(see Fig. 6), except that the broad onset occurs around 3.5 ev.

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Sauter Theory of the Photoelectric Effect*

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Results of Sauter are expressed in the form of a transition matrix which determines the photoelectric effect cross section for arbitrary x-ray polarization and arbitrary initial and final orientations of the electron spin. The structure of the matrix elements accounts for curious properties of the cross section in terms of interference between orbital and spin currents. Expansion of the wave functions into powers of $Z/137$ simplifies the calculation of the transition matrix, reduces it to a special case of the bremsstrahlung theory in Born approximation, and explains discrepancies between results of earlier calculations. Analytical and graphical data are given on the photoemission of polarized electrons by circularly polarized x-rays.

1. INTRODUCTION

UNCERTAINTIES regarding the significance of theoretical results on the photoelectric effect and discrepancies between experimental results have stimulated an effort to clarify the content of the theory and to develop further its application. In the course of this work it has emerged that the theories of the photoelectric effect and of bremsstrahlung coincide, in essence, to lowest order in $Z/137$. This paper reports the results of analysis and calculations on the photoelectric effect. Separate papers deal with the mathematical justification of the expansion which establishes the connection with bremsstrahlung,[1] with applications of this connection[2–4] and with a detailed analysis of spin effects in the absorption or emission of radiation.[5]

An important relativistic calculation of the cross section for the photoelectric effect in the K shell of atoms was carried out by Sauter in 1931.[6,7] The calculation involved an expansion into powers of the atomic number Z and has accordingly often been classed as a Born approximation, although this term is properly applied in a more restricted sense. Because Sauter did not follow the usual rather simple method of Born approximation calculations, his results are not physically transparent.[8] Sauter himself felt unable to "read out" of his calculation results on the probability of electron spin reorientation which were implicity contained in it (reference 7, p. 485). Spin orientation and its relation to circular polarization of the x-rays have attracted increasing attention in recent years,[9] and will be considered in some detail in this paper.

It may be noted that the integral cross sections for the photoelectric effect calculated by Sauter for high-Z materials exceed by a factor ~ 2 those obtained numerically by Hulme *et al.*, with exact Coulomb-field wave functions[10,11] and those obtained experimentally at relativistic energies. (The discrepancy is much larger still at lower energies, e.g., at 50 kev.) On the other hand, the Hulme procedure has never been applied extensively or to verify whether any of the more

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[1] K. W. McVoy and U. Fano, this issue [Phys. Rev. **116**, 1168 (1959)].

[2] U. Fano, following paper [Phys. Rev. **116**, 1156 (1959)].

[3] Fano, Koch, and Motz, Phys. Rev. **112**, 1679 (1958).

[4] J. W. Motz and R. C. Placious, Phys. Rev. **112**, 1039 (1958).

[5] Fano, McVoy, and Albers, this issue [Phys. Rev. **116**, 1159 (1959)].

[6] F. Sauter, Ann. Physik **9**, 217 (1931).

[7] F. Sauter, Ann. Physik **11**, 454 (1931).

[8] An independent derivation of Sauter's results by A. Sommerfeld, *Atombau and Spektrallinien* (F. Vieweg und Sohn, Braunschweig, 1939), second edition, Vol. 2, p. 482 ff., proved of little advantage in this respect.

[9] See in particular, K. W. McVoy, Phys. Rev. **108**, 365 (1957).

[10] Hulme, McDougall, Buckingham, and Fowler, Proc. Roy. Soc. (London) **149**, 454 (1935).

[11] See in particular, W. Heitler, *Quantum Theory of Radiation* (Oxford University Press, Oxford, 1954), third edition, p. 209 ff.

detailed results of Sauter should be attributed to inadequate approximation.

Two qualitative features of the Sauter results are somewhat surprising. One is that the differential cross section for ejection of photoelectrons in the direction of the incident x-rays vanishes. This result would follow for a spinless K-shell electron from the transverse character of x-rays and the conservation of angular momentum, but the possibility of a spin flip makes forward emission consistent with the conservation requirements. Forward emission has in fact been observed[12] and Sauter himself verified that his formulas do yield forward emission when evaluated numerically prior to an approximate expansion.[13]

The other surprising result concerns the preferential direction of photoelectric emission under the influence of linearly polarized x-rays. Maximum emission might be expected in the plane containing the electric vector and the direction of propagation of the x-rays. However, according to Sauter this occurs only at low energies, whereas at energies of the order of 1 Mev and at large angles with respect to the x-ray direction ejection occurs with maximum probability in the plane of the magnetic vector. Direct experimental evidence on this point has thus far been contradictory.[14,15]

Still another remarkable phenomenon, contained implicitly in the Sauter theory and emphasized in reference 9, is a strong correlation between any circular polarization of high-energy x-rays and the helicity (longitudinal spin polarization) of the photoelectrons. This effect has an analog in the bremsstrahlung process.[16,17] It is explained only in part by the conservation of angular momentum in spin-flip processes and it will be shown to be closely related to the other effects of x-ray polarization.

In order to facilitate the interpretation and extension of Sauter's result, two steps were taken. Sauter's results were expressed in the form of a transition matrix[18] rather than of a cross section averaged over spin orientations; each element of the transition matrix is the probability amplitude that a photon of specified polarization be absorbed by a K-shell electron of given spin orientation in a transition to a state of given final momentum and spin orientation. Alternative forms of the transition matrix, corresponding to different choices of x-ray polarization and spin orientation, are given and discussed in Secs. 2 and 3. The spin and polarization effects discussed above can be identified in the structure of the matrix elements and traced, in part, to interference between contributions from the action of x-rays upon orbital and spin currents.

A second step of simplification of Sauter's theory is carried out in Sec. 4 by expanding the initial and final wave functions of the electron into powers of $Z/137$ before the calculation of matrix elements, instead of calculating the matrix elements first and then expanding them to lowest order in $Z/137$. The expansion of the K-shell wave function $[\exp(-r/a_Z)\sim 1-r/a_Z]$ has only a restricted, *ad hoc*, mathematical significance; it may be regarded as a symbolic procedure whose significance and justification are given in reference 1. The first two terms of the expansion represent a K-shell state as a zero-energy free-particle state perturbed to first order by the nuclear attraction; the binding energy due to this attraction is disregarded because it is of order $(Z/137)^2$. The calculation of the transition matrix for the photoeffect becomes thereby equivalent to the corresponding calculation, in Born approximation, for a bremsstrahlung process in which the electron is left with zero kinetic energy. The calculation shows then that the forward emission of photoelectrons vanishes in the Sauter approximation because of cancellation between the contributions of two Feynman diagrams. It also shows that the results of reference 9 differ from Sauter's because reference 9 disregarded the Feynman diagram corresponding to nuclear perturbation of the final-state wave function.[19] One can also analyze, simultaneously for the photoelectric effect and bremsstrahlung, the calculation of matrix elements to see how the dependence of the process on x-ray polarization and spin orientation derives from the mechanics of the Dirac electron; this is done in reference 5.

Because a significant contribution to the matrix element for the photoelectric effect has been disregarded in reference 9, the data on the cross section given in that reference must be rectified. This has been done independently by Olsen,[20] but some data are nevertheless presented analytically and graphically in Sec. 5.

