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K SHELL INTERNAL CONVERSION COEFFICIENTS AT THRESHOLD

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Abstract: Coulomb field effects on K shell internal conversion coefficients for threshold values of the gamma-ray energy are investigated using exact wave functions to describe both the bound and the continuum state electrons. Exact results for the internal conversion coefficients are obtained in terms of gamma functions and confluent hypergeometric functions. To facilitate numerical evaluation, the exact result is expanded in a series in αZ and the first three terms of this series are retained. The dominant terms are identical to the expressions obtained by Drell and by Dancoff and Morrison, in the non-relativistic approximation. Terms of order αZ times the dominant term are shown to be zero but the $\alpha^2 Z^2$ corrections to the non-relativistic results are seen to bring the analytical results into closer agreement with the numerical results of Spinrad. The effects of finite nuclear size and screening are also considered.

1. Introduction

Non-relativistic formulas for K shell internal conversion coefficients (hereafter referred to as ICC's) have been derived by Drell [1]) and by Dancoff and Morrison [2]). Spinrad [3]) computed numerically the K shell ICC's at threshold values of the gamma-ray energy and compared his results with those obtained from the non-relativistic formulas. The ratios of the non-relativistic results to the numerical results of Spinrad tend towards unity for small Z, as they should, but for higher Z values the ratios can be as large as 4 (electric transitions) or as low as $\frac{1}{5}$ (magnetic transitions); the deviations are strongly L dependent, where L is the angular momentum of the radiated field.

The purpose of this paper is to investigate the origin of these deviations and to ascertain how they depend on L. To this end we use exact relativistic Coulomb wave functions to calculate the ICC's at threshold.

In sect. 2 we write down the ICC's for the K shell in terms of radial integrals. At threshold, we find that the integrals can be evaluated analytically thus giving an exact answer for the ICC's. To facilitate numerical evaluation, the exact result is expanded in a series in αZ and the first three terms are retained. Sect. 3 is devoted to a discussion of the effects of screening and finite nuclear size. Finally, in sect. 4, we discuss all the results obtained. A table of ICC's, derived from our analytical formulas, is presented. These results are also compared graphically with the results of Spinrad [3]).

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2. Pure Coulomb Field Effects

The ICC's will be denoted by $\beta_L^{(\lambda)}$ where $\lambda = 0, 1$ refers to magnetic and electric multipole radiation respectively. The expression for an angular momentum eigenstate of the electron is [4])

$$\psi_{jlm} = \begin{pmatrix} ig_\kappa(r)\Omega_{jlm}(\hat{r}) \\ f_\kappa(r)\sigma\cdot\hat{r}\Omega_{jlm}(\hat{r}) \end{pmatrix}, \tag{1}$$

where $\kappa = \mp(j+\frac{1}{2})$ for $j = l\pm\frac{1}{2}$. In particular, we consider the case when the electron is initially bound in the K shell and denote the radial functions by g_K and f_K (g_κ and f_κ will refer to the continuum state). Then the $\beta_L^{(\lambda)}$ can be written in terms of radial integrals as follows:

$$\beta_L^{(1)} = \frac{\alpha\omega}{8\pi}\left\{\frac{L}{2L+1}(|R_1+R_2+2iR_3|^2)_{j_2=L+\frac{1}{2};\, l_2=L;\, \kappa=L-1} + \frac{L^2}{(2L+1)(L+1)}\left(\left|R_1+R_2-i\left(\frac{1}{L}R_3+\frac{2L+1}{L}R_4\right)\right|^2\right)_{j_2=L-\frac{1}{2};\, l_2=L;\, \kappa=L}\right\}, \tag{2}$$

$$\beta_L^{(0)} = \frac{\alpha\omega}{8\pi}\frac{1}{2L+1}\{L(|R_5+R_6|^2)_{j_2=L+\frac{1}{2};\, l_2=L+1;\, \kappa=L+1} + (L+1)(|R_5+R_6|^2)_{j_2=L-\frac{1}{2};\, l_2=L-1;\, \kappa=-L}\}, \tag{3}$$

