

Elastic Scattering of Photons by a Hydrogen Atom

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An exact analytic expression is derived for the Kramers-Heisenberg matrix element describing the elastic scattering of photons by a hydrogen atom in the dipole approximation. The method followed consists in writing the matrix element in terms of the Coulomb-field Green's function in momentum space and using for this an integral representation originally derived by Schwinger. Various integrations then yield the matrix element in terms of a hypergeometric function of the Gauss type ${}_2F_1$ with parameters and variable depending on the photon energy. Different limiting cases are considered. Finally, a very accurate numerical computation of the result is reported. The procedure used in the computation was to sum the series expansions of the hypergeometric functions occurring in the different equivalent conveniently chosen forms of the matrix element. The results presented cover all values of the photon energy.

I. MATRIX ELEMENT

LOW-ENERGY elastic scattering of photons by atoms is dominated by Rayleigh scattering from bound atomic electrons. The differential cross section for this process is given by¹

$$d\sigma = r_0^2 |\mathfrak{M}|^2 d\Omega, \quad (1)$$

where $r_0 = e^2/m^2$ and \mathfrak{M} is the Kramers-Heisenberg matrix element³ equal in the case of a single atomic electron and the dipole approximation to

$$\mathfrak{M} = \mathbf{s} \cdot \mathbf{s}'$$

$$-m^{-1} \mathbf{S} \left[\frac{(\mathbf{s}' \cdot \mathbf{P})_{0n} (\mathbf{s} \cdot \mathbf{P})_{n0}}{E_n - (E_0 + \omega + i\epsilon)} + \frac{(\mathbf{s} \cdot \mathbf{P})_{0n} (\mathbf{s}' \cdot \mathbf{P})_{n0}}{E_n - (E_0 - \omega)} \right]. \quad (2)$$

Here ω denotes the energy of the elastically scattered photon, \mathbf{s} and \mathbf{s}' are its initial and final polarizations, \mathbf{P} is the momentum operator, E_n are the energy eigenvalues of the hydrogen atom and E_0 is the energy of the ground state. The infinitesimal positive quantity ϵ prevents the occurrence of a singularity when $\omega > |E_0|$.

In spite of its considerable age, there have been few attempts to evaluate the Kramers-Heisenberg matrix element, even in the simplest case of a hydrogen atom. Thus for values $\omega \ll |E_0|$, Podolsky and later Dalgarno and Kingston⁴ have calculated the first terms of the expansion of \mathfrak{M} in powers of ω . Mittleman and Wolf,⁵ following a method of Schwartz, have given an evaluation of \mathfrak{M} for values of ω up to the first resonance $\omega < \frac{3}{4}|E_0|$. More recently, Constantinescu and the

author⁶ have evaluated the matrix element for all values of ω by an approximate method.

In the present work we shall first derive an exact analytic formula for the Kramers-Heisenberg matrix element by means of expressing it in terms of the Green's function for the Coulomb field. This has received considerable attention lately. Integral representations have been given for it and even its closed form expression has been found by Hostler and Pratt.⁷ We shall write the matrix element (2) in terms of the Fourier transform of the Green's function and use for this an integral representation originally derived by Schwinger.⁸⁻⁹

The general Green's function (defined in the complex Ω plane cut along the positive real axis) can be written in the form of the eigenfunction expansion

$$G(\mathbf{r}_2, \mathbf{r}_1; \Omega) = \mathbf{S} \sum_n [u_n(\mathbf{r}_2) u_n^*(\mathbf{r}_1) / (E_n - \Omega)]. \quad (3)$$

Therefore (2) is equivalent to¹⁰

$$\mathfrak{M} = \mathbf{s} \cdot \mathbf{s}' - \sum_{i,j} [s'_i s_j \Pi_{ij}(\Omega_1) + s_i s'_j \Pi_{ij}(\Omega_2)], \quad (4)$$

where

$$\Pi_{ij}(\Omega) = m^{-1} \iint u_0^*(\mathbf{r}_2) P_{2i} G(\mathbf{r}_2, \mathbf{r}_1; \Omega) \times P_{1j} u_0(\mathbf{r}_1) d\mathbf{r}_1 d\mathbf{r}_2, \quad (5)$$

and Ω_1, Ω_2 are given by

$$\begin{aligned} \Omega_1 &= E_0 + \omega + i\epsilon = -|E_0| + \omega + i\epsilon, \\ \Omega_2 &= E_0 - \omega = -|E_0| - \omega. \end{aligned} \quad (6)$$

¹ W. Heitler, *The Quantum Theory of Radiation* (Oxford University Press, New York, 1954), p. 192.

² We use the natural system of units, such that $\hbar = c = 1$; then $e^2 Z = \alpha Z$.

³ H. A. Kramers and W. Heisenberg, *Z. Physik* **31**, 681 (1925).

⁴ B. Podolsky, *Proc. Natl. Acad. Sci. (U.S.)* **4**, 253 (1928); A. Dalgarno and A. E. Kingston, *Proc. Roy. Soc. (London)* **A259**, 424 (1960). These calculations actually refer to the refractive index of hydrogen n , the quantity \mathfrak{M}/ω^2 being proportional to $n^2 - 1$.

⁵ M. H. Mittleman and F. A. Wolf, *Phys. Rev.* **128**, 2686 (1962).

⁶ D. H. Constantinescu and M. Gavrilă, *Revue Roumaine Phys.* **12**, 121 (1967).

⁷ L. Hostler and R. H. Pratt, *Phys. Rev. Letters* **10**, 469 (1963); *L. Hostler, J. Math. Phys.* **5**, 591 (1964).

⁸ J. Schwinger, *J. Math. Phys.* **5**, 1606 (1964).

⁹ Essentially the same result has been obtained also by S. Okubo and D. Feldman, *Phys. Rev.* **117**, 292 (1960); L. Hostler, *J. Math. Phys.* **5**, 1235 (1964), and V. G. Gorshkov, *Zh. Eksperim. i Teor. Fiz.* **47**, 352 (1964) [English transl.: *Soviet. Phys.—JETP* **20**, 234 (1965)].

¹⁰ Depending on the method of derivation one may consider either (2) as the primary result and (4) its consequence, or vice versa.

Because of the rotational invariance of the ground state eigenfunction $u_0(r)$ and of the Green's function G , it may be shown that $\Pi_{ij}(\Omega)$ is proportional to the unit tensor and hence

$$\mathfrak{N} = (\mathbf{s} \cdot \mathbf{s}') M, \quad (7)$$

where

$$M = 1 - P(\Omega_1) - P(\Omega_2), \quad (8)$$

with

$$P(\Omega) = (3m)^{-1} \iint G(\mathbf{r}_2, \mathbf{r}_1; \Omega) [\mathbf{P}_2 u_0(r_2)]^* \cdot [\mathbf{P}_1 u_0(r_1)] d\mathbf{r}_1 d\mathbf{r}_2. \quad (9)$$

Taking the Fourier transforms of the functions involved, $P(\Omega)$ becomes

$$P(\Omega) = (3m)^{-1} \iint (\mathbf{p}_2 \cdot \mathbf{p}_1) u_0^*(\mathbf{p}_2) G(\mathbf{p}_2, \mathbf{p}_1; \Omega) u_0(\mathbf{p}_1) \times d\mathbf{p}_1 d\mathbf{p}_2, \quad (10)$$

containing the Green's function in momentum space $G(\mathbf{p}_2, \mathbf{p}_1; \Omega)$.