No effort has been made in this paper to proceed beyond the Sauter approximation, even though it yields absolute cross sections of very low accuracy for heavy atoms. The next higher order of approximation has recently been calculated.[21]

2. TRANSITION MATRIX DERIVED FROM SAUTER'S CALCULATION

The state of a K-shell electron perturbed by x-rays is described in the Sauter theory[6,7] by means of a 4-com-

[12] A. Hedgran and S. Holtberg, Phys. Rev. **94**, 498 (1954); Arkiv Fysik **9**, 245 (1955).
[13] F. Sauter and H. O. Wüster, Z. Physik **141**, 83 (1955).
[14] W. McMaster and F. Hereford, Phys. Rev. **95**, 723 (1954).
[15] D. Brini *et al.*, Nuovo cimento **6**, 98 (1957).
[16] K. W. McVoy, Phys. Rev. **106**, 828 (1957); **111**, 1333 (1958).
[17] K. W. McVoy and F. J. Dyson, Phys. Rev. **106**, 1360 (1957).
[18] We thank Dr. H. Mendlowitz for suggesting this procedure and for numerous discussions.

[19] The perturbation vanishes in the nonrelativistic limit. It was also disregarded in an unpublished calculation which was mentioned in references 9, 14, and 15.
[20] H. Olsen, *Festskrift til Egil Hylleraas* (Bruns, Trondheim, 1958). We thank Dr. Olsen for an advance copy of his paper.
[21] M. Gavrila, Phys. Rev. **113**, 514 (1959).

ponent Dirac wave function. This wave function includes an outgoing spherical wave which represents the current of ejected photoelectrons. Polar coordinates (r,θ,φ) are utilized with the direction of the incident x-ray beam as polar axis. Spin orientation states with magnetic quantum numbers $\pm\frac{1}{2}$ are referred to this polar axis.

As emphasized by Lenard,[22] it is sufficient to consider a single state which, in the absence of x-ray perturbation, has a spin orientation represented by a specific value of the magnetic quantum number m_0; other states are related to it by symmetry transformations. The quantum number m_0 of the initial state of the photoelectron is observable because it coincides with the quantum number of the "hole" left in the K shell after photoelectric emission and thereby influences the polarization of the characteristic x-rays or Auger electrons which are emitted subsequently.

It is also sufficient to consider incident x-rays polarized linearly in a single plane, provided one considers the emission of photoelectrons as a function of the azimuth difference between the meridian planes containing the directions of the photoelectron and of the linear polarization. Sauter considers x-rays with the electric field at the azimuth $\varphi=\frac{1}{2}\pi$.

If we call ψ_{Km_0} the wave function of unperturbed K-shell electrons with spin orientations $m_0=\pm\frac{1}{2}$, Sauter's wave functions may be indicated respectively by $\psi_{K\frac{1}{2}}+\psi_1$ and $\psi_{K-\frac{1}{2}}+\psi_2$, where ψ_1 and ψ_2 indicate the outgoing spherical waves resulting from the perturbation by the x-rays. Sauter represents ψ_1 and ψ_2 in the form

$$\psi_1=\begin{bmatrix} i(F_2e^{-i\varphi}+G_2e^{i\varphi}) \\ -(F_1+G_1e^{2i\varphi}) \\ -(F_4e^{-i\varphi}+G_4e^{i\varphi}) \\ i(F_3+G_3e^{2i\varphi}) \end{bmatrix},\qquad \psi_2=\begin{bmatrix} i(F_1+G_1e^{-2i\varphi}) \\ F_2e^{i\varphi}+G_2e^{-i\varphi} \\ -(F_3+G_3e^{-2i\varphi}) \\ -i(F_4e^{i\varphi}+G_4e^{-i\varphi}) \end{bmatrix}, \tag{1}$$

where each F and G is a function of the polar coordinates r and θ and the dependence on φ characterizes the photoelectron's orbital angular momentum about the polar axis.

Complicated analytical expressions of F and G are obtained in reference 7 and are then evaluated asymptotically for $r\rightarrow\infty$ and by expansion into powers of $Z/137$ and $Z/137\beta$, to lowest order in these parameters. As usual, β indicates here the velocity of the ejected electron, in units of c; units such that $\hbar=c=1$ will be used throughout this paper. Notice that $Z/137\beta\ll1$ only if the photon energy greatly exceeds the K absorption edge. The result to first order in $1/r$, reference 7, Eq. (28), is

$$\begin{aligned}
F_1&=f(r)B(\theta)(-i)\frac{E-m}{m}\sin\theta,\quad G_1=0,\\
F_2&=f(r)B(\theta)\left(i\frac{E-m}{m}\cos\theta-i\frac{E-2m}{m}\frac{E+m}{p}\right),\\
G_2&=f(r)B(\theta)\left(-i\frac{E+m}{p}\right),\\
F_3&=f(r)B(\theta)\left(-\frac{E-2m}{m}\sin\theta\right),\\
G_3&=f(r)B(\theta)(-\sin\theta),\\
F_4&=f(r)B(\theta)\left(-\frac{E-2m}{m}\cos\theta+\frac{E-m}{m}\frac{p}{E+m}\right),\\
G_4&=f(r)B(\theta)(-\cos\theta),
\end{aligned}\tag{2}$$

where

$$f(r)=e^{ipr}/r, \tag{3}$$

$$B(\theta)=r_0\frac{Z^{\frac{5}{2}}}{2\sqrt{2}137^2}\left(\frac{m}{E-m}\right)^{\frac{5}{2}}\frac{\beta^2\sin\theta}{(1-\beta\cos\theta)^2}, \tag{4}$$

E, p, and m are the energy, momentum, and mass of the photoelectron, Z the atomic number, and $r_0=e^2/mc^2$ the "electron radius." The factor B is normalized so that the outgoing wave represents the effect of perturbation by an incident x-ray flux of 1 photon $\text{cm}^{-2}\,\text{sec}^{-1}$.

If the electron had been treated by the Schrödinger method and its wave function for large r were of the form $\psi_1=f(r)g(\theta,\varphi)$, with the conventions adopted above, the differential cross section for photoelectric emission of K-shell electrons per unit solid angle in the direction (θ,φ) would be simply

$$d\sigma(\theta,\varphi)/d\Omega=2\beta|g(\theta,\varphi)|^2. \tag{5}$$

The Dirac wave functions given by (1)–(4) may also be expressed in the form $f(r)g(\theta,\varphi)$, where $g(\theta,\varphi)$ indicates a spinor with components $g_i(\theta,\varphi)$. The cross section obtained by Sauter has accordingly the form

$$d\sigma(\theta,\varphi)/d\Omega=2\beta\sum_i|g_i(\theta,\varphi)|^2, \tag{6}$$

considering that the $\sum_i|g_i|^2$ has the same value for the two initial K-electron states with $m_0=\pm\frac{1}{2}$.

