Retardation corrections to the angular distributions for the free-bound transitions in H-like atoms^{\star}

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Received 4 June 1999

Abstract. The non-relativistic matrix elements and cross-sections of the radiative recombination for Hlike atoms are calculated by considering the retardation corrections up to the first order in αZ . These corrections are evaluated for the transitions to the spherical states using recursion relations which lead to fast and accurate calculations of the cross-sections.

PACS. 32.80.Fb Photoionzation of atoms and ions – 34.80.Kw Electron-ion scattering; excitation and ionization

1 Introduction

In the radiative recombination process (RR) an ion captures a free incident electron and a photon is emitted. This process is the inverse of the photoeffect and the RR differential and total cross-sections can be derived by detailed balance from the photoeffect ones. For this reason, we compare the results obtained in this paper with others reported in literature for either the photoeffect or the radiative recombination.

The photoeffect has been treated since the early days of quantum mechanics and the corresponding theoretical studies developed simultaneously with the improvement of the atomic models. The pioneering theoretical study of the radiative recombination process was carried out in the twenties by Kramers [1], Oppenheimer [2], Wessel [3], Stueckelberg and Morse [4], Stobbe [5]. Stobbe gave the most extensive study by deriving, in the dipole approximation, the expression for the RR cross-section for arbitrary hydrogenic (n, l) states. Since then, the theoretical efforts intensified in the 50's because of the importance of this process for the plasma physics with applications in the astrophysics and thermonuclear fusion, for the accelerator physics, mesonic-atom physics and antimatter production [6-16].

There is some scarcity of experimental data on the RR but many information can be derived from the experiments on the photoeffect, studied extensively in the context of photoabsorption and photoelectron spectroscopy. After the first experimental identification of the radiative recombination [17], this process has been more extensively

studied both experimentally and theoretically. Concerning the recombination of one electron with bare ions, described by the simplest theoretical models, the first experimental results have become available only in the 90's for the cases of He^{2+} , C^{6+} , F^{9+} ions [18,19]; these data showed a good agreement with the Stobbe formulae [5]. Other experiments with highly charged partially stripped atoms were accomplished and were in a reasonable agreement with the theoretical results for RR on bare ions with a judicious choice of the effective charge [20–22]. Recently, data for the recombination on D^+ and He^+ were obtained [23]. These experiments were done for low relative energies (up to about 10 eV). At such low center-of-mass electron energies the nonrelativistic dipole approximation is successful. This explains the considerable work done to obtain from Stobbe formulae [5] simple low energy analytical results. Thus, detailed studies of the cross-section formulae in the dipole approximation were performed, their main goal being the calculus efficiency, namely the fast computation, with minimum errors, of as many as possible shell contributions to the total cross-sections [15, 16, 23].

In all these direct studies on RR, whether experimental or theoretical, the main task was to measure or to compute the total cross-section corresponding to one shell or summed over all shells. Rather lately the interest for the detailed transitions on (n, l) subshells has appeared, especially since the experiments concerning the state-selective laser-induced RR process became available [24,25]. Thus, Pajek and Schuch [26] studied systematically the state selective RR of the free electrons with bare ions in the lowenergy limit. In the same paper a detailed discussion of the emitted photon angular distribution was given using dipole approximation, *i.e.* omitting the retardation which does not produce observable effects for such low energies.

 $^{^{\}star}$ Work supported partially by CNCSU under Contract No. 17/60/1998.

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The retardation corrections are the contributions to the matrix elements and differential cross-sections due to the different nonzero powers of $\mathbf{k} \cdot \mathbf{r}$ occurring in the expansion of the photon plane wave; replacing the $\exp(-i\mathbf{k}\cdot\mathbf{r})$ by unity gives, as it is well-known, the standard dipole approximation. These retardation corrections are proportional to powers of αZ . Their effect is the shift of the photon angular distribution peak towards forward or backward with respect to the direction of the incident electron in RR process. A corresponding shift of the photoelectron angular distribution peak occurs for the photoeffect. Classically, this effect is related to the tendency of the radiation of an accelerated charged particle to concentrate towards the velocity direction with increasing particle energy. In a semiclassical picture, the classical charged particle accelerated by the Colombian field of a nucleus, losing energy by radiation, might be captured on a stationary orbit ceasing thus to radiate. A more subtle physical picture was given by Sommerfeld [27] who showed that for the K-shell photoeffect the retardation may be derived from the momentum conservation law applied to the electronphoton system. Moreover, considering the distribution of the electron momentum in the bound state, Sommerfeld accounted for the correct quantum result. This picture may be extended to the photoeffect or the radiative recombination on the higher shells, some specific features of these effects being explained by the characteristics of the various bound state electron momentum distributions.

Particularly, the second term of the photon plane wave expansion yields correction only to the emitted photon differential cross-section. The αZ term does not contribute to the total cross-section (its integral over angles vanishes). The first term beyond dipole approximation is ~ $(\alpha Z)^2$ being of the same order as the first relativistic correction. In fact, the total cross-section is quite well described in nonrelativistic dipole approximation, for a large range of atomic number Z (Z between 1 and 80) and incident photon energy up to 50 keV [28,29].

Remarkable theoretical results on the radiative recombination for completely or partially ionized atoms in the nonrelativistic approach were reported by Belkić *et al.* in a larger context [30–32]. They gave exact nonrelativistic formulae, including thus all the retardation corrections. These formulae are expressed by polynomial hypergeometric Appell functions of two arguments or polynomial hypergeometric Lauricella functions of three arguments. However, only the first order retardation correction to the differential cross-section, in the nonrelativistic approach, is physically useful because the higher order terms, *i.e.* $\sim (\alpha Z)^n$, with $n \geq 2$, are of the same order of magnitude as those due to the relativistic corrections.

The first retardation correction was considered for the photoeffect long ago by Sommerfeld and Schur [33,34] who derived simple analytical formulae for the cross-sections corresponding to the K and L shells of an H-like atom. In the 60–70's the retardation problem was reconsidered, both experimentally and theoretically. The most extensive experiments were firstly reported for the krypton and neon photoeffect [35,36], for an energy range between 100 eV

and 2000 eV; this is a range where the retardation effects become observable and the nonrelativistic formulation works well.

A detailed discussion of the retardation effects, based on numerical calculations performed within the framework of the relativistic Dirac and Hartree-Fock-Slater formulation, was given by Tseng *et al.* [37]. Although the atomic photoeffect was the subject of this paper, their results are also useful for the RR studies and we recover some of them in the particular point Coulomb case.

