

## Radiative corrections to atomic photoeffect and tip bremsstrahlung. III

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The radiative corrections to the photoeffect from the  $K$  shell were evaluated recently by McEnnan and Gavrilă assuming a hydrogenlike atomic model. The result was expressed in the form of a corrective factor  $[1 + (\alpha/\pi)\delta]$  multiplying the basic photoeffect differential cross section. An expression for  $\delta$ , correct to lowest order in  $\alpha$  and  $\alpha Z$ , was derived in analytic form in terms of a large number of single and double integrals over Feynman parameters, requiring numerical integration.  $\delta$  depends on the photon energy  $\omega$ , on the electron-ejection angle  $\theta$ , and on the energy threshold  $\Delta E$  below which we allow the additional (soft) photon, emitted together with the ejected electron to go undetected. The  $\Delta E$  dependence of  $\delta$  reflects the inseparable connection between the  $K$ -shell photoeffect and the Compton effect from the  $K$  shell with (soft) photons emitted in the range  $\Delta E$ . It was shown that the same expression for  $\delta$ , with an appropriate redefinition of the variables, also radiatively corrects the bremsstrahlung spectrum at its high-energy tip. In the present work we have carried out the computation of  $\delta$ . It covers the  $\omega$  energy range from 0.5 keV to 50 MeV at all relevant angles. The relative error was kept below 0.001, except at high energies where it was only 0.01. We find that  $(-\alpha\delta/\pi)$  is always positive and increases with  $\theta$  and  $\omega$ . At energies of about 500 keV,  $(\alpha\delta/\pi)$  becomes of the order of 1% and at 5 MeV it has grown to about 5%, when taking  $\Delta E = 0.01mc^2$ . By integrating over the angles we have derived the quantity  $\Delta$  which radiatively corrects the total photoelectric cross section, in the form of a factor  $[1 + (\alpha/\pi)\Delta]$ . We also infer by exponentiation the correct form of  $\delta$  and  $\Delta$  in the limit  $\Delta E \rightarrow 0$ . Finally, we derive the expression for the cross section describing the energy spectrum of the electrons emitted in the vicinity of the photoelectric peak, which is the basic information coming from coincidence experiments.

### I. INTRODUCTION

Over the years evaluations of radiative corrections have been performed for many atomic bound-state problems and scattering processes, in some cases to high orders. Nevertheless, it was only recently that the radiative corrections to the atomic photoeffect were first considered. Possible reasons for such a delay are several. For example, at higher energies, where radiative corrections might be expected to become significant, the photoeffect is quite difficult to observe and in the past experimental results were subject to large errors. At the same time, the accuracy of the earlier theoretical calculations of the basic photoeffect cross section at high energies have been rather low.

In recent years our knowledge of the photoeffect has improved considerably due to advances in both

theory and experiment. Increasingly accurate numerical computations in the relativistic energy range (photon energy of the order of the electron rest energy or larger) have yielded values of the basic cross section which are probably accurate to a few percent. This same degree of accuracy has been attained in recent experiments at these relativistic energies. Within experimental errors, measurements of the cross section agree with the theoretical calculations. Since one expects the radiative corrections to be of the order of a few percent of the basic cross section at high energies, the point is being approached at which their existence may become apparent. Therefore, it seemed timely to attempt their evaluation.

The calculation of the radiative corrections to the atomic photoeffect was carried out for the case of the  $K$  shell by McEnnan and Gavrilă<sup>1,2</sup> (Ref. 2

will be denoted in the following by I). The corrected cross section  $d\sigma_K(\Delta E)/d\Omega$  was expressed in the form of a factor  $1 + (\alpha/\pi)\delta$  multiplying the basic cross section  $d\sigma^{(0)}/d\Omega$  ( $\Delta E$  represents the photon energy resolution, see Sec. II).  $\delta$ , correct to lowest order in  $\alpha$  and  $\alpha Z$ , was given in terms of closed form functions and a large number of integrals, which could not be performed analytically. A numerical evaluation of these integrals required a substantial computational effort that could not be made at the time.

It has also been shown<sup>1,3</sup> that the radiative corrections to electron bremsstrahlung in the field of an atom, at the high-energy end of the photon spectrum ("tip bremsstrahlung"), can be expressed to lowest order by the same fractional correction  $\delta$  as that occurring for the photoeffect. (Henceforth, Ref. 3 will be denoted by II.)

In this paper we present the numerical evaluation of  $\delta$  and interpret the results. We hope that this work will stimulate an experimental search for these corrections. At present this still appears to be a task of considerable complexity but the situation will undoubtedly improve in the future due to the ever increasing accuracy of the detection methods.

The outline of our paper is as follows. In Sec. II we review the analytic results derived in papers I and II. We shall present these in a rather self-contained manner, emphasizing those aspects needed for the understanding of the physics. Next, in Sec. III, we describe the computation of  $\delta$ , and its features at low and high energies. The numerical results obtained for  $\delta$ , and its angular-integrated counterpart are presented in Tables I and II, respectively, and are commented on in Sec. IV. In Sec. V we discuss some extensions of our results. Firstly, by applying the exponentiation procedure a more general expression for  $d\sigma_K(\Delta E)/d\Omega$ , valid also for  $\Delta E \rightarrow 0$ , is obtained. This allows the derivation of the energy distribution of the ejected electrons, described by the cross section  $d^2\sigma/d\epsilon d\Omega$ , where  $\epsilon$  is the energy loss of the electron with respect to the value predicted by the energy conservation equation. Some comments are made on the connection to experiment. Finally, the  $\alpha Z$  and screening corrections to our results are briefly considered. In the Appendix an Errata is given for the previous three papers, Ref. 1, 2, and 3.

## II. ANALYTIC FORMULATION

The atomic model adopted in I for the description of the  $K$ -shell photoeffect was that of an in-

dependent electron under the influence of a Coulomb field of a nucleus of charge  $Z$ . (Possible electron-screening corrections to this model are considered in Sec. V.) At high photon energies and for arbitrary values of  $Z$ , where the relativistic Dirac theory is required, the photoeffect cross section cannot be expressed in simple analytic form even for this model, and a numerical computation has to be carried out. (The current status of the theory of the atomic photoeffect, for high-incident photon energies, is summarized in the review article by Pratt *et al.*<sup>4</sup>) However, for light elements ( $\alpha Z \ll 1$ ) and high photoelectron velocities ( $\alpha Z/\beta \ll 1$ ), Sauter was able to obtain an analytic approximation to the relativistic cross section, correct to lowest order in  $\alpha Z$  [i.e.,  $\alpha(\alpha Z)^5$ ].<sup>4,5</sup>

The radiative corrections to the  $K$ -shell photoeffect were calculated in I to lowest order in the radiation field, and with the same limiting conditions,  $\alpha Z \ll 1$  and  $\alpha Z/\beta \ll 1$ , as the Sauter result. The matrix elements were expressed in the Furry picture of QED. In this picture, the wave functions and the electron propagators contain all effects of the potential so that the resulting matrix elements are exact in  $\alpha Z$ . Neglecting second and higher orders in  $\alpha Z$  and  $\alpha Z/\beta$ , the ground state can be expressed in terms of the Pauli approximation, and the final state in terms of a Born expansion, respectively. Two terms in the Born expansion were retained to get a consistent lowest-order result in  $\alpha Z$ . For the electron propagators in the Coulomb field, it was argued that it is consistent to use a Born expansion with the first two terms retained, as was done for the final state. By applying the renormalization program of QED, the ultraviolet divergences were eliminated. The infrared divergences were avoided in the usual manner by attributing a finite mass  $\lambda$  to the photon. This allowed the calculation of a finite "virtual-photon correction" to the photoeffect cross section. Elimination of the fictitious mass  $\lambda$  was done as usually by recognizing that any physical process can be accompanied by the emission of photons. Only events in which the secondary photons are emitted below a certain energy threshold  $\Delta E$  are considered. If  $\Delta E$  is not excessively small (see Sec. VA), there is an appreciable probability for the emission of only *one* photon in the range  $\Delta E$ . This is the process if Compton scattering by a bound  $K$ -shell electron, in which the energy of the final photon is less than  $\Delta E$ . For reasons of calculational convenience the assumption  $\Delta E \ll 1mc^2$  was adopted and terms vanishing in the limit  $\Delta E \rightarrow 0$

were dropped (soft-photon approximation). Further, for consistency, a mass  $\lambda$  was attributed to the photon. In this way the Compton cross section could easily be derived. Finally, the incoherent addition of the latter to the cross section contributed by the virtual photons considered before results in the physical, corrected photoeffect cross section, which is independent of  $\lambda$  although it is dependent upon  $\Delta E$ . Note that, due to the conservation of energy, the emission of a soft photon of energy less than  $\Delta E$  implies an energy loss for the ejected electron of not more than  $\Delta E$ .<sup>6,7</sup>

