Threshold Values of Internal Conversion Coefficients for the K-Shell

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(Received February 28, 1955)

Corrected relativistic calculations for the internal conversion coefficients of K-shell electrons at threshold energies of the gamma rays are presented. A comparison is made with nonrelativistic formulas.

INTRODUCTION

CALCULATIONS of the K-shell internal conversion coefficients for threshold values of the gamma-ray energy in an unperturbed central Coulomb field were previously reported in a very brief communication.[1] Since that time, results of low-energy experiments which have been brought to the author's attention have indicated that these results were in error. In addition, it was pointed out[2] that these old calculations were in disagreement with results obtained from the Dancoff-Morrison[3,4] and Drell[5] formulations, even in the limit of low Z where these should be exact.

As a result of these indications, the previous work was rechecked, with the consequence that errors in formulation were discovered. Consequently, the whole problem was reformulated and the formulation checked by using two independent derivations. The problem was then programmed for computation on AVIDAC[6]; the programming was checked by comparing intermediate results with previously computed numbers, by using library routines wherever possible, and by multiple scrutiny of program and code. Numerical results were checked by running the problem several times on AVIDAC during periods of reliable operation.

It must be emphasized that the computations here are, as described previously, of interest as mathematical limits to the function which correctly describes internal conversion in the absence of screening. For example, the threshold energies used are the values computed for the unscreened single-electron atom, rather than the K-shell cutoff energies which are significantly different for large Z. The validity of various simplified methods for taking screening into account must ultimately depend on experiment. Since internal conversion coefficients generally show a more rapid variation with energy than with Z, however, it seems reasonable to expect that the correlation of conversion coefficient with gamma-ray energy at threshold (k in the tables) will be somewhat better than a correlation with Z.

[1] B. I. Spinrad and L. B. Keller, Phys. Rev. **84**, 1056 (1951).
[2] Church, Herbst, and Monahan, Argonne National Laboratory Quarterly Report ANL-5174, February, 1954, pp. 69–71 (unpublished).
[3] S. Dancoff and P. Morrison, Phys. Rev. **55**, 122 (1939).
[4] M. Hebb and G. Uhlenbeck, Physics **5**, 605 (1938).
[5] S. D. Drell, Phys. Rev. **75**, 132 (1949).
[6] AVIDAC is the automatically sequenced, electronic, digital computing machine now in service at Argonne National Laboratory. A report on its design and programming is in preparation.

FORMULATION

The computations were formulated in two ways. In the first method, the general formulas for conversion coefficients given by Rose, Goertzel *et al.*,[7] were reduced to the limit as p, the momentum of the outgoing electron, approaches zero. In the second method, the wave functions of the outgoing electron[8] were reduced to the zero-momentum limit before substitution into the radial integrals of reference 7. Essentially, then, the computation of the radial integrals, which is the major mathematical labor, was checked by comparing results of direct substitution of the reduced wave functions into Eqs. (13c–f) and (17b,c) of reference 7 with results obtained by reducing Eqs. (21) through (29) of that paper to the zero-momentum limit.

The presentation of the formulas used in computation is made in the Appendix.

RESULTS AND DISCUSSION

The results obtained are presented in tabular form in Table I. The concentration of points at low Z is due to a desire to check these results against the Dancoff-Morrison and Drell formulations in the limit as $Z\rightarrow 0$. At $Z=0$, their formulas are exact.

The computations which yielded Table I were performed to seven significant-figure precision. Table I has been rounded off to give six significant figures, although there is a possibility that successive truncation errors in the complicated arithmetical computations may have penetrated to the fifth figure in some cases.

The comparison formulas used were obtained from them by substituting into the general equations given in references 3 and 5 the gamma-ray energy at threshold, as a function of Z. The equations so obtained were then rearranged as series in ascending powers of Z, and the first term was retained. Identical results were obtained by finding the limiting form of the exact calculations given in the Appendix for $Z\rightarrow 0$.

A comparison of the ratios of the results obtained in Table I to the results obtained from the approximate equations (11a) and (11c) is made in graphical form in Figs. 1 and 2 for electric and magnetic conversion, respectively. The smoothness of the ratios, as seen in Figs. 1 and 2, indicates that interpolation to intermediate Z can be conveniently performed on these

[7] Rose, Goertzel, Spinrad, Harr, and Strong, Phys. Rev. **83**, 79 (1951).
[8] M. E. Rose, Phys. Rev. **51**, 484 (1937).

