2 1962

Angular Distribution of Relativistic Atomic K-Shell Photoelectrons*

T. A. WEBER

Institute for Atomic Research and Department of Physics
Iowa State University, Ames, Iowa

and

C. J. MULLIN

University of Notre Dame, Notre Dame, Indiana

Abstract

Using the high energy limit of the exact Coulomb wave function for the outgoing electron, the differential cross section, correct to three orders in αZ , is calculated for the K-shell photoeffect. An analytic expression, exact in αZ , is obtained for the differential cross section for the special case in which the electron emerges in the forward direction.

MASTER

Angular Distribution of Relativistic Atomic K-Shell Photoelectrons***T. A. WEBER****Institute for Atomic Research and Department of Physics****Iowa State University, Ames, Iowa****and****C. J. MULLIN****University of Notre Dame, Notre Dame, Indiana****Abstract**

Using the high energy limit of the exact Coulomb wave function for the outgoing electron, the differential cross section, correct to three orders in aZ , is calculated for the K-shell photoeffect. An analytic expression, exact in aZ , is obtained for the differential cross section for the special case in which the electron emerges in the forward direction.

I. INTRODUCTION

Using the first Born approximation, M. Gavrila¹ calculated the differential and total cross sections for the K-shell photoeffect to two orders in aZ . It is apparent from Gavrila's work that the aZ correction is significant even for fairly small values of Z . More recently R. H. Pratt² made numerical calculations of the total cross section using the high energy limit of the exact Coulomb wave function for the ejected electron.

Pratt also derived an approximate formula which gives the total cross section as a function of Z . This formula compares favorably with the exact numerical results for all values of Z .

In this paper, the differential cross section for the relativistic K-shell photoeffect is calculated by using the high energy limit of the exact Coulomb wave function for the ejected electron. While this result is correct to three orders in αZ , (i. e., to terms of relative order $\alpha^2 Z^2$), it is not a strict expansion in this parameter. We have used Pratt's work as a guide to determine what factors should be left unexpanded. Upon integration over the solid angles of the outgoing electron we then obtain precisely Pratt's approximate formula for the total cross section. One might then conjecture that our result would give an accurate approximate formula for the angular distribution. However, in the forward direction the terms of relative order 1 and αZ vanish, and the resulting cross section is valid only to the first non-vanishing order in αZ . This non-vanishing term makes a contribution of relative order $\alpha^2 Z^2$ to the total cross section. Since the terms of relative order $\alpha^2 Z^2$ make a very small contribution to Pratt's expression for the total cross section, we cannot use a comparison with Pratt's result for the total cross section to justify the validity of our differential cross section for electron ejection angles near the forward direction. Therefore, for this special case of photoelectrons emerging in the forward direction, we calculate the differential cross section correct to all orders in αZ .

Figure 1 shows the angular distribution of the ejected photoelectrons. Figure 2 gives the differential cross section exact in αZ for the special case of forward emission as a function of Z .

II. MATRIX ELEMENT

Neglecting radiative corrections, the matrix element for the photoeffect is

$$M = - \left(\frac{2\pi\alpha}{k} \right)^{1/2} \int \psi_2^* \underline{\alpha} \cdot \underline{\epsilon} e^{i\underline{k} \cdot \underline{r}} \psi_1(\underline{r}) d\underline{r} \quad (1)$$

where $\underline{k}$ is the momentum of the incident photon and $\underline{\epsilon}$ is its polarization direction. ψ_1 is the wave function of the bound atomic electron, and ψ_2 is the wave function of an electron in the continuum states of a Coulomb field.

