Compton Scattering by *K*-Shell Electrons. II. Nonrelativistic Dipole Approximation

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The dipole approximation of the nonrelativistic cross section for Compton scattering by electrons bound in the ground state of a hydrogenlike atom, obtained by the present author, is computed and discussed. In this approximation the cross-section differential with respect to the angles and energy of the scattered photon is proportional to $C_1+C_2\cos^2\theta$, where θ is the scattering angle of the photon. The coefficients C_1, C_2 are combinations of Appell functions F_1, depending on the atomic number Z and the energies of the initial and final photons κ_1, κ_2 by means of the dimensionless variables $k_i=\kappa_i/Z^2\mathcal{R}$, $i=1,2$, where $\mathcal{R}$ is the rydberg. In order to compute the Appell functions, these were first continued analytically and expressed in terms of other hypergeometric functions of two variables, which under our circumstances admit convergent series expansions. These were then summed numerically. The incident photon energies considered lie in the interval $1.05\leq k_1\leq 20$. For each value k_1 the coefficients C_1 and C_2 were computed for a number of values of k_2 $(0\leq k_2\leq k_1-1)$. Special attention was given to the end points $k_2=0$ and $k_2=k_1$. C_1 and C_2 turn out to be monotonically decreasing functions of k_2 presenting the infrared-divergent behavior $1/k_2$ for $k_2\to 0$. The limitations of the result due to retardation corrections are considered.

I. ANALYTIC EXPRESSIONS OF MATRIX ELEMENT AND CROSS SECTIONS

In a previous paper (I)[1] we derived an exact analytic expression for the nonrelativistic matrix element of Compton scattering by an electron bound in the ground state of a hydrogenlike atom. The matrix element was obtained in terms of generalized hypergeometric functions of four variables of the type F_D. It was shown that the result simplifies considerably in the dipole approximation, when κ_1/λ and therefore also κ_2/λ are small enough and can be neglected with respect to 1. In this case the matrix element reduces to a combination of hypergeometric functions of two variables of Appell's type F_1. The result is contained in Eqs. (1), (75)–(77), and (80)–(82) of I.

In this work we present the numerical evaluation of the dipole approximation of the matrix element and cross sections. We have computed the Appell functions $F_1(x, y)$ involved by series summation. This is the fastest and most accurate method available. However, this can not be done directly because the variables x and y do not satisfy the necessary convergence conditions ($|x|<1$, $|y|<1$). Therefore an analytic continuation of the F_1 functions in terms of convergent series expansions must first be carried out. This is presented in Sec. II. The limiting cases $\kappa_2\to 0$ and $\kappa_2\to\kappa_1-E_0$ (the high-energy end of the spectrum) are considered separately in Sec. III. Finally, the numerical results are presented and discussed in Sec. IV.

We shall start by redefining the matrix element of the process Eq. (75) of I, according to

$$M=(|N|/N)(\lambda^2/2m)^{1/2}\mathfrak{M}\ , \tag{1}$$

where N is given by Eq. (24) of I. If we redefine all the quantities occurring in Eqs. (75)–(77) of I in the same manner, we get

$$M=A(\vec{s}_1\cdot\vec{s}_2)+E(\vec{s}_1\cdot\vec{n})(\vec{s}_2\cdot\vec{n})\ , \tag{2}$$

$$A=-[P(\Omega_1)+P(\Omega_2)],\quad E=-[T(\Omega_1)+T(\Omega_2)]. \tag{3}$$

Further, we shall introduce new, dimensionless energy variables for the photons, defined by

$$k_i=(2m/\lambda^2)\kappa_i=\kappa_i/Z^2\mathcal{R}\ ,\quad i=1,\ 2 \tag{4}$$

where $\mathcal{R}$ is the rydberg. Then the differential cross section of Eq. (1) of I becomes

$$d^3\sigma=r_0^2\,(k_2/k_1)\,|M|^2\,dk_2\,d\Omega_2\,d\Omega\ . \tag{5}$$

However, we are primarily interested in the cross section Eq. (83) of I, referring to the case when the ejected electron is not recorded, the incident photon beam is unpolarized and the final photon polarization is not detected. From Eq. (2) we get

$$\int|M|^2\,d\Omega=\tfrac{4}{15}\pi\,|E|^2 + 4\pi(\vec{s}_1\cdot\vec{s}_2)^2\left[|A|^2+\tfrac{2}{15}|E|^2+\tfrac{2}{3}\,\mathrm{Re}(A^*E)\right],$$

and hence Eq. (83) of I becomes

$$d^2\sigma=\tfrac{1}{2}r_0^2\,(C_1+C_2\cos^2\theta)\,dk_2\,d\Omega_2\ , \tag{6}$$

with

$$C_1=4\pi(k_2/k_1)\left[|A|^2+\tfrac{2}{5}|E|^2+\tfrac{2}{3}\,\mathrm{Re}(A^*E)\right], \tag{7}$$

$$C_2=4\pi(k_2/k_1)\left[|A|^2+\tfrac{2}{15}|E|^2+\tfrac{2}{3}\,\mathrm{Re}(A^*E)\right]. \tag{8}$$