The aim of the present paper is the study of the first order correction to the RR of the free electrons with bare ions. We give analytical formulae for the corrected differential cross-sections in closed forms in terms of Gordon's integrals for the RR on arbitrary (n, l) subshells. We make a discussion of the dependence of the results upon Z, incident electron energy and n, l quantum numbers. We hope our results to be useful for planing and analyzing experiments for both RR and photoeffect.

This article is organized as follows: in Section 2 we provide some of the theoretical background needed for our treatment. This part contains basic relations and formulas. In Section 3 we obtain the corrected differential crosssection formula expressed in terms of Gordon integrals. The method for the computation of these Gordon integrals is detailed in the Appendix. Finally, in Section 4 we make some concluding remarks and discussion.

2 General formulae

The nonrelativistic matrix element describing the transition from the state $|\kappa\rangle$ of the continuous spectrum to the spherical bound state $|n, l, m\rangle$ with the emission of a photon of polarization **s** and wave vector **k** is given by

$$M_{nlm;\boldsymbol{\kappa}}(\mathbf{s}) = \mathbf{s} \cdot \mathbf{D}(n, l, m; \boldsymbol{\kappa}), \tag{1}$$

$$\mathbf{D}(n,l,m;\boldsymbol{\kappa}) = -\mathrm{i}\hbar \int \mathrm{d}^3 x \,\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}} \Psi_{nlm}^*(\mathbf{r}) \boldsymbol{\nabla} \Psi_{\kappa}(\mathbf{r}) \qquad (2)$$

where κ is the wave vector of the incoming electron. The bound state reads as follows

$$\Psi_{nlm}(r,\theta,\varphi) = g_{nlm}r^{l}e^{-\varepsilon r}F(-n+l+1,2l+2;2\varepsilon r) \times P_{l}^{m}(\cos\theta)e^{im\varphi},$$
(3)

$$g_{nlm} = \frac{(2\varepsilon)^{l+3/2}}{(2l+1)!} \sqrt{\frac{(2l+1)(n+l)!(l-|m|)!}{8\pi n(n-l-1)!(l+|m|)!}},$$
(4)

$$P_l^m(u) = \frac{(-1)^{(|m|-m)/2}(1-u^2)^{\frac{|m|}{2}}}{2^l l!} \frac{\mathrm{d}^{l+|m|}(u^2-1)^l}{\mathrm{d}u^{l+|m|}}$$
(5)

where $\varepsilon = 1/na$, $a = \hbar^2/Zm_e e^2$ is the first Bohr radius of an H-like atom and $F(\alpha, \gamma; z)$ is the confluent hypergeometric function. The continuous spectrum eigenfunction element may be written as

is given by

$$\Psi_{\kappa}(\mathbf{r}) = \sum_{\lambda=0}^{\infty} f_{\lambda}(\kappa) r^{\lambda} \mathrm{e}^{-\mathrm{i}\kappa r} F(\mathrm{i}n' + \lambda + 1, 2\lambda + 2; 2\mathrm{i}\kappa r) \\ \times P_{l}(\cos\theta), \tag{6}$$

$$f_{\lambda}(\kappa) = \frac{\mathrm{i}^{\lambda}(2\kappa)^{\lambda}\mathrm{e}^{\pi n'/2}}{(2\lambda)!}\Gamma(\lambda + 1 - \mathrm{i}n')$$

where the z-axis is chosen in the direction of the incoming electron momentum and we use, throughout this paper, the following notations:

$$n' = \frac{1}{\kappa a} = \frac{1}{q} = \sqrt{\frac{|E_1|}{E}} \tag{7}$$

where E is the incident electron energy and $E_1 = -Z^2 Ry$ is the ground-state energy of the atom.

By introducing in equation (2) the series expansion of $\exp(-i\mathbf{k} \cdot \mathbf{r})$ one obtains the multipole expansion of the matrix element represented by an αZ power series. In this expansion we retain only the first two terms, resulting thus the approximation

$$\mathbf{D}(n,l,m;\boldsymbol{\kappa}) = \mathbf{D}^{(0)}(n,l,m;\boldsymbol{\kappa}) + \mathbf{D}^{(1)}(n,l,m;\boldsymbol{\kappa})$$
(8)

where

$$\mathbf{D}^{(0)}(n,l,m;\boldsymbol{\kappa}) = -\mathrm{i}\hbar \int \mathrm{d}^3 x \, \Psi_{nlm}^*(\mathbf{r}) \boldsymbol{\nabla} \Psi_{\boldsymbol{\kappa}}(\mathbf{r}), \quad (9)$$

is the standard dipole approximation and

$$\mathbf{D}^{(1)}(n,l,m;\boldsymbol{\kappa}) = -\hbar \int \mathrm{d}^3 x \, (\mathbf{k} \cdot \mathbf{r}) \Psi_{nlm}^*(\mathbf{r}) \boldsymbol{\nabla} \Psi_{\boldsymbol{\kappa}}(\mathbf{r}) \quad (10)$$

represents the first retardation correction.

The angular differential cross-section of the RR on the spherical state (n, l, m) for a nonpolarized emitted photon is

$$\frac{\mathrm{d}\sigma_{nlm}(\boldsymbol{\kappa})}{\mathrm{d}\Omega(\mathbf{k})} = \frac{1}{4\pi} \frac{r_0^2}{\alpha\hbar^2 a} \frac{1+n^2 q^2}{n^2 q} \sum_{\mathbf{s}} |\mathbf{s} \cdot \mathbf{D}(n,l,m;\boldsymbol{\kappa})|^2.$$
(11)

In this paper we use for **D** the approximation (8), and, consequently, in the right hand side of equation (11) only the terms up to the first order in αZ must be retained.