For the bound state, the K-shell hydrogen-like wave function is used.

$$\psi_1(\underline{r}) = N e^{-\lambda r} (mr)^{\delta-1} \left(1 + \frac{\lambda}{m(1+\delta)} \underline{\hat{r}} \right) u(\underline{r}) \quad (2)$$

where $\lambda = \alpha Z m$

$$w_1 = m\delta = m(1 - \alpha^2 Z^2)^{1/2}$$

and
$$|N|^2 = \frac{(1+\delta)(\alpha Z m)^3 (2\alpha Z)^{2(\delta-1)}}{\pi \Gamma(2\delta+1)}$$

This wave function has been expressed in terms of the plane wave spinor $u(\underline{p}_1)$ in order to facilitate the evaluation of the spin summations. In all results the momentum $\underline{p}_1$ is set equal to zero.

Since we are restricting ourselves to high energy incident photons, the final energy of the electron will be much greater than its rest mass energy m . Now in the limit $pr \rightarrow \infty$, the exact Coulomb wave function reduces to a distorted plane wave. For a final state this is

$$\psi_2(\underline{r}) = e^{i\underline{P} \cdot \underline{r}} (pr + \underline{p} \cdot \underline{r})^{i\mathcal{V}} u_2(\underline{p}) \quad (3)$$

where $\mathcal{V} = \alpha Z$.

We are justified in using this wave function for the final state of the electron provided that in the neighborhood of the origin there is no

contribution to the matrix element when the exact Coulomb wave function is used. That this is so has recently been demonstrated.^{3,4}

III. DIFFERENTIAL CROSS SECTION

The differential cross section for two K-shell electrons is

$$d\sigma = \frac{P^W}{(2\pi)^2} \sum |M|^2 d\Omega \quad (4)$$

where Σ represents the sum over initial and final electron spin states.

Using the matrix element given by Eq. (1) together with Eqs. (2) and (3) we obtain

$$\begin{aligned} \sum |M|^2 = & \frac{2\pi\alpha^2}{k} |M|^2 \left\{ |I_1|^2 + \frac{\Lambda^2}{m^2(1+\delta)^2} \underline{I}_2 \cdot \underline{I}_2 \right. \\ & \left. + \frac{2\Lambda}{m(1+\delta)} \Re(\hat{\underline{p}} \cdot \underline{I}_2 - 2\underline{\epsilon} \cdot \hat{\underline{p}} \underline{\epsilon} \cdot \underline{I}_2) I_1 \right\} \quad (5) \end{aligned}$$

$$\text{where } I_1 = -\frac{2}{3\lambda} I \quad (6-a)$$

$$\underline{I}_2 = \nabla_{\delta} I \quad (6-b)$$

and

$$I = \int e^{-\lambda t} (m t)^{\delta-1} e^{-i\underline{q} \cdot \underline{r}} (p t + \underline{p} \cdot \underline{r})^{-i\delta} \frac{d\underline{r}}{r} \quad (6-c)$$

$$\text{with } \underline{q} = \underline{p} - \underline{k}$$

The basic integral I has been calculated correct to three orders in αZ .⁵

(The procedure used in the evaluation of I is outlined in the appendix.)

Using this result and performing the differentiations indicated by Eqs.

(6-a) and (6-b) we obtain

$$\begin{aligned}
I_1 = & C \left\{ \frac{1}{g^2 + \lambda^2} \left(\frac{2\lambda}{g^2 + \lambda^2} + \frac{i\nu}{\lambda - i\hat{p} \cdot \hat{q}} - \frac{2i\nu\lambda}{g^2 + \lambda^2} \right) \right. \\
& - \frac{(1-\delta)}{g^2} \left[-\frac{\pi}{2g} + \frac{3\lambda}{g^2} - \frac{2\lambda}{g^2} \ln \frac{q}{m} \right. \\
& - \frac{\nu}{2g} \left(2i\pi \ln 2 - L_2(\hat{p} \cdot \hat{q}) + L_2(-\hat{p} \cdot \hat{q}) \right. \\
& + \ln \hat{p} \cdot \hat{q} \ln \frac{1 + \hat{p} \cdot \hat{q}}{1 - \hat{p} \cdot \hat{q}} - i\pi \ln \frac{1 + \hat{p} \cdot \hat{q}}{\hat{p} \cdot \hat{q}} \\
& \left. \left. \left. - \frac{2}{\hat{p} \cdot \hat{q}} \ln \frac{\hat{p} \cdot \hat{q}}{m} - 2i\pi + \frac{\pi^2}{2} + \frac{i\pi}{\hat{p} \cdot \hat{q}} \right) \right] \right\} \quad (7)
\end{aligned}$$