From Eq. (6), we find for the spectral distribution of photons scattered in all space, defined in Eq. (84) of I,

$$d\sigma = 2\pi r_0^2 (C_1 + \tfrac{1}{3} C_2) dk_2 \,. \tag{9}$$

Taking into account Eqs. (81) and (82) of I and the redefinition of Eq. (1), we get

$$P(\Omega) = \frac{64}{[2\pi(1-e^{-2\pi|n|})]^{1/2}} \left(\frac{1-i\sigma}{1+i\sigma}\right)^n \frac{1}{(1-i\sigma)^2(1+\sigma^2)} \frac{\tau^5}{(1+\tau)^4(2-\tau)} F_1(2-\tau;\, 3-n,\, 1+n;\, 3-\tau;\, x,\, y) \,, \tag{10}$$

$$T(\Omega) = \frac{128}{[2\pi(1-e^{-2\pi|n|})]^{1/2}} \left(\frac{1-i\sigma}{1+i\sigma}\right)^n \frac{(n+1)(n+2)\sigma^2\tau^4}{(1+\sigma^2)^3(1+\tau)^4}$$
$$\times \left[\frac{1}{2-\tau} F_1(2-\tau;\, 3-n,\, 3+n;\, 3-\tau;\, x,\, y) - \left(\frac{1-\tau}{1+\tau}\right)^2 \frac{1}{4-\tau} F_1(4-\tau;\, 3-n,\, 3+n;\, 5-\tau;\, x,\, y)\right] , \tag{11}$$

where F_1 is one of the Appell functions.[2] We have abbreviated here

$$\sigma = p/X \,. \tag{12}$$

Using this and Eq. (19) of I, the variables x, y given by Eq. (80) of I can be written

$$x = (1-\tau)(1+i\sigma)/(1+\tau)(1-i\sigma) \,,$$
$$y = (1-\tau)(1-i\sigma)/(1+\tau)(1+i\sigma) \,. \tag{13}$$

The energy-conservation equation (21) of I becomes now

$$(p/\lambda)^2 = k_1 - k_2 - 1 \,. \tag{14}$$

From here it follows that the range of variation of k_2 is $0 \leq k_2 \leq k_1 - 1$. Equation (14) yields also

$$n = \lambda/ip = -i(k_1 - k_2 - 1)^{-1/2} \,. \tag{15}$$

II. METHOD OF EVALUATION

As mentioned before, we want to carry out the numerical evaluation of the Appell functions F_1 by series summation. To this end we need to know the position of the complex variables x, y in their respective planes and how it depends on k_1, k_2. This will allow us to choose the right analytic continuation of the F_1 functions, in terms of convergent series. Now, the variables x, y behave quite differently in the two cases required Ω_1, Ω_2 [see Eq. (9) of I]. We shall therefore consider them separately.

Let us begin with the *evaluation of* $P(\Omega_1)$, $T(\Omega_1)$. In this case, from Eqs. (19) and (22) of I and Eq. (12) and (14) we get

$$\tau_1 = \frac{i}{(k_1-1)^{+1/2}} \,, \quad \sigma_1 = i\left(\frac{k_1 - k_2 - 1}{k_1 - 1}\right)^{1/2} \,. \tag{16}$$

Denoting by x_1, y_1 the values of the variables Eq. (13) corresponding to this case, one easily finds that

$$|y_1| = 1/|x_1| \,, \quad \arg y_1 = \arg x_1 \,. \tag{17}$$

Moreover, since k_2 varies in the interval $0 \leq k_2 \leq k_1 - 1$, we have $0 \leq |x_1| \leq 1$, and therefore $\infty > |y_1| \geq 1$. We also have $-\pi \leq \arg x_1 < 0$.

The formula of analytic continuation we need in the present case is[3]

$$F_1(a;\, b_1,\, b_2;\, c;\, x,\, y) = \frac{\Gamma(c)\Gamma(b_2-a)}{\Gamma(b_2)\Gamma(c-a)} (-y)^{-a} F_1\left(a;\, b_1,\, 1+a-c;\, a-b_2+1;\, \frac{x}{y} \,,\, \frac{1}{y}\right)$$
$$+ \frac{\Gamma(c)\Gamma(a-b_2)}{\Gamma(a)\Gamma(c-b_2)} (-y)^{-b_2} G_2\left(b_1,\, b_2;\, 1+b_2-c,\, a-b_2;\, -x,\, -\frac{1}{y}\right) . \tag{18}$$

This contains the function $G_2(a_1, a_2; b_1, b_2; x_1, x_2)$ which also belongs to the class of hypergeometric functions of two variables. Equation (18) is valid provided that $b_2 - a$ is not an integer, and the principal branch of the complex powers of $(-y)$ is taken ($|\arg(-y)| < \pi$).

On account of what has been said for x_1, y_1 the variables x_1/y_1, $1/y_1$, $-x_1$, $-1/y_1$ occurring on the right-hand side of Eq. (18) are smaller in modulus than 1. In this case the corresponding functions F_1 and G_2 can be expanded in convergent double series of their variables. In fact, as we shall presently see, no double series expansion is needed for F_1 because it reduces in our case to a simpler form.