3 Matrix elements and cross-sections

By specifying in the following only the argument m of the matrix element, the first approximation of the matrix $\mathbf{D}^{(0)}(m) = -\mathrm{i}m_e\omega \int \mathrm{d}^3 x \Psi_{nlm}^*(\mathbf{r}) \mathbf{r} \Psi_{\boldsymbol{\kappa}}(\mathbf{r})$ $= -\mathrm{i}m_e\omega g_{nlm} \sum_{\lambda=0}^{\infty} f_{\lambda}(\kappa)$

$$\times \int_{0}^{\infty} \mathrm{d}r \, r^{l+\lambda+3} \mathrm{e}^{-(\varepsilon+\mathrm{i}\kappa)r} F(-n+l+1, 2l+2; 2\varepsilon r)$$

$$\times F(\mathrm{i}n'+\lambda+1, 2\lambda+2; 2\mathrm{i}\kappa r)$$

$$\times \int_{0}^{\pi} \mathrm{d}\theta \sin\theta \int_{0}^{2\pi} \mathrm{d}\varphi \mathrm{e}^{-\mathrm{i}m\varphi} \frac{\mathbf{r}}{r} P_{\lambda}(\cos\theta) P_{l}^{m}(\cos\theta)$$

and the first retardation correction to the dipole matrix element is given by

$$\mathbf{D}^{(1)}(m) = -\hbar k g_{nlm} \sum_{\lambda=0}^{\infty} f_{\lambda}(\kappa) \int_{0}^{2\pi} \mathrm{d}\varphi \mathrm{e}^{-\mathrm{i}m\varphi}$$

$$\times \int_{0}^{\infty} \mathrm{d}r \, r^{l+\lambda+3} \mathrm{e}^{-(\varepsilon+\mathrm{i}\kappa)r} F(-n+l+1,2l+2;2\varepsilon r)$$

$$\times \int_{0}^{\pi} \mathrm{d}\theta \sin\theta P_{l}^{m}(\cos\theta) \big[\sin\theta_{\gamma}\cos\left(\varphi-\varphi_{\gamma}\right)\sin\theta$$

$$+ \cos\theta_{\gamma}\cos\theta \big] \big\{ \frac{\mathbf{r}}{r} \big[\big(\frac{\lambda}{r}-\mathrm{i}\kappa\big)F(\mathrm{i}n'+\lambda+1,2\lambda+2;2\mathrm{i}\kappa r) \big]$$

$$+ \frac{\mathrm{i}\kappa(\mathrm{i}n'+\lambda+1)}{\lambda+1} F(\mathrm{i}n'+\lambda+2,2\lambda+3;2\mathrm{i}\kappa r) \big] P_{\lambda}(\cos\theta)$$

$$-\mathbf{e}_{\theta}\sin\theta \frac{1}{r} F(\mathrm{i}n'+\lambda+1,2\lambda+2;2\mathrm{i}\kappa r) \frac{\mathrm{d}}{\mathrm{d}\cos\theta} P_{\lambda}(\cos\theta) \big\}$$

$$(13)$$

where

$$\hbar\omega = c\hbar k = \hbar^2 (1 + n^2 q^2) / (2m_e n^2 a^2)$$
(14)

is the emitted photon energy,

 $\mathbf{e}_{\theta} = \cos\theta\cos\varphi\mathbf{e}_x + \cos\theta\sin\varphi\mathbf{e}_y - \sin\theta\mathbf{e}_z$

and θ_{γ} , φ_{γ} are the photon emission angles.

By performing the integration over φ in equations (12, 13) we see that $\mathbf{D}^{(0)}$ and $\mathbf{D}^{(1)}$ are different from zero only for $m = 0, \pm 1$ and for $m = 0, \pm 1, \pm 2$, respectively.

Because the order of the first nonzero term in the αZ power series expansion of the matrix element is 0 for |m| = 0, 1 and is 1 for |m| = 2, the first two terms of the αZ power series of the cross-section correspond only to |m| = 0, 1. So, according to the first order approximation, we retain in the matrix element $\mathbf{D}^{(1)}$ only the terms corresponding to $m = 0, \pm 1$.

In this approximation the only nonzero matrix elements are $D_x^{(0)}(\pm 1), D_y^{(0)}(\pm 1), D_z^{(0)}(0)$ and

$$D_x^{(0)}(1) = D_x^{(0)}(-1) = iD_y^{(0)}(1) = -iD_y^{(0)}(-1).$$
(15)

(12)

For the retardation corrections one obtains the relations

$$D_{y}^{(1)}(0) = \tan \varphi_{\gamma} D_{x}^{(1)}(0), \quad D_{y}^{(1)}(1) = -iD_{x}^{(1)}(1),$$

$$D_{x}^{(1)}(-1) = D_{x}^{(1)}(1), \quad D_{y}^{(1)}(-1) = iD_{x}^{(1)}(1),$$

$$D_{z}^{(1)}(1) = e^{-i\varphi_{\gamma}} \tan \theta_{\gamma} D_{x}^{(1)}(1),$$

$$D_{z}^{(1)}(-1) = D_{z}^{(1)}(1)|_{\varphi_{\gamma} \to -\varphi_{\gamma}}.$$
(16)

Thus, our problem is reduced to the calculation of only six terms and after carrying out the integration over θ , we write separately the contributions from the $\lambda = l, l \pm 1, l \pm 2$ partial waves using the following notations:

$$\begin{split} D_x^{(0)}(1) &= \pi \hbar k g_{l0} D_{0x1}, \\ D_{0x1} &= f_{l-1} D_{0x1}^{(l-1)} + f_{l+1} D_{0x1}^{(l+1)}; \\ D_z^{(0)}(0) &= \pi \hbar k g_{l0} D_{0z0}, \\ D_{0z0} &= f_{l-1} D_{0z0}^{(l-1)} + f_{l+1} D_{0z0}^{(l+1)}; \\ D_x^{(1)}(0) &= \pi \hbar k g_{l0} D_{1x0} \sin \theta_\gamma \cos \varphi_\gamma, \\ D_{1x0} &= f_{l-2} D_{1x0}^{(l-2)} + f_l D_{1x0}^{(l)} + f_{l+2} D_{1x0}^{(l+2)}; \\ D_x^{(1)}(1) &= \pi \hbar k g_{l0} D_{1x1} \cos \theta_\gamma, \\ D_{1x1} &= f_{l-2} D_{1x1}^{(l-2)} + f_l D_{1x1}^{(l)} + f_{l+2} D_{1x1}^{(l+2)}; \\ D_{z}^{(1)}(0) &= \pi \hbar k g_{l0} D_{1z0} \cos \theta_\gamma, \\ D_{1z0} &= f_{l-2} D_{1z0}^{(l-2)} + f_l D_{1z0}^{(l)} + f_{l+2} D_{1z0}^{(l+2)}; \end{split}$$

$$D_{z}^{(1)}(1) = \pi \hbar k g_{l0} D_{1z0} e^{-i\varphi_{\gamma}} \sin \theta_{\gamma},$$

$$D_{1z1} = f_{l-2} D_{1z1}^{(l-2)} + f_{l} D_{1z1}^{(l)} + f_{l+2} D_{1z1}^{(l+2)}.$$
 (17)