$$\begin{aligned}
I_2 = & C \left\{ \frac{1}{g^2 + \lambda^2} \left(\frac{2(i\nu-1)}{g^2 + \lambda^2} q - \frac{\nu}{\lambda - i\hat{p} \cdot \hat{q}} \hat{p} \right) \right. \\
& \left. + \frac{(1-\delta)}{g^4} (1 - 2 \ln \frac{q}{m}) q \right\} \quad (8)
\end{aligned}$$

where

$$C = 4\pi \left(\frac{m}{2p} \right)^{i\nu} \Gamma(\delta) \Gamma(1-i\nu) \left(\frac{\lambda^2 + g^2}{m(\lambda - i\hat{p} \cdot \hat{q})} \right)^{i\nu}$$

and $L_2(x)$ is Euler's dilogarithm.⁶ Using these results we can write the different cross section in the form

$$d\sigma = \sigma_0 F d\Omega \quad (9)$$

where $\sigma_0 = 4\alpha (aZ)^5 \frac{W}{m^3}$

and where F is correct to three orders in aZ . However, considerable simplifications can be made in F if we confine our attention to the region where $\hat{p} \approx \hat{k}$. It is easily seen that the outgoing electrons are confined to a cone in the forward direction of half width of order (m/W) because of the high power of q in the denominator. For θ in this region, $\hat{p} \cdot \hat{q} = \gamma m$ to highest order in W , and $(\hat{e} \cdot \hat{p})^2$ will be of order (m^2/W^2) so that the term dependent on the polarization direction can be neglected. Thus we obtain

$$F = v^{2(\gamma-1)} e^{-\pi v + 2v \sin^{-1} v} \left\{ \frac{2}{u^4} - \frac{2}{u^6} + v\pi \left(\frac{1}{u^4} - \frac{1}{u^6} \right) + \frac{v^2}{2} \left[\frac{6}{u^4} - \frac{2}{3} \frac{\pi^2}{u^4} - 4 \frac{\ln^2 u}{u^4} + \frac{3}{u^6} + \frac{11}{12} \frac{\pi^2}{u^6} + 4 \frac{\ln^2 u}{u^6} - \frac{8}{u^8} + 2 \left(\frac{1}{u^6} - \frac{1}{u^8} \right) \left(L_2\left(\frac{1}{u}\right) - L_2\left(\frac{1}{u}\right) + \ln u \ln \frac{u+1}{u-1} - \frac{\pi^2}{2} \right) \right] \right\}$$

where $\mu^2 = \frac{g^2 + \lambda^2}{m^2} \approx 1 + \frac{W^2}{m^2} \theta^2$.

The factor which is left unexpanded in ϵZ is precisely the same factor which appears in Pratt's approximate formula for the total cross section. In the forward direction $\mu = 1$ so that the first two orders of ϵZ ($\mathcal{D} = \epsilon Z$) drop out leaving our result valid only to lowest non-vanishing order in this region. However the basic integral I given in Eq. (6-c) can be evaluated exactly for the case $\underline{p} = \underline{k}$ and is given in the Appendix Eq. (A-8). Using the results given by Eq. (A-8) and performing the differentiations indicated in Eqs. (6-a) and (6-b) we obtain

$$I_1 = C \left\{ F_1 + \frac{1}{2-i\mathcal{D}} \frac{t_2 - t_1}{t_2} F_2 \right\} \quad (11)$$

$$I_2 = C \hat{\underline{D}} \left\{ -i F_1 + \frac{i}{2-i\mathcal{D}} \frac{t_2 + t_1}{t_2} F_2 \right\} \quad (12)$$

