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Photoelectric Effect in Pb at High Energies

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A formula for the photoelectric absorption cross section for the K shell is derived using the Furry or Sommerfeld-Maue approximate wave function. The surviving terms at the high-energy limit are given explicitly and the value for the cross section is found for Pb by numerical integration. The exact wave function is rewritten so as to simplify the derivation of the Furry approximation.

INTRODUCTION

THERE appears to be a recent revival of interest in the high-energy photoelectric effect. A paper[1] has appeared in which an approximate continuum Coulomb wave function was used to calculate the cross section for large photon energies. This function, given by Schiff[2] and others, is asymptotic at great distances to the Furry[3] or Sommerfeld-Maue[4] wave function (as employed by Bethe and Maximon[5] to calculate bremsstrahlung). This latter function, it has been argued, gives exact results at the high-energy limit in certain calculations, the reason for which may be seen upon comparison with the exact solution when both are expanded in spherical waves. The respective terms are asymptotically equal for large l (angular momentum). But in certain cases, such as bremsstrahlung[5] and the photoelectric effect,[6] the contribution to the matrix element of a fixed partial sum of (exact) spherical waves is negligible for large k (initial photon energy). Now Prange and Pratt have shown that their function (less accurate than Furry's) yields for the photoelectric cross section at high energies precisely the result of Hall (who used the exact wave function), namely the factor $1/k$ multiplied by a certain function of Z given by Hall as a double integral. This argues independently for the correctness of a calculation based upon the Furry wave function, since it should be bracketed between the exact calculation of Hall and that of Prange and Pratt. A new derivation of the Furry function is given in the Appendix.

CALCULATION OF THE CROSS SECTION

Such a calculation has been performed for the K shell using the continuum wave function

$$\Psi_f = N \exp(i\mathbf{p}\cdot\mathbf{r})[1-(i\boldsymbol{\alpha}\cdot\nabla/2E)] \times F(-ia_1;1;-i(pr+\mathbf{p}\cdot\mathbf{r}))u(\mathbf{p}).$$

The notation is basically that of Bethe and Maximon, the confluent hypergeometric function corresponding to ingoing waves. $a=e^2Z/\hbar c\cong Z/137$, $a_1=Ea/p$. E and $\mathbf{p}$ are in units of mc^2, $\mathbf{r}$ is in units of $\hbar/mc$. $u(\mathbf{p})$ is a spinor coefficient associated with a free particle of momentum $\mathbf{p}$. The bound state of the K electron is given by

$$\Psi_i = N' r^{\sigma-1}\exp(-ar)g(\Theta,\Phi),$$

$$g(\Theta,\Phi)=\begin{bmatrix}1\\0\\iA\cos\Theta\\iA\sin\Theta\exp(i\Phi)\end{bmatrix}.$$

The initial electron spin is in the $+z$ direction, to which the angles Θ,Φ refer. $\sigma=(1-a^2)^{\frac{1}{2}}$, $A=(1-\sigma)a^{-1}$, and N' is a normalizing constant. We may omit the details of the summation of the squared matrix element over the two final spin states of the electron, which may be accomplished using a projection operator. It is then convenient to write the differential absorption cross section for a photon of polarization $\mathbf{e}$ with direction of propagation $\mathbf{k}$ as

$$d\sigma(\theta)=(3/16\pi^2)N^2N'^2(137)^{\sigma+\frac{3}{2}}\sigma_0(Ep/k)\mathbf{U}^*\cdot\mathbf{D}\cdot\mathbf{U}d\Omega.$$

θ is the scattering angle and σ_0 the Thomson cross section $8\pi e^4/3m^2c^4$. Here

$$\mathbf{U}=\begin{bmatrix}\int d^3\mathbf{r}\, F(ia_1;1;i(pr+\mathbf{p}\cdot\mathbf{r}))\exp i(\mathbf{q}\cdot\mathbf{r}-ar)r^{\sigma-1}g(\Theta,\Phi)\\ (i/2E)\int d^3\mathbf{r}\,\nabla F(ia_1;1;i(pr+\mathbf{p}\cdot\mathbf{r}))\exp i(\mathbf{q}\cdot\mathbf{r}-ar)r^{\sigma-1}g(\Theta,\Phi)\end{bmatrix}$$