In what concerns the function G_2, when $|x_1| < 1$, $|x_2| < 1$ this admits the following expansion[4]:

$$G_2(a_1, a_2; b_1, b_2; x_1, x_2)$$
$$= \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} (a_1)_m (a_2)_n (b_1)_{n-m} (b_2)_{m-n} \frac{x_1^m}{m!} \frac{x_2^n}{n!} \,. \tag{19}$$

As usual, we have denoted $(a)_p = \Gamma(a+p)/\Gamma(a)$, which holds for $p \gtrless 0$. We shall transform Eq. (19), taking into account that the coefficients occurring in it can be written

$$(b_1)_{n-m} = (-1)^m (b_1 - m)_n / (1 - b_1)_m , \tag{20}$$

$$(b_2)_{m-n} = (-1)^n (b_2)_m / (1 - b_2 - m)_n . \tag{21}$$

Inserting these into Eq. (19), the sum over n can be recognized to be a ${}_2F_1$ function and one finds[5]

$$G_2(a_1, a_2; b_1, b_2; x_1, x_2) = \sum_{m=0}^{\infty} \frac{(a_1)_m (b_2)_m}{(1-b_1)_m} \frac{(-x_1)^m}{m!} \times {}_2F_1(a_2, b_1 - m, 1 - b_2 - m; -x_2) . \tag{22}$$

Equations (10) and (11) show that the Appell functions we need are of the following form:

$$F(\alpha, \beta, \gamma) \equiv F_1(\alpha - \tau; \beta - n, \gamma + n; \alpha + 1 - \tau; x, y) , \tag{23}$$

with α, β, γ positive integers. In the case we are now considering $\tau = \tau_1$, $x = x_1$, $y = y_1$.

Transforming Eq. (23) according to Eq. (18) one gets on the right-hand side the function

$$F_1\left(\alpha - \tau_1; \beta - n, 0; \alpha - \gamma + 1 - n - \tau_1; \frac{x_1}{y_1}, \frac{1}{y_1}\right) = {}_2F_1\left(\alpha - \tau_1, \beta - n, \alpha - \gamma + 1 - n - \tau_1; \frac{x_1}{y_1}\right) . \tag{24}$$

This equality follows readily from the integral representation Eq. (47) of I. Therefore we have

$$F(\alpha, \beta, \gamma) = \frac{\Gamma(\alpha + 1 - \tau_1)\,\Gamma(\gamma - \alpha + n + \tau_1)}{\Gamma(\gamma + n)} (-y_1)^{\tau_1 - \alpha} {}_2F_1 + \frac{\alpha - \tau_1}{\alpha - \gamma - n - \tau_1} (-y_1)^{-\gamma - n} G_2 , \tag{25}$$

where ${}_2F_1$ stands for the Gauss function appearing in Eq. (24) and

$$G_2 \equiv G_2(\beta - n, \quad \gamma + n; \quad \gamma - \alpha + n + \tau_1, \quad \alpha - \gamma - \tau_1 - n; \quad -x_1, -1/y_1) . \tag{26}$$

The series expansion in powers of (x_1/y_1) of the ${}_2F_1$ function in Eq. (24) is rapidly convergent and very convenient for numerical computation. Further, by expanding Eq. (26) according to Eq. (22) one gets

$$G_2 = (\alpha - \gamma - \tau_1 - n) \sum_{r=0}^{\infty} \frac{(\beta - n)_r}{(\alpha - \gamma - \tau_1 - n + r) r!} b_r x_1^r , \tag{27}$$

where

$$b_r = {}_2F_1(\gamma + n, \ \gamma - \alpha + n + \tau_1 - r, \ 1 - \alpha + \gamma + \tau_1 + n - r; \ 1/y_1) . \tag{28}$$

The coefficients b_r can be calculated from the recurrence relation[6,7]

$$b_r = \left(\frac{1 - \alpha + \tau_1 - r}{1 - \alpha + \gamma + n + \tau_1 - r} \frac{1}{y_1} + 1\right) b_{r-1} - \frac{2 - \alpha + \tau_1 - r}{2 - \alpha + \gamma + n + \tau_1 - r} \frac{1}{y_1} b_{r-2} \tag{29}$$

once b_0, b_1 have been determined from the series expansion Eq. (28). For k_2 approaching $k_1 - 1$, when $|x_1|$, $|y_1|$ approach 1, the convergence of the series Eqs. (27) and (28) becomes poor and the summation time consuming. Because of that, the largest value of k_2 we have considered was $k_2 = 0.98(k_1 - 1)$ and a different procedure was needed to evaluate the case $k_2 = k_1 - 1$.

Let us now describe the *evaluation* of $P(\Omega_2)$, $T(\Omega_2)$. From Eqs. (19) and (22) of I and Eqs. (12) and (14) it follows that

$$\tau_2 = \frac{1}{(k_2 + 1)^{+1/2}} , \qquad \sigma_2 = \left(\frac{k_1 - k_2 - 1}{k_2 + 1}\right)^{1/2} . \tag{30}$$

Further, Eq. (13) shows that in the present case the variables x_2, y_2 have the properties

$$|x_2| = |y_2| < 1, \quad y_2^* = x_2 . \tag{31}$$

The fact that x_2, y_2 are in the unit circle centered at the origin makes the evaluation of the Appell functions F_1 straightforward. One can use their double series expansion, which we shall write in the form[8]

$$F_1(a; b_1, b_2; c; x, y) = \sum_{p=0}^{\infty} \frac{(a)_p (b_1)_p}{(c)_p} \frac{x^p}{p!} {}_2F_1(a + p, \ b_2, \ c + p; y). \tag{32}$$

The ${}_2F_1$ functions occurring here can be determined from their series expansion about the origin.[7]

The functions F_1 needed are again of the type considered in Eq. (23), this time with $\tau = \tau_2$, $x = x_2$, $y = y_2$.

The methods we have outlined enable the computation of the scattering amplitudes Eq. (3) over nearly the whole spectrum of k_2.