The summation over squared spinor components in (6) makes no use of the information which is contained in ψ_1 regarding the spin orientation of the ejected electron and which could be represented by other expressions bilinear in g_i and g_i^*. One method of analyzing this information consists of expanding the spinor $g(\theta,\varphi)$ into a superposition of two spinors $u_m(\theta,\varphi)$ with $m=\pm\frac{1}{2}$, corresponding to outgoing electrons whose spin—in the rest frame of reference—is directed either way along the z axis. These spinors are determined as solutions of the Dirac equation for free electrons of momentum $\mathbf{p}=(p,\theta,\varphi)$, because the spherical wave ψ_1

[22] A. Lenard, Phys. Rev. **107**, 1712 (1957).

approximates a plane wave with this momentum to lowest order in $1/r$ in the neighborhood of the point (r,θ,φ).[23] In the representation of Dirac matrices adopted by Sauter the plane wave spinors are

$$u_{\frac{1}{2}}(\theta,\varphi)=\left(\frac{E+m}{2E}\right)^{\frac{1}{2}}\begin{bmatrix}1\\0\\ [p/(E+m)]\cos\theta\\ -i[p/(E+m)]\sin\theta e^{i\varphi}\end{bmatrix},$$

$$u_{-\frac{1}{2}}(\theta,\varphi)=i\left(\frac{E+m}{2E}\right)^{\frac{1}{2}}\begin{bmatrix}0\\1\\ i[p/(E+m)]\sin\theta e^{-i\varphi}\\ -[p/(E+m)]\cos\theta\end{bmatrix}. \quad (7)$$

We then set

$$\psi_1(r,\theta,\varphi)=f(r)g(\theta,\varphi)$$
$$=f(r)\sum_{m=\pm\frac{1}{2}}u_m(\theta,\varphi)h_{m\frac{1}{2}}(\theta,\varphi), \quad (8)$$

where $h_{m\frac{1}{2}}=\sum_i u_{mi}{}^*g_i$, since the spinors u_m are normalized to 1, and where the subscript $\frac{1}{2}$ has been added as a reminder that the wave function ψ_1 and the spinor g pertain to the initial K-shell state with spin quantum number $m_0=\frac{1}{2}$. Combining the preceding equations, and proceeding similarly for the Sauter wave function ψ_2 with $m_0=-\frac{1}{2}$, one finds

$$h_{mm_0}(\theta,\varphi)=B(\theta)\left(\frac{2E}{E-m}\right)^{\frac{1}{2}}T_{mm_0y}(\theta,\varphi), \quad (9)$$

where the subscript y of the matrix T_{mm_0y} indicates the electric field direction of the incident x-rays, where

$$T_{mm_0y}(\theta,\varphi)=\begin{array}{c|cc} m\diagdown m_0 & \frac{1}{2} & -\frac{1}{2}\\ \hline \frac{1}{2} & e^{i\varphi}-[1-a(\theta)]e^{-i\varphi} & b(\theta)\\ -\frac{1}{2} & b(\theta) & -e^{-i\varphi}+[1-a(\theta)]e^{i\varphi}\end{array}, \quad (10)$$

and where the functions

$$a(\theta)=\frac{E-m}{m}\left(1-\frac{p\cos\theta}{E+m}\right),\quad b(\theta)=\frac{E-m}{m}\frac{p\sin\theta}{E+m}, \quad (11)$$

are shown in Fig. 1.

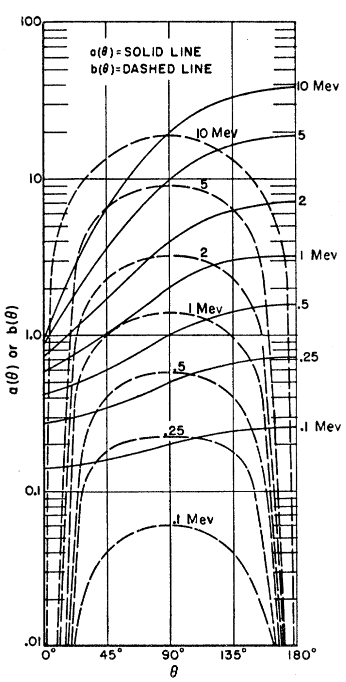

FIG. 1. The functions $a(\theta)$ and $b(\theta)$, for various values of the incident photon energy in Mev.

Equations (9) and (10) include all the information contained in the Sauter theory for $Z/137\beta\ll 1$. The transition matrix T_{MM_0P}, for arbitrary polarization P of the incident x-rays and for spin quantum numbers M,M_0 referred to arbitrary axes of reference, is obtained from (10) by means of coordinate changes and unitary transformations. Thus, for linear polarization parallel to the x axis ($P=x$) and with spins referred to the polar axis, as above, we have

$$T_{mm_0x}(\theta,\varphi)$$
$$=e^{im\frac{1}{2}\pi}T_{mm_0y}(\theta,\varphi+\tfrac{1}{2}\pi)e^{-im_0\frac{1}{2}\pi}$$
$$=i\begin{vmatrix}e^{i\varphi}+[1-a(\theta)]e^{-i\varphi} & b(\theta)\\ -b(\theta) & e^{-i\varphi}+[1-a(\theta)]e^{i\varphi}\end{vmatrix}, \quad (12)$$

where the rows and columns are labelled as in (10). For circular polarization with helicity $\delta=\pm1$ ($P=\delta$) we have the double matrix

$$(1/\sqrt{2})T_{mm_0\delta}(\theta,\varphi)$$
$$=-\tfrac{1}{2}i[T_{mm_0x}(\theta,\varphi)+i\delta T_{mm_0y}(\theta,\varphi)]$$
$$=\begin{vmatrix}e^{i\varphi} & b(\theta)\\ 0 & [1-a(\theta)]e^{i\varphi}\end{vmatrix}\quad \text{for } \delta=1$$
$$=\begin{vmatrix}[1-a(\theta)]e^{-i\varphi} & 0\\ b(\theta) & e^{-i\varphi}\end{vmatrix}\quad \text{for } \delta=-1. \quad (13)$$

To obtain the transition matrix for circular polarization

[23] The 4-component wave function ψ_1 can be resolved into a combination of only two basic spinors because it obeys a wave equation with a positive energy eigenvalue E.

and for spins referred to the direction (θ,φ) of photoemission (electron helicity eigenstates, $M=\epsilon$, $M_0=\epsilon_0$), one transforms (13) with the unitary matrix

$$U_{\epsilon m}=\begin{vmatrix}\cos\frac{1}{2}\theta\, e^{i\frac{1}{2}\varphi} & -\sin\frac{1}{2}\theta\, e^{-i\frac{1}{2}\varphi}\\ i\sin\frac{1}{2}\theta\, e^{i\frac{1}{2}\varphi} & i\cos\frac{1}{2}\theta\, e^{-i\frac{1}{2}\varphi}\end{vmatrix}. \quad (14)$$