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[1] R. E. Prange and R. H. Pratt, Phys. Rev. **108**, 139 (1957).
[2] L. I. Schiff, Phys. Rev. **103**, 443 (1956).
[3] W. H. Furry, Phys. Rev. **46**, 391 (1934).
[4] A. Sommerfeld and A. W. Maue, Ann. Physik **22**, 629 (1935).
[5] H. A. Bethe and L. C. Maximon, Phys. Rev. **93**, 768 (1954).
[6] H. Hall, Revs. Modern Phys. **8**, 358 (1936).

is displayed as a vector of four components (labelled o, x, y, z) each of which has four subcomponents answering to the spinor indices 1, 2, 3, 4 of $g(\Theta,\Phi)$. $\mathbf{q}=\mathbf{k}-\mathbf{p}$ is the recoil momentum. Similarly, D may be written as the dyadic

$$\mathsf{D}=(2E)^{-1}(\boldsymbol{\alpha}\cdot\mathbf{e})\begin{pmatrix}(H+E) & (H+E)\boldsymbol{\alpha}\\ \boldsymbol{\alpha}(H+E) & \boldsymbol{\alpha}(H+E)\boldsymbol{\alpha}\end{pmatrix}(\boldsymbol{\alpha}\cdot\mathbf{e}),$$

where $H=\boldsymbol{\alpha}\cdot\mathbf{p}+E-\beta$. The Dirac matrices $\boldsymbol{\alpha}$, β will be used in the representation of Bethe and Maximon, and in addition we shall use the 4×4 matrices

$$\boldsymbol{\sigma}=\begin{pmatrix}\boldsymbol{\sigma}' & 0\\ 0 & \boldsymbol{\sigma}'\end{pmatrix}\quad\text{and}\quad \epsilon=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},$$

where $\boldsymbol{\sigma}'$ are the 2×2 Pauli matrices. D is thus in detail a 16×16 Hermitian matrix. Define $\mathbf{I}$ as the unit dyadic and $\mathsf{E}=2(\mathbf{ee})-\mathbf{I}$. Then, after some matrix algebra (which the dyadic notation simplifies considerably) we arrive at an expression linear in the Dirac matrices.

$$\mathsf{D}=(2E)^{-1}\left[\begin{array}{l|l}\boldsymbol{\alpha}\cdot\mathsf{E}\cdot\mathbf{p} & \\ \quad & \mathbf{p}+i\boldsymbol{\sigma}\cdot\mathsf{E}\times\mathbf{p}+(E-\beta)(\boldsymbol{\alpha}\cdot\mathsf{E})\\ +(E-\beta) & \\ \hline \mathbf{p} & (\boldsymbol{\alpha}\cdot\mathsf{E})\mathbf{p}+\mathbf{p}(\mathsf{E}\cdot\boldsymbol{\alpha})\\ -i\boldsymbol{\sigma}\cdot\mathsf{E}\times\mathbf{p} & -(\boldsymbol{\alpha}\cdot\mathsf{E}\cdot\mathbf{p})\mathbf{I}+i\epsilon\mathbf{p}\times\mathbf{I}\\ +(\boldsymbol{\alpha}\cdot\mathsf{E})(E-\beta) & +(E+\beta)(\mathbf{I}-i\boldsymbol{\sigma}\cdot\mathsf{E}\times\mathbf{I})\end{array}\right].$$

When we average over the two photon polarizations, remembering that $\mathbf{e}$ occurs only in E, we may use $\mathsf{E}'=-(\mathbf{ff})$, where $\mathbf{f}$ is the unit vector along $\mathbf{k}$. We find that