The integrals over r in the terms D_{0x1} , D_{0z0} , D_{1x0} , ... may be represented by the Gordon integrals [38]:

$$J_{\gamma}^{sp}(\alpha, \alpha'; \eta, \eta') = \int_{0}^{\infty} e^{-\frac{1}{2}(\eta + \eta')z} z^{\gamma - 1 + s} \\ \times F(\alpha, \gamma; \eta z) F(\alpha', \gamma - p; \eta' z) dz, \ s, p \ge 0.$$
(18)

Obtaining this representation is an essential step in developing the analytical calculations. Finally, after a tedious calculation, the matrix elements are represented by the following five combinations of Gordon integrals:

$$J^{(l-2)} = J^{04}_{2l+2}(-n+l+1, \mathrm{i}n'+l-1; 2\varepsilon, 2\mathrm{i}\kappa) -\frac{\mathrm{i}n'+l-1}{l-1}J^{03}_{2l+2}(-n+l+1, \mathrm{i}n'+l; 2\varepsilon, 2\mathrm{i}\kappa), \quad (l \ge 2),$$

$$J^{(l-1)} = J^{12}_{2l+2}(-n+l+1, in'+l+1; 2\varepsilon, 2i\kappa), \quad (l \ge 1),$$

$$J^{(l)} = J^{20}_{2l+2}(in'+l+1, -n+l+1; 2i\kappa, 2\varepsilon) - \frac{in'+l+1}{l+1}J^{11}_{2l+3}(in'+l+2, -n+l+1; 2i\kappa, 2\varepsilon), \quad (l \ge 0),$$

$$J^{(l+1)} = J^{12}_{2l+4}(\mathrm{i}n'+l+2, -n+l+1; 2\mathrm{i}\kappa, 2\varepsilon), \quad (l \ge 0),$$

$$J^{(l+2)} = i\kappa \ J^{04}_{2l+6}(in'+l+3, -n+l+1; 2i\kappa, 2\varepsilon) - (2l+5) \ J^{03}_{2l+5}(in'+l+3, -n+l+1; 2i\kappa, 2\varepsilon), \quad (l \ge 0).$$
(19)

The results are listed below:

$$\begin{split} D_{0x1}^{(l-1)} &= -\frac{i}{\lambda_c} \frac{2\sqrt{l(l+1)}}{(2l-1)(2l+1)} J^{(l-1)}, \\ D_{0x1}^{(l+1)} &= \frac{i}{\lambda_c} \frac{2\sqrt{l(l+1)}}{(2l+1)(2l+3)} J^{(l+1)}, \\ D_{0z0}^{(l-1)} &= -\frac{i}{\lambda_c} \frac{4l}{(2l-1)(2l+1)} J^{(l-1)}, \\ D_{0z0}^{(l+1)} &= -\frac{i}{\lambda_c} \frac{4(l+1)}{(2l+1)(2l+3)} J^{(l+1)} \\ D_{1x0}^{(l-2)} &= \frac{-2l(l-1)i\kappa}{(2l-3)(2l-1)(2l+1)} J^{(l-2)}, \\ D_{1x0}^{(l)} &= \frac{4(l^2+l-1)i\kappa}{(2l-1)(2l+1)(2l+3)} J^{(l)} \\ D_{1x0}^{(l+2)} &= \frac{-2(l+1)(l+2)}{(2l+1)(2l+3)(2l+5)} J^{(l+2)} \\ D_{1z0}^{(l-2)} &= -2D_{1x0}^{(l-2)}, \\ D_{1z0}^{(l-2)} &= -2D_{1x0}^{(l-2)}, \\ D_{1z0}^{(l-2)} &= -2D_{1x0}^{(l+2)} \\ D_{1x1}^{(l-2)} &= \frac{2(l-1)\sqrt{l(l+1)}i\kappa}{(2l-3)(2l-1)(2l+1)} J^{(l-2)} \\ D_{1x1}^{(l)} &= \frac{2\sqrt{l(l+1)}i\kappa}{(2l-1)(2l+1)(2l+3)} J^{(l)} \\ D_{1x1}^{(l)} &= \frac{-2(l+2)\sqrt{l(l+1)}}{(2l-1)(2l+1)(2l+3)} J^{(l+2)} \end{split}$$

and

$$D_{1z1} = D_{1x1}.$$
 (21)

Thus, the calculation of the Gordon integrals involved in the matrix elements remains the main task. In the Appendix we present a method for the evaluation of these integrals based on a set of functions which satisfy simple recursive relations.

The polarization sums are given by

$$\sum_{\mathbf{s}} |\mathbf{s} \cdot \mathbf{D}(0)|^2 = \pi^2 \hbar^2 k^2 g_{l0}^2 \{ |D_{0z0}|^2 \sin^2 \theta_{\gamma} + 2\mathcal{R}e [D_{0z0}^* (D_{1z0} - D_{1x0})] \cos \theta_{\gamma} \sin^2 \theta_{\gamma} \}, \quad (22)$$

 $\langle \alpha \rangle$

$$\sum_{\mathbf{s}} \left| \mathbf{s} \cdot \mathbf{D}(1) \right|^2 = \pi^2 \hbar^2 k^2 g_{l0}^2 \left\{ \left| D_{0x1} \right|^2 (2 - \sin^2 \theta_\gamma) \right. \\ \left. + 4 \mathcal{R} e \left[D_{0x1}^* D_{1x1} \right] \cos \theta_\gamma \right. \\ \left. - 2 \mathcal{R} e \left[D_{0x1}^* (D_{1x1} + D_{1z1}) \right] \cos \theta_\gamma \sin^2 \theta_\gamma \right\}$$