[In this matrix the phases are adjusted in accordance with those of the Sauter spinors (7).] One finds

$$(1/\sqrt{2})T_{\epsilon\epsilon_0\delta}(\theta,\varphi)=(1/\sqrt{2})\textstyle\sum_{mm_0}U_{\epsilon m}T_{mm_0\delta}(\theta,\varphi)U^{-1}{}_{m_0\epsilon_0}$$

$$=e^{i\varphi}\begin{vmatrix}1-\frac{1}{2}a(\theta)(1-\cos\theta)-\frac{1}{2}b(\theta)\sin\theta & -\frac{1}{2}i[a(\theta)\sin\theta+b(\theta)(1+\cos\theta)]\\ \frac{1}{2}i[a(\theta)\sin\theta-b(\theta)(1-\cos\theta)] & 1-\frac{1}{2}a(\theta)(1+\cos\theta)+\frac{1}{2}b(\theta)\sin\theta\end{vmatrix}\quad\text{for }\delta=1$$

$$=e^{-i\varphi}\begin{vmatrix}1-\frac{1}{2}a(\theta)(1+\cos\theta)+\frac{1}{2}b(\theta)\sin\theta & \frac{1}{2}i[a(\theta)\sin\theta-b(\theta)(1-\cos\theta)]\\ -\frac{1}{2}i[a(\theta)\sin\theta+b(\theta)(1+\cos\theta)] & 1-\frac{1}{2}a(\theta)(1-\cos\theta)-\frac{1}{2}b(\theta)\sin\theta\end{vmatrix}\quad\text{for }\delta=-1. \quad (15)$$

The total cross section (6) is given in terms of T by

$$\frac{d\sigma_P(\theta,\varphi)}{d\Omega}=\beta B^2(\theta)\frac{2E}{E-m}\sum_{MM_0}|T_{MM_0P}(\theta,\varphi)|^2; \quad (16)$$

the partial cross section for photoemission of an electron with spin M is

$$\frac{d\sigma_{MP}(\theta,\varphi)}{d\Omega}=\beta B^2(\theta)\frac{2E}{E-m}\sum_{M_0}|T_{MM_0P}(\theta,\varphi)|^2. \quad (17)$$

3. DISCUSSION OF THE TRANSITION MATRIX

The matrices T are unnormalized transition matrices. Their elements are proportional to probability amplitudes of electron transitions from a K-shell state with spin orientation M_0 to an unbound state in which the electron travels away in the direction (θ,φ) with spin orientation M, the transition being produced by the absorption of a photon with polarization P. The dependence on φ of the matrix elements in (13) has the simple form

$$e^{i(\delta+m_0-m)\varphi}. \quad (18)$$

The difference of the initial and final state quantum numbers $\delta+m_0$ and m in the exponent represents the quantum number that identifies the photoelectron's orbital angular momentum about the z axis, as anticipated at the beginning of this section. Accordingly, the terms with $\exp(\pm i\varphi)$ in the diagonal elements of the linear polarization matrices (10) and (12) represent the separate contributions of the circularly polarized components into which the linear polarization can be resolved.[24]

All probability amplitudes for the emission of a photoelectron in the forward direction $(\theta=0)$ vanish owing to the factor $\sin\theta$ in the coefficient $B(\theta)$, Eq. (4), which multiplies all the matrices T. As noted in the introduction, photoemission must vanish at $\theta=0$ whenever the orbital motion of the photoelectron receives a nonzero angular momentum about the polar axis. In the scheme of Eq. (13), this angular momentum is $(\delta+m_0-m)\hbar$. Therefore the matrix elements corresponding to spin flip $(m\neq m_0)$ need not vanish at $\theta=0$ for transitions with $\delta+m_0-m=0$. In fact, these matrix elements vanish *quadratically* at $\theta=0$ owing to the additional factor $\sin\theta$ in the expression (11) of $b(\theta)$. A further analysis of this result is achieved by a recalculation of the matrix elements in Sec. 4 and reference 5.

Another remarkable feature of the Sauter results is the fact that photoelectrons with kinetic energies $\sim 2m$ are less likely to be directed along the electric than along the magnetic field of the x-rays, for $\theta\sim\frac{1}{2}\pi$. This result is observed by comparing the transition matrices

$$T_{mm_0x}(\theta,0)=i\begin{vmatrix}2-a(\theta) & b(\theta)\\ -b(\theta) & 2-a(\theta)\end{vmatrix}$$

$$T_{mm_0x}(\theta,\tfrac{1}{2}\pi)=\begin{vmatrix}-a(\theta) & ib(\theta)\\ -ib(\theta) & a(\theta)\end{vmatrix}. \quad (19)$$

In these two matrices all spin-flip elements $(m\neq m_0)$ have the same magnitude, $b(\theta)$, as one would expect. On the other hand, the nonflip elements have magnitudes $|2-a(\theta)|$ and $a(\theta)$, respectively. Consider now the behavior of $a(\theta)$ in Fig. 1. This function is always positive, it increases with increasing θ, and it increases rapidly with increasing photon energy $E-m$. Therefore the ratio of matrix elements

$$[2-a(\theta)]/a(\theta), \quad (20)$$

whose square is the probability ratio of nonflip photoemission at the azimuths of the electric and magnetic fields, is very large at low energies and small θ and thereafter it decreases as θ or $E-m$ increases. In particular this ratio is less than 1 at $\theta=\frac{1}{2}\pi$ provided $E-m>m$; it passes through zero at $\theta=\frac{1}{2}\pi$ and $E-m=2m$ and eventually approaches -1 for very high energies. Therefore the photoemission at any given θ is largest at the electric field azimuth at low energies, at the magnetic field azimuth at higher energies, and eventually becomes uniform in the high-energy limit.

This variation of the ratio (20) may be called an

[24] It can be verified that the terms with $\exp(\pm i\varphi)$ originate respectively from the terms G and F in (1) and that these terms stem, in turn, in reference 6, from the circularly polarized components of the x-rays.

effect of destructive interference between the contributions 2 and $-a(\theta)$ to the nonflip transition matrix elements $T_{\frac{1}{2}\frac{1}{2}x}(\theta,0)$ and $T_{-\frac{1}{2}-\frac{1}{2}x}(\theta,0)$. This interference effect will presumably remain significant in a theory more accurate than Sauter's, because the corresponding effect in bremsstrahlung has been clearly observed experimantally.[4] Because both $a(\theta)$ and $b(\theta)$ vanish in the limit of low photon energy, at which limit the transition matrices take the form to be expected for the photoemission of a spinless particle, one may surmise that the contributions $a(\theta)$ and $b(\theta)$ to (19) and the resulting behavior of the ratio (20) stem from the electron spin. This surmise is confirmed by the recalculation of the transition matrix in reference 5.

In summary, a detector capable of observing only nonflip photoemission would yield zero response for that combination of electron energy and direction in the xz plane which makes $2-a(\theta)=0$. A detector insensitive to spin orientation observes only a minimum in the xz plane.

The correlation between the circular polarization of the x-rays and the spin orientation of the photoelectron, which was mentioned in the introduction, is displayed in the transition matrix (13), where the elements whose δ and m have equal signs are larger than those with opposite sign (except $\theta>\frac{1}{2}\pi$ at very high energy). We have indeed two separate effects: (1) The spin-flip elements vanish when δ and m have opposite sign. (Since in this case $\delta+m_0-m=2$, the matrix elements could differ from zero provided two units of angular momentum were absorbed by the orbital motion of the photoelectron.) (2) The non-spin-flip elements with δ and m of opposite sign are reduced by destructive interference between the contributions proportional to 1 and to $-a(\theta)$. This effect is thereby related to the reduction of the ratio (20) for linearly polarized x-rays.