The units used throughout I, II, and the present paper are "natural units,"  $\hbar=c=m_e=1$ . Consequently, momenta are measured in units of  $mc$ , energies in units of  $mc^2$ , and the cross sections in squares of the Compton wavelength. (Notations will be the same as in I and II.) Neglecting terms of order  $(\alpha Z)^2$ , the energy conservation equation is

$$E_f = 1 + \omega, \quad (1)$$

where  $\omega$  and  $E_f = (1 - \beta^2)^{-1/2}$  are the energy of the incident photon and the kinetic energy of the ejected electron, respectively. The variables  $\kappa$  and

$$\delta = \Lambda + \left[ \frac{2 - \tau}{\tau} - \frac{8}{\kappa\tau} \right]^{-1} \text{Re}[R_1 + (1 - \tau)R_2 - (\kappa - \tau - 8)R_3 - 2R_4]. \quad (5)$$

The  $R_n$  are functions of only  $\kappa$  and  $\tau$ , and are defined by Eqs. (5.8), (5.14)–(5.16), (5.20), (5.22)–(5.27), and Tables I–III of paper I. The function  $\Lambda$ , on the other hand, depends on  $\tau$  and  $\Delta E$ , but is angle independent. It is defined by Eq. (6.8) in I, and because of its form we may separate the  $\Delta E$ -dependent part of  $\delta$  as

$$\delta = \delta_0 + \delta_1, \quad (6)$$

where

$$\delta_1 = A \ln \Delta E, \quad (7)$$

$$A = -2 + \frac{1}{\beta} \ln \frac{1 + \beta}{1 - \beta}, \quad (8)$$

and  $\delta_0$  is  $\Delta E$  independent.

The quantities  $R_n$  contain elementary functions together with 50 Feynman-parameter integrals which cannot be expressed analytically in general. Each of these integrals is well defined for all (finite) values of  $\kappa$  and  $\tau$ . They are of the form [see Eqs. (5.23)–(5.27) in I]:

$$G_n^{\tau\kappa} = \int_0^1 dy \Gamma_n^{\tau\kappa}(\kappa, \tau; y) g_{n\tau}(\kappa, \tau; y), \quad (9)$$

$\tau$  are defined by

$$\kappa = 2\omega E_f (1 - \beta \cos \theta) \simeq |\vec{p} - \vec{k}|^2, \quad \tau = 2\omega, \quad (2)$$

where  $\vec{k}$  and  $\vec{p}$  are the momenta of the photon and electron, respectively, and  $\theta$  is the angle between  $\vec{p}$  and  $\vec{k}$ .

The radiatively corrected differential cross section derived in I for the  $K$ -shell photoeffect, summed over the electron and photon polarizations, which allows for the emission of one soft photon in the range  $\Delta E \ll 1$ , is [see Eq. (6.14) in I (Refs. 8–10)]

$$\frac{d\sigma_K(\Delta E)}{d\Omega} = \frac{d\sigma_K^{(0)}}{d\Omega} \left[ 1 + \frac{\alpha}{\pi} \delta \right], \quad (3)$$

where  $d\sigma_K^{(0)}/d\Omega$  is the Sauter cross section,

$$\frac{d\sigma_K^{(0)}}{d\Omega} = \alpha(\alpha Z)^5 \frac{8 |\vec{p}|^3 \sin^2 \theta}{\omega |\vec{p} - \vec{k}|^8} \times [4 + (\omega - 1) |\vec{p} - \vec{k}|^2]. \quad (4)$$

The radiative correction  $\delta$ , given by Eq. (6.15) in I, has the form

$$H_n^{\tau\kappa} = \int_0^1 \int_0^1 dx dy \theta_n^{\tau\kappa}(\kappa, \tau; x, y) h_{n\tau}(\kappa, \tau; x, y), \quad (10)$$

$$J_n^{\tau\kappa} = \int_0^1 \int_0^1 dx dy K_n^{\tau\kappa}(\kappa, \tau; x, y) j_{n\tau}(\kappa, \tau; x, y), \quad (11)$$

where the factors in the integrands are given in Tables I–III of I. Nevertheless, in the nonrelativistic limit  $\omega \ll 1$ , and in the high-energy limit  $\omega \gg 1$  at finite momentum transfer  $\sqrt{\kappa}$ , simple analytic forms could be obtained for these integrals and hence for  $\delta$  [see Eqs. (7.1) and (7.2) in I].

In the nonrelativistic case one finds:

$$\delta = \beta^2 \left[ -\frac{19}{45} + \frac{2}{3} \ln(2\Delta E) \right] - \frac{4}{3} \beta^3 \cos \theta \ln \beta + \frac{559}{720} \beta^3 \cos \theta + O(\beta^4 \ln \beta). \quad (12)$$

In Eq. (12) we include the order  $\beta^3$  term which was not given previously in Eq. (7.1) in I. Since the calculation of  $\delta$  is based on the Born approximation, Eq. (12) will be physically valid only a sufficiently high (nonrelativistic) values of  $\beta$ .

In the high-energy limit the result is

$$\delta = 2(\ln \tau - 1) [\ln(2\Delta E) - \frac{1}{2} \ln \tau] - \ln \kappa \ln \tau + O(1). \quad (13)$$

The  $O(1)$  term with respect to the energy in Eq. (13) is a function of  $\kappa$ ; it could not, unfortunately, be obtained analytically. Equation (13) approximates the exact  $\delta$  on condition that  $\kappa$  can be neglected with respect to  $\tau$ , i.e.:  $\tau \gg \kappa \geq 1$ . (Note that at high energies  $\kappa \geq 1$ .)

The total cross section corresponding to Eq. (3) can be written as

$$\sigma_K = \sigma_K^{(0)} \left[ 1 + \frac{\alpha}{\pi} \Delta \right], \quad (14)$$

where  $\sigma_K^{(0)}$  is the total Sauter cross section, and the expression for  $\Delta$  is

$$\Delta = \frac{1}{\sigma_K^{(0)}} \int \delta \frac{d\sigma_K^{(0)}}{d\Omega} d\Omega. \quad (15)$$

In general, since  $\delta$  is only given in numerical form, the integration over the angles in Eq. (15) must be evaluated numerically. However, in the high-energy limit, by using Eq. (13) and the high energy-limit of  $d\sigma_K^{(0)}/d\Omega$ , an analytic expression can be derived for  $\Delta$ , see Eq. (7.6) in I:

$$\Delta = 2(\ln\tau - 1)(\ln 2\Delta E - \frac{1}{2}\ln\tau) - \frac{3}{2}\ln\tau + \overline{O(1)}. \quad (16)$$

As does  $\delta$  itself,  $\Delta$  contains the not analytically determined term of order one in the high-energy limit,  $\overline{O(1)}$ .

The radiative corrections to the case of tip bremsstrahlung are the subject of II.<sup>11</sup> Tip bremsstrahlung is that process in which an incoming electron is accelerated in the atomic potential and radiates all its kinetic energy in the form of one photon, thereby being left (quasi) at rest. This is a case which cannot be handled by the usual Born-approximation techniques since the velocity of the final electron  $\beta_2$  is (quasi) zero ( $\alpha Z/\beta_2 \gg 1$ ). Apart from atomic binding effects, i.e., neglecting terms of order  $(\alpha Z)^2$ , tip bremsstrahlung and photoeffect are essentially inverse processes and the energy conservation equation, Eq. (1), still applies. This idea was used by Fano and collaborators, and by Pratt (see II) to derive a simple relation between the differential cross sections for tip bremsstrahlung  $(d^2\sigma^{(0)}/d\omega d\Omega)_{\text{TB}}$  and photoeffect  $(d\sigma_K^{(0)}/d\Omega)$ , which holds to first order in  $\alpha Z$ , see Eq. (6) in II. In II it was proven that this relation remains valid when including radiative corrections to lowest order in  $\alpha$ . The fractional radiative correction  $\delta$  to the tip bremsstrahlung cross section,<sup>12</sup> defined as

$$\left[ \frac{d^2\sigma}{d\omega d\Omega} \right]_{\text{TB}} = \left[ \frac{d^2\sigma^{(0)}}{d\omega d\Omega} \right]_{\text{TB}} \left[ 1 + \frac{\alpha}{\pi} \delta \right], \quad (17)$$

is the same as for the photoeffect, see Eq. (3).