where

$$C = \frac{4\pi \Gamma(2+\delta-i\mathcal{D})}{m^2 (1-i\mathcal{D})} \left(\frac{m}{2p} \right)^{i\mathcal{D}} t_2^{-\delta+i\mathcal{D}-2}$$

$$F_1 = {}_2F_1 \left(1, 1+\delta-i\mathcal{D}; 2-i\mathcal{D}; \frac{t_2 - t_1}{t_2} \right)$$

$$F_2 = {}_2F_1 \left(2, 2+\delta-i\mathcal{D}; 3-i\mathcal{D}; \frac{t_2 - t_1}{t_2} \right).$$

The quantities t_1 , t_2 , and t_3 are defined by the equations following Eq. (A-3) of the appendix. The differential cross section for $\theta = 0$ can now be written to all orders in ϵZ .

$$d\sigma = \frac{32\pi\alpha W}{m^6\gamma^2} |\Gamma(1+\delta-i\nu)|^2 |N|^2 e^{-\pi\nu+2\nu\sin^{-1}\nu} \\ \times \left| F_1 + \frac{(1+\delta+i\nu)}{(2-i\nu)(\delta-i\nu)} F_2 \right|^2 d\Omega \quad (13)$$

Using standard relations between hypergeometric functions, we can write the cross section in terms of one hypergeometric function.

$$d\sigma = \frac{8\pi\alpha W}{m^6\gamma^4} |\Gamma(1+\delta-i\nu)|^2 |N|^2 e^{-\pi\nu+2\nu\sin^{-1}\nu} \\ \times \left| (1-i\nu)\left(\frac{\nu-i\delta}{\nu+i\delta}\right)^\delta - (1-i\nu-2\delta)_2 F_1\left(1-i\nu, 1-\delta; 2-i\nu; \frac{2\delta}{\delta-i\nu}\right) \right|^2 \quad (14)$$

Since the modulus of $\frac{2\gamma}{\gamma-1}$ is greater than 1, the hypergeometric function must be analytically continued in order to represent the function in its usual series expansion. This is accomplished by a standard relation.⁷

Thus writing $d\sigma = \sigma_0 F_0 d\Omega$,

we find

$$F_0 = \frac{(1+\delta)}{\nu^2\gamma^2} \frac{|\Gamma(\delta-i\nu)|^2}{\Gamma(2\delta)} (2\nu)^{2(\delta-1)} e^{-\pi\nu+2\nu\sin^{-1}\nu} \\ \times \left| 1 - \frac{(1-2\delta-i\nu)}{2\delta^2(\delta+i\nu)} \left[\frac{\Gamma(1-i\nu)\Gamma(1+\delta)}{\Gamma(1+\delta-i\nu)} \left(\frac{2\delta}{\delta-i\nu}\right)^{i\nu} \left(\frac{i\nu+\delta}{i\nu-\delta}\right)^{-\delta} \right. \right. \\ \left. \left. - {}_2F_1\left(1, i\nu; 1+\delta; \frac{\delta+i\nu}{2\delta}\right) \right] \right|^2 \quad (15)$$

This expression is now in a form suitable for a numerical calculation.

IV. TOTAL CROSS SECTION

For the total cross section we must perform the $d\Omega$ integration over terms of the form $(\underline{p} \cdot \underline{q})^l / (q^2 + \lambda^2)^n$ or over functions whose series representation has terms of this type. It is easily shown that to highest order in W , $\underline{p} \cdot \underline{q}$ can be set equal to Ym in the integral

$$\int (\underline{p} \cdot \underline{q})^l / (q^2 + \lambda^2)^n d\Omega$$

provided $n > l + 1$. This condition is met in our differential cross section so that we may take F given by Eq. (10) to be integrated over $d\Omega$. The integrals over the dilogarithm functions are easily carried out by integration by parts. The total cross section for two K-shell electrons is

$$\sigma = \pi \sigma_0 \frac{m^2}{W^2} \beta^{-2(1-\gamma)} e^{-\pi \gamma + 2 \pi \alpha^{-1} \gamma} \times \left\{ 1 - \frac{4\pi}{15} \gamma + \gamma^2 \left[2 + \frac{1}{2} - \ln 2 + \pi^2 \left(\frac{1}{16} - \frac{1}{6} - \frac{4}{45} \right) \right] \right\} \quad (16)$$

This is precisely the result that R. H. Pratt obtained.