Denoting a global factor by

$$Q_{nl} = \frac{\pi r_0^2}{4\alpha} \frac{g_{l0}^2 k^2 (1+n^2 q^2)}{n^2 q a},$$

we may write the differential cross-section for the recombination on the (n, l) subshell in the following form:

$$\frac{\mathrm{d}\sigma_{nl}}{\mathrm{d}\Omega} = Q_{nl} \left[A_{nl} + B_{nl} \left(1 + \gamma_{nl} \cos \theta_{\gamma} \right) \sin^2 \theta_{\gamma} + C_{nl} \cos \theta_{\gamma} \right]$$
(23)

where

$$A_{nl} = 4 |D_{0x1}|^2, \quad B_{nl} = |D_{0z0}|^2 - 2 |D_{0x1}|^2,$$

$$C_{nl} = 8 \mathcal{R} e [D_{0x1}^* D_{1x1}], \qquad (24)$$

$$\gamma_{nl} = \frac{2}{B_{nl}} \mathcal{R} e [D_{0z0}^* (D_{1z0} - D_{1x0}) - 4D_{0x1}^* D_{1x1}].$$

As it is seen from the last equations, the first retardation correction contributes with terms containing the factor $\cos \theta_{\gamma}$. This shape of the corrected cross-section was predicted already by Tseng *et al.* [37] using general arguments, but no explicit expressions were given for the coefficients A_{nl} , B_{nl} , ... except for the results obtained by Sommerfeld and Schur [33] and Schur [34] for the K and L shells. From the equations (20, 24) we see that all the coefficients A_{n0} and C_{n0} are zero, the only remaining terms being those proportional to $\sin^2 \theta_{\gamma}$ and $\cos \theta_{\gamma} \sin^2 \theta_{\gamma}$. We point out that for the analytical or numerical calculations it is useful to factorize f_l and $\rho^{in'}$ in equations (17) with the following contribution to the global factor in the crosssection

$$\begin{split} |f_l \rho^{\mathrm{i}n'}|^2 &= \frac{2\pi (2\kappa)^{2l}}{[(2l)!]^2} \frac{\Pi_l^2 \exp[-\frac{4}{q}\arctan{(nq)}]}{q(1-\mathrm{e}^{-2\pi/q})},\\ \Pi_l &= \begin{cases} \prod_{s=1}^l \sqrt{s^2 + n'^2}, \ l > 0\\ 1, \qquad l = 0 \end{cases}. \end{split}$$

4 Results and discussion

Equations (23) were used to create a short computer program that efficiently calculates the angular distributions for arbitrary values of (n, l) including the first order retardation corrections.

The precision of our calculations is insured by the stable character of the calculation of the $Y_j^{(k,\gamma)}$ – functions defined in the Appendix. However, for very high values of (n, l) the calculation using the equations (20) is stopped due to computing overflow. Our tests show that, for a given n, the overflow is associated with the very small cross-section values corresponding to high values of l but these cases may be eliminated from the calculations. The computing overflows are eliminated even for n of the order of a thousand by imposing a very weak condition like ignoring those values of l for which the integrated cross-section σ_{nl} is smaller then $10^{-30}\sigma_{n0}$.

The cross-section for the transition to the (n, l) subshell is given by

$$\sigma_{nl} = \frac{4\pi}{3} Q_{nl} \left[3 A_{nl} + 2 B_{nl} \right]. \tag{25}$$

To compute the cross-section $\sigma_n = \sum_l \sigma_{nl}$ for the transition to the *n* shell, we point out that it is much more suitable to use the sum over the cross-sections corresponding to the transitions in the Stark states [29],

$$\sigma_n(\boldsymbol{\kappa}) = \frac{2^8 \pi^2 r_0^2 \mathrm{e}^{-(4/q) \arctan nq}}{3\alpha q^2 (1 + n^2 q^2) (1 - \mathrm{e}^{-2\pi/q})} \times \sum_{j=0}^{n-1} \left[(1 + n^2 q^2) (Y_j + Y_{j-1})^2 + 4 \left(\frac{n-j-1}{j+1}\right) Y_j^2 \right]$$
(26)

where $Y_j(\rho) = Y_j^{(1,2)}(\rho)$. Our numerical tests, using also asymptotic formulae for higher values of n, proved that the formula (26) is characterized by a very high numerical stability and can be successfully used even for n of the order of one thousand. For example, for q = 0.5 and n =8000 the asymptotic formula for the Gaunt factor given by equation (56) of [29] and the formula (26) give values of σ_n with 5 coincident digits.

In Table 1 we represent the contributions to the total cross-section $\sigma = \sum_{n=1}^{\infty} \sigma_n$ of the different *n*-shells by the ratios $\sigma^{(N)}/\sigma$ where

$$\sigma^{(N)} = \sum_{n=1}^{N} \sigma_n.$$
(27)

The total cross-section σ is calculated by the formula

$$\sigma = \sum_{n=1}^{n_0} \sigma_n + \sum_{n=n_0+1}^{n_1} \sigma_n^{(a)} + \int_{n_1+1}^{\infty} \sigma_n^{(a)} dn \qquad (28)$$

where in the first sum σ_n is given by equation (26) and for $\sigma_n^{(a)}$ in the second sum and in the integral the asymptotic formula for the Gaunt factor [39] is used. The values for n_0 and n_1 are chosen such that a given precision for σ is assured. In this table are also given the values of the incident electron energy for given value of q^2 and various values of the atomic number Z (Z = 1, 26, 42). One may see from Table 1 that at low incident electron energies the high n values give notable contributions to the total cross-section. Although, for a given Z, these contributions decrease when the incident electron energy increases, an examination of Table 1 shows that in the considered energy range, where the nonrelativistic approach is valid, at least the first ten shells must be considered.

Table 1. The weights $\sigma^{(N)}/\sigma$, $\sigma^{(N)} = \sum_{n=1}^{N} \sigma_n$, representing the contributions of the first N shells to the total cross-section σ of the radiative recombination with the bare ions in the dipolar approximation. In the last three columns are indicated the values of the incident electron energy corresponding to the values 1, 26 and 43 of the atomic number Z for given ratio $q^2 = E/|E_1|$. The number in parentheses is the power of ten multiplying the entry.