The calculation of the Kramers-Heisenberg matrix element is thus reduced to the evaluation of $P(\Omega)$, which will be carried out in Sec. II.

The differential cross section for unpolarized incident photons and arbitrary polarization of the scattered photon, yielded by Eqs. (1) and (2), has the well known form

$$d\sigma = r_0^2 \frac{1}{2} (1 + \cos^2\theta) |M|^2 d\Omega, \quad (11)$$

where θ is the scattering angle.

II. CALCULATION OF $P(\Omega)$

The Schwinger integral representation for the Coulomb-Green's function in momentum space may be written as¹¹

$$G(\mathbf{p}_2, \mathbf{p}_1; \Omega) = \frac{m\kappa}{2\pi^2\lambda} \frac{ie^{i\pi\kappa}}{2\sin\pi\kappa} \int_1^{(0+)} \rho^{-\kappa} \frac{d}{d\rho} \{ [(1-\rho^2)/\rho] [(\mathbf{p}_2 - \mathbf{p}_1)^2 - (\mathbf{p}_1^2 - 2m\Omega)(\mathbf{p}_2^2 - 2m\Omega)(1-\rho)^2/8m\Omega\rho]^{-2} \} d\rho. \quad (12)$$

Here $\lambda = \alpha Z m$ and

$$\kappa = i\lambda/(2m\Omega)^{1/2}, \quad \text{Im}(2m\Omega)^{1/2} > 0. \quad (13)$$

The integration contour in (12) begins at $\rho=1$ (where one should take $\rho^{-\kappa}=1$), runs along the real axis to a point closely on the right of $\rho=0$, encircles the origin in the counter-clockwise sense and runs back to $\rho=1$ on the real axis. The integral representation (12) then

describes the Green's function in the whole complex (Ω) plane cut along the positive real axis.

The ground-state energy eigenfunction of the hydrogen atom in momentum space is

$$u_0(\mathbf{p}) = (8\lambda^5/\pi^2)^{1/2} (\mathbf{p}^2 + \lambda^2)^{-2}. \quad (14)$$

Inserting (12) and (14) into (10) and interchanging the order of integrations, one finds

$$P(\Omega) = -\frac{2\lambda^4}{3\pi^4} \kappa \frac{ie^{i\pi\kappa}}{2\sin\pi\kappa} \int_1^{(0+)} \rho^{-\kappa} \frac{d}{d\rho} \left\{ \frac{1-\rho^2}{\rho} Q \right\} d\rho, \quad (15)$$

where

$$Q = \iint \frac{[(\mathbf{p}_2 - \mathbf{p}_1)^2 - \mathbf{p}_1^2 - \mathbf{p}_2^2]}{(\mathbf{p}_2^2 + \lambda^2)^2 [(\mathbf{p}_2 - \mathbf{p}_1)^2 - (\mathbf{p}_1^2 - 2m\Omega)(\mathbf{p}_2^2 - 2m\Omega)(1-\rho)^2/8m\Omega\rho]^2 (\mathbf{p}_1^2 + \lambda^2)^2} d\mathbf{p}_1 d\mathbf{p}_2. \quad (16)$$

The integrand of Eq. (16) depends only on the variables $\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_{12} = |\mathbf{p}_1 - \mathbf{p}_2|$. Therefore one can use the integration formula¹²

$$\iint F(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_{12}) d\mathbf{p}_1 d\mathbf{p}_2 = 8\pi^2 \iiint F(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_{12}) \mathbf{p}_1 \mathbf{p}_2 \mathbf{p}_{12} d\mathbf{p}_1 d\mathbf{p}_2 d\mathbf{p}_{12}. \quad (17)$$

Denoting

$$\alpha = (1-\rho)^2/4\rho, \quad (18)$$

$$X^2 = -2m\Omega, \quad (19)$$

one gets

$$Q = 8\pi^2 X^4 \iiint \frac{(\mathbf{p}_{12}^2 - \mathbf{p}_1^2 - \mathbf{p}_2^2) \mathbf{p}_1 \mathbf{p}_2 \mathbf{p}_{12}}{(\mathbf{p}_2^2 + \lambda^2)^2 [X^2 \mathbf{p}_{12}^2 + \alpha(\mathbf{p}_1^2 + X^2)(\mathbf{p}_2^2 + X^2)]^2 (\mathbf{p}_1^2 + \lambda^2)^2} d\mathbf{p}_1 d\mathbf{p}_2 d\mathbf{p}_{12}. \quad (20)$$

¹¹ See Eq. (3') of Ref. 8. Our Green's function Eq. (3) has the opposite sign of the one of Schwinger.

¹² See, for example, P. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), Part II, p. 1737.

This may be expressed as

$$Q = 8\pi^2 X^2 \left\{ \frac{1}{4\lambda^2} \frac{\partial^2 I}{\partial \lambda \partial \mu} - \alpha J + (X^2 + \alpha X^2 - \alpha \lambda^2) \frac{1}{\lambda} \frac{\partial J}{\partial \lambda} - [\alpha(X^2 - \lambda^2)^2 - 2\lambda^2 X^2] \frac{1}{4\lambda^2} \frac{\partial^2 J}{\partial \lambda \partial \mu} \right\}_{\lambda=\mu}, \quad (21)$$

where I and J are the parameter-dependent integrals

$$I(\lambda, \mu; X^2) = \iiint \frac{p_1 p_2 p_{12}}{(p_2^2 + \mu^2) [X^2 p_{12}^2 + \alpha(p_1^2 + X^2)(p_2^2 + X^2)] (p_1^2 + \lambda^2)} d p_1 d p_2 d p_{12}, \quad (22)$$

$$J(\lambda, \mu; X^2) = \iiint \frac{p_1 p_2 p_{12}}{(p_2^2 + \mu^2) [X^2 p_{12}^2 + \alpha(p_1^2 + X^2)(p_2^2 + X^2)]^2 (p_1^2 + \lambda^2)} d p_1 d p_2 d p_{12}. \quad (23)$$

Here λ and μ vary in the neighborhood of $\alpha Z m$, whereas X^2 of Eq. (19) may be a complex number.

We begin with the evaluation of $I(\lambda, \mu; X^2)$. In Eq. (22), the integral over the variable p_{12}

$$(|p_1 - p_2| \leq p_{12} \leq p_1 + p_2)$$

can be immediately carried out. The result is

$$I = \frac{1}{8X^2} \int_{-\infty}^{+\infty} \frac{p_2}{(p_2^2 + \mu^2)} f(p_2; X^2) d p_2, \quad (24)$$

with

$$f(p_2; X^2) = \int_{-\infty}^{+\infty} \frac{p_1}{(p_1^2 + \lambda^2)} \times \ln \frac{X^2(p_1 + p_2)^2 + \alpha(p_1^2 + X^2)(p_2^2 + X^2)}{X^2(p_1 - p_2)^2 + \alpha(p_1^2 + X^2)(p_2^2 + X^2)} d p_1. \quad (25)$$

The symmetry of the integrand of I with respect to the variables p_1 and p_2 has allowed us to extend the integration intervals from $0 \leq p_1, p_2 \leq \infty$ to $-\infty \leq p_1, p_2 \leq \infty$.