where α is the fine-structure constant and ω is the transition energy †. The radial integrals are given by

$$R_1 = \int_0^\infty g_\kappa g_K G_L r^2 \mathrm{d}r, \tag{4a}$$

$$R_2 = \int_0^\infty f_\kappa f_K G_L r^2 \mathrm{d}r, \tag{4b}$$

$$R_3 = \int_0^\infty f_\kappa g_K G_{L-1} r^2 \mathrm{d}r, \tag{4c}$$

$$R_4 = \int_0^\infty g_\kappa f_K G_{L-1} r^2 \mathrm{d}r, \tag{4d}$$

$$R_5 = \int_0^\infty f_\kappa g_K G_L r^2 \mathrm{d}r, \tag{4e}$$

$$R_6 = \int_0^\infty g_\kappa f_K G_L r^2 \mathrm{d}r, \tag{4f}$$

where

$$G_L(\omega r) = (2\pi)^{\frac{1}{2}} i^L \frac{1}{\sqrt{(\omega r)}} H_{L+\frac{1}{2}}^{(1)}(\omega r), \tag{5}$$

and $H_{L+\frac{1}{2}}^{(1)}(r)$ is the Hankel function of the first kind. By a simple change in notation,

† In our units $\hbar = c = 1$.

we find that these results are identical to those obtained by Rose [5]). Note that the corresponding results, given in eqs. (39.25) and (39.28) of Akhiezer and Berestetsky [4]), are in error; furthermore, there is a sign mistake in eq. (10.13) of the same reference.

The exact continuum-state wave functions are given by [6])

$$f_\kappa = -i\sqrt{(W-m)}\,\frac{e^{\frac{1}{2}\pi\nu}}{\sqrt{(\pi p)}}\,\frac{|\Gamma(\gamma+i\nu)|}{2\Gamma(2\gamma+1)}\,(2pr)^\gamma\,\frac{1}{r} \times\{e^{-ipr+i\eta}(\gamma+i\nu)F(\gamma+1+i\nu;\,2\gamma+1;\,2ipr)-\text{c.c.}\}, \tag{6}$$

$$g_\kappa = \sqrt{(W+m)}\,\frac{e^{\frac{1}{2}\pi\nu}}{\sqrt{(\pi p)}}\,\frac{|\Gamma(\gamma+i\nu)|}{2\Gamma(2\gamma+1)}\,(2pr)^\gamma\,\frac{1}{r} \times\{e^{-ipr+i\eta}(\gamma+i\nu)F(\gamma+1+i\nu;\,2\gamma+1;\,2ipr)+\text{c.c.}\}, \tag{7}$$

where $F(a;b;x)$ is the confluent hypergeometric function, $\Gamma(Z)$ is the gamma function and c. c. denotes complex conjugate. The energy, momentum, and mass of the electron are denoted by W, p, and m respectively;

$$\nu = \frac{\alpha Z W}{p}, \qquad \gamma = \sqrt{(\kappa^2-\alpha^2 Z^2)},$$

and

$$e^{2i\eta} = \frac{-\kappa+\dfrac{i\alpha Z m}{p}}{\gamma+\dfrac{i\alpha Z W}{p}}.$$

These equations simplify considerably at threshold i.e., when p tends to zero.

Making use of the relations [7])

$$\lim_{a\to\infty} F\left(a;\,c;\,-\frac{x}{a}\right) = \Gamma(c)x^{\frac{1}{2}(1-c)}J_{c-1}(2\sqrt{x}), \tag{8}$$

and

$$\lim_{|y|\to 0} e^{\frac{1}{2}\pi|y|}|\Gamma(x+iy)| = \sqrt{(2\pi)}|y|^{x-\frac{1}{2}} \qquad (x,\,y \text{ real}), \tag{9}$$