Here  $(d^2\sigma^{(0)}/d\omega d\Omega)_{\text{TB}}$  is the basic tip bremsstrahlung cross section, which can be derived to lowest order in  $\alpha Z$  from the Sauter cross section Eq. (4) by multiplication with  $\omega^2/(\alpha Z)^2 p^2$ . The  $\vec{p}$ ,  $E_f$ , and  $\vec{k}$ ,  $\omega$  entering the expression of  $\delta$  now characterize the incoming electron and the radiated photon, respectively. Equation (17) specifically applies to the tip of the spectrum ( $\beta_2 \simeq 0$ ), a case not covered by other Born-type radiative corrections calculations to bremsstrahlung (see II).

By integrating over the angles Eq. (17), the tip value of the spectral distribution is

$$\left[ \frac{d\sigma}{d\omega} \right]_{\text{TB}} = \left[ \frac{d\sigma^{(0)}}{d\omega} \right]_{\text{TB}} \left[ 1 + \frac{\alpha}{\pi} \Delta \right], \quad (18)$$

where  $(d\sigma^{(0)}/d\omega)_{\text{TB}}$  corresponds to  $(d^2\sigma^{(0)}/d\omega d\Omega)_{\text{TB}}$  and, to lowest order in  $\alpha Z$ ,  $\Delta$  coincides with the one given in Eq. (15).

### III. COMPUTATION

The radiative correction  $\delta$  is a function of three variables: the photon energy  $\omega$ , the emission angle  $\theta$  (or, alternatively, the momentum transfer squared  $\kappa$ ), and the energy resolution  $\Delta E$ . The dependence of  $\delta$  on  $\Delta E$  is such that the values  $\delta$  and  $\delta'$  corresponding to the two values  $\Delta E$  and  $\Delta E'$ , are related by [see Eqs. (6)–(8)]

$$\delta' = \delta + A \ln \left[ \frac{\Delta E'}{\Delta E} \right]. \quad (19)$$

This equation allows the calculation of  $\delta$  for any  $\Delta E$  once a computation has been carried out for some specific  $\Delta E$ . We have chosen this reference value to be  $\Delta E = 0.01$ .

Some of the quantities contained in  $\delta$ , Eq. (5), are expressed in terms of simple functions which can be easily evaluated. Such quantities are  $\Lambda$ , see Eq. (6.8) in I, and the  $P_n$ ,  $M_n$ , and  $F_n$  appearing in the  $R_n$  ( $n = 1, \dots, 4$ ) of Eq. (5), see Eqs. (5.8)–(5.22) and (6.15) in I. Both the  $\Lambda$  and  $M_n$  explicitly depend upon the Euler dilogarithm  $L_2(z)$ , which is a quantity frequently appearing in radiative corrections calculations. (Detailed accounts of this function are given in Refs. 13 and 14.) From Eq. (6.15) in I it is apparent that in our case only the real part of  $L_2(z)$  is needed, which is given by [see

Eqs. (5.19) and (5.21) in I]

$$\operatorname{Re}L_2(z) = - \int_0^z \frac{\ln|1-x|}{x} dx .$$

For any real  $z$ ,  $L_2(z)$  can be expressed in terms of logarithms and another function  $L_2(x)$  of a different variable, contained in the range  $(0, \frac{1}{2})$ . For the latter one can use a rapidly convergent series expansion.

The other quantities contained in the  $R_n$  of  $\delta$  are the integrals  $G_n^{\mathcal{R}}$ ,  $H_n^{\mathcal{R}}$ , and  $J_n^{\mathcal{R}}$ . The functions  $g_{\mathcal{R}}(y)$ ,  $h_{\mathcal{R}}(x,y)$ , and  $j_{\mathcal{R}}(x,y)$  appearing in the integrands exhibit a number of common traits. For example, some of the  $g_{\mathcal{R}}(y)$  have a logarithmic singularity at  $y=0$ , and some of the  $j_{\mathcal{R}}(x,y)$  have a logarithmic singularity at  $x=0$ . These singularities are integrable and, if one chooses a quadrature formula which avoids evaluating the integrands at  $x=0$  or  $y=0$ , these points present no numerical difficulties. Also, many of the functions  $g_{\mathcal{R}}(y)$ ,  $h_{\mathcal{R}}(x,y)$ , and  $j_{\mathcal{R}}(x,y)$  contain in their denominators the quantities

$$\begin{aligned} q_y^2 &= 1 - \kappa y^2, \\ q_x^2 &= -\kappa\kappa + [\tau y(1-y) - \kappa y](1-x)^2 \\ &\quad + \kappa y(1-x) + 1, \end{aligned}$$

which can vanish within the domain of integration.<sup>15</sup> In the case of  $q_y^2$  this happens for a certain point  $y_0$  of the integration interval  $(0,1)$ , defined by  $q_y^2(y_0)=0$ . In the case of the  $q_x^2$ , this occurs along a line  $y_0=y_0(x)$  crossing the integration square, defined by  $q_x^2[x, y_0(x)]=0$ . Nevertheless, the functions  $g_{\mathcal{R}}$ ,  $h_{\mathcal{R}}$ , and  $j_{\mathcal{R}}$  are not singular at these points due to the fact that the numerators also vanish. Thus, the singularities are only apparent. This can easily be seen by expanding the functions involved in powers of  $q_y^2$  and  $q_x^2$ , assumed to be small. To evaluate those integrands containing in their denominators  $q_y^2$  or  $q_x^2$  near the points  $(x,y)$  for which  $|q_x^2| < 10^{-7}$ , we replaced the numerically evaluated functions  $g_{\mathcal{R}}$ ,  $h_{\mathcal{R}}$ , or  $j_{\mathcal{R}}$  by their series expansions in  $q_x^2$  or  $q_y^2$ .

An open-panel integration method was chosen in the form of a simple (case of  $y$  integrations) or composite (case of  $x$  and  $y$  integrations) third-order Gaussian quadrature with a predetermined step size, to minimize program complexity and to avoid evaluating logarithmic singular integrands at the end points  $x=0$  or  $y=0$ . The step size was varied, in general, in the different parts of the integrations domains depending upon the energy  $\omega$ .

The desired level of accuracy in the computation

was achieved by repeating the integration with decreasing step sizes. The procedure was stopped at the point when the difference in results between two consecutive integrations was smaller than the error allowed. In fact, rather than checking the accuracy for each integral separately, we preferred to check it for the combination  $R_1 + (1-\tau)R_2 - (\kappa-\tau-8)R_3 - 2R_4$  explicitly appearing in  $\delta$ , thereby preventing the loss of significant figures due to the cancellation between various terms.

To test the accuracy and correctness of the numerical code we have performed a number of checks. For example, we have compared the numerical results with those derived analytically for the low- and high-energy limits. We did not consider it sufficient to compare with the overall limiting results for  $\delta$  given in Eqs. (12) and (13) because not all of the 50 integrals [Eqs. (9)–(11)] contribute to these limits and, further, considerable cancellation occurs. Instead, we have tested *each* of the integrals against its low- and high-energy analytic limits. The test against the high-energy limits required the use of more refined integration procedures than those needed for the values of  $\omega$  physical interest.