V. CONCLUSION

We have written the differential cross section for the relativistic photoeffect in the form

$$d\sigma = \sigma_0 F d\Omega \quad \text{where}$$

$\sigma_0 = 4a(\epsilon Z)^5 W/m^3$ and F is given correct to three orders in ϵZ by Eq. (10) or exactly in ϵZ for $\theta = 0$ by Eq. (15). In Fig. 1 we plot F vs. (W/m) , and the dashed curves are extrapolations to the exact value for $\theta = 0$. Since F is good only to lowest non-vanishing order in ϵZ in the region where $\theta \simeq 0$, it is not surprising that for $Z = 79$ this lowest order result and the exact result (marked with an x) are greatly different. The cross section for $\theta = 0$, correct to all orders in ϵZ , is given as a function of Z in Fig. 2. By comparing Figs. 1 and 2 one can estimate the behavior of the differential cross sections for angles near $\theta = 0$.

APPENDIX

The basic integral necessary in the work of this paper is

$$I = \int e^{-\lambda r} (mr)^{\gamma-1} e^{-i\lambda \underline{r} \cdot \underline{t}} (\underline{p} + \underline{p} \cdot \underline{t})^{-1} \frac{d\underline{t}}{t}. \quad (A-1)$$

Using Hankel's representation

$$\frac{1}{\Gamma(z)} = \frac{1}{2\pi i} \int_{-\infty}^{0+} e^t t^{-z} dt, \quad |\arg t| \leq \pi$$

and setting $t = \xi s$ where ξ is real positive, we obtain

$$\xi^{z-1} = \frac{\Gamma(z)}{2\pi i} \int_{-\infty}^{0+} e^{\xi s} s^{-z} ds. \quad (A-2)$$

Using this representation for $(mr)^{\gamma-1}$ and $(\underline{p} + \underline{p} \cdot \underline{t})^{-1}$ in the integral I , the integration over $\underline{t}$ becomes trivial and we obtain

$$I = \frac{\Gamma(1-i\nu)\Gamma(\delta)}{2\pi m p} \int_{-\infty}^{0+} \frac{t^{-\gamma}}{t_0 - t} dt \lim_{R \rightarrow \infty} \int_{-R}^{0+} \frac{s^{i\nu-1}}{s - s_0(t)} ds \quad (A-3)$$

where

$$S_0(t) = \frac{m}{2p} \left[\frac{(t_1 - t)(t_2 - t)}{t_3 - t} \right]$$

$$t_1 = t_2^* = \frac{\lambda - i\hat{p}}{m}$$

$$t_3 = \frac{\lambda - i\hat{p} - \hat{p}}{m}$$

We can close the path of integration for s with a circle of radius R .

As $R \rightarrow \infty$ there will be no contribution from the integration along the circle. Reversing the path of integration and applying Cauchy's theorem we obtain

$$I = -2i \frac{\Gamma(1-i\hat{p})\Gamma(\hat{p})}{m^2} \left(\frac{m}{2p}\right)^{i\hat{p}} \int_{-\infty}^{\infty} \frac{t^{-\hat{p}}}{(t_1 - t)(t_2 - t)} \left[\frac{(t_1 - t)(t_2 - t)}{t_3 - t} \right]^{i\hat{p}} dt \quad (A-4)$$