Whenever $1-a(\theta)=0$, one whole row of each 2×2 matrix in (13) vanishes. No electron is then ejected with spin opposite to that of a circularly polarized photon; the degree of spin polarization of the photoelectrons equals the degree of circular polarization of the x-rays (see Fig. 3 in Sec. 5). This condition is fulfilled for one angle $0<\theta\leq\pi$ whenever the photon energy exceeds $\frac{2}{3}mc^2$. In particular, circularly polarized x-rays of energy mc^2 yield *100% transverse spin polarization* of the photoelectrons ejected at 90°, according to the present (Sauter) approximation. It seems plausible that the matrix elements indicated by $1-a(\theta)$ in (13) would in fact vanish, in an exact theory, at some value of θ whenever the photon energy is sufficiently high. On the other hand the matrix elements equal to zero in (13) would probably not vanish in an exact theory; an experimental determination of the maximum attainable degree of spin polarization would provide an estimate of the actual departure from the Sauter approximation.

Notice finally that the elements of the matrices T are related to one another by a relationship equivalent to Lenard's,[22] namely,

$$(-1)^{m-m_0}T_{-m-m_0P'}(\theta,-\varphi)=T_{mm_0P}(\theta,\varphi),\quad(21)$$

where the polarization P' is obtained from P by reflection of the polarization vectors on the xz plane. This reflection leaves the polarization x unchanged, changes y into $y'=-y$ and thereby reverses the sign of the matrix (10), and changes δ into $\delta'=-\delta$. Equation (21) expresses the fact that the transition probability amplitudes are invariant under the following combination of operations: (a) reflection of all polar vectors on the xz plane, which changes φ into $-\varphi$ and P into P', and (b) rotation of all spins by 180° about the y axis, which changes (m,m_0) into $(-m,-m_0)$ and multiples T by $(-1)^{m-m_0}$. This invariance derives from the well known invariance under the following separate operations, whose combination is equivalent to the combination of (a) and (b), namely: (A) inversion of all polar vectors, but not of spins, at the origin of coordinates, (B) simultaneous rotation of all polar and spin vectors by 180° about the y axis.[25]

4. EXPANSION OF THE K-SHELL WAVE FUNCTION. CONNECTION BETWEEN PHOTOEFFECT AND BREMSSTRAHLUNG

The interaction of an electron with radiation of wave vector $\mathbf{k}$ and polarization vector $\mathbf{e}$ may be represented by the Dirac operator

$$\boldsymbol{\alpha}\cdot\mathbf{e}\; e^{i\mathbf{k}\cdot\mathbf{r}}.\quad(22)$$

The probability amplitude for the photoeffect in the K shell is proportional to the matrix element of (22) between a K-shell and a free-electron state. In the calculation of this matrix element a K-shell state with spin quantum number $m_0=\frac{1}{2}$ is usually represented by the Coulomb-field Dirac wave function

$$\Psi_{K\frac{1}{2}}(r,\theta,\varphi)=[8\pi\Gamma(2\gamma+1)]^{-\frac{1}{2}}\left(\frac{2Zm}{137}\right)^{\gamma+\frac{1}{2}}r^{\gamma-1}\times e^{-Zmr/137}\begin{bmatrix}(1+\gamma)^{\frac{1}{2}}\\0\\i(1-\gamma)^{\frac{1}{2}}\cos\theta\\i(1-\gamma)^{\frac{1}{2}}\sin\theta e^{i\varphi}\end{bmatrix},\quad(23)$$

where

$$\gamma=(1-Z^2/137^2)^{\frac{1}{2}}.\quad(24)$$

The calculations we are considering in this paper are approximate ones, in which the matrix elements are expanded into powers of Z and only the lowest significant power is retained. To simplify the calculation and make it more transparent we shall expand the wave function (23) prior to calculation of the matrix element.

[25] The theorem in reference 22 is restricted to Born approximation matrix elements because only in this approximation and with appropriate phase conventions the sign reversal of φ can be expressed as a complex conjugation and sign reversal of the matrix element.

Interchanging the order of the operations of matrix calculation and expansion should be regarded as an illustrative device, in that the expansion of the wave function has very limited validity *per se* but must be judged in connection with its intended application.

A detailed analysis of the expansion, of its significance, and of its mathematical justification has required considerable effort and is given in reference 1; it leads specifically to the following results. The factor $r^{\gamma-1}$ in (23) can be disregarded in calculations to first order in $Z/137$ because $\gamma-1=O(Z^2/137^2)$. After this factor is dropped, only the values of the wave function and of its first derivative at $r=0$ are relevant, to first order in $Z/137$, because the photoelectric process takes place near the nucleus.[26] That is, the approximate form of the wave function to be utilized must be realistic only near the nucleus. This form is found to be

$$\Psi_{K\frac{1}{2}}(r,\theta,\varphi)=\Psi_{K\frac{1}{2}}{}^{(0)}+\frac{Z}{137}\Psi_{K\frac{1}{2}}{}^{(1)}+\cdots$$

$$\sim\left(\frac{1}{\pi}\left(\frac{Zm}{137}\right)^3\right)^{\frac{1}{2}}\left\{\begin{bmatrix}1\\0\\0\\0\end{bmatrix}+\frac{Z}{137}\begin{bmatrix}-mr\\0\\\frac{1}{2}i\cos\theta\\\frac{1}{2}i\sin\theta e^{i\varphi}\end{bmatrix}\right\}. \quad (25)$$

A final state in which, following a photon absorption, the electron travels away with momentum $\mathbf{p}$ and spin quantum number m may now be represented, in analogy with (25), by the usual Born approximation wave function

$$\Psi_{\mathbf{p}m}(\mathbf{r})\sim\left[e^{i\mathbf{p}\cdot\mathbf{r}}-\frac{Z}{137}\frac{1}{2\pi^2}\times\int d\mathbf{p}'\,e^{i\mathbf{p}'\cdot\mathbf{r}}\frac{E(p)+\boldsymbol{\alpha}\cdot\mathbf{p}'+\beta m}{(p^2-p'^2)|\mathbf{p}-\mathbf{p}'|^2}\right]u_m(\mathbf{p}), \quad (26)$$

where $u_m(\mathbf{p})$ is given by (7) in the Sauter representation.

The relationship of the expansions (25) and (26) is brought out by noticing that

$$\Psi_{K\frac{1}{2}}{}^{(0)}(\mathbf{r})=\pi^{-\frac{1}{2}}(Zm/137)^{\frac{3}{2}}u_{\frac{1}{2}}(0)$$

and by expanding $\Psi_{K\frac{1}{2}}{}^{(1)}(\mathbf{r})$ into momentum eigenstates. This expansion is part of the procedure discussed in reference 1. One finds

$$\Psi_{K\frac{1}{2}}(\mathbf{r})=\left[\frac{1}{\pi}\left(\frac{Zm}{137}\right)^3\right]^{\frac{1}{2}}\left[1-\frac{Z}{137}\frac{1}{2\pi^2}\times\int d\mathbf{p}''\,e^{i\mathbf{p}''\cdot\mathbf{r}}\frac{m+\boldsymbol{\alpha}\cdot\mathbf{p}''+\beta m}{-p''^2|\mathbf{p}''|^2}\right]u_{\frac{1}{2}}(0). \quad (27)$$

[26] The minimum nuclear recoil momentum q_m, under the limitation $Z/137\beta\ll 1$ of the Sauter approximation obeys the condition $m>q_m\gg mZ/137$. That is, the corresponding de Broglie wavelength is much smaller than the K-shell radius.