In what follows we shall describe in more detail our integration procedures for low and high energies. At *low and intermediate*  $\omega$ , i.e., from about 0.5 keV to about 1 MeV, the integrands in Eqs. (9)–(11) are slowly varying functions of their variables  $x$  and  $y$ . A rather small number of integration points uniformly distributed in the integration domain sufficed to yield  $\delta$  with a relative error which is, we are confident, smaller than  $10^{-3}$ . When testing the nonrelativistic limit, however, one has to go to much lower energies. We have considered the sequence  $\beta=0.1$ ,  $\beta=0.1$ ,  $\beta=0.001$  and have followed the convergence of the numerical results to their corresponding analytical counterparts. For  $\beta=0.001$  agreement was achieved to better than  $10^{-3}$  in all cases.<sup>16</sup>

At *high energies*  $\omega$ , above about 1 MeV, changes are required in the integration procedures in order to achieve the desired accuracy with a minimum of computer time. This is due to the fact that now the integrands in Eqs. (9)–(11) cease to be smooth functions. Thus, for example, in the extreme case  $\tau \rightarrow \infty$  with  $\kappa$  held fixed,  $(p_x^2)^{-1}$  vanishes in all points of the integration square of the  $(x,y)$  plane, except for the points  $(0,0)$  and  $(0,1)$  where it tends to 1. Similarly  $(p_x^2 - x\tau)^{-1}$ ,  $(q_x^2 + \kappa x)^{-1}$ ,  $(q_x^2)^{-1}$  vanish in all points of the integration square except on its three sides  $y=0$ ;  $x=1$ ;  $y=1$ . The situation

is further complicated by the factors  $\theta_n^{\tau_s}$  and  $K_n^{\tau_s}$  which can vanish on the sides of the square, thereby producing local maxima and/or minima. In these areas the value of the integrands may vary considerably within a distance of  $1/\tau$ , and this variation is sharper the larger  $\tau$ . To deal with

these variations of the integrands we chose to subdivide the integration square into three areas: (1) the vicinities of the points (0,0) and (0,1); (2) a strip along the sides  $y=0$ ;  $x=1$ ;  $y=1$  of the square; (3) the remainder of the square. The integration grid varied from area to area, with the

TABLE I. Values of the radiative correction  $-(\alpha/\pi)\delta$  as a function of the emission angle  $\theta$  (in degrees) and incident photon energy  $\omega$  (in keV). We have taken  $\Delta E=0.01mc^2$ . Numbers in parentheses denote powers of 10.

$\theta \backslash \omega$	0.5	1	10	50	100	200	300	400	500
0	1.270(-5)	2.477(-5)	2.141(-4)	9.142(-4)	1.721(-3)	3.276(-3)	4.785(-3)	6.254(-3)	7.679(-3)
15	1.274(-5)	2.486(-5)	2.161(-4)	9.301(-4)	1.757(-3)	3.371(-3)	4.950(-3)	6.502(-3)	8.021(-3)
30	1.285(-5)	2.513(-5)	2.220(-4)	9.757(-4)	1.866(-3)	3.620(-3)	5.351(-3)	7.049(-3)	8.697(-3)
45	1.301(-5)	2.557(-5)	2.314(-4)	1.046(-3)	2.025(-3)	3.957(-3)	5.836(-3)	7.629(-3)	9.307(-3)
60	1.323(-5)	2.613(-5)	2.434(-4)	1.133(-3)	2.216(-3)	4.330(-3)	6.322(-3)	8.139(-3)	9.762(-3)
75	1.349(-5)	2.679(-5)	2.573(-4)	1.231(-3)	2.422(-3)	4.707(-3)	6.777(-3)	8.569(-3)	1.010(-2)
90	1.376(-5)	2.749(-5)	2.720(-4)	1.333(-3)	2.629(-3)	5.068(-3)	7.194(-3)	8.930(-3)	1.035(-2)
105	1.403(-5)	2.819(-5)	2.866(-4)	1.430(-3)	2.826(-3)	5.404(-3)	7.565(-3)	9.227(-3)	1.055(-2)
120	1.429(-5)	2.884(-5)	3.000(-4)	1.519(-3)	2.999(-3)	5.701(-3)	7.883(-3)	9.461(-3)	1.069(-2)
135	1.450(-5)	2.940(-5)	3.115(-4)	1.593(-3)	3.146(-3)	5.948(-3)	8.139(-3)	9.634(-3)	1.080(-2)
150	1.467(-5)	2.983(-5)	3.202(-4)	1.650(-3)	3.256(-3)	6.130(-3)	8.327(-3)	9.750(-3)	1.086(-2)
165	1.477(-5)	3.010(-5)	3.257(-4)	1.685(-3)	3.325(-3)	6.245(-3)	8.442(-3)	9.814(-3)	1.089(-2)
180	1.481(-5)	3.019(-5)	3.276(-4)	1.697(-3)	3.348(-3)	6.284(-3)	8.481(-3)	9.835(-3)	1.090(-2)

  

$\theta \backslash \omega$	600	662	700	800	900	1000	1100	1200	1332
0	9.060(-3)	9.893(-3)	1.040(-2)	1.169(-2)	1.294(-2)	1.416(-2)	1.534(-2)	1.648(-2)	1.794(-2)
5						1.430(-2)	1.551(-2)	1.668(-2)	1.818(-2)
10						1.466(-2)	1.592(-2)	1.715(-2)	1.873(-2)
15	9.506(-3)	1.041(-2)	1.095(-2)	1.237(-2)	1.375(-2)	1.509(-2)	1.640(-2)	1.767(-2)	1.930(-2)
30	1.028(-2)	1.124(-2)	1.181(-2)	1.327(-2)	1.467(-2)	1.601(-2)	1.731(-2)	1.856(-2)	2.016(-2)
45	1.087(-2)	1.178(-2)	1.233(-2)	1.371(-2)	1.503(-2)	1.632(-2)	1.758(-2)	1.882(-2)	2.042(-2)
60	1.123(-2)	1.208(-2)	1.260(-2)	1.392(-2)	1.523(-2)	1.654(-2)	1.784(-2)	1.914(-2)	2.083(-2)
75	1.147(-2)	1.228(-2)	1.279(-2)	1.412(-2)	1.549(-2)	1.687(-2)	1.826(-2)	1.965(-2)	2.145(-2)
90	1.165(-2)	1.247(-2)	1.298(-2)	1.438(-2)	1.584(-2)	1.732(-2)	1.880(-2)	2.026(-2)	2.216(-2)
105	1.182(-2)	1.265(-2)	1.319(-2)	1.468(-2)	1.623(-2)	1.780(-2)			
120	1.196(-2)	1.283(-2)	1.340(-2)	1.497(-2)	1.661(-2)	1.825(-2)			
135	1.208(-2)	1.299(-2)	1.358(-2)	1.523(-2)	1.694(-2)	1.864(-2)	2.031(-2)	2.195(-2)	2.403(-2)
150	1.216(-2)	1.311(-2)	1.372(-2)	1.543(-2)	1.719(-2)	1.893(-2)			
165	1.221(-2)	1.318(-2)	1.381(-2)	1.556(-2)	1.734(-2)	1.911(-2)			
180	1.223(-2)	1.320(-2)	1.384(-2)	1.560(-2)	1.739(-2)	1.917(-2)	2.091(-2)	2.259(-2)	2.474(-2)

  

$\theta \backslash \omega$	1400	1500	1600	1700	1800	1900	2000	2754	5000
0	1.867(-2)	1.972(-2)	2.074(-2)	2.173(-2)	2.270(-2)	2.364(-2)	2.456(-2)	3.083(-2)	4.496(-2)
5	1.893(-2)	2.002(-2)	2.108(-2)	2.211(-2)	2.312(-2)	2.411(-2)	2.508(-2)	3.176(-2)	4.735(-2)
10	1.953(-2)	2.068(-2)	2.180(-2)	2.289(-2)	2.396(-2)	2.501(-2)	2.603(-2)	3.308(-2)	4.918(-2)
15	2.012(-2)	2.130(-2)	2.244(-2)	2.356(-2)	2.465(-2)	2.571(-2)	2.674(-2)	3.382(-2)	4.981(-2)
30	2.096(-2)	2.211(-2)	2.323(-2)	2.433(-2)	2.540(-2)	2.644(-2)	2.747(-2)	3.453(-2)	5.062(-2)
45	2.124(-2)	2.241(-2)	2.357(-2)	2.470(-2)	2.581(-2)	2.690(-2)	2.796(-2)	3.530(-2)	5.210(-2)
60	2.169(-2)	2.294(-2)	2.416(-2)	2.535(-2)	2.652(-2)	2.767(-2)	2.879(-2)	3.648(-2)	5.405(-2)
75	2.236(-2)	2.367(-2)	2.496(-2)	2.622(-2)	2.744(-2)	2.864(-2)	2.981(-2)	3.783(-2)	5.609(-2)
90	2.312(-2)	2.449(-2)	2.583(-2)	2.714(-2)	2.842(-2)	2.966(-2)	3.087(-2)		
135	2.508(-2)	2.657(-2)	2.803(-2)	2.944(-2)	3.081(-2)	3.214(-2)	3.344(-2)		

TABLE I. (Continued.)