we find

$$f_\kappa = 8\mu\sqrt{(\alpha Z)}\,\frac{J_{2\gamma}(x)}{x^2}, \tag{10a}$$

and

$$g_\kappa = -\frac{\gamma-\kappa}{\alpha Z}f_\kappa+\frac{4\mu}{\sqrt{(\alpha Z)}}\,\frac{J_{2\gamma+1}(x)}{x^2}, \tag{10b}$$

where $\mu = m\alpha Z$, $x = \sqrt{(8\mu r)}$ and $J_n(x)$ is the cylindrical Bessel function of the first kind. These results are not valid as $r \to \infty$. However, as $r \to \infty$ we get no contribution to the radial integrals due to the presence of the factor $e^{-\mu r}$ which appears in the bound state wave function. The exact ground state wave functions are given by [8])

$$g_K = N_K x^{2(\gamma_K-1)} 2\mu^{\frac{3}{2}} e^{-\frac{1}{2}x^2}, \tag{11}$$

and

$$f_K = -\Lambda g_K, \tag{12}$$

where

$$N_K = \sqrt{\frac{1+\gamma_K}{\Gamma(2\gamma_K+1)}}\, 2^{-2(\gamma_K-1)}, \qquad \Lambda = \sqrt{\frac{1-\gamma_K}{1+\gamma_K}},$$

and

$$\gamma_K = (1-\alpha^2 Z^2).$$

Thus we can write

$$R_1 = -\frac{\gamma-\kappa}{\alpha Z} R_5 + R_{1a}, \tag{13a}$$

$$R_{1a} = \frac{1}{2\alpha Z}\int_0^\infty \left\{\frac{xJ_{2\gamma+1}(x)}{J_{2\gamma}(x)}\right\} f_\kappa g_K G_L r^2 \mathrm{d}r, \tag{13b}$$

$$R_2 = -\Lambda R_5, \tag{13c}$$

$$R_3 = (R_5)_{G_L \to G_{L-1}}, \tag{13d}$$

$$R_4 = \frac{\Lambda}{\alpha Z}(\gamma-\kappa)R_3 - \Lambda(R_{1a})_{G_L\to G_{L-1}}, \tag{13e}$$

$$R_6 = \frac{\Lambda}{\alpha Z}(\gamma-\kappa)R_5 - \Lambda R_{1a}. \tag{13f}$$

Making use of the series expansion for the Hankel function, we find

$$R_5 = -i2\pi\sqrt{\alpha Z} N_K \frac{\mu}{\omega}\sum_{v=0}^{L}\frac{(L+v)!}{v!(L-v)!}\left(\frac{4i\mu}{\omega}\right)^v \times \int_0^\infty e^{-\frac{1}{2}x^2(1-i\omega/\mu)} x^{-2v+1+2(\gamma_K-1)} J_{2\gamma}(x)\mathrm{d}x. \tag{14}$$

At threshold, the photon energy ω is equal to the binding energy:

$$\omega = m(1-\sqrt{1-\alpha^2 Z^2}). \tag{15}$$

After evaluation of the integrals we obtain

$$R_5 = a\sum_{v=0}^{L} bF_a, \tag{16}$$

$$R_3 = a\sum_{v=0}^{L-1}\frac{L-v}{L+v} bF_a, \tag{17}$$

$$R_{1a} = ac\sum_{v=0}^{L}(\gamma-v+\gamma_K) bF_b, \tag{18}$$

$$(R_{1a})_{G_L \to G_{L-1}} = ac \sum_{v=0}^{L-1} (\gamma - v + \gamma_K) \frac{L-v}{L+.} bF_b, \tag{19}$$

where

$$a = -i2^{\gamma+3\gamma_K} \pi \sqrt{\alpha Z} N_K \frac{\mu}{\omega} \mu^{-\frac{1}{2}} \frac{1}{\Gamma(2\gamma+1)} \left(1 - \frac{i\omega}{\mu}\right)^{-(\gamma+\gamma_K)}, \tag{20}$$