The expressions

$$E_{\pm} = X^2(p_1 \pm p_2)^2 + \alpha(p_1^2 + X^2)(p_2^2 + X^2), \quad (26)$$

occurring in Eq. (25) may be written as

$$E_+ = (X^2 + \alpha X^2 + \alpha p_2^2)(p_1 - \pi_+)(p_1 - \pi_-),$$

$$E_- = (X^2 + \alpha X^2 + \alpha p_2^2)(p_1 + \pi_+)(p_1 + \pi_-), \quad (27)$$

where

$$\pi_{\pm} = \frac{-p_2 X^2 \pm i \alpha \beta X (p_2^2 + X^2)}{X^2 + \alpha X^2 + \alpha p_2^2}, \quad (28)$$

and

$$\beta = [(1 + \alpha)/\alpha]^{1/2} = (1 + \rho)/(1 - \rho). \quad (29)$$

We will suppose provisionally that X^2 is real positive. This is always true for α of Eq. (18) when ρ varies along the integration contour of (12). Then whatever p_2 real, the root π_+ is always in the upper complex half-plane (p_1), whereas π_- is always in the lower half-plane (p_1).

With the above notation we have

$$f(p_2; X^2) = \int_{-\infty}^{+\infty} \frac{p_1}{p_1^2 + \lambda^2} \left[\ln \frac{p_1 - \pi_+}{p_1 + \pi_-} + \ln \frac{p_1 - \pi_-}{p_1 + \pi_+} \right] d p_1. \quad (30)$$

This may be evaluated by means of the residue theorem. Indeed, the critical points of the first logarithm lie in the upper half-plane (p_1), so that one can close the contour of integration by an arc at infinity in the lower half-plane. The opposite can be done in the case of the second logarithm. One finds

$$f(p_2; X^2) = 2\pi i \ln(i\lambda - \pi_-)/(i\lambda + \pi_+). \quad (31)$$

Introducing (31) into (24), one gets

$$I = \frac{\pi i}{4X^2} \int_{-\infty}^{+\infty} \frac{p_2}{(p_2^2 + \mu^2)} \times \ln \frac{\lambda(X^2 + \alpha X^2 + \alpha p_2^2) + \alpha \beta X (p_2^2 + X^2) - i p_2 X^2}{\lambda(X^2 + \alpha X^2 + \alpha p_2^2) + \alpha \beta X (p_2^2 + X^2) + i p_2 X^2} d p_2. \quad (32)$$

The expressions

$$F_{\pm} = \lambda(X^2 + \alpha X^2 + \alpha p_2^2) + \alpha \beta X (p_2^2 + X^2) \pm i p_2 X^2, \quad (33)$$

occurring in Eq. (32) may be written

$$F_- = \alpha(\lambda + \beta X)(p_2 - \rho_+)(p_2 - \rho_-),$$

$$F_+ = \alpha(\lambda + \beta X)(p_2 + \rho_+)(p_2 + \rho_-), \quad (34)$$

with

$$\rho_+ = i\beta X,$$

$$\rho_- = -iX(X + \beta\lambda)/(\lambda + \beta X). \quad (35)$$

The root ρ_+ is in the upper complex half-plane (p_1), whereas ρ_- is in the lower one.

Hence the integral I of Eq. (32) can be written successively

$$I = \frac{\pi i}{4X^2} \int_{-\infty}^{+\infty} \frac{p_2}{p_2^2 + \mu^2} \left[\ln \frac{p_2 - \rho_+}{p_2 + \rho_-} + \ln \frac{p_2 - \rho_-}{p_2 + \rho_+} \right] d p_2$$

$$= \frac{\pi^2}{2X^2} \ln \frac{i\mu + \rho_+}{i\mu - \rho_-}. \quad (36)$$

The integration has been performed similarly to the

one in Eq. (30). Taking into account Eqs. (35), we get the result

$$I(\lambda, \mu; X^2) = \frac{\pi^2}{2X^2} \ln \frac{(\lambda + \beta X)(\mu + \beta X)}{\lambda\mu + \beta X(\lambda + \mu) + X^2}. \quad (37)$$

We have derived Eq. (37) supposing that $X^2 > 0$. We will now indicate how it can be shown that the result is true for any X^2 in the complex (X^2) plane cut along the negative real axis [i.e., by Eq. (19), for any Ω in the (Ω) plane cut along the positive real axis].

We first notice that the integrand of $f(\mathbf{p}_2; X^2)$ given by Eq. (25) is an analytic function of X^2 , except for a line of critical points yielded by the equations $E_{\pm} = 0$ [see Eq. (26)]. It is easy to see that because $\mathbf{p}_1, \mathbf{p}_2$ are real and $\alpha > 0$, this line of critical points coincides with the real negative axis of the (X^2) plane. Next, we remark that the integral $f(\mathbf{p}_2, X^2)$ is convergent for every complex X^2 . Moreover, it can be shown that whatever the value of \mathbf{p}_2 , $f(\mathbf{p}_2; X^2)$ is also uniformly convergent in a circular (arbitrarily big) domain $|X^2| \leq R$ which does not contain a strip of finite (arbitrarily small) width situated along the real negative axis of the (X^2) plane.

The integral $f(\mathbf{p}_2; X^2)$ is thus an analytic function of X^2 in the cut (X^2) plane, whatever the real value of \mathbf{p}_2 . The same is true also for the integrand of $I(\lambda, \mu; X^2)$ in Eq. (24). $I(\lambda, \mu; X^2)$ is convergent for any complex X^2 , because one can show that for $|\mathbf{p}_2| \rightarrow \infty$, $f(\mathbf{p}_2; X^2)$ is always of order $1/\mathbf{p}_2$. Besides, $I(\lambda, \mu; X^2)$ is also uniformly convergent in any finite domain of the cut (X^2) plane. Consequently, it is an analytic function of X^2 in the cut plane.

Now the right-hand side of Eq. (37) is itself an analytic function of X^2 . Therefore the equality (38) we established for $X^2 > 0$ holds by analytic continuation everywhere in the cut (X^2) plane. This proves our statement.

By continuity, one sees that for complex X^2 in Eq. (37) one must understand by X the square root of X^2 for which

$$\operatorname{Re} X > 0. \quad (38)$$

Also, the principal value of the logarithm of Eq. (37) should be taken.