TABLE I. Threshold values of K-shell internal conversion coefficients.[a]

A. Electric multipoles

k (mc^2 units)	Z	α_1	α_2	α_3	α_4	α_5
0.00002663	1	1.89502(7)	3.07795(11)	1.97352(15)	7.13197(18)	1.68289(22)
0.00010652	2	1.18428(6)	4.80813(9)	7.70579(12)	6.96062(15)	4.10543(18)
0.00023967	3	2.33888(5)	4.21917(8)	3.00427(11)	1.20572(14)	3.15963(16)
0.00066582	5	3.02954(4)	1.96577(7)	5.03385(9)	7.26570(11)	6.84786(13)
0.00170609	8	4.61655(3)	1.16770(6)	1.16510(8)	6.55299(9)	2.40686(11)
0.0026664	10	1.88861(3)	3.05138(5)	1.94397(7)	6.98183(8)	1.63762(10)
0.0107085	20	1.16835(2)	4.64159(3)	7.24914(4)	6.38675(5)	3.67723(6)
0.024259	30	2.26901(1)	3.88934(2)	2.61155(3)	9.90373(3)	2.45728(4)
0.043553	40	7.01220(0)	6.45825(1)	2.32648(2)	4.74275(2)	6.33931(2)
0.068947	50	2.78769(0)	1.53738(1)	3.33305(1)	4.10686(1)	3.33417(1)
0.100957	60	1.29709(0)	4.52694(0)	6.33805(0)	5.10154(0)	2.74308(0)
0.140322	70	6.71873(−1)	1.52266(0)	1.46042(0)	8.31641(−1)	3.27786(−1)
0.188113	80	3.76149(−1)	5.63962(−1)	4.05247(−1)	1.85118(−1)	6.11577(−2)
0.233459	88	2.46902(−1)	2.77935(−1)	1.78623(−1)	7.58180(−2)	2.27476(−2)
0.286423	96	1.67115(−1)	1.61666(−1)	1.04270(−1)	4.12401(−2)	1.06695(−2)

B. Magnetic multipoles

k (mc^2 units)	Z	β_1	β_2	β_3	β_4	β_5
0.00002663	1	1.83974(4)	1.24191(9)	2.22055(13)	1.80155(17)	8.30293(20)
0.00010652	2	4.60131(3)	7.76405(7)	3.47011(11)	7.03761(14)	8.10789(17)
0.00023967	3	2.04643(3)	1.53426(7)	3.04697(10)	2.74585(13)	1.40571(16)
0.00066582	5	7.38356(2)	1.99116(6)	1.42254(9)	4.61222(11)	8.49547(13)
0.00170609	8	2.89989(2)	3.04848(5)	8.49251(7)	1.07395(10)	7.71655(11)
0.0026664	10	1.86527(2)	1.25253(5)	2.22953(7)	1.80190(9)	8.27558(10)
0.0107085	20	4.86496(1)	8.03482(3)	3.52677(5)	7.04250(6)	8.00028(7)
0.024259	30	2.32537(1)	1.65881(3)	3.16119(4)	2.75014(5)	1.36366(6)
0.043553	40	1.45535(1)	5.59317(2)	5.79573(3)	2.75595(4)	7.49006(4)
0.068947	50	1.07857(1)	2.49430(2)	1.58022(3)	4.62831(3)	7.77724(3)
0.100957	60	9.11391(0)	1.34218(2)	5.56398(2)	1.07733(3)	1.20284(3)
0.140322	70	8.69887(0)	8.32455(1)	2.34933(2)	3.14107(2)	2.43774(2)
0.188113	80	9.49930(0)	5.81850(1)	1.14045(2)	1.08016(2)	5.99073(1)
0.233459	88	1.15504(1)	4.73879(1)	6.95823(1)	5.04608(1)	2.16247(1)
0.286423	96	1.65777(1)	4.16743(1)	4.54694(1)	2.52489(1)	8.38363(0)

[a] The numbers in the parentheses are the powers of 10 by which the corresponding numbers are to be multiplied.

ratios; and their smooth approach to unity for low Z values is a further check on the correctness of the computations.