Comparison of (27) with (26) shows that

$$\Psi_{K\frac{1}{2}}(\mathbf{r})=\left[\frac{1}{\pi}\left(\frac{Zm}{137}\right)^3\right]^{\frac{1}{2}}\Psi_{0\frac{1}{2}}(\mathbf{r}),$$

$$\text{to first order in } Z/137. \quad (28)$$

It follows from this relation among wave functions that the calculation of the matrix element of the interaction (22) in the Sauter theory of the photoelectric effect coincides with the corresponding calculation in the Born approximation theory of bremsstrahlung. More specifically, the photoelectric effect corresponds to the high-energy limit of bremsstrahlung at which the in-

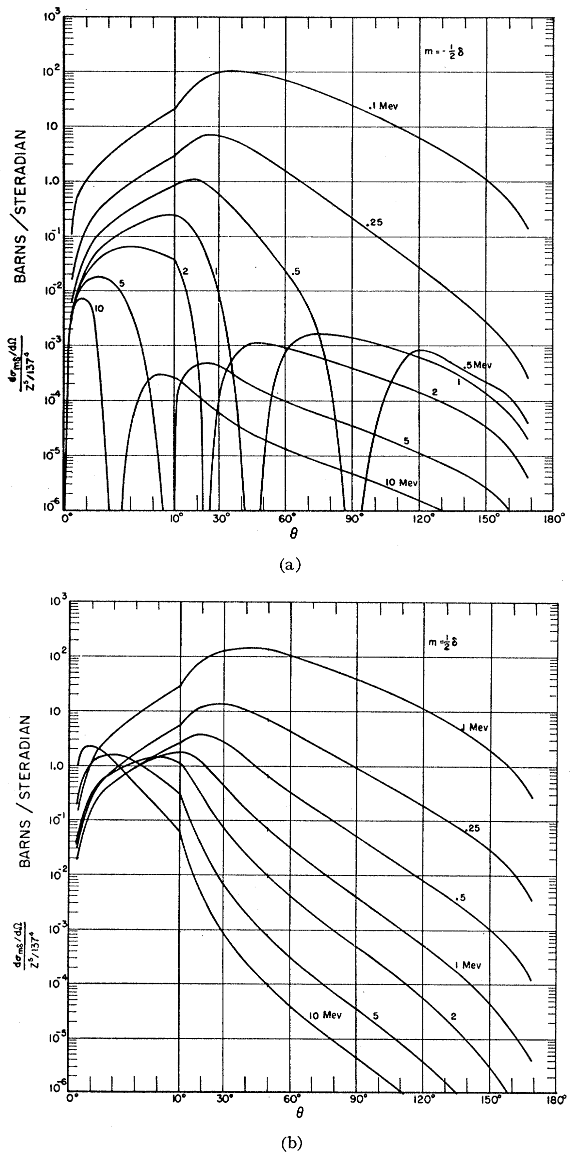

FIG. 2. Differential cross sections for photoemission, by circularly polarized x-rays, of electrons with spin parallel or opposite to the direction of incidence.

cident electron radiates all of its kinetic energy and is left with zero momentum.

The relation between the Sauter calculation of the photoelectric effect and that of reference 9 may be indicated at this point. The matrix element of the interaction (22) calculated with the wave functions (27) and (26) separate out into terms of different order in $Z/137$. The combination of the lowest order term of (27) with the lowest order term of (26) yields a zero contribution to the matrix element, because the momenta $\mathbf{k}$ and $\mathbf{p}$ of the photon and electron cannot be equal consistently with energy conservation. The combination of the second term of (27) with the lowest order term of (26) yields a contribution to the matrix element arising from the component $\mathbf{p}''=\mathbf{p}-\mathbf{k}$ of the Fourier integral of (27). This contribution is of order

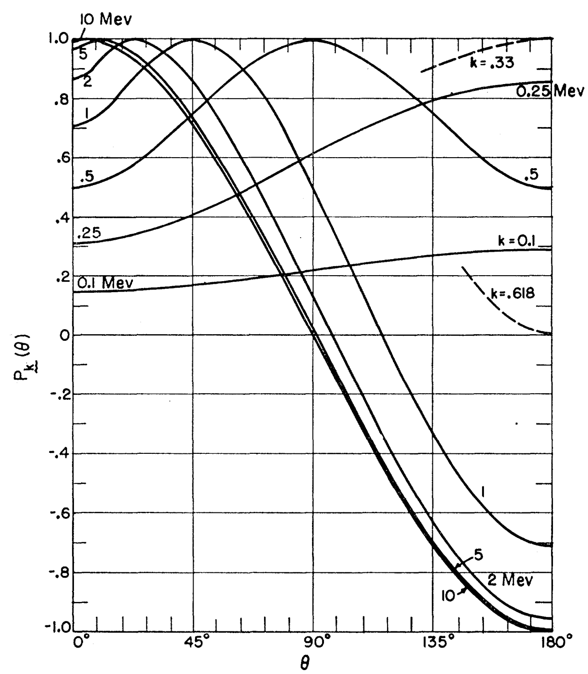

FIG. 3. Degree of electron spin polarization parallel to the circular polarization of the incident x-rays, as a function of the angle of emission.

$Z/137$ and was considered in reference 9. However, this reference disregarded the second term of (26) and thereby the contribution it yields in combination with the lowest order term of (27). This contribution arises from the component $\mathbf{p}'=\mathbf{k}$ in the Fourier integral of (26) and is again of first order in $Z/137$. The combination of the second term of (26) with the second term of (27) is of order $(Z/137)^2$ and is accordingly disregarded in the Sauter approximation.