$\theta$ \ / \ $\omega$	6756	$10^4$	$2 \cdot 10^4$	$5 \cdot 10^4$
0	5.319(-2)	6.49(-2)	8.81(-2)	1.23(-1)
1		6.56(-2)	9.05(-2)	1.32(-1)
2		6.70(-2)	9.39(-2)	1.37(-1)
3		6.85(-2)	9.60(-2)	1.39(-1)
5	5.676(-2)	7.05(-2)	9.80(-2)	1.39(-1)
10	5.864(-2)	7.21(-2)	9.87(-2)	1.39(-1)
15	5.914(-2)	7.24(-2)	9.89(-2)	1.40(-1)
30	6.012(-2)	7.39(-2)	1.02(-1)	1.48(-1)
45	6.210(-2)	7.67(-2)	1.07(-1)	
60	6.452(-2)			

most dense mesh in area (1), followed by areas (2) and (3). This allowed us to concentrate the integration points in those areas where the integrands varied most rapidly, thereby attaining the desired accuracy with minimal computer time. For energies less than 5 MeV we still could achieve a relative error of about  $10^{-3}$ . However, at still higher energies, the computation time increases dramatically, so that we could keep the errors only at the  $10^{-2}$  level.

In order to test the high-energy limit of the computation we have considered very large values of  $\tau$ , such as  $\tau=10^3$  and  $\tau=10^4$ . Extreme numerical precautions had to be taken in these cases. We were able to verify that the computed values of the integrals approached their analytic limits.<sup>17</sup>

To conclude, we mention that for the numerical integration of  $\Delta$  from Eq. (15) we have used for  $d\sigma_K^{(0)}/d\Omega$  its analytical form and for  $\delta$  an accurate interpolation polynomial derived from the minimax principle. Thus, the error on  $\Delta$  is about the same as on  $\delta$ . Since an equation similar to Eq. (19) holds also for  $\Delta$ , it is sufficient to consider the case of  $\Delta E=0.01$ .

#### IV. RESULTS

We have computed the radiative corrections to the photoeffect (under the limitations discussed in Sec. II) for a wide range of incident photon energies and emission angles, covering all situations of practical interest. In Table I we present our results for  $(\alpha/\pi)\delta$  as a function of  $\omega$  and  $\theta$ , given that  $\Delta E=0.01mc^2$ . The range of incident photon energies extends from 0.5 keV to 50 MeV. For energies up to 1.3 MeV the range of  $\theta$  was from  $0^\circ$  to  $180^\circ$ . For higher energies, due to limitations on computer time, we give results for  $(\alpha/\pi)\delta$  at only

those angles for which the Sauter cross section is large, and neglect the angular range over which the Sauter cross section has decreased 3 orders of mag-

TABLE II. Values of the radiative correction  $-(\alpha/\pi)\Delta$  as a function of the photon energy  $\omega$ . We have taken  $\Delta E=0.01mc^2$ . Numbers in parentheses denote powers of 10.

$\omega$	$-(\alpha/\pi)\Delta$
0.5 keV	1.372(-5)
1	2.735(-5)
10	2.629(-4)
50	1.193(-3)
100	2.226(-3)
200	4.072(-3)
300	5.742(-3)
400	7.306(-3)
500	8.797(-3)
600	1.169(-2)
662	1.110(-2)
700	1.164(-2)
800	1.298(-2)
900	1.429(-2)
1000	1.555(-2)
1100	1.682(-2)
1200	1.803(-2)
1332	1.959(-2)
1400	2.036(-2)
1500	2.148(-2)
1600	2.256(-2)
1700	2.362(-2)
1800	2.465(-2)
1900	2.566(-2)
2000	2.664(-2)
2754	3.35(-2)
5000	4.84(-2)
10 MeV	6.97(-2)
20	9.44(-2)
50	1.32(-1)

nitude from its peak value.<sup>18</sup> (At such large energies and angles the photoeffect cannot be detected by present experimental techniques.) In Table II we give our results for the  $\omega$  dependence of the integrated correction  $(\alpha/\pi)\Delta$  for a sample of the incident photon energies. We estimate that the values given in Table I and II are accurate to about the last digit displayed (see the discussion in Sec. III).

Table I combined with Eq. (19) shows that, for  $\Delta E/E_f \ll 1$ ,  $(\alpha/\pi)\delta$  is always negative and decreases with increasing  $\theta$ . This agrees with both the low- and high-energy limiting forms, Eqs. (12) and (13). Consequently, the radiative corrections decrease the basic photoeffect cross section.

The variation of  $(\alpha/\pi)\delta$  is rather weak over the angular range of the peak of the Sauter cross section. This means that the corrective term  $(\alpha/\pi)\delta d\sigma_K^{(0)}/d\Omega$ , has an angular dependence similar to that of the Sauter cross section  $d\sigma_K^{(0)}/d\Omega$  itself (i.e., has a sharp maximum shifting towards zero angle with increasing energy). Below 500 keV,  $(\alpha/\pi)\delta$  decreases smoothly as  $\theta$  increases; above this energy a slight shoulder sets in.<sup>19</sup>

As the photon energy increases,  $(\alpha/\pi)\delta$  increases in magnitude (becomes more negative). At low energies, below a few keV, it is very small, less than 0.02%. The agreement with the analytic, nonrelativistic formula of Eq. (12) is quite good in this case.<sup>20</sup> (For  $\omega \leq 5$  keV, the agreement is to within 1%, but for  $\omega = 100$  keV it is only to within 30%.) At energies of about 500 keV,  $(\alpha/\pi)\delta$  becomes of the order of 1%, and at 5 MeV it has grown to about 5%.

At very high energies one may compare the numerical results with Eq. (13). This comparison is hindered by the fact that the terms of  $O(1)$  with respect to  $\tau$  contained in Eq. (13) could not be determined analytically. Note that these terms are, in fact, of the form

$$O(1) = \phi(\kappa) + \mathcal{R}, \quad (20)$$

where  $\phi$  is an unknown function of  $\kappa$ , and  $\mathcal{R}$  contains terms of order  $1/\tau$  or higher, vanishing in the limit  $\tau \rightarrow \infty$  at finite  $\kappa$  [e.g.,  $\kappa/\tau, \kappa(\ln^2\tau)/\tau$ , etc.].

To circumvent this difficulty we have subtracted the values of the analytic expression contained in  $\delta$  of Eq. (13) from the numerical results, thus obtaining the unknown term  $O(1)$ . This was done at the two highest energies of our calculation,  $\omega = 20$  MeV ( $\tau = 78$ ) and  $\omega = 50$  MeV ( $\tau = 196$ ). The results are given in Table III. By comparing them we find in both cases that, for the lower values of  $\sqrt{\kappa}$ ,  $O(1)$  is very well represented by  $3\sqrt{\kappa}$ . As  $\sqrt{\kappa}$  increases beyond a certain value (about 3.03 for  $\omega = 20$  MeV, and 3.57 for  $\omega = 50$  MeV) the agreement deteriorates. This is not surprising in view of the fact that the corrective term  $\mathcal{R}$  in Eq. (20) contains terms which can become large when  $\kappa$  increases towards  $\tau$ . Consequently, we infer from Table III that, to a good approximation,

$$\phi(\kappa) = 3\sqrt{\kappa}. \quad (21)$$

By combining Eqs. (13), (20), and (21) we now have an improved formula for the high-energy limit. Note that the relative error the  $\mathcal{R}$  of Eq. (20) transmits to  $\delta$  decreases with the energy.

We may proceed similarly in the case of the high-energy expression of  $\Delta$  given by Eq. (16). Here we can write the unknown  $\overline{O(1)}$  term as

$$\overline{O(1)} = c + \mathcal{S},$$

where  $c$  is a constant and  $\mathcal{S}$  is a function of  $\tau$  vanishing for  $\tau \rightarrow \infty$ . The value of  $c$  can be calculated analytically given the form of  $\phi(\kappa)$  of Eq. (21). The result is  $c = 5\sqrt{2} = 7.07$ . This is quite consistent with the values obtained by subtracting the analytic part of Eq. (16) from the numerical results for  $\Delta$  at 20 and 50 MeV given in Table II. We thus find  $\overline{O(1)} = 6.84$  and  $\overline{O(1)} = 7.19$ , respectively.

## V. DISCUSSION

### A. Exponentiation

When considering our corrected photoeffect cross section  $d\sigma_K(\Delta E)/d\Omega$  of Eqs. (3), (6), and (7), we find that for  $\Delta E \rightarrow 0$  it has the unphysical

TABLE III. Momentum-transfer dependence of the quantity  $O(1)$  appearing in Eq. (13), as derived from the comparison with the numerical data at  $\omega = 20$  MeV and  $\omega = 50$  MeV.