$$\mathsf{D}'=(2E)^{-1}\left[\begin{array}{l|l}-(\boldsymbol{\alpha}\cdot\mathbf{f})(\mathbf{f}\cdot\mathbf{p}) & \\ \quad & \mathbf{p}-i(\boldsymbol{\sigma}\cdot\mathbf{f})(\mathbf{f}\times\mathbf{p})-(E-\beta)(\boldsymbol{\alpha}\cdot\mathbf{f})\mathbf{f}\\ +(E-\beta) & \\ \hline \mathbf{p} & -(\boldsymbol{\alpha}\cdot\mathbf{f})(\mathbf{fp}+\mathbf{pf})\\ +i(\boldsymbol{\sigma}\cdot\mathbf{f})(\mathbf{f}\times\mathbf{p}) & +(\boldsymbol{\alpha}\cdot\mathbf{f})(\mathbf{f}\cdot\mathbf{p})\mathbf{I}+i\epsilon\mathbf{p}\times\mathbf{I}\\ -\mathbf{f}(\boldsymbol{\alpha}\cdot\mathbf{f})(E-\beta) & +(E+\beta)(\mathbf{I}+i(\boldsymbol{\sigma}\cdot\mathbf{f})(\mathbf{f}\times\mathbf{I}))\end{array}\right].$$

The averaged cross section for a K electron with spin in the $-z$ direction is the same, so we need only to double this result to find the total absorption by the K shell. A single function I provides all components of $\mathbf{U}$:

$$\mathbf{U}=\begin{bmatrix}-\partial/\partial a\\ 0\\ A\partial/\partial q_z\\ A(\partial/\partial q_x+i\partial/\partial q_y)\end{bmatrix}\begin{Bmatrix}I(\mathbf{p},\mathbf{q},a,\sigma)\\ (ip/2E)\nabla_{\mathbf{p}}I(\mathbf{p},\mathbf{q},a,\sigma-1)\end{Bmatrix},$$

where

$$I(\mathbf{p},\mathbf{q},a,\sigma)=\int d^3\mathbf{r}F(ia_1;1;i(pr+\mathbf{p}\cdot\mathbf{r}))\exp(i\mathbf{q}\cdot\mathbf{r}-ar)r^{\sigma-2}.$$

Particular values for $\mathbf{p}$ and $\mathbf{q}$ are not substituted until all differentiations are performed. We next make the replacement

$$r^{\sigma-1}=[\Gamma(1-\sigma)]^{-1}\int_0^\infty x^{-\sigma}\exp(-xr)dx,$$

and interchange the order of integration. After some transformations of a contour integral (guided in part by the method of Nordsieck[7]) we arrive at

$$I(\mathbf{p},\mathbf{q},a,\sigma)=4\pi[\Gamma(1-\sigma)]^{-1}\int_0^\infty dx x^{-\sigma}(x-p_1)^{ia_1-1}(x-p_2)^{-ia_1}(x-p_3)^{ia_1-1}(x-p_4)^{-ia_1}.$$

[7] A. Norsieck, Phys. Rev. 93, 785 (1954).

For purposes of differentiation, **p**, **q**, a are contained only in

$$p_1=-a-iq, \qquad p_2=-a+i(p-k),$$
$$p_3=-a+iq, \qquad p_4=-a+i(p+k).$$

Principal values of the arguments of $(x-p_i)$ are to be used.

It is now a matter of estimating the orders of magnitude of I and its derivatives as $k\to\infty$. After a laborious sorting of terms there remains only

$$\sigma_K=(3Z^5\sigma_0/2(137)^4k)\left(\frac{2^{2\sigma+3}a^{2\sigma-4}|\Gamma(1-ia)|^2}{(1+A^2)\Gamma(2\sigma+1)[\Gamma(1-\sigma)]^2}\right)\int_\sigma^\infty qK(q)dq,$$

as the term of lowest order, the integration being performed over q instead of θ. Here

$$K(q)=(a^2/4)(1+A^2)|K_1(q)|^2+(1+a^2)A^2q^2|K_2(q)|^2+(1+a^2)|K_3(q)+aK_2(q)|^2$$
$$+\mathrm{Re}\{-(A-i)(1+ia)a[\bar{K}_3(q)+a\bar{K}_2(q)]K_1(q)$$
$$+(A-i)(1+ia)aA\sigma\bar{K}_2(q)K_1(q)-2A(1+a^2)\sigma[\bar{K}_3(q)+a\bar{K}_2(q)]K_2(q)\}.$$

