from parabolic to spherical basis.

In [57], the so-called phase-space distribution method was used to calculate the classical form factors for $nlm \to n'l'm$ transitions. It was shown that the classical form factors can be considered as effective averaged versions of their quantum counterparts.

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Appendix A

Diagonal form factors for nS states, $n \le 6$

$$
\begin{aligned}
F_{100}^{100} &= \frac{16}{(4+q^2)^2}\,, \\
F_{200}^{200} &= \frac{1-3\cdot q^2+2\cdot q^4}{(1+q^2)^4}\,, \\
F_{300}^{300} &= \frac{16\left(3^9\cdot q^8-6^6\cdot q^6+2^7\cdot 3^5\cdot q^4-2^8\cdot 3^1\cdot 7^1\cdot q^2+2^8\right)}{(4+9q^2)^6}\,, \\
F_{400}^{400} &= \frac{1}{(1+4q^2)^8}\Big[2^{14}\cdot q^{12}-23\cdot 2^{11}\cdot q^{10}+83\cdot 2^9\cdot q^8-43\cdot 5\cdot 2^6\cdot q^6 \\
&\quad +109\cdot 2^4\cdot q^4-4\cdot 19\cdot q^2+1\Big]\,, \\
F_{500}^{500} &= \frac{16}{(4+25q^2)^{10}}\Big[5^{17}\cdot q^{16}-2^4\cdot 5^{16}\cdot q^{14}+37\cdot 2^5\cdot 3^2\cdot 5^{12}\cdot q^{12} \\
&\quad -113\cdot 10^{10}\cdot q^{10}+373\cdot 2^9\cdot 3\cdot 5^8\cdot q^8-29\cdot 11\cdot 2^{12}\cdot 5^6\cdot q^6 \\
&\quad +271\cdot 3\cdot 2^{13}\cdot 5^3\cdot q^4-2^{19}\cdot 5^2\cdot q^2+2^{16}\Big]\,, \\
F_{600}^{600} &= \frac{1}{(1+9q^2)^{12}}\Big[2\cdot 3^{21}\cdot q^{20}-37\cdot 5\cdot 3^{18}\cdot q^{18}+73\cdot 3^{19}\cdot q^{16} \\
&\quad -859\cdot 2^5\cdot 3^{13}\cdot q^{14}+263\cdot 5\cdot 2^4\cdot 3^{12}\cdot q^{12}-149\cdot 7\cdot 2^3\cdot 3^{11}\cdot q^{10} \\
&\quad +23\cdot 17\cdot 5\cdot 2^3\cdot 3^8\cdot q^8-1249\cdot 2^2\cdot 3^6\cdot q^6+383\cdot 2\cdot 3^4\cdot q^4 \\
&\quad -29\cdot 15\cdot q^2+1\Big]\,. \qquad \text{(A.1)}
\end{aligned}
$$

For $n \le 4$, they agree with the results of [58].

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