As indicated in the introduction, the approximate connection between the photoelectric effect and bremsstrahlung established by (28) has applications described in references 2, 3, and 4. It also makes applicable to the photoeffect the calculation of the bremsstrahlung

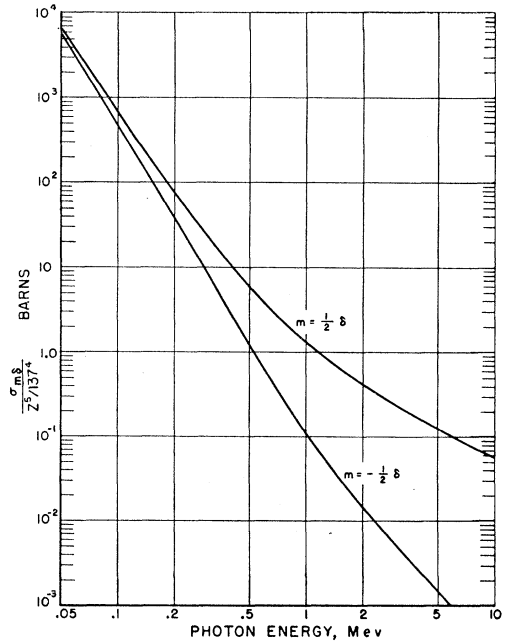

FIG. 4. Integral cross sections for photoemission, by circularly polarized x-rays, of electrons with spin parallel or opposite to the direction of incidence.

matrix elements of reference 5, in which the contribution of different effects in the mechanics of the Dirac electron are kept separate. This calculation identifies the terms containing $a(\theta)$ and $b(\theta)$ in the transition matrices of Sec. 2 as contributed by the action of x-rays upon the spin current of the electron. It also shows that the combinations of the first term of (26) with the second term of (27) and of the second term of (26) with the first one of (27) contribute separately finite amounts to $B(\theta)b(\theta)$ at $\theta=0$, but that the two contributions cancel out.

5. CROSS SECTIONS

Olsen[27] has given an explicit formula for the cross section (17), $d\sigma_{MP}(\theta,\varphi)/d\Omega$, for ejection of an electron in

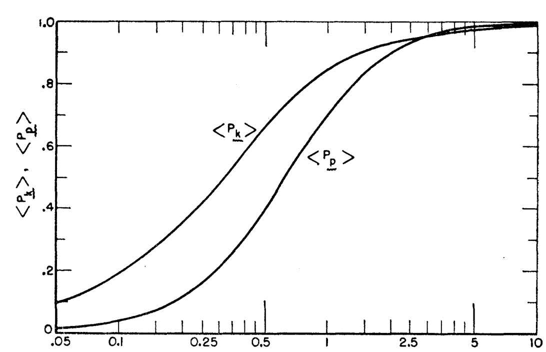

FIG. 5. Average degree of electron spin polarization in the direction of incidence ($\langle P_{\mathbf{k}}\rangle$) and in the direction of emission ($\langle P_{\mathbf{p}}\rangle$).

[27] Reference 20, Eq. (16); the factor ϵ should be deleted in this equation.

the direction (θ,φ) and with spin quantum number $M=\frac{1}{2}$ referred to an arbitrary axis **s** by a photon with any given polarization P. Here we give data for the special case of helicity eigenstates $(M=\epsilon=\pm\frac{1}{2})$ and of circular polarization $(P=\delta=\pm 1)$ to replace the data of reference 9. We also give data for the case of spin orientation in the direction of the incident x-rays $(M=m=\pm\frac{1}{2})$, and for circular polarization, because the results of Sec. 2 indicate that analytical expressions are simpler in this case and, therefore, possibly more fundamental.

Equations (17) and (13) yield

$$d\sigma_{m\delta}(\theta,\varphi)=C(\theta)[1+b^2(\theta)]d\Omega,\quad \text{for } m=\tfrac{1}{2}\delta, \tag{29a}$$

$$d\sigma_{m\delta}(\theta,\varphi)=C(\theta)[1-a(\theta)]^2 d\Omega,\quad \text{for } m=-\tfrac{1}{2}\delta, \tag{29a}$$

where

$$C(\theta)=4\frac{E}{E-m}\beta B^2(\theta)$$

$$=\frac{1}{2}\frac{Z^5}{137^4}r_0^2\left(\frac{m}{k}\right)^5\frac{k+2m}{k+m}\,\frac{\beta^3\sin^2\theta}{(1-\beta\cos\theta)^4}, \tag{30}$$

and $a(\theta)$, $b(\theta)$ are given by (11). Figure (2a) and (2b) show $d\sigma_{m\delta}/d\Omega$ as a function of θ for various values of $k=E-m$. Figure 3 shows the degree of spin polarization in the direction of the photon momentum **k**.

$$P_{\mathbf{k}}(\theta)=\frac{[1+b^2(\theta)]-[1-a(\theta)]^2}{[1+b^2(\theta)]+[1-a(\theta)]^2}. \tag{31}$$

Notice that $P_{\mathbf{k}}$ attains 1 at one value of θ provided $k\geqslant\frac{2}{3}m$, as discussed in Sec. 3. The corresponding integral

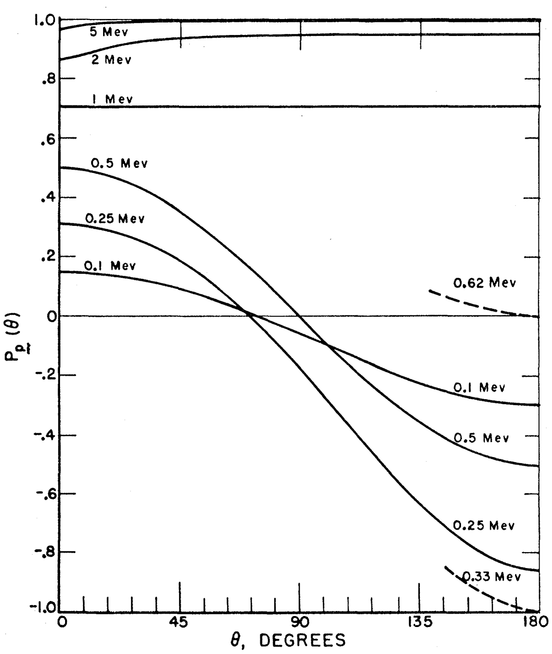

FIG. 6. Degree of electron spin polarization with helicity equal to that of the incident x-rays, as a function of the angle of emission.

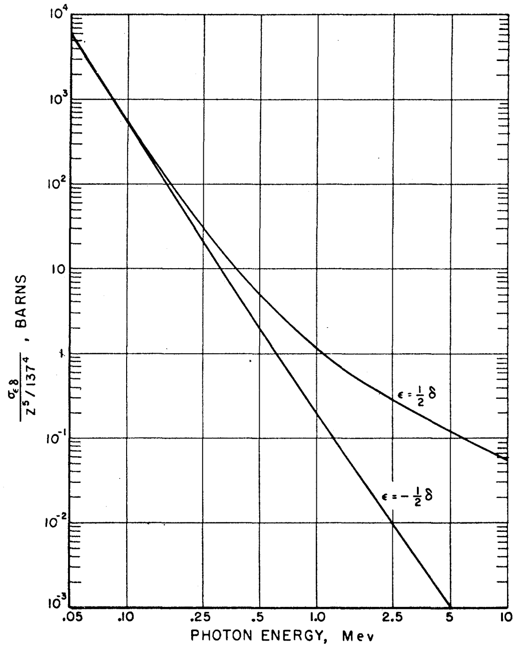

FIG. 7. Integral cross section for photoemission, by circularly polarized x-rays, of electrons with helicity equal or opposite to that of the x-rays.