$$K_1(q)=\int_0^\infty x^{-\sigma}[(x+a)^2+q^2]^{ia-1}(x+a-i\sigma)^{-ia-1}dx,$$

$$K_2(q)=\int_0^\infty x^{-\sigma}[(x+a)^2+q^2]^{ia-2}(x+a-i\sigma)^{-ia}dx,$$

$$K_3(q)=\int_0^\infty x^{1-\sigma}[(x+a)^2+q^2]^{ia-2}(x+a-i\sigma)^{-ia}dx.$$

It will be noticed that this result would be changed, even at the high-energy limit, by the effect of electronic screening upon the ground state; for, since q represents physically the recoil momentum of the atom, the lower limit of the integral is simply the ionization energy of a K electron, which is altered by screening.

The above integrals $K_i(q)$ were performed in the case of lead for the range $q=0.80(0.05)1.40(0.10)2.00$ on the electronic computer of the University of Manchester, and the final integration over momentum was performed by a planimeter as far as $q=2$, beyond which point the asymptotic formula $K(q)\sim(0.789)/q^4$ was used. This result is apparent from an inspection of the functions $K_i(q)$ for large q.

The resulting cross section was found to be

$$\sigma_K=[3Z^5\sigma_0/2(137)^4k](0.235).$$

The well-known approximate formula of Hall,[6]

$$\sigma_K=[3Z^5\sigma_0/2(137)^4k]\exp[-a\pi+2a^2(1-\ln a)],$$

yields for the constant in question the value 0.451. The figure 0.235 is in good agreement with another numerical calculation using the formula of Prange and Pratt,[8] which has given the value 0.222. It seems significant that the Hall formula is also about twice as large as the exact figure for $Z=137$, which has been conveniently evaluated by Prange and Pratt.

A recent paper[9] has given a derivation of the cross section for the K shell using the Born approximation for the continuum wave functions which, in the extreme relativistic limit, agrees with Hall's formula to first order in a.

APPENDIX

I should also like to point out that it is possible to rewrite the exact continuum wave function in a much simpler form,[10] which makes nearly trivial the passage to the Furry approximation $\{$where we set $[(l+1)^2-a^2]^{\frac{1}{2}}=l+1\}$. Heretofore this has been a rather cumbersome procedure.[3,5] In this expression for the exact solution, the gradient term $\boldsymbol{\alpha}\cdot\nabla/2E$ (typical of the Furry approximation), already makes its appearance. It turns out that many of the recurrence relations for confluent hypergeometric functions of the type $F(l+1-ia_1;\ 2l+3;\ -2ipr)$ apply as well to functions of the type $F([(l+1)^2-a^2]^{\frac{1}{2}}-ia_1;\ 2[(l+1)^2-a^2]^{\frac{1}{2}}+1;\ -2ipr)$. A sketch of the method follows.

Let Ψ be the solution of $(E+a/r+i\boldsymbol{\alpha}\cdot\nabla-\beta)\Psi=0$ which behaves at great distances like a plane wave in the $+z$ direction with $\sigma_z=+1$. Then it is known that

$$\Psi\sim\Psi^{(0)}+\exp i[pr+a_1\ln(2pr)]u_1(\theta,\phi)/pr,$$

where $u_1(\theta,\phi)$ is a certain spinor function of angle and $\Psi^{(0)}=\psi^{(0)}u$ with

$$\psi^{(0)}=\Gamma(1-ia_1)\exp(a_1\pi/2+ipr\cos\theta)\times F(ia_1;1;ipr(1-\cos\theta))$$

(the continuum solution of the Schrödinger equation

[8] R. H. Pratt and T. Erber (private communication).

[9] M. Gavrila, Phys. Rev. **113**, 514 (1959).