$\omega$ (MeV) \ $\sqrt{\kappa}$	0.988	0.995	1.54	2.03	3.03	3.57	5.24	6.98
20	2.93		4.66	6.11	8.67			15.84
50		3.01				10.50	13.69	



feature that it becomes negative and diverges logarithmically. The case when for some reason a transition probability calculated by perturbation theory becomes large and/or negative indicates that the limits of validity of the theory have been violated. In order to be able to also encompass the  $\Delta E \rightarrow 0$  case, a higher order in  $\alpha$  calculation of the radiative corrections is needed.

The calculation of I involved only *one* virtual and *one* real soft photon (see the diagrams in Figs. 3 and 6 of I). It was thus implied that among the undetected soft-photon emissions occurring in the range  $\Delta E$ , the one for a single photon has a probability dominating the others (see Sec. II). Actually, for extremely small values of  $\Delta E$ , the probability for emission of several photons becomes comparable to that for single-photon emission, even though the latter is of lower order in  $\alpha$ . We have thus to deal with generalized forms of the Compton effect in which, for example,  $n$  photons of total energy within the range  $\Delta E$  are emitted. This is characterized by a cross section  $d\sigma^{(n)}(\Delta E)/d\Omega$ , which we shall assume includes virtual-photon radiative corrections to *all* orders. (The result is kept finite and mathematically well defined at the expense of introducing the finite photon mass  $\lambda$ .) These partial cross sections  $d\sigma^{(n)}(\Delta E)/d\Omega$  have then to be summed over *all*  $n$  values ( $n=0,1,2,\dots$ ; the  $n=0$  case has also to be included) in order to get the global cross section  $d\sigma(\Delta E)/d\Omega$  for the photoeffect with the emission of an arbitrary number of undetected soft photons, of total energy in the interval  $\Delta E$ :

$$\frac{d\sigma(\Delta E)}{d\Omega} = \sum_{n=0}^{\infty} \frac{\sigma^{(n)}(\Delta E)}{d\Omega}. \quad (22)$$

Alternatively, Eq. (22) can be viewed as the cross section corresponding to an energy loss of the ejected electron smaller than  $\Delta E$ , with all possible soft-photon events accounted for.

To deal in general with a sum like Eq. (22), is a formidable problem. However, the aspects related to its infrared behavior have been extracted in an elegant manner for a general elementary process (e.g., see Yennie, Frautschi, and Suura, Ref. 21, Sec. 4). Thus it can be shown that  $d\sigma(\Delta E)/d\Omega$  is finite in the limit  $\lambda \rightarrow 0$ , i.e., free of infrared divergences to all orders in  $\alpha$  (real photon divergences cancel those related to virtual photons) and that this is a consequence of their cancellation to lowest order in  $\alpha$ . Moreover, the lowest-order result [such as our Eq. (3)] enables us to obtain the  $\Delta E$  dependence of the global  $d\sigma(\Delta E)/d\Omega$  for  $\Delta E \ll 1$ , by a

procedure which has been termed “exponentiation,” because the  $\Delta E$ -dependent terms add up to give an exponential (see also Refs. 22 and 23). We shall now apply this procedure to the case of the photoeffect.

To this end it is useful to divide  $\delta$  as was done in Eqs. (6)–(8). Then, following Ref. 21, we infer the corrected cross section for the photoeffect, assuming  $\Delta E \ll 1$ , to be<sup>24</sup>

$$\frac{d\sigma_K(\Delta E)}{d\Omega} = \frac{d\sigma_K^{(0)}}{d\Omega} e^{(\alpha/\pi)\delta_1} \left[ 1 + \frac{\alpha}{\pi}\delta_0 \right]. \quad (23)$$

Whereas the exponentiation of  $(\alpha/\pi)\delta_1$  follows from the general proof, it is not clear if also some terms of  $\delta_0$  should be included under the exponential. Since only the case when  $(\alpha/\pi)\delta_0$  is rather small is of practical interest, we have written its contribution to Eq. (23) to first order only, as it appeared in Eq. (3). The quantity  $\delta_0$  can be obtained directly from Table I since, by its definition in Eqs. (6)–(8), we have  $\delta_0 = \delta - A \ln 0.01$ .

$d\sigma_K(\Delta E)/d\Omega$  of Eq. (23) is a generalization of our original Eq. (3), valid now for any  $\Delta E \ll 1$ , and in particular for  $\Delta E \rightarrow 0$ . The result is not only free of singularities for  $\Delta E \rightarrow 0$ , but actually vanishes in the limit. Indeed, from Eq. (7) we have

$$e^{(\alpha/\pi)\delta_1} = (\Delta E)^{(\alpha/\pi)A}. \quad (24)$$

Since  $A > 0$  for all  $\beta$ ,<sup>25</sup> this factor vanishes for  $\Delta E \rightarrow 0$ , as does the cross section Eq. (23). This fact has an important implication. It means that a “pure” photoeffect (i.e., the case when the emitted electron would lose no energy in the form of photons) cannot occur in reality. This is entirely similar to what happens in electron scattering by a potential, where a purely elastic collision (with no photons emitted) cannot occur as well.<sup>21</sup>

For not too small values of  $\Delta E$ , such that

$$\left| \frac{\alpha}{\pi} A \ln \Delta E \right| \ll 1, \quad (25)$$

Eq. (23) reduces to our Eq. (3). In view of the smallness of  $\alpha A/\pi$ , the condition Eq. (25) can be violated only under extreme circumstances. Thus, even for  $\omega$  as high as 10 MeV,  $\Delta E$  would have to be of the order of  $10^{-15}$  in order that the quantity on the left-hand side of Eq. (25) be 0.4. This indicates that for our problem exponentiation can be neglected from a quantitative point of view.

Because the factor Eq. (24) is angle independent,

the considerations above can be extended to the angle-integrated cross section Eq. (14).

### B. Electron energy distribution in theory and experiment

So far we have described the physics of our process in terms of the energy-resolution-type cross section  $d\sigma_K(\Delta E)/d\Omega$ . However, one may adopt an alternative point of view. Since in the final state of the process the emission of the electron is accompanied by that of photons, the electron (of final energy  $E$ ) will suffer some energy loss  $\epsilon = E_f - E$  ( $0 < \epsilon < E_f$ ) with respect to the value  $E_f$  predicted by the photoeffect energy conservation Eq. (1). The energy-loss distribution can be represented by a cross section of the form  $d^2\sigma_K/d\epsilon d\Omega$ . Evidently, the connection

$$\frac{d\sigma_K(\Delta E)}{d\Omega} = \int_0^{\Delta E} \frac{d^2\sigma_K}{d\epsilon d\Omega} d\epsilon \quad (26)$$

should hold.

We are now interested in deriving the expression of  $d^2\sigma_K/d\epsilon d\Omega$ , since this is the quantity primarily obtained in experiments rather than  $d\sigma_K(\Delta E)/d\Omega$ .  $d^2\sigma_K/d\epsilon d\Omega$  can be derived from Eq. (26) by simply taking the derivative of  $d\sigma_K(\Delta E)/d\Omega$  with respect to  $\Delta E$ . Using the expression derived in Eq. (23) we thus find

$$\frac{d^2\sigma_K}{d\epsilon d\Omega} = \frac{\alpha}{\pi} A \epsilon^{\alpha(A/\pi)-1} \frac{d\sigma_K^{(0)}}{d\Omega} \left[ 1 + \frac{\alpha}{\pi} \delta_0 \right]. \quad (27)$$

This form of the energy spectrum is valid only for sufficiently small  $\epsilon$  ( $\epsilon \ll 1$ ). In cases of physical interest Eq. (27) represents a decreasing function of  $\epsilon$ ,<sup>26</sup> which is singular for  $\epsilon \rightarrow 0$ , but the singularity is evidently integrable.

Notice that we could not have used our original Eq. (3) to derive  $d^2\sigma_K/d\epsilon d\Omega$  because of the undesirable feature that, for  $\Delta E \rightarrow 0$ , Eq. (3) becomes singular, in contradicton to Eq. (26).

The basic information yielded by photoeffect coincidence experiments (i.e., the ejected electron is detected in coincidence with the  $K$  x rays) is the energy spectrum of electrons in the vicinity of the photoelectric peak. For the case of angle-resolved experiments, the experimental spectrum, denoted by  $d^2\bar{\sigma}_K/d\epsilon d\Omega$ , can be obtained from the theoretical one in Eq. (27) by convoluting the latter with the (sample + spectrometer) transmission function, allowing for the energy spread in the initial beam, etc. The convolution is possible because the singu-

larity at  $\epsilon=0$  of  $d^2\sigma_K/d\epsilon d\Omega$  is integrable.