cross sections are given by

$$\sigma_{m\delta}=4\pi\frac{Z^5}{137^4}r_0^2\left(\frac{m}{k}\right)^{7/2}\left(\frac{k+2m}{m}\right)^{\frac{1}{2}}\left\{\frac{4}{3}\frac{k+m}{m}+\left(\frac{k}{m}\right)^2+\frac{2k}{k+2m}\left(1-\frac{1}{2\beta}\ln\frac{1+\beta}{1-\beta}\right)\right\},\quad \text{for } m=\tfrac{1}{2}\delta, \tag{32a}$$

$$\sigma_{m\delta}=4\pi\frac{Z^5}{137^4}r_0^2\left(\frac{m}{k}\right)^{7/2}\left(\frac{k+2m}{m}\right)^{\frac{1}{2}}\left\{-\frac{5}{3}+\frac{4m}{k+2m}+\left[1-\frac{2km}{(k+m)(k+2m)}\right]\frac{1}{2\beta}\ln\frac{1+\beta}{1-\beta}\right\},\quad \text{for } m=-\tfrac{1}{2}\delta, \tag{32b}$$

with $\beta=k^{\frac{1}{2}}(k+m)^{\frac{1}{2}}/(k+m)$. They are plotted as functions of the photon energy k in Fig. 4. Figure 5 shows the "average" spin polarization

$$\langle P_{\mathbf{k}}\rangle=\frac{\sigma_{\frac{1}{2}\delta,\delta}-\sigma_{-\frac{1}{2}\delta,\delta}}{\sigma_{\frac{1}{2}\delta,\delta}+\sigma_{-\frac{1}{2}\delta,\delta}}. \tag{33}$$

The differential cross sections pertaining to eigenstates of helicity of the outgoing electron are obtained from (17) and (15); they are[28]

[28] *Note added in proof.*—We are very grateful to Dr. H. Banerjee for pointing out to us that the sign of the last term of (34) in the manuscript of this paper was originally incorrect, being at variance with results published by him in Nuovo cimento, **10**, 863 (1958) and **11**, 220 (1959). The error arose from an inconsistency in the phases of (7) and (14). Equations (14), (15), (34), (35), (36), Figs. 5, 6, and 7, and the relevant discussion have now been corrected.

$$d\sigma_{\epsilon\delta}=C(\theta)\{\tfrac{1}{2}[1+b^2(\theta)+(1-a(\theta))^2] +(-1)^{\epsilon-\frac{1}{2}\delta}\tfrac{1}{2}[1+b^2(\theta)-(1-a(\theta))^2]\cos\theta -(-1)^{\epsilon-\frac{1}{2}\delta}b(\theta)[1-a(\theta)]\sin\theta\}d\Omega. \quad (34)$$

The corresponding degree of polarization (helicity) is

$$P_{\mathrm{p}}(\theta) =\frac{\{1+b^2(\theta)-[1-a(\theta)]^2\}\cos\theta-2b(\theta)[1-a(\theta)]\sin\theta}{1+b^2(\theta)+[1-a(\theta)]^2} =\left(\frac{k}{k+2m}\right)^{\frac{1}{2}}\frac{1+\frac{1}{2}(k+m)(k^2-2m^2)(1-\beta\cos\theta)}{1+\frac{1}{2}k(k^2-m^2)(1-\beta\cos\theta)}, \quad (35)$$

and is plotted in Fig. 6. As expected, $P_{\mathrm{p}}(\theta)$ and $P_{\mathrm{k}}(\theta)$ are nearly equal at small θ, where the cross section is largest at relativistic energies, and have opposite sign at $\theta\sim 180°$. It is remarkable that $P_{\mathrm{p}}(\theta)$ approaches 1 for all values of θ in the high-energy limit.

The integral cross sections pertaining to helicity eigenstates are given by

$$\sigma_{\epsilon\delta}=2\pi\frac{Z^5}{137^4}r_0^2\left(\frac{m}{k}\right)^2\left(\frac{k+2m}{k}\right)^{\frac{3}{2}} \times\left\{\frac{4}{3}+\frac{k^2-m^2}{m(k+2m)}\left(1-\frac{m^2}{(k+m)^2}\frac{1}{2\beta}\ln\frac{1+\beta}{1-\beta}\right) +(-1)^{\epsilon-\frac{1}{2}\delta}\left(\frac{k}{k+2m}\right)^{\frac{1}{2}}\left[\frac{4}{3}+\frac{k+m}{k}\frac{k^2-2m^2}{m(k+2m)} \times\left(1-\frac{m^2}{(k+m)^2}\frac{1}{2\beta}\ln\frac{1+\beta}{1-\beta}\right)\right]\right\}, \quad (36)$$

and are shown in Fig. 7. The corresponding "average" degree of polarization $\langle P_{\mathrm{p}}\rangle$ is shown in Fig. 5.

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High-Frequency Limit of Bremsstrahlung in the Sauter Approximation

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The expansion in powers of $Z/137$ utilized in the Sauter theory of the photoelectric effect yields a nonzero cross section proportional to Z^3 at the high-frequency limit of the bremsstrahlung spectrum, and also at the low electron energy limit of the pair production spectrum. These cross sections are related to the Sauter photoelectric cross section by detailed balancing. The results apply equally when the effects of spin orientations and x-ray polarization are considered.

THE x-ray emission by electrons is calculated most simply in the Born approximation.[1] However this approximation breaks down completely at the upper end of the x-ray frequency spectrum, because it involves an expansion in powers of $Z/137\beta_0$ and of $Z/137\beta$, where β_0 and β are the electron velocities (in units of c) before and after a radiative collision with a nucleus of atomic number Z. The high-frequency end of the spectrum arises from collisions in which the electron emerges with $\beta=0$, so that $Z/137\beta=\infty$ instead of being $\ll 1$ as required by the approximation method. Procedures have been proposed to compensate this failure of the simple theory through corrections derived by comparing the exact and the Born approximation results in the nonrelativistic limit.[1,2]

This paper presents a modified Born approximation, which applies at $\beta\sim 0$ and involves an expansion in powers of $Z/137\beta_0$ and $Z/137$ instead of $Z/137\beta$. The modified ("Sauter"[3]) approximation yields, like the earlier corrections, a simple renormalization of the Born approximation results. Whereas the earlier corrections were tentative extrapolations and were intended to apply throughout the range $0\leq\beta<1$, the correction introduced here has a more definite foundation and applies only for $\beta\lesssim Z/137$. The result obtained in this paper for the high-energy limit of the bremsstrahlung is directly applicable to the low electron energy limit of pair production and is related by detailed balancing to the cross section for the photoelectric emission of atomic electrons calculated in the same approximation. No attempt is made here to take into account the terms of

[1] See, e.g., W. Heitler, *Quantum Theory of Radiation* (Oxford University Press, Oxford, 1954), third edition, pp. 242–247.

[2] G. Elwert, Ann. Physik **34**, 178 (1939); E. Guth, Phys. Rev. **59**, 329 (1941); P. Kirkpatrick and L. Wiedemann, Phys. Rev. **67**, 321 (1945). In addition, F. Nagasaka, thesis, University of Notre Dame, 1955 (unpublished), and M. V. Mihailovic, Nuovo cimento **9**, 331 (1958), have carried out calculations at the high-frequency limit using Sommerfeld-Maue wave functions; however, they do not discuss the significance of these wave functions at $\beta=0$.

[3] F. Sauter, Ann. Physik **9**, 217 (1931) and **11**, 454 (1931).