Let us now pass to the *evaluation of* $J(\lambda, \mu; X^2)$ of Eq. (23). Performing the integration over the variable \mathbf{p}_{12} , it can be written as [see Eqs. (26) and (27)]:

$$J = [16i\alpha\beta X^3]^{-1} \int_{-\infty}^{+\infty} \frac{\mathbf{p}_2}{(\mathbf{p}_2^2 + \mu^2)(\mathbf{p}_2^2 + X^2)} g(\mathbf{p}_2; X^2) d\mathbf{p}_2, \quad (39)$$

where

$$g(\mathbf{p}_2; X^2) = \int_{-\infty}^{+\infty} \frac{\mathbf{p}_1}{\mathbf{p}_1^2 + \lambda^2} \{[(\mathbf{p}_1 + \pi_-)^{-1} - (\mathbf{p}_1 - \pi_+)^{-1}] + [(\mathbf{p}_1 - \pi_-)^{-1} - (\mathbf{p}_1 + \pi_+)^{-1}]\} d\mathbf{p}_1, \quad (40)$$

and π_{\pm} are given by Eq. (28). We have again extended the integration variables for $\mathbf{p}_1, \mathbf{p}_2$ to $-\infty < \mathbf{p}_1, \mathbf{p}_2 < \infty$.

Supposing that $X^2 > 0$, for any real \mathbf{p}_2 we get

$$g(\mathbf{p}_2; X^2) = 2\pi i [(\mathbf{p}_2 - \pi_-)^{-1} - (\mathbf{p}_2 + \pi_+)^{-1}], \quad (41)$$

or, taking into account Eqs. (34) and (35),

$$g(\mathbf{p}_2; X^2) = \frac{2\pi}{i\alpha} \frac{X^2 + \alpha X^2 + \alpha \mathbf{p}_2^2}{X^2 + 2\lambda\beta X + \beta^2 X^2} \times \{[(\mathbf{p}_2 - \rho_+)^{-1} - (\mathbf{p}_2 + \rho_-)^{-1}] + [(\mathbf{p}_2 + \rho_+)^{-1} - (\mathbf{p}_2 - \rho_-)^{-1}]\}. \quad (42)$$

Then

$$J = -i\pi^2/4\alpha^2\beta X^3 (X^2 + 2\lambda\beta X + \beta^2 X^2) (X^2 - \mu^2) \times \{(X^2 + \alpha X^2 - \alpha\mu^2) [(i\mu + \rho_+)^{-1} - (i\mu - \rho_-)^{-1}] - X^2 [(iX + \rho_+)^{-1} - (iX - \rho_-)^{-1}]\}. \quad (43)$$

After some elementary calculations this becomes

$$J(\lambda, \mu; X^2) = \frac{\pi^2}{4\alpha^2\beta(1+\beta)X^2} \times (\lambda + X)^{-1} (\mu + X)^{-1} [\lambda\mu + \beta X(\lambda + \mu) + X^2]^{-1}. \quad (44)$$

Equation (44) has been derived by supposing that $X^2 > 0$. Proceeding as in the case of $I(\lambda, \mu; X^2)$ of Eq. (37), it may be shown that the result is true for any X^2 in the complex (X^2) plane cut along the real negative axis.

We next need the quantities appearing in the expression for Q in Eq. (21). We will give only their final forms obtained by noting that on account of Eqs. (13), (19), and (38), we have

$$\kappa = \lambda/X, \quad (45)$$

and that α and β are given by Eqs. (18) and (29). Thus

$$\left(\frac{\partial^2 I}{\partial \lambda \partial \mu}\right)_{\lambda=\mu} = \frac{2\pi^2}{X^4(1+\kappa)^4} \frac{\rho}{[1-\xi\rho]^2}, \quad (46)$$

$$\alpha J_{\lambda=\mu} = \frac{\pi^2}{2X^6(1+\kappa)^4} \frac{\rho(1-\rho)}{(1+\rho)(1-\xi\rho)}, \quad (47)$$

$$\left(\frac{\partial J}{\partial \lambda}\right)_{\lambda=\mu} = -\frac{4\pi^2}{X^7(1+\kappa)^7} \frac{\rho^2[\kappa(1-\kappa)\rho + (1+\kappa)^2]}{(1-\rho^2)(1-\xi\rho)^2}, \quad (48)$$

$$\left(\frac{\partial^2 J}{\partial \lambda \partial \mu}\right)_{\lambda=\mu} = \frac{8\pi^2\rho^2}{X^8(1+\kappa)^{10}(1-\rho^2)(1-\xi\rho)^3} \times [\kappa^2(1-\kappa)^2\rho^2 + (1+\kappa)^2(1+2\kappa-2\kappa^2)\rho + (1+\kappa)^4]. \quad (49)$$

In the above, we have set

$$\xi = [(1-\kappa)/(1+\kappa)]^2. \quad (50)$$

Introducing Eqs. (46)-(49) into Eq. (21), one finds

$$Q = \frac{32\pi^4}{\lambda^4} \frac{\kappa^4}{(1+\kappa)^{10}} \frac{\rho^3[(1-\kappa)^2\rho - 3(1+\kappa)^2]}{(1-\rho^2)(1-\xi\rho)^3}. \quad (51)$$

Carrying now Q into Eq. (15), we obtain

$$P(\Omega) = 128 \frac{\kappa^5}{(1+\kappa)^8} \frac{e^{i\pi\kappa}}{2 \sin \pi\kappa} \int_1^{(0+)} \rho^{1-\kappa} (1-\xi\rho)^{-4} d\rho. \quad (52)$$

$P(\Omega)$ can be expressed in terms of the Gauss hypergeometric function ${}_2F_1$. Indeed there exists the following integral representation¹³:

$${}_2F_1(a, b, c; \xi) = -\frac{i\Gamma(c)e^{-i\pi a}}{\Gamma(a)\Gamma(c-a)2\sin\pi a} \times \int_1^{(0+)} \rho^{a-1}(1-\rho)^{c-a-1}(1-\xi\rho)^{-b} d\rho, \quad (53)$$

provided that $\text{Re}c > \text{Re}a$. This allows us to rewrite $P(\Omega)$ in the final form

$$P(\Omega) = 128[\kappa^5/(1+\kappa)^3(2-\kappa)] {}_2F_1(2-\kappa, 4, 3-\kappa; \xi), \quad (54)$$

with ξ given by Eq. (50).

Using well-known properties of the hypergeometric function we will give some equivalent forms to our result in Eq. (54), which will be needed in Sec. III. Firstly, one can write^{14,15}

$$P(\Omega) = [2\kappa^2/(1+\kappa)^2(2-\kappa)] {}_2F_1(1, -1-\kappa, 3-\kappa; \xi). \quad (55)$$

Then¹⁶

$$P(\Omega) = \frac{1}{2}[\kappa/(2-\kappa)] {}_2F_1[1, 4, 3-\kappa; \xi/(\xi-1)]. \quad (56)$$

Finally, one can express $P(\Omega)$ by means of a series expansion in $(1-\xi)$. To this end we use the formula for the analytic continuation of a hypergeometric series of variable ξ to a series of variable $(1-\xi)$. It should be noted that in our case the ${}_2F_1$ function appearing in (55) has an integer difference between the third parameter and the sum of the first two. Using the adequate formula of analytic continuation for this case,¹⁷ one finds

$$P(\Omega) = \frac{2}{3} \frac{\kappa^2(1+5\kappa+7\kappa^2+11\kappa^3)}{(1+\kappa)^5} + \frac{64}{3} \frac{\kappa^6}{(1-\kappa^2)^3} \xi^\kappa [\psi(m-\kappa) + \ln(1-\xi)] - \frac{64}{3} \frac{\kappa^6(1-\kappa)}{(1+\kappa)^7} \sum_{p=0}^{\infty} \frac{(2-\kappa)_p}{p!} (1-\xi)^p \times \left[\psi(p+1) - \left(\frac{1}{m-\kappa} + \frac{1}{m+1-\kappa} \cdots + \frac{1}{p+1-\kappa} \right) \right]. \quad (57)$$

Here m is an integer which may be taken equal to 0 or 1. In writing (57) we have taken into account Eq.