III. LOW- AND HIGH-ENERGY ENDS OF SPECTRUM

The two ends of the scattered photon spectrum, $k_2 = 0$ and $k_2 = k_1 - 1$, should be given special attention. For $k_2 = 0$ we know from the general case with retardation that one of the amplitudes is singular [see Paper I, Sec. IV]. For $k_2 = k_1 - 1$ the quantity n appearing in the parameters of the Appell functions of Eqs. (10) and (11) tends to infinity [see Eq. (15)].

Obviously, in order to obtain the limit $k_2 \to 0$ of the scattering amplitudes we have to take the dipole approximation of the results derived in I, Sec. IV. From Eqs. (63)–(71) of I and the redefinition implied by Eq. (1), we get the following dominant behavior:

$$P_0(\Omega_1) \simeq -4[2\pi(1-e^{-2\pi|n|})]^{-1/2} \times n^5(n-1)^{-3}(n+1)^{-1}\left(\frac{n-1}{n+1}\right)^n , \tag{33}$$

$$T_0(\Omega_1) \simeq (2/k_2)(1-n)n^{-3}P_0(\Omega_1) , \tag{34}$$

$$P_0(\Omega_2) \simeq -n^{-1}P_0(\Omega_1) , \tag{35}$$

$$T_0(\Omega_2) \simeq 2(2+n)n^{-1}(n+1)^{-1}P_0(\Omega_1) . \tag{36}$$

$T_0(\Omega_1)$ again displays the $1/k_2$ singularity for $k_2 \to 0$, characteristic of the infrared divergence.

In order to treat the limit $k_2 \to k_1 - 1$ (or $p \to 0$), we shall consider the general form of our F_1 functions, given in Eq. (23). This we shall transform according to[9]

$$F(\alpha,\beta,\gamma) = (1-y)^{-\alpha+\tau} F_1\left(\alpha-\tau;\ \alpha+1-\beta-\gamma-\tau,\ \beta-n;\ \alpha+1-\tau;\ \frac{y}{y-1},\ \frac{y-x}{y-1}\right). \tag{37}$$

Now

$$\frac{y-x}{y-1} = \frac{2(1-\tau)}{(1+n)(1-i\sigma)} , \tag{38}$$

$$\frac{y}{(y-1)} = \frac{n(\tau-1)(1-i\sigma)}{2\tau(1+n)} . \tag{39}$$

For $p \to 0$ ($|n| \to \infty$) the dominant behavior of Eqs. (38) and (39) is

$$(y-x)/(y-1) \simeq 2(1-\tau)/n \to 0 , \tag{40}$$

$$y/(y-1) \simeq (\tau-1)/2\tau . \tag{41}$$

Equations (38)–(41) hold for both cases X_1 and X_2.

While the variable Eq. (40) tends to zero, the parameter $\beta - n \simeq -n$ of F_1 in Eq. (37) tends to infinity. This is a case of "confluence" for the Appell function F_1, taking place according to the general formula

$$\lim_{\epsilon\to 0} F_1(a;\ b,\ 1/\epsilon;\ c;\ \xi,\ \epsilon\eta) = \phi_1(a,\ b,\ c;\ \xi,\ \eta) . \tag{42}$$

The limit ϕ_1 is one of the confluent hypergeometric functions of two variables introduced by Humbert.[10] In our case, on account of Eqs. (40) and (41) we have to take[11]

$$\epsilon = -(1/n) , \quad \xi = (\tau-1)/2\tau, \quad \eta = 2(\tau-1) . \tag{43}$$

It then follows from Eqs. (37) and (42)

$$\lim_{p\to 0} F(\alpha,\beta,\gamma) = [2\tau/(1+\tau)]^{\tau-\alpha} \times \phi_1(\alpha-\tau,\ \alpha+1-\beta-\gamma-\tau,\ \alpha+1-\tau;\ \xi,\ \eta) . \tag{44}$$

Returning now to Eqs. (10) and (11) these contain the factor

$$[(1-i\sigma)/(1+i\sigma)]^n = [(1-\epsilon\tau)/(1+\epsilon\tau)]^{1/\epsilon} .$$

The limit of this factor for $p \to 0$ ($\epsilon \to 0$) is $e^{-2\tau}$. With this and Eq. (44) we find the following limits for Eqs. (10) and (11):

$$P_m(\Omega) = \frac{16}{(2\pi)^{1/2}} e^{-2\tau}\left(\frac{2\tau}{1+\tau}\right)^\tau \frac{\tau^3}{(1+\tau)^2(2-\tau)} \times \phi_1(2-\tau,\ -1-\tau,\ 3-\tau;\ \xi,\ \eta) , \tag{45}$$

$$T_m(\Omega) = \frac{32}{(2\pi)^{1/2}} e^{-2\tau}\left(\frac{2\tau}{1+\tau}\right)^\tau \frac{\tau^4}{(1+\tau)^2} \times\left(\frac{(1-\tau)^2}{4\tau^2(4-\tau)}\ \phi_1(4-\tau,\ -1-\tau,\ 5-\tau;\ \xi,\ \eta) - \frac{1}{2-\tau}\ \phi_1(2-\tau,\ -3-\tau,\ 3-\tau;\ \xi,\ \eta)\right) , \tag{46}$$

with ξ, η given by Eq. (43).