q^2	σ_1 (barns)	$\frac{\sigma^{(1)}}{\sigma}$	$\frac{\sigma^{(2)}}{\sigma}$	$\frac{\sigma^{(3)}}{\sigma}$	$\frac{\sigma^{(4)}}{\sigma}$	$\frac{\sigma^{(5)}}{\sigma}$	$\frac{\sigma^{(10)}}{\sigma}$	E(1) (keV)	E(26) (keV)	E(42) (keV)
0.01	16674	0.31	0.47	0.58	0.66	0.72	0.87	1(-4)	0.09	0.24
0.05	3249	0.42	0.62	0.74	0.81	0.86	0.95	7(-4)	0.5	1.2
0.1	1573	0.48	0.69	0.80	0.87	0.90	0.97	1(-3)	0.9	2.4
0.5	251	0.65	0.84	0.91	0.94	0.96	0.99	7(-3)	4.6	12.0
1.0	99	0.72	0.88	0.94	0.96	0.97	0.99	1(-2)	9.2	24.0
1.5	54	0.75	0.90	0.95	0.97	0.98	0.99	2(-2)	13.8	36.0
2.0	35	0.77	0.91	0.95	0.97	0.98	1.00	3(-2)	18.4	48.0



Fig. 1. The branching ratios $p(n,l) = \sigma_{nl}/\sigma_n$ for the population of the (n,l) subshells versus incident electron energy parameter $q = \sqrt{E/|E_1|}$ for n = 3, 4. The curves corresponding to the various subshells are labelled by the quantum numbers n, l.

Let us define the branching ratio for the population of the (n, l) subshell as

$$p(n,l) = \frac{\sigma_{nl}}{\sigma_n} \,. \tag{29}$$

Figure 1 shows the q-dependence of the branching ratios for n = 3 and n = 4 and the contributions of the transitions for different (n, l) subshells. For $q \to 0$ the dominant contribution is given by the (n, n/2) subshell for even nor (n, (2n+1)/2) subshell for odd n and with increasing q the transition to the s state becomes dominant.

Figure 2 shows the corrected angular distribution summed on the first N shells for two N values: N = 1and N = 100, for a given q^2 value. The first retardation correction depends on q^2 and also on Z. In Figure 2 three curves corresponding to Z = 26, 42 and 74 are plotted. The results obtained with the dipole approximation are also plotted (dotted line); as one knows, these depend only on q^2 . The contributions to the sum from higher n shells are significant, as it is seen by comparing the curves corresponding to the two different values of N.

Based on these observations we can conclude that some efforts are justified in order to obtain a detailed description of the radiative recombination for arbitrary (n, l) subshells in spite of the fact that experimental information on the relative contributions from these individual states for RR with bare ions is scanty, especially for intermediate energies.

We have compared our angular distributions for the K shell recombination with the results of the exact



Fig. 2. Comparison between the angular distribution for the recombination on the K-shell and that corresponding to the transitions on the first 100 shells for different values of the atomic number Z and a given value of the incident electron energy parameter $q^2 = E/|E_1|$ (Eq. (7)). The results corresponding to the conventional dipole approximation, which depend only on q^2 , are represented by points and those including the first retardation corrections are represented by full lines.

relativistic numerical calculations from the tables for the relativistic K shell photoeffect [40]. There is a very good agreement for $Z \leq 42$ and $E \leq 10$ keV. We cannot perform such a comparison for higher transitions because of the lack of available relativistic numerical data for angular distributions in these cases.

Because the cross-section for the recombination is proportional to the photoeffect one, some ratios as for example $(4\pi/\sigma)d\sigma/d\Omega$ and $(d\sigma/d\Omega)/(d\sigma/d\Omega)_{\theta_{\gamma}=\pi/2}$, are the same for both processes. Moreover, the comparisons of theoretical and experimental results for such ratios are preferable [37].

We report the analytic expressions for the recombination (photoeffect) on the first three shells for

$$\frac{4\pi}{\sigma_{nl}}\frac{\mathrm{d}\sigma_{nl}}{\mathrm{d}\Omega} = a_{nl} + b_{nl}(1 + \gamma_{nl}\cos\theta_{\gamma})\sin^2\theta_{\gamma} + c_{nl}\cos\theta_{\gamma}.$$
(30)

The coefficients a_{nl}, b_{nl}, c_{nl} and γ_{nl} , expressed in terms of the parameter¹

$$\gamma = |E_n|/E_\gamma,\tag{31}$$

 E_n being the bound state energy and $E_{\gamma}-$ the photon energy, are

$$\begin{aligned} a_{10} &= 0, \ b_{10} = \frac{3}{2}, \ \gamma_{10} = 4\beta, \ c_{10} = 0; \\ a_{20} &= 0, \ b_{20} = \frac{3}{2}, \ \gamma_{20} = 4(1-\gamma)\beta; \\ a_{21} &= \frac{3}{8\gamma+3}, \ b_{21} = \frac{12\gamma}{8\gamma+3}, \\ \gamma_{21} &= \frac{11\gamma+1}{2\gamma}\beta, \ c_{21} = \frac{6}{8\gamma+3}\beta; \\ a_{30} &= 0, \ b_{30} = \frac{3}{2}, \ \gamma_{30} = -\frac{4(4\gamma-3)}{4\gamma+3}\beta, \ c_{30} = 0; \\ a_{31} &= \frac{3(3\gamma+1)}{28\gamma^2+26\gamma+3}, \ b_{31} = \frac{3\gamma}{2}\frac{28\gamma+17}{28\gamma^2+26\gamma+3}, \\ \gamma_{31} &= -\frac{4}{\gamma}\frac{24\gamma^3-24\gamma^2-26\gamma-1}{28\gamma+17}\beta, \\ c_{31} &= -6\frac{4\gamma^2-2\gamma-1}{28\gamma^2+26\gamma+3}\beta; \\ a_{32} &= \frac{9}{2}\frac{1}{6\gamma+5}, \ b_{32} = \frac{3}{4}\frac{12\gamma+1}{6\gamma+5}, \\ \gamma_{32} &= 8\frac{84\gamma^2+32\gamma+1}{(12\gamma+1)(8\gamma+1)}\beta, \ c_{32} = 18\frac{6\gamma+1}{(8\gamma+1)(6\gamma+5)}\beta. \end{aligned}$$
(32)

The results (32) for the K and L shells may be compared with the formulae given by Sommerfeld and Schur [33] and Schur [34] respectively. As far as we know, the Mshell analytical result was firstly reported in [41].