¹³ See for example: A. Erdélyi, W. Magnus, F. Oberhettinger, and F. Tricomi, *Higher Transcendental Functions* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. I, p. 114; Eq. (3) and p. 60. This work will be referred to in the following as HTF.

¹⁴ HTF, p. 105, Eq. (2).

¹⁵ This result has been originally derived by the author using in Eq. (9) the Coulomb-Green's function in closed form found by Hostler and Pratt (Ref. 7).

¹⁶ HTF, p. 105, Eq. (3).

¹⁷ HTF, p. 110, Eq. (12). See also p. 16, Eq. (10).

(50) and

$$\sum_{p=0}^{\infty} \frac{(2-\kappa)_p}{p!} (1-\xi)^p = \xi^{\kappa-2}.$$

The arguments of the powers involved are fixed by

$$|\arg(1-\xi)| < \pi, \quad |\arg\xi| < \pi. \quad (58)$$

III. DISCUSSION OF ANALYTIC RESULT

Now that $P(\Omega)$ is determined, Eq. (8) yields the matrix element M by specializing the values of Ω . In this section we shall consider the expression of M in different limiting cases and make a comparison with previous results. The photon energy will be measured subsequently in $Z^2 \times \text{Rydberg}$ units setting

$$k = [\omega/(\lambda^2/2m)] = (\omega/Z^2 \cdot \text{Ry}). \quad (59)$$

We shall designate by subscripts 1 and 2 the values of κ and ξ corresponding by Eqs. (13) and (50) to Ω_1, Ω_2 of Eqs. (6).

There are two distinct cases to be discussed: $0 \leq k < 1$ and $1 \leq k < \infty$.

If the photon energy is below the photoelectric threshold ($0 \leq k < 1$), κ_1 is positive real and

$$\kappa_1 = 1/(1-k)^{1/2}, \quad 1 \leq \kappa_1 < \infty, \quad 0 \leq \xi_1 < 1. \quad (60)$$

As regards κ_2 , it is positive real for all values of k ($0 \leq k < \infty$) and

$$\kappa_2 = 1/(1+k)^{1/2}, \quad 1 \geq \kappa_2 > 0, \quad 0 \leq \xi_2 < 1. \quad (61)$$

For $0 \leq k < 1$ we have

$$1 \geq \kappa_2 > \frac{1}{2}\sqrt{2}, \quad 0 \leq \xi_2 < 0.029437. \quad (62)$$

The values of κ_1 and κ_2 being real, M itself is real.

Formula (2) discloses the existence of singularities of the matrix element for $k=1-(1/n^2)$, $n=2, 3, \dots$. These singularities are nonphysical, a consequence of the neglect in the theory of the finite width of the energy levels. When M is expressed as in Eq. (8) they are contained in $P(\Omega_1)$, which, on account of (55), has simple poles at $\kappa_1=2$ and $\kappa_1=3, 4, \dots$ (that is, $3-\kappa_1=0, -1, -2, \dots$). Between two consecutive poles, for increasing values of κ_1 , $P(\Omega_1)$ increases from $-\infty$ to $+\infty$, whereas M decreases from $+\infty$ to $-\infty$ passing through zero [$P(\Omega_2)$ varies slowly in the interval].

We shall now consider the expansion of M in powers of k . At the same time this will yield a procedure for determining the negative order sum rules for the hydrogen atom.

Starting from Eq. (9) for $P(\Omega)$ and making use of (3), (6), and (60), it is not difficult to see that we can write the expansion

$$P(\Omega_1) = \frac{1}{2} \sum_{p=0}^{\infty} S(-p) k^p, \quad (63)$$

containing the negative order sum rules for the hydrogen atom

$$S(-p) = \mathbf{S} \frac{f_{n0}}{[1-(E_n/E_0)]^p}. \quad (64)$$

Here f_{n0} is the oscillator strength of the transition $0 \rightarrow n$. By introducing the result (56) for $P(\Omega)$ into (63) and taking into account (60), it follows that

$$[2(1-k)^{1/2}-1]^{-1} {}_2F_1(1, 4, 3-(1-k)^{-1/2}; -[1-(1-k)^{1/2}]^2/4(1-k)^{1/2}) = \sum_{p=0}^{\infty} S(-p)k^p. \quad (65)$$

Expanding the left-hand side of this equality into powers of k , one obtains the expression of the sum rules to any negative order. It is apparent that the series (65) converges for $k < \frac{3}{4}$.

Dalgarno and co-workers^{4,18} have given general methods for the calculation of sum rules and have derived the values of $S(-p)$ up to $p=6$. We have checked these values by the procedure outlined above and have calculated further¹⁹

$$\begin{aligned} S(-7) &= \frac{9}{2} \frac{243}{654} \frac{157}{208}, \\ S(-8) &= \frac{289}{63} \frac{165}{700} \frac{453}{992}, \\ S(-9) &= \frac{45}{7} \frac{464}{644} \frac{213}{119} \frac{273}{040}, \\ S(-10) &= \frac{7}{917} \frac{175}{294} \frac{468}{284} \frac{425}{800} \frac{411}{800}. \end{aligned} \quad (66)$$

Similarly, one can write for $P(\Omega_2)$ the expansion

$$P(\Omega_2) = \frac{1}{2} \sum_{p=0}^{\infty} S(-p)(-k)^p, \quad (67)$$

which has the same coefficients as (63) and is convergent for $k < 1$. Combining (63) and (67) according to (8) and taking into account that $S(0) = 1$, one gets

$$M = - \sum_{p=1}^{\infty} S(-2p)k^{2p}. \quad (68)$$

M vanishes like k^2 for $k \rightarrow 0$.

The case $0 < k < \frac{3}{4}$ has been considered also by Mittleman and Wolf.⁵ They write the matrix element as in our Eq. (8) and derive an alternative exact expression for $P(\Omega)$, following a method of Schwartz. In order to establish the connection between their result and ours, we remark that for $0 < k < \frac{3}{4}$, κ_1 and κ_2 satisfy the inequalities $\text{Re}(3-\kappa) > \text{Re}(2-\kappa) > 0$. This allows us to use in both cases a standard integral representation for the hypergeometric function occurring in Eq. (54),²⁰ so that

$$P(\Omega) = 128 \frac{\kappa^5}{(1+\kappa)^8} \int_0^1 \rho^{1-\kappa} (1-\xi\rho)^{-4} d\rho.$$

¹⁸ A. Dalgarno, Rev. Mod. Phys. 35, 522 (1963).

¹⁹ This calculation was carried out by Mrs. V. Florescu.

²⁰ HTF, p. 59, Eq. (10).