For the evaluation of the functions ϕ_1 we start from the expansion[10]

$$\phi_1(a,\ b,\ c;\ \xi,\ \eta) = \sum_{r=0}^{\infty} \frac{(a)_r}{(c)_r}\ \frac{\eta^r}{r!}\ {}_2F_1(a+r,\ b,\ c+r;\ \xi) , \tag{47}$$

which holds for any ξ, η.[7] This we shall use in the modified form

$$\phi_1(a,\ b,\ c;\ \xi,\ \eta) = (1-\xi)^{-b} \times \sum_{r=0}^{\infty} \frac{(a)_r}{(c)_r}\ \frac{\eta^r}{r!}\ {}_2F_1(c-a,\ b,\ c+r;\ \xi)/(\xi-1) . \tag{48}$$

In the *case of* $P_m(\Omega_1)$, $T_m(\Omega_1)$, τ is given by Eq. (16) and the variables ξ_1, η_1 are complex. We have

$$\xi_1/(\xi_1-1)=(1-\tau_1)/(1+\tau_1),\quad \eta_1=2(\tau_1-1)\,, \tag{49}$$

and therefore

$$|\xi_1/(\xi_1-1)|=1,\quad |\eta_1|>2\,.$$

Thus, the variable of ${}_2F_1$ in Eq. (48) is situated right on the circle of convergence of its series expansion about the origin. Nevertheless, because a certain condition concerning its parameters is fulfilled, the series expansion is still absolutely convergent.[12] Consequently, it can be used for the computation of ${}_2F_1$.

In the *case of* $P_m(\Omega_2)$, $T_m(\Omega_2)$, τ is given by Eq. (30), which now becomes

$$\tau_2 = k_1^{-1/2}\,. \tag{50}$$

The corresponding variables ξ_2, η_2 are real and satisfy the inequalities

$$0<\xi_2/(\xi_2-1)<1,\quad -2<\eta_2<0.$$

Therefore we can again evaluate the ${}_2F_1$ functions of Eq. (48) by summing their series expansions. Note that $P_m(\Omega_2)$ and $T_m(\Omega_2)$ are real.

IV. RESULTS OF COMPUTATION AND DISCUSSION

With retardation included, the differential cross section $d^2\sigma/d\kappa_2 d\Omega_2$ of Eq. (83) of I has a complicated angular dependence which is intricately connected to the dependence on κ_1, κ_2, and Z. However, in the dipole approximation the angular dependence reduces to the simple expression given in Eq. (6). Moreover, the dependence of the coefficients C_1 and C_2 on κ_1, κ_2, Z is concentrated in the two dimensionless variables k_1, k_2 given by Eq. (4). Their range of variation is: $k_1>1$ and $0\leq k_2\leq k_1-1$. However, instead of k_2 we shall use in the following ξ, defined as

$$\xi = k_2/(k_1-1)\,. \tag{51}$$

This has the property that it varies in the interval $0\leq\xi\leq 1$, whatever the value of k_1.

We shall now comment on the computation. First we have computed the quantities $P(\Omega_1)$, $T(\Omega_1)$, $P(\Omega_2)$, $T(\Omega_2)$ according to the methods described in Secs. II and III and then the coefficients C_1, C_2 from Eqs. (3), (7), and (8).

Since we are working here in the nonrelativistic dipole approximation, the validity of the results is restricted by the conditions that $\alpha Z \ll 1$ and $\kappa_1 \ll \lambda$ or $k_1 \ll 2/\alpha Z$. Therefore we have considered only low values of k_1, extending from 1.05 to 20. For every k_1 we have computed the coefficients C_1, C_2 for a number of values of ξ extending from $\xi=0.001$ to $\xi=1.0$. The series involved were summed with a relative error smaller than 10^{-5}; this is the error also for C_1, C_2. The computational errors are therefore much smaller than the corrections of a physical nature affecting the result (retardation, relativity and screening).

A number of tests were carried out to check the computation. First, in order to check the values for $P(\Omega_1)$, $T(\Omega_1)$, $P(\Omega_2)$, $T(\Omega_2)$, the alternative expansion of the Appell functions

$$F_1(a;b_1,b_2;c;x_1,x_2)=(1-x_0)^{c-a-b_1-b_2}\times\sum_{n=0}^{\infty}\frac{(a)_n}{(c)_n}\,{}_2F_1(c-a,c-b_1-b_2,c+n;x_0)\times\sum_{r=0}^{\infty}\frac{(b_1)_r(b_2)_{n-r}}{r!(n-r)!}\left(\frac{x_1-x_0}{1-x_0}\right)^r\left(\frac{x_2-x_0}{1-x_0}\right)^{n-r} \tag{52}$$

was used. This is the Taylor expansion of F_1 about the points $x_1=x_2=x_0$[13]; it is convergent if

$$\frac{|x_1-x_0|}{|1-x_0|}<1 \quad\text{and}\quad \frac{|x_2-x_0|}{|1-x_0|}<1\,.$$

For our purposes we have taken $x_0=(1-\tau)/(1+\tau)$ with τ equal to τ_1 or τ_2, as needed. For any k_1 the convergence conditions are fulfilled only if ξ is situated in the neighborhood of 1. The numerical results obtained in this way for the scattering amplitudes agree with the ones of the main computation within the relative error of 10^{-5}.

Secondly, the main program for $P(\Omega_1)$, $T(\Omega_1)$, $P(\Omega_2)$, $T(\Omega_2)$ was applied to the case of the very small value $k_2=10^{-6}$ and several values of k_1. The results were compared with those one obtains from the exact formulas for $k_2=0$ given by Eqs. (49)–(52). It was found that the former agree with the latter to a large number of digits.