When ignoring the energy spread in the initial beam,  $d^2\bar{\sigma}_K/d\epsilon d\Omega$  essentially vanishes for  $\epsilon \leq -\Gamma$ , where  $\Gamma$  is the half-width of the transmission function, then rises sharply to finite maximum around  $\epsilon = \Gamma$ , to decrease more slowly for  $\epsilon > \Gamma$ . One may calculate the area under the curve  $d^2\bar{\sigma}_K/d\epsilon d\Omega$  from  $\epsilon = -\Gamma$  to some  $\epsilon = \Delta E$  of our choice ( $\Delta E < E_f$ ). This will give the number of counts in this energy interval. If  $\Delta E$  is chosen such that  $\Delta E \gg \Gamma$  (and, on the other hand,  $\Delta E \ll 1$ ), it follows that

$$\int_{-\Gamma}^{\Delta E} \frac{d^2\bar{\sigma}_K}{d\epsilon d\Omega} d\epsilon \simeq \frac{d\sigma_K(\Delta E)}{d\Omega}, \quad (28)$$

where on the right-hand side we now have our theoretical cross section Eq. (3). Thus, the condition  $\Delta E \gg \Gamma$  indicates the limitation to be imposed on  $\Delta E$  under which our Eq. (3) can be compared directly with the experimental data.<sup>27</sup>

The above discussion for the differential cross section Eq. (3) can be readily extended to the case of the total cross section Eq. (14).

### C. $\alpha Z$ and screening corrections

Our calculation was based on a hydrogenlike model and was carried out to lowest order in  $\alpha Z$ . We shall now briefly comment on its limitations and suggest possible improvements.

We first notice that for small  $Z$  atoms, consistency requires that the basic Sauter cross section  $d\sigma_K^{(0)}/d\Omega$  should be replaced in Eq. (3) by its first order in  $\alpha Z$  corrected version,  $d\sigma_K^{(1)}/d\Omega$  (in this case  $\alpha Z$  is not very different from  $\alpha$ ). An expression for  $d\sigma_K^{(1)}/d\Omega$  was derived by Gavrilu,<sup>5</sup> see also Nagel.<sup>28</sup> Unfortunately,  $d\sigma_K^{(1)}/d\Omega$  can itself be applied only to very low values of  $Z$ , because it turns out that the effective-expansion parameter of the basic cross section is not  $\alpha Z$ , but rather  $\pi\alpha Z$  (see Ref. 4). However, it is possible that by replacing  $d\sigma_K^{(0)}/d\Omega$  by Pratt's modification of the Sauter-Gavrilu formula,<sup>29</sup> or by a numerical evaluation of the basic (Coulomb) cross section,<sup>30</sup> the validity of Eq. (3) may be substantially extended towards higher  $Z$  values, at the high energies we are considering.

The electron-screening corrections to the Coulomb field model were analyzed for the basic photoeffect cross section by Pratt and collaborators (e.g., see Ref. 4). By applying their "normalization screening theory," which is valid for tightly bound electrons and high photon energies, the screening

corrections appear as constants multiplying the Coulomb cross sections. The natural question arises if this procedure could be extended to the case of the radiative corrections. An inspection of the matrix elements of Fig. 3 in I, shows that this is indeed the case for some of them, but that the rest would require a more elaborate analysis. If indeed the screening corrections could be factored out as in the normalization screening theory for *all* matrix elements, the replacement in Eq. (3) of  $d\sigma_K^{(0)}/d\Omega$  by the Coulomb cross section corrected for screening (or, equivalently, by a numerical evaluation for a realistic self-consistent potential) may correct, approximately, both for screening *and* for higher  $Z$  effects (as discussed above). However, an independent study would be required to analyze the extent to which such a procedure would be applicable.

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#### APPENDIX

In the following we would like to correct some misprints contained in papers I and II.

*Paper I.* Following Eq. (2.2), the expression of  $E_i$  should read  $E_i = (1 - a^2)^{+1/2}$ . In Eq. (5.21), the imaginary part of  $L_2(1 + \tau)$  should be  $-i\pi \ln(1 + \tau)$ . Further, Eq. (7.3) should read

$$(\alpha/\pi)\delta \simeq 0.009(\ln 2\Delta E - 1.50) - 0.011.$$

This changes slightly the numerical estimates following Eq. (7.3), but we shall not correct them here since they are superseded by the present computation.

In Eq. (7.4) the notation  $\kappa$  was inadvertently used for the momentum transfer, whereas throughout the paper  $\kappa$  represents the *square* of the momentum transfer [see Eq. (5.6)]. Then, at the end of the Appendix, after Eq. (A.8), the expression "physical photoeffect cross section" should read "physical (renormalized) photoeffect matrix element."

*Paper II.* In the first sentence of the paragraph beginning after Eq. (4), the word "including" should be replaced by "excluding." In Eq. (7) a factor  $\alpha$  should be added to the right-hand side. Further, in the second line of Eq. (15) the factor  $-|\vec{p} - \vec{k}|$  should be replaced by  $-\ln|\vec{p} - \vec{k}|$ . Then, in Ref. 15 the phrase "is equal to 1 for any  $\alpha Z \rightarrow 0$  . . ." should read "is equal to 1 for any  $\alpha Z$ , and, for  $\alpha Z \rightarrow 0$  . . ."

Finally we would like to add that in Eq. (12) of Ref. 1 of the present paper, the high-energy expression of  $\delta$  was incorrectly stated, and should read as given in Eq. (7.2) in I. Also, the sentence following Eq. (12) should be deleted.

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<sup>1</sup>M. Gavrilu and J. McEnnan, Phys. Lett. **59A**, 441 (1977).

<sup>2</sup>J. McEnnan and M. Gavrilu, Phys. Rev. A **15**, 1537 (1977).

<sup>3</sup>J. McEnnan and M. Gavrilu, Phys. Rev. A **15**, 1557 (1977).

<sup>4</sup>R. H. Pratt, A. Ron, and H. K. Tseng, Rev. Mod. Phys. **45**, 273 (1973).

<sup>5</sup>M. Gavrilu, Phys. Rev. **113**, 514 (1959).

<sup>6</sup>This connection is important, because what is typically measured in photoeffect experiments is the energy distribution of the emitted electrons, rather than anything related to the secondary photons (see Sec. V B).

<sup>7</sup>The (general) theoretical procedure described above for handling the infrared problem has a direct experimen-

tal justification. Indeed, because of the finite resolution  $\Delta E$  of the detection equipment (e.g., the electron spectrometer), events in which one or more photons of total energy smaller than  $\Delta E$  should be emitted during the basic process cannot be distinguished from the latter. Consequently, the experimentally meaningful cross section is obtained, as is done in theory, by adding the cross section for the basic process to that for the events in which one or more photon emissions have taken place in the interval  $\Delta E$  [see Eq. (22) below]. Physically,  $\Delta E$  can be chosen at will. Thus, it can be arbitrarily small, but finite. On the other hand, it cannot exceed some maximum value, in our case  $E_f$ , the kinetic energy of the outgoing electron, see Eq. (1). For the case when  $\Delta E$  is not small with respect to 1 see Ref. 9.

<sup>8</sup>More precisely, the cross section Eq. (3) was summed over the magnetic substates of the  $K$  shell and the

spin orientations of the ejected electron, and averaged over the polarizations of the incident photons.

<sup>9</sup>The restriction  $\Delta E \ll 1$  on Eq. (3) can be eliminated since the cross section  $d\sigma_{\kappa}(\Delta E')/d\Omega$  for some value  $\Delta E'$  larger than  $\Delta E$  can be obtained by adding to Eq. (3) the cross section for Compton scattering  $d^2\sigma_{\kappa}'/d\omega'd\Omega$  integrated over the final (hard) photon energy  $\omega'$  from  $\Delta E$  to  $\Delta E'$ . [See also the discussion by M. Gavrilă, Phys. Rev. A **6**, 1348 (1972), Sec. VI.] For consistency the relativistic Born-approximation calculation for  $d^2\sigma_{\kappa}'/d\omega'd\Omega$  should be used. This was carried out by V. G. Gorshkov, A. I. Mikhailov, and S. G. Sherman, Zh. Eksp. Teor. Phys. **64**, 1128 (1973) [Sov. Phys.-JETP **37**, 572 (1973)].