ACKNOWLEDGMENTS

The author would like to acknowledge his indebtedness to Dr. G. David Jackson of the Radiation Laboratory, McGill University, for his stimulating discussion on this problem; Dr. Joseph Cook of the Mathematics and Computing Section, Physics Division, Argonne National Laboratory, for his assistance in checking formulation; Mrs. Ruth Freshour of that Section for the programming of the problem for AVIDAC; Miss Mildred Schlapkohl of the Reactor Engineering Division, Argonne National Laboratory, for miscellaneous computation; and finally, Mrs. Lorraine B. Keller, co-author of reference 1, whose work was extensively used in checking the present problem.

APPENDIX

The following formulas were used in the computation. These are presented as they were used in programming the problem, so that extensive rearrangement of terms and redisignation of symbols will be noted on comparison with reference 7

$$\gamma=[1-(\alpha Z)^2]^{\frac{1}{2}}=1-k, \tag{1}$$

where k is gamma-ray energy at threshold, in m_0c^2 units.

$$N^2=2\pi\alpha(1+\gamma)^{1+\gamma}2^{\gamma}/(\alpha Z)^2\Gamma(2\gamma+1), \tag{2}$$

$$\gamma_J'=[(J+\tfrac{1}{2})^2-(\alpha Z)^2]^{\frac{1}{2}}, \tag{3}$$

$$D_J^2=(2\gamma+2)^{\gamma_J'}[\Gamma(\gamma_J'+\gamma)/\Gamma(2\gamma_J'+1)]^2, \tag{4}$$

$$x=-1-\gamma-i\alpha Z, \tag{5}$$

$$F_{J,0}=F(\gamma_J'+\gamma;2\gamma_J'+1;x), \tag{6a}$$

$$G_{J,0}=2\gamma_J'F(\gamma_J'+\gamma;2\gamma_J';x), \tag{6b}$$

when F is the confluent hypergeometric function.

$$F_{J,\nu}=\{[\alpha Z+i(1+\gamma)]/2\alpha Z\nu(\gamma_J'+\gamma-\nu)(\gamma_J'-\gamma+\nu)\}\times[G_{J,\nu-1}-(\gamma_J'+\gamma-\nu+x)F_{J,\nu-1}], \tag{7a}$$

$$G_{J,\nu}=\{[\alpha Z+i(1+\gamma)]/2\alpha Z\nu(\gamma_J'+\gamma-\nu)\}\times[G_{J,\nu-1}-xF_{J,\nu-1}], \tag{7b}$$

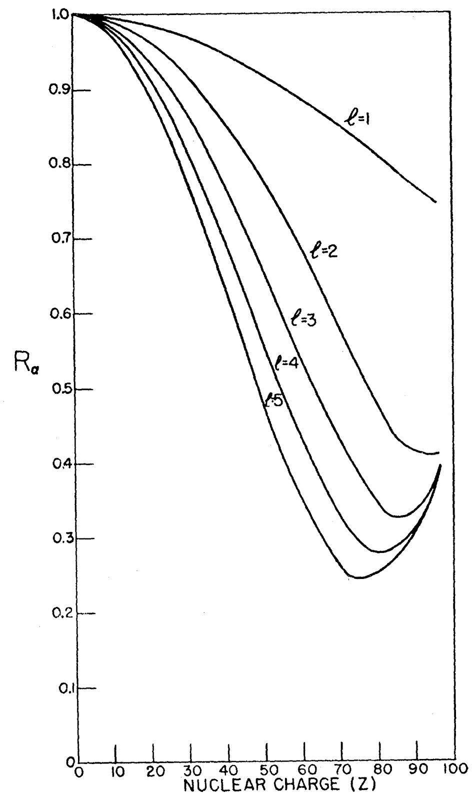

FIG. 1. Ratio ($R\alpha$) of "exact" electric internal conversion coefficients at threshold to low-Z limiting form.