By considering the incident electron moving in the field of an effective nuclear charge and expanding the bound state wave function of an atom on the basis of Slater-type orbitals [42], it may be shown that the cross-sections for the recombination, as well as for the photoeffect, with the partially stripped atoms with the first retardation corrections are represented by expressions of the same form as in the equation (23) [43]. As a test, we fitted the experimental data obtained by Krause [35] for the normalized angular distribution of Kr 3*d* photoelectrons, corresponding to 1.2536 keV for the incident photon energy, by

$$J = \frac{100}{\left(\mathrm{d}\sigma/\mathrm{d}\Omega\right)_{\pi/2}} \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}$$
$$= 2.35 + 67.65(1 + 0.22\cos\theta)\sin^2\theta + 5.14\cos\theta \quad (33)$$

that is by a function of the form (23). The results obtained with this formula almost coincide with the relativistic Hartree-Fock-Slater ones of Tseng *et al.* [37] which agree with experimental results. These agreements argue for the validity in this case of the cross-section formula only with the first order retardation correction

¹ We choose this parameter with the view of a direct comparison with the results of Sommerfeld and Schur.



Fig. 3. Comparison of the normalized angular distribution $J(\theta) = 100(d\sigma/d\Omega)(\theta)/[(d\sigma/d\Omega)(\pi/2)]$ of Ne 2p (a, b), Kr 3p (c), Kr 3d (d) photoelectrons between the experimental data (points) of Krause [35], the relativistic Hartree-Fock-Slater results of Tseng *et al.* [37] (crosses) and the results from formula (23) for $J(\theta)$ in the corresponding bare ions cases (full line).

(for this example, and also for the following ones, we point out that we obtained data by scanning the graphics from [37] and our representations might be affected by some errors; however, we believe that these possible errors do not affect the conclusions of the graphical comparisons done in the present paper).

It is known that in the case of non-bare ions at low energies a large part of the total cross-section is determined by the transitions to the excited states. The final states have high angular momentum numbers l and practically only the region of space outside the core contributes to the matrix element, so that the total cross-section will be determined by the total ion charge. Some tests for low relative energies in the case of non-bare ions with one residual

electron show an excellent agreement between the experimental data and the results of the calculations based on the theory of RR with bare ions using an effective charge Z_{eff} equal to the total ionic charge [20,44]. By increasing the incident electron energy (or the photon energy in the case of the photoeffect) it is expected to obtain reasonable results using an intermediate effective charge situated between the total ionic charge and the nuclear one. For more complex non-bare ions it is not sure that the bare ion model can be always successfully used. However, using the formula (23) for the calculation of the normalized angular distribution $J(\theta)$ for the atomic photoeffect, we obtain some reasonable results compared with the experimental ones. Figure 3 shows for four cases the comparisons



Fig. 4. Comparison of the normalized angular distribution $J(\theta) = 100(d\sigma/d\Omega)(\theta)/[(d\sigma/d\Omega)(\pi/2)]$ of Ne 2p (a) and Kr 3d (b) photoelectrons between the experimental data (points) of Krause [35], the relativistic Hartree-Fock-Slater results of Tseng *et al.* [37] (crosses) and the results from a formula of the type (23) corresponding to Slater-type orbitals [43] for various effective charges: 7 and 8 for neon and 12 and 14 for krypton (full lines).

of the normalized angular distributions of photoelectrons between the experimental data of Krause [35], the relativistic Hartree-Fock-Slater results of Tseng et al. [37] and our results obtained by using equation (23) and considering the ratios of the corresponding bare ions cross-sections. These results could be explained by the approximate validity in these cases of the property that at high energies the screening manifests only through wave function normalizations [37]. Moreover, the formula (23) with modified coefficients obtained in [43] by using Slater-type orbitals gives excellent results in the above cases for intermediate values of Z_{eff} . Thus, for example, the theoretical results of Tseng et al. [37] for the normalized angular distribution $J(\theta)$ of Ne 2p photoelectrons are well reproduced for $Z_{\rm eff} = 8$ and a better agreement with the experimental values is achieved for $7 \leq Z_{\rm eff} < 8$. Similar results are obtained for the Kr 3d photoelectrons. In Figure 4 some of these results, which will be justified and detailed elsewhere, are shown.

An interesting feature of the formula (23), not extensively studied but already pointed out by Tseng *et al.* [37], is that, for some (n, l) transitions, by decreasing the incident electron energy (the incident photon energy in the case of the photoeffect), the photon (photoelectron) angular distribution, first peaked forward, will shift towards 90° and begin to peak backward [37]. We note that, at least in the point Coulomb case, the angle θ_{\max} , corresponding to the distribution peak, reaches the value 90° for a Z independent value γ_0 of the parameter γ defined by the equation (31). Figure 5 represents the variation of $\cos \theta_{\max}$ versus β for Z = 42, l = 0 and various n. For Z = 42 the magnitude of the displacement backward from 90° is about 0.5°. This displacement increases with increasing Z so that, for example, for Z = 74 it is about 1°.



Fig. 5. The forward and backward shifts of the maximum of the RR cross-section. The function $\cos \theta_{\max}$ is plotted against $\beta = v/c$ where v is the velocity of the incident electron.

This peaking towards backward is not present for all transitions. Thus, based on an analysis of the analytical expressions of the corresponding cross-sections, we remark that this effect appears, for example, for the transitions $(n \ge 3, l = 0), (n \ge 7, l = 1), (n \ge 15, l = 2)$ but we could not give a general rule. However, this backward shift remains a pure theoretical problem because a too high angular resolution is necessary for an experimental evidence.

Appendix: Gordon integrals calculation

Using the recurrence relations [45]

$$J_{\gamma}^{sp}(\alpha, \alpha'; \eta, \eta') = \frac{\gamma - 1}{\eta} \\ \times \left[J_{\gamma-1}^{s, p-1}(\alpha, \alpha'; \eta, \eta') - J_{\gamma-1}^{s, p-1}(\alpha - 1, \alpha'; \eta, \eta') \right],$$

$$J_{\gamma}^{s+1,0}(\alpha, \alpha'; \eta, \eta') = \frac{4}{\eta'^2 - \eta^2} \\ \times \left\{ \left[\frac{\gamma}{2} (\eta' - \eta) - \eta' \alpha' + \eta \alpha - \eta s \right] J_{\gamma}^{s0}(\alpha, \alpha'; \eta, \eta') \right. \\ \left. + s(\gamma - 1 + s - 2\alpha) J_{\gamma}^{s-1,0}(\alpha, \alpha'; \eta, \eta') \right. \\ \left. + 2\alpha s J_{\gamma}^{s-1,0}(\alpha + 1, \alpha'; \eta, \eta') \right\},$$
(A.1)

all the Gordon integrals in equations (19) may be expressed by

$$J_{\gamma}^{00}(-j, \mathrm{i}n'+k; 2\varepsilon, 2\mathrm{i}\kappa) = J_{\gamma}^{00}(\mathrm{i}n'+k, -j; 2\mathrm{i}\kappa, 2\varepsilon)$$
$$= \frac{(-1)^{j}\Gamma(\gamma)\rho^{\mathrm{i}n'+k}}{(j+1)(\varepsilon+\mathrm{i}\kappa)^{\gamma}} {}_{2}F_{1}(-j, \mathrm{i}n'+k, \gamma; 1-\rho^{2}) \quad (A.2)$$

where

$$\rho = \frac{\varepsilon + i\kappa}{\varepsilon - i\kappa} = \frac{1 + inq}{1 - inq},$$

$$\rho^{in'} = \exp[-\frac{2}{q}\arctan(nq)], \qquad (A.3)$$

 γ is a natural number and k an integer one [45].