Changing the integration variable according to

$$\rho = \frac{1+\kappa}{1-\kappa} \frac{t-\kappa}{t+\kappa},$$

$P(\Omega)$ transforms into the expression given by Mittleman and Wolf:

$$P(\Omega) = 16 \frac{\kappa^4}{(\kappa^2-1)^2} \left(\frac{1-1/\kappa}{1+1/\kappa} \right)^\kappa \int_1^\kappa \frac{1-t^2/\kappa^2}{(1+t)^4} \left(\frac{1+t/\kappa}{1-t/\kappa} \right)^\kappa dt.$$

If the photon energy is above the photoelectric threshold ($1 \leq k < \infty$), κ_1 is positive imaginary and

$$\kappa_1 = i/(k-1)^{1/2}, \quad \infty > |\kappa_1| > 0, \quad |\xi_1| = 1. \quad (69)$$

For increasing values of k , ξ_1 moves on the unit circle centered at the origin of the ξ plane, in the counter-clockwise sense, starting from $\xi = 1$ for $k = 1$ ($|\kappa_1| \rightarrow \infty$), passing through $\xi = -1$ for $k = 2$ ($\kappa_1 = i$) and returning to $\xi = 1$ for $k \rightarrow \infty$ ($|\kappa_1| \rightarrow 0$). The situation is presented in Fig. 1.

As already mentioned, κ_2 is given by (61); above the threshold we have

$$\frac{1}{2}\sqrt{2} \geq \kappa^2 > 0, \quad 0.029437 \leq \xi_2 < 1.$$

The imaginary value of κ_1 makes $P(\Omega_1)$, and therefore also M , complex. This is connected to the fact that when $k > 1$, absorption of the photon may take place by photoeffect.

We now show that the imaginary part of M can be expressed in terms of elementary functions. Indeed, noting that

$$\kappa_1^* = -\kappa_1, \quad \xi_1^* = 1/\xi_1,$$

one has

$$\begin{aligned} \text{Im}P(\Omega_1) &= \{P(\Omega_1) - [P(\Omega_1)]^*\} / 2i \\ &= \frac{\kappa_1^2}{i} \left[\frac{{}_2F_1(1, -1-\kappa_1, 3-\kappa_1; \xi_1)}{(1+\kappa_1)^2(2-\kappa_1)} \right. \\ &\quad \left. - \frac{{}_2F_1(1, -1+\kappa_1, 3+\kappa_1; 1/\xi_1)}{(1-\kappa_1)^2(2+\kappa_1)} \right]. \end{aligned} \quad (70)$$

The square bracket in Eq. (70) may be transformed

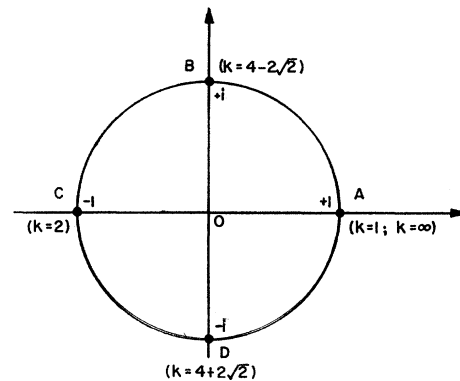


FIG. 1. Position of variable ξ_1 given by Eqs. (50) and (69) in complex ξ plane for different values of k .

using the formula of analytic continuation of a hypergeometric series of variable ξ to a series of variable $1/\xi$.²¹ Hence,

$$\operatorname{Im}P(\Omega_1) = -\frac{64\pi}{3} \frac{\kappa_1^6}{(1-\kappa_1^2)^3} \frac{\exp(-\pi|\kappa_1|)}{1-\exp(-2\pi|\kappa_1|)} \times \left[-\left(\frac{1-\kappa_1}{1+\kappa_1}\right)^2 \right]^{\kappa_1}, \quad (71)$$

with

$$\left| \arg \left\{ -\left(\frac{1-\kappa_1}{1+\kappa_1}\right)^2 \right\} \right| < \pi. \quad (72)$$

Defining

$$\eta = 1/(k-1)^{1/2} = -i\kappa_1, \quad (73)$$

one has, on account of (72),

$$\arg \left\{ -\left(\frac{1-\kappa_1}{1+\kappa_1}\right)^2 \right\} = -\pi + 4 \arctan_0 \eta^{-1}.$$

Therefore, because $P(\Omega_2)$ is real,

$$\operatorname{Im}M = -\operatorname{Im}P(\Omega_1) = -\frac{64}{3}\pi \frac{\eta^6}{(1+\eta^2)^3} \frac{\exp[-4\eta \arctan_0(1/\eta)]}{1-\exp(-2\pi\eta)}. \quad (74)$$

This agrees with the result yielded by the optical theorem.⁶

We shall determine next the value of M at the threshold $k=1$. This corresponds to $\kappa_1 \rightarrow i\infty$ so that we are interested in the expansion of $P(\Omega_1)$ in powers of $1/\kappa_1$. Because ξ_1 varies in the neighborhood of 1, expression (57) should be used with $m=0$.

For the term in the second line of Eq. (57) we note that on account of (58) we have

$$\begin{aligned} \xi_1^{\kappa_1} &= [(1-\kappa_1)/(1+\kappa_1)]^{2\kappa_1} \\ &= \exp[-4|\kappa_1| \arctan_0(1/|\kappa_1|)] \\ &= e^{-4} + O(1/\kappa_1^2), \end{aligned}$$

and that the *asymptotic* expansion of $\psi(-\kappa_1)$ reads²²

$$\psi(-\kappa_1) = \ln|\kappa_1| - i\pi/2 + O(1/\kappa_1).$$

The series contained in the third line of Eq. (57) can itself be expanded in powers of $1/\kappa_1$, yielding to lowest order

$$\sum_{p=0}^{\infty} = \tau(-4) + O(\kappa_1^{-1}), \quad (75)$$

where

$$\tau(z) = \sum_{p=0}^{\infty} \frac{\psi(p+1)}{p!} z^p. \quad (76)$$

In order to calculate $\tau(z)$ we remark that²³

$$\psi(p+1) = C + \int_0^1 \frac{t^p - 1}{t-1} dt, \quad (77)$$

where C is the Euler constant. Introducing (77) into the series expansion of $\tau(z)$ and interchanging the sum and the integral, one finds

$$\begin{aligned} \tau(z) &= e^z \left(-C + \int_0^1 \frac{\exp[z(t-1)] - 1}{t-1} dt \right) \\ &= -e^z \left(C + \sum_{k=1}^{\infty} \frac{(-z)^k}{k \cdot k!} \right). \end{aligned} \quad (78)$$