Finally, the alternative expansion of the ϕ_1 function[10]

$$\phi_1(a,b,c;\xi,\eta)=\sum_{r=0}^{\infty}\frac{(a)_r(b)_r}{(c)_r}\,\frac{\xi^r}{r!}\,{}_1F_1(a+r,c+r;\eta) \tag{53}$$

was used to check the results for $P_m(\Omega_1)$, $T_m(\Omega_1)$, $P_m(\Omega_2)$, $T_m(\Omega_2)$. This holds for $|\xi|<1$ and any η. With ξ, η given by Eqs. (43), (16), and (50) the expansion is convergent for sufficiently small k_1. In this range the results thus obtained agreed within the relative error of 10^{-5} with the ones one gets from Eqs. (45) and (46).

We give in Table I examples of the variation of the quantities $P(\Omega_1)$, $T(\Omega_1)$, $P(\Omega_2)$, $T(\Omega_2)$. The values for $\xi=0$ were obtained from Eqs. (33)–(36), the values for $\xi=1$ from Eqs. (45)–(48), and the rest of the values by applying the methods described in Sec. II. Notice that for smaller values k_1, like $k_1=2$, the quantities listed in Table I, with the exception of $\mathrm{Im}P_1$, are monotonically increasing or decreasing functions of ξ. However, when k_1 becomes larger (see the illustrative example of $k_1=10$) only $\mathrm{Re}P_1$, $\mathrm{Re}P_2$, $\mathrm{Re}T_1$, retain their monotonical variation, the rest of the quantities presenting maxima and minima.

TABLE I. Typical behavior of scattering amplitudes.

ξ	ReP_1	ImP_1	ReP_2	ImP_2	ReT_1	ImT_1	ReT_2	ImT_2
				$k_1=2$				
0.000	−0.0830	0.0000	0.0000	0.0830			0.0830	−0.2490
0.001	−0.0831	−0.0001	0.0000	0.0830	−165.4727	166.7403	0.0828	−0.2490
0.100	−0.0905	−0.0047	0.0063	0.0827	−1.4308	2.0110	0.0698	−0.2483
0.200	−0.0971	−0.0068	0.0129	0.0826	−0.6190	1.1328	0.0554	−0.2479
0.300	−0.1044	−0.0078	0.0200	0.0824	−0.3415	0.8288	0.0394	−0.2473
0.400	−0.1125	−0.0077	0.0279	0.0819	−0.1935	0.6698	0.0211	−0.2458
0.500	−0.1217	−0.0064	0.0367	0.0809	−0.0944	0.5675	0.0000	−0.2427
0.600	−0.1325	−0.0034	0.0468	0.0788	−0.0167	0.4909	−0.0249	−0.2364
0.700	−0.1452	0.0022	0.0587	0.0749	0.0517	0.4244	−0.0547	−0.2248
0.800	−0.1604	0.0125	0.0727	0.0677	0.1185	0.3556	−0.0909	−0.2033
0.900	−0.1792	0.0320	0.0897	0.0536	0.1895	0.2665	−0.1356	−0.1608
0.980	−0.1982	0.0691	0.1061	0.0264	0.2549	0.1351	−0.1794	−0.0793
1.000	−0.2052	0.1063	0.1106	0.0000	0.2777	0.0190	−0.1917	0.0000
				$k_1=10$				
0.000	−0.00148	−0.00197	−0.00592	0.00444			0.02519	−0.01334
0.001	−0.00148	−0.00198	−0.00590	0.00444	−14.82640	4.96679	0.02515	−0.01332
0.100	−0.00161	−0.00241	−0.00432	0.00427	−0.15652	0.06575	0.02282	−0.01282
0.200	−0.00176	−0.00285	−0.00360	0.00445	−0.08315	0.04080	0.02224	−0.01336
0.300	−0.00195	−0.00336	−0.00312	0.00481	−0.05902	0.03320	0.02223	−0.01443
0.400	−0.00222	−0.00397	−0.00270	0.00533	−0.04713	0.03031	0.02248	−0.01599
0.500	−0.00262	−0.00474	−0.00226	0.00605	−0.04003	0.02969	0.02281	−0.01814
0.600	−0.00324	−0.00575	−0.00168	0.00704	−0.03506	0.03070	0.02301	−0.02113
0.700	−0.00432	−0.00712	−0.00072	0.00844	−0.03071	0.03334	0.02262	−0.02534
0.800	−0.00642	−0.00905	0.00116	0.01048	−0.02505	0.03799	0.02030	−0.03143
0.900	−0.01150	−0.01149	0.00588	0.01319	−0.01273	0.04445	0.01112	−0.03957
0.980	−0.02375	−0.00943	0.01765	0.01176	0.01885	0.03771	−0.01774	−0.03528
1.000	−0.03043	0.00306	0.02416	0.00000	0.03694	0.00006	−0.03501	0.00000

Table II contains some of our results for the coefficients C_1, C_2.[14] In most cases the accuracy of the computation is higher than is reported. We have omitted the last digits of the results without rounding off.

It is apparent from Table II that the coefficients C_1, C_2 are monotonically decreasing functions of ξ. This happens although they are constructed from quantities which do not all have this type of behavior, as was shown in Table I. C_1 is always larger than C_2. This was to be expected from the comparison of Eqs. (7) and (8). For small values of ξ (e.g., $\xi = 0.001$) one notices that $C_1 \simeq 3C_2$. Again, this was to be expected from Eqs. (7) and (8) and the fact that for small ξ the amplitude E is the dominant one. For larger k_1 (e.g., $k_1 > 5$) and ξ in the vicinity of 1, Table II shows that C_1 and C_2 become nearly equal.