$d^2\sigma_{\kappa}'/d\omega'd\Omega$  is of order  $\alpha^2(\alpha Z)^5$  as is the contribution of the  $\delta$  term in Eq. (3).

<sup>10</sup>It was shown in I and II that the result of Eq. (3) can be extended in a simple manner to any  $nS_{1/2}$  subshell [see eq. (6.17) in I].

<sup>11</sup>A discussion of tip bremsstrahlung in terms of various approximations was given by H. K. Tseng and R. H. Pratt, Pittsburgh University, Physics Department, Report PITT 130, May 1974 (unpublished); and by R. H. Pratt and H. K. Tseng, Phys. Rev. A **11**, 1797 (1975). See also L. Maximon, Natl. Bur. Stand. (U.S.) Tech. Note 955 (1977).

<sup>12</sup>The cross sections appearing here have been averaged over the initial, and summed over the final spin states of the electron, and also summed over the emitted photon polarizations.

<sup>13</sup>K. Mitchell, Philos. Mag. **40**, 351 (1949).

<sup>14</sup>L. Lewin, *Dilogarithms and Associated Functions* (Macdonald, London, 1958).

<sup>15</sup>Note that the other quantities appearing in the denominators of  $g_{rs}$ ,  $h_{rs}$ ,  $j_{rs}$  of Eqs. (9)–(11) do not vanish in the integration domains, since for all  $x, y$ :  $p_y^2 > 1$ ,  $p_y^2 - y\tau > 1$ ,  $q_y^2 + y\kappa > 1$ ,  $p_x^2 > 1$ ,  $p_x^2 - x\tau > 1$ ,  $q_x^2 + \kappa x > 1$ ,  $k_y^2 > 1$ .

<sup>16</sup>Although  $\delta$  of Eq. (12) vanishes like  $\beta^2$ , this does not hold for the integrals Eqs. (9)–(11). In fact, some of them increase like  $\ln\tau/\tau$ ,  $\ln\kappa/\kappa$ ,  $1/\tau$ ,  $1/\kappa$ , or tend to constants. (Remember that, to lowest order in  $\beta$ ,  $\tau^2 \simeq \kappa^2 \simeq \beta^2$ .) The fact that, nevertheless,  $\delta$  is of order  $\beta^2$  in the nonrelativistic limit is due to the coefficient  $[(2-\tau)/\tau - 8/\kappa\tau]^{-1}$  appearing Eq. (5), which is of order  $\beta^4$ . To check the computation of the integrals Eqs. (9)–(11), we have extracted analytically their dominant behavior for  $\beta \rightarrow 0$ . When the terms of  $O(1)$  could be determined, comparison with the numerical results was made directly. When this was not the case, differences of the results for  $\beta=0.01$  and  $\beta=0.001$  were compared, so that the unknown terms of  $O(1)$  were eliminated.

<sup>17</sup>Technically, we have used the following procedure. From the analytic work related to paper I we knew the dominant behavior for large  $\tau$  and finite  $\kappa$  (i.e.,  $\tau \gg \kappa \geq 1$ ) of the individual integrals Eqs. (9)–(11). This is of the general form:  $A \ln^2\tau + B \ln\tau$

$+ C + O(\ln^2\tau/\tau)$ , where  $A, B, C$  are functions of  $\kappa$ , independent of  $\tau$ . Unfortunately, in most cases only the coefficients  $A$  and  $B$  could be determined analytically but not  $C$ . Consequently, in order to check the computation of a specific integral, we subtracted from its values at  $\tau=10^3$  and  $\tau=10^4$  the corresponding values of  $A \ln^2\tau + B \ln\tau$ , thereby obtaining two results for  $C + O(\ln^2\tau/\tau)$ . If these results agreed to within 5%, which is the estimated contribution of the neglected  $O(\ln^2\tau/\tau)$  terms, we considered that the computation had converged to the analytical limit.

<sup>18</sup>Recall that the Sauter angular distribution, as well as the more accurate results (e.g., the Coulomb cross section for arbitrary  $Z$ , or the cross sections derived from screened Coulomb potentials), all peak at decreasing angles as the energy increases. Thus, for  $\omega$  larger than 1 MeV the peak lies already below  $12^\circ$ . For a discussion of the high-energy limit of the angular distribution of the basic cross section (Coulomb potential, arbitrary  $Z$ ), see, B. Nagel, Ark. Fys. (Sweden) **24**, 151 (1963). When the Sauter cross section is given in terms of the momentum transfer  $\sqrt{\kappa}$ , the relevant values of  $\sqrt{\kappa}$  are smaller than about 5. [See Fig. 1 of the quoted paper by Nagel; note that in the high-energy limit our  $\sqrt{\kappa}$  is related to the  $\xi$  defined there by  $\sqrt{\kappa} = (1 + \xi^2)^{1/2}$ .]

<sup>19</sup>At 1 MeV it is in the vicinity of  $45^\circ$ , at 5 MeV around  $25^\circ$ , and at 20 MeV at about  $10^\circ$ . Its presence can be recognized more easily on a graphical representation of  $(\alpha/\pi)\delta$ .

<sup>20</sup>The agreement with the numerical results is substantially improved by our Eq. (12) in comparison to Eq. (7.1) in I.

<sup>21</sup>D. R. Yennie, S. C. Frautschi, and H. Suura, Ann. Phys. (N. Y.) **13**, 379 (1961).

<sup>22</sup>L. C. Maximon, Rev. Mod. Phys. **41**, 193 (1969).

<sup>23</sup>A. C. Hearn, P. K. Kuo, and D. R. Yennie, Phys. Rev. **187**, 1950 (1969).

<sup>24</sup>The line of reasoning followed by Yennie, Frautschi, and Suura in Ref. 21 is somewhat different from the one adopted here. These authors apply the exponentiation procedure to a general energy-loss cross section, of the type of our  $d^2\sigma/d\epsilon d\Omega$ , and derive an analog of our Eq. (27). (Their result is more general with respect to the virtual photon corrections but, on the other hand, is expressed in terms of unknown quantities.) Equation (23) appears then as a consequence of Eq. (27). McEnnan and Gavrilă followed in I the traditional approach of calculating to lowest order the energy-resolution cross section  $d\sigma(\Delta E)/d\Omega$  of Eq. (3) rather than a  $d^2\sigma/d\epsilon d\Omega$ . We therefore have to infer by exponentiation Eq. (23) in order to obtain Eq. (27).

<sup>25</sup>This can be seen on the series expansion of  $A$  in powers of  $\beta$  ( $0 \leq \beta < 1$ ).

<sup>26</sup> $A$  is an increasing function of  $\beta$ . For  $\beta \rightarrow 0$ ,  $A$  tends to zero as  $\beta^2$ ; and for  $\beta \rightarrow 1$ ,  $A$  has a logarithmic singularity. For physically relevant  $\beta$ ,  $\alpha A/\pi$  is small-

er than 1 and, in fact, is quite small: even for  $\omega=10$  MeV,  $\alpha A/\pi$  is only  $1.2 \cdot 10^{-2}$ . Nevertheless, for *exceedingly* high  $\beta$ ,  $\alpha A/\pi$  can become larger than 1 and arbitrarily large. (This would indicate the breakdown of our lowest order in  $\alpha$  perturbation theory, i.e., higher-order contributions in  $\alpha$  should be taken into account. An entirely similar situation occurs in the electron scattering case, see Refs. 21–23, where the quantity  $A$  defined there can also become extremely large.) Thus, for values of  $\beta$  for which  $0 < \alpha A/\pi < 1$ , Eq. (27) represents a decreasing function of  $\epsilon$ . For exceedingly high  $\beta$ , however, when  $\alpha A/\pi > 1$ , Eq. (27) yields an increasing function of  $\epsilon$ , vanishing at

$\epsilon=0$ .

<sup>27</sup>For a similar situation in electron-proton scattering see Fig. 1 of the paper by Y. S. Tsai, Phys. Rev. 122, 1898 (1961).

<sup>28</sup>B. Nagel, Ark. Fys. (Sweden) 18, 1 (1960).

<sup>29</sup>See Ref. 4, Eq. (6.1.8). The case of the total cross section was considered there, but a similar composite formula can be written for the differential cross section.

<sup>30</sup>See, for example, S. Hultberg, B. Nagel, and P. Olsson, Ark. Fys. (Sweden) 38, 1 (1968); or H. K. Tseng, R. H. Pratt, S. Yu, and A. Ron, Phys. Rev. A 17, 1061 (1978).