This may be expressed in terms of the exponential integral $E_1(z)$;

$$E_1(z) = \int_z^{\infty} \frac{e^{-u}}{u} du = -C - \ln z - \sum_{k=1}^{\infty} \frac{(-z)^k}{k(k!)}, \quad (79)$$

where the principal value of the logarithm is to be taken. Thus

$$\tau(z) = e^z [\ln z + E_1(z)]. \quad (80)$$

Consequently,²⁴

$$\tau(-4) = e^{-4} [\ln 4 + \operatorname{Re}E_1(-4)]. \quad (81)$$

Summing up the contributions to $P(\Omega_1)$ one gets the result

$$P(\Omega_1) = \frac{1}{3} \{ 22 + 64[e^{-4} \operatorname{Re}E_1(-4)] \} + i\frac{64}{3}\pi e^{-4} + O(\kappa_1^{-1}), \quad (82)$$

containing the first term of the *asymptotic* expansion of $P(\Omega_1)$ in $1/\kappa_1$.²⁵ The imaginary part of Eq. (82) agrees with the one obtained from Eq. (74). Using the tabulated value $e^{-4} \operatorname{Re}E_1(-4) = -e^{-4} \operatorname{Ei}(4) = -0.3595520$, the real part of $P(\Omega_1)$ at the threshold is

$$\operatorname{Re}P(\Omega_1) = -0.3371095. \quad (83)$$

The value of $P(\Omega_2)$ at the threshold ($\kappa_2 = \frac{1}{2}\sqrt{2}$, $\Omega^2 = -\lambda^2/m$) can be readily obtained from (55). One finds

$$P(-\lambda^2/m) = 0.259629. \quad (84)$$

Combining (83) and (84), we find the threshold value of

$$\operatorname{Re}M = 1.077480. \quad (85)$$

For the imaginary part of M one finds from (82) or (74)

$$\operatorname{Im}M = -1.227526. \quad (86)$$

We consider finally the expression of M for large values of k . This corresponds to $|\kappa_1|$, $\kappa_2 \rightarrow 0$, so that one must expand $P(\Omega)$ in powers of κ . As ξ varies in the neighborhood of 1, Eq. (57) for $P(\Omega)$ should again be used, this time with $m=1$.

The expansion of the term in the first line of Eq. (57) is immediate. In the case of the term in the second

²⁴ $\tau(z)$ is uniform; for $z < 0$ one has

$$\ln z + E_1(z) = \ln|z| + \operatorname{Re}E_1(z) = \ln|z| - \operatorname{Ei}(|z|).$$

²⁵ The next term can be shown to be

$$(1/\kappa_1^2) \left\{ \frac{1}{3} [122 + 320[e^{-4} \operatorname{Re}E_1(-4)]] + i\pi(320/9)e^{-4} \right\} + O(\kappa_1^{-3}).$$

²¹ HTF, p. 107, Eq. (34) and p. 105, Eq. (14).

²² HTF, p. 47, Eq. (7).

²³ HTF, p. 16, Eq. (13).

line we remark that the logarithm may be written

$$\begin{aligned}\ln(1-\xi) &= \ln[4\kappa/(1+\kappa)^2] \\ &= \ln|\kappa| + (\ln 4 + i\varphi) - 2(\kappa - \frac{1}{2}\kappa^2) + O(\kappa^3),\end{aligned}$$

where, because of (58), $\varphi = \pi/2$ for $\kappa = \kappa_1$ and $\varphi = 0$ for $\kappa = \kappa_2$. Moreover, the expansion of $\psi(1-\kappa)$ reads²⁶

$$\psi(1-\kappa) = -C - \zeta(2)\kappa - \zeta(3)\kappa^2 + O(\kappa^3),$$

where ζ is the Riemann function. Finally, the expansion of the series of Eq. (57) in powers of κ is

$$\sum_{p=0}^{\infty} = -[(1+C) + (5+8C)\kappa + (17+28C)\kappa^2 + O(\kappa^3)].$$

Summing up the contributions to $P(\Omega)$, one obtains

$$\begin{aligned}P(\Omega) &= \frac{2}{3}[\kappa^2 - 3\kappa^4 + 16\kappa^5 + (-23 + 32\ln 4 + 32i\varphi)\kappa^6 \\ &\quad - (16 + 32\zeta(2))\kappa^7 + (101 - 32\ln 4 - 32\zeta(3) - 32i\varphi)\kappa^8 \\ &\quad + 32\kappa^6(1-\kappa^2)\ln|\kappa|] + O(\kappa^9; \kappa^9\ln|\kappa|).\end{aligned}\quad (87)$$

When combined with Eqs. (69) and (61), the preceding result gives the expansions in powers of $1/k$ for $P(\Omega_1)$ and $P(\Omega_2)$. The resulting expression for M is

$$\begin{aligned}M &= 1 + \frac{16}{3}\frac{1}{k^2} - \frac{32}{3}\frac{1+i}{k^{5/2}} + \frac{32}{3}\frac{i\pi}{k^3} \\ &\quad + \frac{16}{3}\frac{[7+4\zeta(2)](1-i)}{k^{7/2}} - \frac{64}{3}\frac{9-16\ln 2-2\zeta(3)-2i\pi}{k^4} \\ &\quad - \frac{256}{3}\frac{\ln k}{k^4} + O(k^{-9/2}; k^{-9/2}\ln k).\end{aligned}\quad (88)$$

Because this expansion is slowly convergent it can be applied with good accuracy only for large values of k .²⁷ The imaginary part of M in Eq. (88) agrees to the order considered with the one derived from Eq. (74).

IV. NUMERICAL COMPUTATION

We now briefly describe the computation of the matrix element M in Eq. (8). This has been done by summing the series of the hypergeometric functions ${}_2F_1$ occurring in the expressions for $P(\Omega_1)$ and $P(\Omega_2)$. Different equivalent expressions for $P(\Omega)$ had to be used on different intervals of k in order to ensure as rapid a convergence as possible to the series involved. The module of the error with which $P(\Omega_1)$, $P(\Omega_2)$, and M were computed is less than 10^{-7} . For larger Z values and higher photon energies this is much smaller than the corrections of a physical nature (relativity and retardation) affecting Eq. (2).

²⁶ HTF, p. 45, Eq. (5).

²⁷ It should be remembered, however, that the dipole approximation limits the validity of the calculation to $k \ll 1/\alpha Z$. Indeed the retardation corrections are of order $(\alpha Z k)^2$.

We begin by considering the *computation of $P(\Omega_1)$* . If $0 \leq k \leq 1$, $P(\Omega_1)$ presents an infinite number of resonances for $k = 1 - (1/n^2)$, $n = 2, 3, \dots$. We have computed $P(\Omega_1)$ up to the fourth resonance $k < 24/25$. We did not approach too closely the resonances because then Eq. (2) breaks down (due to the neglect of the finite width of the energy levels). For the interval considered, the computation of $P(\Omega_1)$ was based on Eq. (55) combined with Eqs. (60) and (50). Indeed for $k < 24/25$ we have $\xi_1 < 4/9$, so that the hypergeometric series occurring in Eq. (55) converges rapidly.

If $k \geq 1$, $P(\Omega_1)$ is complex and we have computed its real and imaginary parts up to $k = 50$. As already mentioned in this case the variable ξ_1 moves on the unit circle of the complex ξ plane as shown in Fig. 1. Its position on the circle is decisive as to which of the alternative expressions of $P(\Omega_1)$ should be used.

The threshold value of $k = 1$ corresponds to the point $\xi = 1$, which is a critical point of the hypergeometric function occurring in Eq. (55). This case has to be handled analytically, which yields the values given by Eqs. (85) and (86).