The spectral distribution yielded by Eq. (6) is itself a decreasing function of ξ, for any scattering angle θ. This is peculiar to the dipole approximation and does not remain true at higher energies k_1. The most important retardation corrections come from the term $\mathcal{O}$ contained in the amplitude $\mathcal{A}$ of the exact matrix element [see Eqs. (14) and (15) of I]. In order to have a better idea of the validity of our results we have calculated the corrections given by this term. To lowest order in the photon momentum transfer $\vec{q} = \vec{\kappa}_1 - \vec{\kappa}_2$ (which is sufficient at the low energies we are considering), $\mathcal{O}$ of Eq. (23) of I becomes proportional to $\vec{p} \cdot \vec{q}$. Then C_1 and C_2 of Eq. (6) are replaced by the angle dependent quantities: $C_i' = C_i + (q^2/\lambda^2)D$ ($i = 1, 2$), where D is a function of p/λ.

The evaluation of the corrective term $(q^2/\lambda^2)D$ shows that it is an increasing function of ξ and that the increase is faster at large scattering angles θ. Besides, its magnitude at $\xi = 1$ is rapidly increasing with k_1. Now, it happens that even when the dipole approximation condition $(\kappa_1/\lambda) \ll 1$ [and therefore $(q/\lambda) \ll 1$] is satisfied, the retardation correction term $(q^2/\lambda^2)D$ may become comparable or larger than C_1, C_2 for $\xi = 1$. For $Z = 1$ this is already the case for $k_1 \simeq 10$, and for larger Z this happens for even lower k_1. However, this occurs only when ξ is close to 1, because for smaller ξ, C_1 and C_2 always dominate $(q^2/\lambda^2)D$. Therefore, at higher energies k_1, for a complete treatment of the $\xi = 1$ end of the spectrum one should take into account also the retardation corrections due to $\mathcal{O}$. However, in order to do this consistently some other corrective terms contained

TABLE II. Values of coefficients C_1, C_2 occurring in the cross section Eq. (6).

ξ	C_1	C_2	C_1	C_2	C_1	C_2	C_1	C_2	C_1	C_2
$k_1=$	1.05		1.50		2		2.50		3	
0.001	827.4431	276.2723	311.2638	103.9274	138.5295	46.2534	72.96382	24.36181	42.87451	14.31532
0.100	11.3240	4.2578	3.2131	1.2454	1.3603	0.5293	0.70038	0.27270	0.40608	0.15800
0.200	6.7518	2.7436	1.6314	0.7182	0.6654	0.2965	0.33667	0.15034	0.19321	0.08614
0.300	5.0939	2.1968	1.0975	0.5398	0.4343	0.2184	0.21653	0.10936	0.12316	0.06208
0.400	4.2021	1.9036	0.8283	0.4494	0.3195	0.1791	0.15723	0.08881	0.08868	0.05002
0.500	3.6314	1.7163	0.6660	0.3945	0.2513	0.1555	0.12222	0.07646	0.06835	0.04277
0.600	3.2285	1.5842	0.5577	0.3575	0.2065	0.1397	0.09932	0.06823	0.05509	0.03795
0.700	2.9254	1.4850	0.4805	0.3309	0.1751	0.1284	0.08335	0.06237	0.04585	0.03452
0.800	2.6871	1.4069	0.4230	0.3108	0.1521	0.1199	0.07171	0.05799	0.03913	0.03197
0.900	2.4938	1.3436	0.3786	0.2951	0.1346	0.1134	0.06298	0.05461	0.03413	0.03000
1.000	2.3329	1.2909	0.3436	0.2825	0.1212	0.1082	0.05633	0.05194	0.03034	0.02845
$k_1=$	4		5		6		7		8	
0.001	18.28532	6.10526	9.34406	3.11987	5.36524	1.79139	3.34245	1.11600	2.21183	0.73850
0.100	0.17057	0.06618	0.08645	0.03343	0.04938	0.01903	0.03066	0.01178	0.02024	0.00775
0.200	0.08024	0.03552	0.04042	0.01774	0.02301	0.01002	0.01425	0.00615	0.00940	0.00403
0.300	0.05061	0.02525	0.02534	0.01248	0.01437	0.00699	0.00888	0.00427	0.00584	0.00277
0.400	0.03605	0.02009	0.01792	0.00984	0.01011	0.00547	0.00622	0.00331	0.00408	0.00214
0.500	0.02746	0.01699	0.01354	0.00825	0.00759	0.00455	0.00465	0.00274	0.00304	0.00176
0.600	0.02185	0.01493	0.01067	0.00719	0.00594	0.00394	0.00361	0.00236	0.00235	0.00151
0.700	0.01794	0.01347	0.00867	0.00644	0.00478	0.00350	0.00288	0.00208	0.00186	0.00133
0.800	0.01511	0.01238	0.00721	0.00588	0.00393	0.00318	0.00235	0.00188	0.00150	0.00119
0.900	0.01300	0.01155	0.00613	0.00546	0.00330	0.00294	0.00195	0.00173	0.00124	0.00109
1.000	0.01143	0.01091	0.00534	0.00513	0.00285	0.00275	0.00167	0.00162	0.00104	0.00102
$k_1=$	9		10		15		20			
0.001	1.53333	0.51196	1.10300	0.36827	0.306180	0.102229	0.121809	0.040670		
0.100	0.01401	0.00535	0.01007	0.00383	0.002790	0.001050	0.001110	0.000414		
0.200	0.00650	0.00276	0.00466	0.00197	0.001292	0.000533	0.000514	0.000208		
0.300	0.00403	0.00190	0.00289	0.00135	0.000798	0.000359	0.000317	0.000139		
0.400	0.00281	0.00146	0.00201	0.00103	0.000553	0.000271	0.000219	0.000104		
0.500	0.00208	0.00119	0.00149	0.00084	0.000405	0.000217	0.000160	0.000082		
0.600	0.00160	0.00101	0.00114	0.00071	0.000307	0.000181	0.000120	0.000068		
0.700	0.00126	0.00089	0.00089	0.00062	0.000236	0.000155	0.000091	0.000057		
0.800	0.00101	0.00079	0.00071	0.00055	0.000182	0.000135	0.000069	0.000049		
0.900	0.00082	0.00072	0.00057	0.00050	0.000142	0.000121	0.000052	0.000043		
1.000	0.00069	0.00067	0.00047	0.00046	0.000113	0.000111	0.000040	0.000039		