[10] R. H. Boyer, thesis, Oxford University, 1957 (unpublished).

for the Coulomb field) and

$$u=[(E+1)/2E]^{\frac{1}{2}}\begin{bmatrix}1\\0\\p/(E+1)\\0\end{bmatrix}.$$

It happens that the exact solution may be written in two terms,

$$\Psi=\Psi^{(1)}+\Psi^{(2)},$$

where

$$\Psi^{(1)}=[(E+1)/2E]^{\frac{1}{2}}\begin{pmatrix}S_1\\pS_1/(E+1)\end{pmatrix},\quad \Psi^{(2)}=[(E+1)/2E]^{\frac{1}{2}}\begin{pmatrix}pS_2/(E+1)\\S_2\end{pmatrix}.$$

We have introduced the two-spinors S_1 and S_2 with the notation $\rho_l=[(l+1)^2-a^2]^{\frac{1}{2}}$:

$$\begin{aligned}S_1=\exp(a_1\pi/2+ipr)\sum_{l=0}^{\infty}(-1)^l\\
\times\Bigg[(-2ipr)^{\rho_l-1}\frac{\Gamma(\rho_l-ia_1)}{\Gamma(2\rho_l+1)}\{(\rho_l-ia_1)F(\rho_l+1-ia_1;\,2\rho_l+1;\,-2ipr)\\
+(l+1-ia_1)F(\rho_l-ia_1;\,2\rho_l+1;\,-2ipr)\}\begin{pmatrix}(l+1)P_l(\cos\theta)\\-e^{i\phi}P_l^{(1)}(\cos\theta)\end{pmatrix}\\
+(-2ipr)^{\rho_{l-1}-1}\frac{\Gamma(\rho_{l-1}-ia_1)}{\Gamma(2\rho_{l-1}+1)}\{(\rho_{l-1}-ia_1)F(\rho_{l-1}+1-ia_1;\,2\rho_{l-1}+1;\,-2ipr)\\
-(l-ia_1)F(\rho_{l-1}-ia_1;\,2\rho_{l-1}+1;\,-2ipr)\}\begin{pmatrix}lP_l(\cos\theta)\\e^{i\phi}P_l^{(1)}(\cos\theta)\end{pmatrix}\Bigg],\end{aligned}$$

$$\begin{aligned}S_2=-ia\exp(a_1\pi/2+ipr)\sum_{l=0}^{\infty}(-1)^l\\
\times\Bigg[(-2ipr)^{\rho_l-1}\frac{\Gamma(\rho_l-ia_1)}{\Gamma(2\rho_l+1)}F(\rho_l-ia_1;\,2\rho_l+1;\,-2ipr)\begin{pmatrix}(l+1)P_l(\cos\theta)\\-e^{i\phi}P_l^{(1)}(\cos\theta)\end{pmatrix}\\
+(-2ipr)^{\rho_{l-1}-1}\frac{\Gamma(\rho_{l-1}-ia_1)}{\Gamma(2\rho_{l-1}+1)}F(\rho_{l-1}-ia_1;\,2\rho_{l-1}+1;\,-2ipr)\begin{pmatrix}lP_l(\cos\theta)\\e^{i\phi}P_l^{(1)}(\cos\theta)\end{pmatrix}\Bigg].\end{aligned}$$

Close inspection of $(-i\boldsymbol{\sigma}'\cdot\nabla/2E)S_1$ shows it to be a sum of three terms:

$$(p/2E)S_1+S_2-(a/2Er)S_2.$$

Thus

$$\begin{aligned}\Psi=[1-(i\boldsymbol{\alpha}\cdot\nabla/2E)-(\boldsymbol{\alpha}\cdot\mathbf{p}/2E)]\Psi^{(1)}\\
+[(\boldsymbol{\alpha}\cdot\mathbf{p}/2E)-(\epsilon p/2E)]\Psi^{(1)}+(a/2Er)\Psi^{(2)}.\end{aligned}$$

If we *now* make the approximation $\rho_l=l+1$, we find that $\Psi^{(1)}=\Psi^{(0)}$ and $[(\boldsymbol{\alpha}\cdot\mathbf{p}/2E)-(\epsilon p/2E)]\Psi^{(0)}=0$, since the second and fourth components of $\Psi^{(0)}$ vanish. If we discard the last term as being negligible for large E, we arrive at the well-known Furry approximation:

$$\Psi=[1-(i\boldsymbol{\alpha}\cdot\nabla/2E)-(\boldsymbol{\alpha}\cdot\mathbf{p}/2E)]\Psi^{(0)}.$$

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