It is apparent that for ξ_1 on the arc BCD of Fig. 1, we have $|\xi_1/(\xi_1-1)| < 1$, so that the hypergeometric series of Eq. (56) is convergent. Because the series is rather slowly convergent near the points B ($k = 1.172$) and D ($k = 6.828$), we have used Eq. (56) to compute $P(\Omega_1)$ only for $1.30 \leq k \leq 5.00$.

To determine $P(\Omega_1)$ outside this interval, we have used Eq. (55), expanding the hypergeometric function it contains about a suitably chosen point. This can be done by taking into account the general formula

$$\begin{aligned}{}_2F_1(a, b, c; z) &= (1-z_0)^{c-a-b} \sum_{p=0}^{\infty} \frac{a_p b_p}{c_p 1_p} \left(\frac{z-z_0}{1-z_0} \right)^p \\ &\quad \times {}_2F_1(c-a, c-b, c+p; z_0),\end{aligned}\quad (89)$$

where z_0 is arbitrary; the series converges if $|z-z_0| < |1-z_0|$. The functions ${}_2F_1(c-a, c-b, c+p; z_0)$ can all be determined by the recurrence relations for contiguous hypergeometric functions from the first two (with $p=0$ and $p=1$).

Taking $z_0 = i$, $z = \xi$, $a = 1$, $b = -1 - \kappa_1$, and $c = 3 - \kappa_1$ in Eq. (89), we get the series expansion of the hypergeometric function occurring in (55) about point $z_0 = i$ which is convergent provided that $|\xi_1 - i| < \sqrt{2}$. This series was used for evaluating $P(\Omega_1)$ on the interval $1.05 \leq k \leq 1.40$ corresponding to ξ_1 in the neighborhood of point B , on arc ABC .²⁸

A similar procedure was applied for the interval $4.00 \leq k \leq 50$, corresponding to ξ_1 in the neighborhood of point D ($z_0 = -i$) on arc CDA .²⁸

²⁸ There is an overlap between this interval and the one considered before ($1.30 \leq k \leq 5.00$). The values obtained for $P(\Omega_1)$ in their common region by the two procedures agreed within less than 10^{-7} in module, thus testing the accuracy of the calculation.

From Eq. (74) it is easy to compute $\text{Im}P(\Omega_1) = -\text{Im}M$. This can then be compared with the values obtained by the methods described above. The agreement is within less than 10^{-7} in absolute value.

As regards the *computation of $P(\Omega_2)$* , this is much simpler because according to (78), we have $0 \leq \xi_2 < 1$ whatever the value of k , so that the computation can be based entirely on Eq. (55).

Some of the results of our computation are listed in Tables I and II.^{29,30} Only the values of the matrix element M are reported here. The general behavior of the matrix element is the one to be expected from a qualitative consideration of Eq. (2). We mention in the following some particular features.

Below the threshold, for small values of k , the results of Table I are, as they should be, in complete agreement with the ones yielded by the series expansion (68). Between every two consecutive resonances, the matrix elements and the cross section vanish for a certain k . The first successive values of k for which this happens are 0.859075, 0.926875, and 0.954935.

TABLE I. Matrix element M for $0 \leq k < 1$.

k	M	k	M
0.000	0.000000	0.830	1.230596
0.040	-0.001804	0.840	0.853766
0.080	-0.007269	0.850	0.451533
0.100	-0.011419	0.860	-0.054939
0.120	-0.016553	0.870	-0.879559
0.160	-0.029936	0.880	-3.150374
0.200	-0.047843		
0.240	-0.070882	0.890	32.260389
0.280	-0.099907	0.894	7.418436
0.300	-0.117022	0.898	4.313409
0.320	-0.136117	0.902	3.043218
0.360	-0.181213	0.906	2.312466
0.400	-0.237667	0.910	1.803441
0.440	-0.309189	0.914	1.394717
0.480	-0.401605	0.918	1.021148
0.500	-0.458448	0.922	0.628449
0.520	-0.524625	0.926	0.136127
0.560	-0.695805	0.930	-0.667435
0.600	-0.950750	0.934	-2.906862
0.640	-1.375285	0.936	-8.169314
0.680	-2.246993		
0.700	-3.177142	0.938	27.981406
0.720	-5.303624	0.940	6.145775
0.740	-15.763602	0.942	3.630968
		0.944	2.593248
0.760	15.382871	0.946	1.978565
0.770	7.538338	0.948	1.529699
0.780	4.890397	0.950	1.143898
0.790	3.535672	0.952	0.755875
0.800	2.691623	0.954	0.287687
0.810	2.094936	0.956	-0.441666
0.820	1.629203	0.958	-2.278530

²⁹ The less accurate numerical results reported by Constantinescu and Gavrilă (Ref. 6) agree within their estimated errors with those of Tables I and II. The agreement is good also with the values obtained for $0 \leq k \leq 0.750$ by Mittleman and Wolf (private communication). See also Ref. 5 and 6.

³⁰ The complete results are contained in M. Gavrilă, Joint Institute for Laboratory Astrophysics, Boulder, Colorado Report 86, 1966 (unpublished).

TABLE II. Matrix element M for $1 \leq k \leq 50$.

k	$\text{Re}M$	$(-\text{Im}M)$
1.000	1.077480	1.227526
1.200	1.187203	0.901823
1.400	1.221606	0.690007
1.600	1.226119	0.544400
1.800	1.218422	0.440031
2.000	1.205980	0.362705
2.400	1.178284	0.258045
2.800	1.153045	0.192414
3.200	1.131855	0.148635
3.600	1.114414	0.118025
4.000	1.100074	0.095814
4.400	1.088218	0.079209
4.800	1.078335	0.066483
5.200	1.070027	0.056525
5.600	1.062983	0.048593
6.000	1.056961	0.042179
6.400	1.051774	0.036922
6.800	1.047276	0.032563
7.200	1.043349	0.028910
7.600	1.039900	0.025821
8.000	1.036855	0.023187
8.400	1.034152	0.020924
8.800	1.031741	0.018965
9.200	1.029582	0.017261
9.600	1.027641	0.015768
10.000	1.025888	0.014455
12.000	1.019235	0.009774
14.000	1.014885	0.006997
16.000	1.011880	0.005226
18.000	1.009713	0.004032
20.000	1.008097	0.003193
24.000	1.005887	0.002126
28.000	1.004482	0.001503
32.000	1.003530	0.001111
36.000	1.002856	0.000850
40.000	1.002359	0.000668
44.000	1.001983	0.000537
48.000	1.001691	0.000439
50.000	1.001569	0.000400

From Table II one sees that above threshold, $\text{Re}M$ is always close to 1 presenting a slight maximum at $k=1.548$. $\text{Im}M$ is negative and decreasing in absolute value. The resulting $|M|^2$ is a monotonically decreasing function of k ; the maximum of $\text{Re}M$ is prevented from manifesting itself because of the rapid decrease of $\text{Im}M$. At threshold $|M|^2 = 2.667783$. For large values of k , $|M|^2$ slowly approaches the value 1.³¹

Our computation extends to $k=50$. At high energies formula (88) for M can be used with good accuracy.²¹

ACKNOWLEDGMENTS

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³¹ In contrast to this, when taking into account retardation, $|M|^2$ of Eq. (1) tends to zero as $k \rightarrow \infty$ for all scattering angles except for forward scattering.