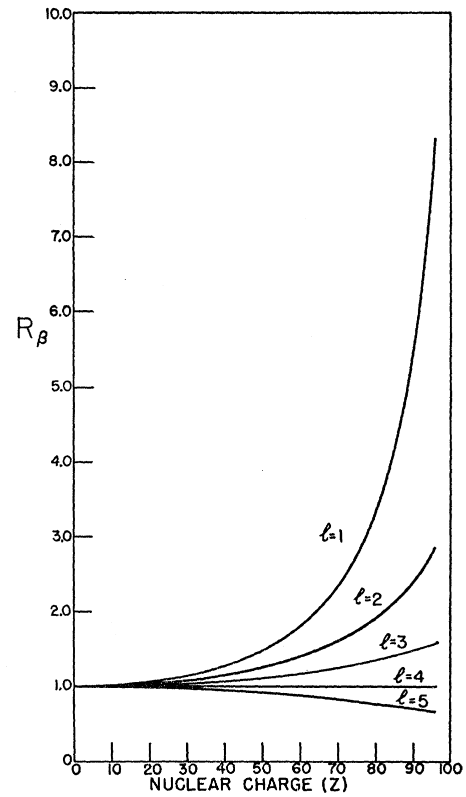

FIG. 2. Ratio ($R\beta$) of "exact" magnetic internal conversion coefficients at threshold to low-Z limiting form.

$$\begin{pmatrix}F^{I,J}\\G^{I,J}\end{pmatrix}=\sum_{\nu=0}^{I}\frac{(I+\nu)!}{(I-\nu)!}\begin{pmatrix}F_{J,\nu}\\G_{J,\nu}\end{pmatrix},\qquad(8)$$

$$W_1{}^J=\left(\frac{J-\frac{1}{2}}{2J}\right)(1+\gamma)D_J{}^2\left|(\tfrac{3}{2}+J-\gamma-\gamma_J{}')F^{J-\frac{1}{2},J}+G^{J-\frac{1}{2},J}+[2i\alpha Z/(1+\gamma)]\times[(\gamma_J{}'-J-\tfrac{1}{2})F^{J-\frac{3}{2},J}-G^{J-\frac{3}{2},J}]\right|^2,\qquad(9a)$$

$$W_2{}^J=\frac{(J+\frac{1}{2})^2}{(J+\frac{3}{2})(2J+2)}(1+\gamma)D_J{}^2\left|(\tfrac{1}{2}-J-\gamma-\gamma_J{}')\times F^{J+\frac{1}{2},J}+G^{J+\frac{1}{2},J}+[i\alpha Z/(1+\gamma)][G^{J-\frac{1}{2},J}/(J+\tfrac{1}{2})+\{2\gamma+1+(1+\gamma-\gamma_J{}')/(J+\tfrac{1}{2})\}F^{J-\frac{1}{2},J}\right|^2,\qquad(9b)$$

$$W_3{}^J=\left(\frac{J-\frac{1}{2}}{2J}\right)\frac{(\alpha Z)^2}{(1+\gamma)}D_J{}^2\times\left|(\gamma_J{}'-\gamma+J+\tfrac{1}{2})F^{J-\frac{1}{2},J}-G^{J-\frac{1}{2},J}\right|^2,\qquad(9c)$$

$$W_4{}^J=\left(\frac{J+\frac{3}{2}}{2J+2}\right)\frac{(\alpha Z)^2}{(1+\gamma)}D_J{}^2\times\left|(\gamma-\gamma_J{}'+J+\tfrac{3}{2})F^{J+\frac{1}{2},J}+G^{J+\frac{1}{2},J}\right|^2.\qquad(9d)$$

In all the foregoing equations, J assumes half odd-integral values.

$$\alpha_l=N^2(W_1{}^{l+\frac{1}{2}}+W_2{}^{l-\frac{1}{2}}),\qquad(10a)$$

$$\beta_l=N^2(W_3{}^{l+\frac{1}{2}}+W_4{}^{l-\frac{1}{2}}).\qquad(10b)$$

As $Z\rightarrow 0$, these equations approach the limiting form of the Dancoff-Morrison and Drell equations at threshold:

$$\alpha_l\doteq 16\pi\alpha[l/(l+1)](l!)^{-2}(2/\alpha Z)^{2l+2}B_l{}^2,\qquad(11a)$$

where

$$B_l=1/(2l+1)F(2;2l+2;-2),\qquad(11b)$$

$$\beta_l\doteq 16\pi\alpha[(l+1)/(2l+1)]\times[(l-1)!]^{-2}(2/\alpha Z)^{2l}C_l^2,\qquad(11c)$$

where

$$C_l^2=1+l^{-1}(l+1)^{-3}B_{l+1}{}^2.\qquad(11d)$$