By expanding the integrand in terms of z , this integral has been evaluated to three orders in z as mentioned earlier. The integral can be evaluated exactly in terms of generalized hypergeometric functions. However, for the special case in which $\hat{p} = \hat{q}$ the integral can be written in terms of hypergeometric functions. In this case $t_1 = t_3$ and

$$I = -2i \frac{\Gamma(1-i\hat{p})\Gamma(\hat{p})}{m^2} \left(\frac{m}{2p}\right)^{i\hat{p}} \int_{-\infty}^{\infty} t^{-\hat{p}} (t_1 - t)^{-1} (t_2 - t)^{i\hat{p}-1} dt \quad (A-5)$$

In this contour of integration, the origin is approached below the cut where the phase of t is $-\pi$, the origin is encircled, and then $-\infty$ is

approached along the top of the cut where the phase of t is π . Splitting the integral into three parts, two along the cut and one around the origin we find the contribution from the origin is zero and the two parts along the cut combine to give

$$I = -4 \sin \pi \delta t_1^{1-\delta} t_2^{i\mathcal{D}-1} \frac{\Gamma(1-i\mathcal{D}) \Gamma(\delta)}{m^2} \left(\frac{m}{2f}\right)^{i\mathcal{D}} \\ \times \int_0^\infty s^{-\delta} (s+1)^{-1} \left(\frac{t_1}{t_2} s+1\right)^{i\mathcal{D}-1} ds \quad (\text{A-6})$$

Now

$${}_2F_1(a, b; c; 1-z) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_0^\infty s^{b-1} (1+s)^{a-c} (1+s\tau)^{-a} ds$$

$$\text{with } \operatorname{Re} c > \operatorname{Re} b > 0, \quad |\arg z| < \pi \quad (\text{A-7})$$

Thus we obtain

$$I = \frac{4\pi \Gamma(1+\delta-i\mathcal{D})}{m^2(1-i\mathcal{D})} \left(\frac{m}{2f}\right)^{i\mathcal{D}} t_2^{-\delta-1+i\mathcal{D}} {}_2F_1\left(1, 1+\delta-i\mathcal{D}; 2-i\mathcal{D}; \frac{t_1-t_2}{t_2}\right) \quad (\text{A-8})$$

FOOTNOTES AND REFERENCES

* Contribution No. 1085. Work was supported in part by the U. S. Atomic Energy Commission.

¹ M. Gavrilă, Phys. Rev. 113, 514 (1959).

² R. H. Pratt, Phys. Rev. 117, 1017 (1960).

³ R. T. Deck, C. J. Mullin, and C. L. Hammer, Phys. Rev. (to be published).

⁴ R. H. Pratt (reference 2) has used a somewhat different argument to justify the use of the distorted plane wave.

⁵ Equations (A-2), (A-10), and (A-21) of reference 3. The integral I given by (A-2) of this work is the same as that given above if we replace $\underline{q}$ by $-\underline{q}$ and $\underline{p}$ by $-\underline{p}$. However the results of the integration are unchanged since the vectors appear only in the combination $\underline{p} \cdot \underline{q}$.

⁶ K. Mitchell, Phil. Mag. 40, 351 (1949), gives nine place tables for $L_2(X)$, $-1 \leq x \leq 1$.

⁷ A. Erdelyi, et al., Higher Transcendental Functions, Bateman Manuscript Project (McGraw-Hill, New York, 1953), Vol. 1, p. 105, Sec. 2.9, Eq. (2) and p. 103, Sec. 2.8, Eq. (34).

⁸ Reference 6, p. 108, Sec. 2.10, Eq. (1).

Fig. 1. F is plotted vs $(W/m)\theta$ for various values of Z . θ is in radians. The dashed curve is the extrapolation to the exact value for $\theta = 0$. The x marks the exact value for $Z = 79$.

Fig. 2. F_0 , the exact value of F for $\theta = 0$, is plotted vs Z .

FIGURE CAPTIONS

Fig. 1. F is plotted vs. $(W/m)\theta$ for various values of Z . θ is in radians.

The dashed curve is the extrapolation to the exact value for $\theta = 0$.

The x marks the exact value for $Z = 79$.

Fig. 2. F_0 , the exact value of F for $\theta = 0$, is plotted vs. Z .

END