in the matrix element $\mathfrak{M}$ of Eqs. (14), (15), and (48)–(52) of I should also be considered. Since the contribution of $\mathcal{O}$ is dominant, it is to be expected that the overall effect of these corrections will be to enhance the cross section in the vicinity of $\xi = 1$, over the value predicted by the dipole approximation.

For the time being, in the low-energy range considered here, there are no other theoretical results for comparison. However, a number of experiments were carried out with light elements ($Z \leq 6$) at low energies, studying the spectral distribution in the vicinity of $\xi = 1$. These were briefly described in I, Sec. I. The experimental conditions were such that $(\kappa_1/\lambda) \geq 0.4$ and therefore the dipole approximation is not fully applicable. From this and the fact that ξ was in the vicinity of 1, it follows that in order to compare with these experiments one would have to take into account also the retardation corrections mentioned above.[15]

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[1]M. Gavrila, preceding paper, Phys. Rev. A 6, 1348 (1972), hereafter denoted by I. We are using the same notations as in I.

[2]See P. Appell and J. Kampé de Fériet, *Fonctions Hypergéométriques et Hypersphériques* (Gauthier-Villars, Paris, 1926).

[3]P. O. M. Olsson, J. Math. Phys. 5, 420 (1964), Eq. (17).

[4]Reference 3, Eq. (4).

[5]It can be shown that this holds for $|x_1| < 1$, whatever x_2. Equation (22) represents the analytic continuation of G_2 defined by Eq. (19) outside the unit circle $|x_2| < |$ of the x_2 complex plane.

[6]This is obtained by combining Eq. (30), p. 103 with Eq. (3), p. 105 of A. Erdelyi *et al.*, *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), Vol. I, and inserting the adequate values of the parameters.

[7]The numerical calculation of ${}_2F_1(a+m, b, c+m; x)$, for varying integer m, from the recurrence relation between contiguous functions must be carried out carefully. The situation depends critically on whether the variable x is larger or smaller in modulus than 1. For $|x| < 1$, when one uses the recurrence relation to *raise* the value of m, this has the tendency of amplifying the inevitable numerical errors on the initial conditions for $m = 0, 1$, yielding eventually absurd results for large m. No difficulties arise if one takes as initial conditions the values of ${}_2F_1$ for some convenient m and one uses the recurrence relation to *lower* the m, because then it has the tendency of damping off the initial errors. [This is also the case of Eqs. (28) and (29), where m decreases from zero through negative integers.] The situation is opposite for $|x| > 1$. The author thanks Dr. L. Maximon for an illuminating discussion on this point.

[8]Reference 2, p. 15, Eq. (15).

[9]We have used Eq. (5_4), p. 30, Ref. 2, combined with the invariance of $F_1(a; b_1, b_2; c; x_1, x_2)$ to the simultaneous interchange of b_1, b_2 and x_1, x_2.

[10]See Ref. 2, p. 124, Eq. (IV); p. 126, case 1; p. 127, Eq. (12).

[11]Our situation is somewhat more complicated than that given in Eq. (42), because ξ and η which appear on its left-hand side are ϵ dependent. Nevertheless, these quantities have finite limits for $\epsilon \to 0$ and it is these limits which should stand on the right-hand side of Eq. (42). This was actually done when writing Eq. (43).

[12]See Sec. 2.1.1. of Ref. 6, where the condition is stated as $\mathrm{Re}(a+b-c) < 0$.

[13]It is obtained by combining the Taylor-expansion formula with Eq. (19), p. 19 and Eq. (25), p. 23 of Ref. 2.

[14]The complete results will be published elsewhere.

[15]Besides, in order to compare our results with experiment they should be corrected for screening.

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Dielectric Model of Diatomic Molecules

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A dielectric model of diatomic molecules has been used to calculate the ground-state force constant and the dipole moment. An attempt is made to use atomic parameters only, but the calculations show that this is not possible with the model. Good agreement with experiment is obtained when one molecular parameter is adjusted, e.g., the position of the bond charge.

I. INTRODUCTION

There has recently been considerable interest in describing diatomic molecules in an approximate but simple way. Such approximations may either be of a computational nature, neglecting certain types of terms which one believes to be unimportant, as in the complete neglect of differen-