Let us define the functions

$$Y_{j}^{(k,\gamma)}(\rho) = (j+1)\rho^{-j} {}_{2}F_{1}(-j, \mathrm{i}n'+k, \gamma; 1-\rho^{2}),$$

$$j = -1, \ 0, \ 1 \ \dots \ (A.4)$$

which satisfy the recursion relation

$$Y_{j}^{(k,\gamma)}(\rho) = -\frac{2(j+1)}{j(j+\gamma-1)} \\ \times \left[j\!+\!k\!-\!1\!+\!\frac{2(n\!-\!j\!-\!k\!+\!1)}{1+n^{2}q^{2}}\right] Y_{j-1}^{(k,\gamma)}(\rho) \\ + \frac{(j+1)(\gamma-2k)}{j(j+\gamma-1)}\rho^{-1}Y_{j-1}^{(k,\gamma)}(\rho) - \frac{j+1}{j+\gamma-1}Y_{j-2}^{(k,\gamma)}(\rho)$$
(A.5)

and the initial conditions

$$Y_{-1}^{(k,\gamma)}(\rho) = 0, \ Y_0^{(k,\gamma)}(\rho) = 1.$$

For $\gamma = 2k$, these are the $Y_j^k(\rho)$ functions used in [29,41]. Let us observe that these functions do not differ es-

sentially from the Jacobi polynomials used by Baratella

et al. [11]. Indeed, the functions $Y_j^{(k,\gamma)}$ may be expressed in terms of Jacobi polynomials $P_a^{(\alpha,\beta)}(z)$ using the relation

$$Y_{j}^{(k,\gamma)}(\rho) = (j+1) \left(\frac{-\gamma}{j}\right)^{-1} \left(\frac{\rho^{2}-1}{\rho}\right)^{j} \times P_{j}^{(-j-in'-k,-j+in'+k-\gamma)} \left(\frac{\rho^{2}+1}{\rho^{2}-1}\right).$$
(A.6)

So, our recursion relations (A.5) are of the same type with those used by Baratella *et al.*

As a result, the quantities $J^{(l-2)}, \ldots, J^{(l+2)}$ can be expressed as combinations of the $Y_j^{(k,\gamma)}(\rho)$:

$$\begin{split} J^{(l-2)} &= -\frac{(2l+1)! F}{16} \Big\{ \frac{1}{n-l} Y_{n-l-1}^{l-1,2l-2} \\ &+ \frac{1}{n-l+4} Y_{n-l+3}^{l-1,2l-2} + \frac{4}{n-l+3} Y_{n-l+2}^{l-1,2l-2} \\ &+ \frac{6}{n-l+2} Y_{n-l+1}^{l-1,2l-2} + \frac{4}{n-l+1} Y_{n-l-1}^{l-1,2l-2} \\ &- \frac{2(l-1+in')(1+inq)}{(l-1)(1+n^2q^2)} \Big[\frac{1}{n-l} Y_{n-l-1}^{l,2l-1} + \frac{1}{n-l+3} Y_{n-l+2}^{l,2l-1} \\ &+ \frac{3}{n-l+2} Y_{n-l+1}^{l,2l-1} + \frac{3}{n-l+1} Y_{n-l-1}^{l,2l-1} \Big] \Big\} \\ J^{(l-1)} &= \frac{na(2l+1)! F}{2(1+n^2q^2)^2} \Big[\frac{1}{n-l} Y_{n-l-1}^{l,2l-1} - \frac{1}{n-l+2} Y_{n-l+1}^{l,2l} \Big], \\ J^{(l)} &= \frac{2i(na)^2(2l+1)! F}{(n-l)q(1+n^2q^2)^3} Y_{n-l-1}^{l+1,2l+2} \\ &\int J^{(l+1)} &= \frac{ia(na)^2(2l+3)! F}{2(n-l)q(1+inq)^2(1+n^2q^2)^2} \\ &\times \Big[\rho^2 Y_{n-l-1}^{l+2,2l+2} - Y_{n-l-1}^{l,2l+2} \Big], \\ J^{(l+2)} &= \frac{-ia^3(2l+5)! F}{16(n-l)q^3(1+inq)^4} \\ &\times \Big[Y_{n-l-1}^{l-1,2l+2} - \rho^4 Y_{n-l-1}^{l+3,2l+2} + 2\rho^3 Y_{n-l-1}^{l+2,2l+2} - 2\rho Y_{n-l-1}^{l,2l+2} \Big] \\ &(A.7) \end{split}$$

where F is a common factor

$$F = \frac{(-1)^{n+l} (na)^{2l+2} \rho^{in'}}{(1+n^2 q^2)^{l-1}} \cdot$$
(A.8)

Let us note that the asymptotic formulae for the electric dipole matrix elements and cross-sections for $q \to 0$ reported in [26] can be obtained from the present paper results using the following asymptotic relations:

$$Y_j^{(k,\gamma)}(\rho) \sim (j+1) \ F(-j,\gamma;4n),$$

$$\begin{split} Y_{n-l-1}^{(l+2,2l+2)}(\rho) &- Y_{n-l-1}^{(l,2l+1)}(\rho) \\ &\sim \frac{4\mathrm{i}n(n-l)(n-l-1)}{l+1}F(-n+l+2,2l+3;4n), \end{split}$$

$$(\rho^2 - 1) Y_{n-l-1}^{(l+2,2l+2)}(\rho)$$

~ $4in(n-l)q \ F(-n+l+1,2l+2;4n).$ (A.9)

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