$$b = \frac{(L+v)!}{v!(L-v)!} \left(\frac{i\mu}{\omega}\right)^v \left(1 - \frac{i\omega}{\mu}\right)^v \Gamma(\gamma - v + \gamma_K), \tag{21}$$

$$c = \frac{2}{\alpha Z} \frac{1}{2\gamma+1} \left(1 - \frac{i\omega}{\mu}\right)^{-1}, \tag{22}$$

$$F_a = F\left(\gamma - v + \gamma_K; 2\gamma+1; \frac{-2}{1 - i\omega/\mu}\right), \tag{23}$$

$$F_b = F\left(\gamma - v + \gamma_K + 1; 2\gamma+2; \frac{-2}{1 - i\omega/\mu}\right). \tag{24}$$

An approximate analytical expression is obtained by carrying out an expansion in powers of αZ. Keeping only terms which will contribute to the result for the ICC's to relative order $\alpha^2 Z^2$ we find

$$\begin{aligned}
R_5 = K \Big\{ & F(k-L+1; 2k+1; -2) - \tfrac{1}{2} i\alpha Z(k-L+1) \\
& \times \Big[-F(k-L+1; 2k+1; -2) + F(k-L+2; 2k+1; -2) \\
& + \frac{2}{2k+1} F(k-L+2; 2k+2; -2) \Big] + (\tfrac{1}{2}\alpha Z)^2 (k-L+1) \\
& \times \Big[\frac{1}{k-L+1} \Big(L(1+k) - \tfrac{1}{2}((1+k)(2+k)+1) - \tfrac{1}{2} L(L-1) - \frac{2(1+k)}{k} \ln 2 + 2\psi(3) \\
& - \frac{2(1+k)}{k} \psi(1+k-L) \Big) F(k-L+1; 2k+1; -2) + (k-L+2) \\
& \times F(k-L+2; 2k+1; -2) + \frac{2(k-L+2)}{2k+1} F(k-L+2; 2k+2; -2) \\
& - \frac{L-1}{2L-1} (k-L+2) F(k-L+3; 2k+1; -2) \\
& - \frac{2(k-L+2)}{2k+1} F(k-L+3; 2k+2; -2) \\
& - \frac{(k-L+2)}{(2k+1)(k+1)} F(k-L+3; 2k+3; -2) \Big] \Big\},
\end{aligned} \tag{25}$$

$$R_{1a} = K\frac{2}{\alpha Z}\frac{k-L+1}{2k+1}\Big\{F(k-L+2;2k+2;\,-2)-\tfrac{1}{2}i\alpha Z(k-L+2)$$

$$\times\Big[-F(k-L+2;2k+2;\,-2)+F(k-L+3;2k+2;\,-2)$$

$$+\frac{1}{k+1}F(k-L+3;2k+3;\,-2)\Big]+(\tfrac{1}{2}\alpha Z)^2(k-L+2)\Big[\frac{1}{k-L+2}\Big(L(2+k)$$

$$-\tfrac{1}{2}((2+k)(3+k)+1)-\tfrac{1}{2}L(L-1)+\frac{4}{k(2k+1)}-\frac{2(1+k)}{k}\ln 2+2\psi(3)$$

$$-\frac{2(1+k)}{k}\psi(1+k-L)-\frac{2(1+k)}{k(k-L+1)}\Big)F(k-L+2;2k+2;\,-2)$$

$$+(k-L+3)F(k-L+3;2k+2;\,-2)+\frac{k-L+3}{k+1}F(k-L+3;2k+3;\,-2)$$

$$-\frac{L-1}{2L-1}(k-L+3)F(k-L+4;2k+2;\,-2)$$

$$-\frac{k-L+3}{k+1}F(k-L+4;2k+3;\,-2)$$

$$-\frac{k-L+3}{(2k+3)(k+1)}F(k-L+4;2k+4;\,-2)\Big]\Big\}, \tag{26}$$

$$R_3 = K\Big\{-\frac{i\alpha Z}{2}\frac{k-L+1}{2L-1}F(k-L+2;2k+1;\,-2)\Big\}, \tag{27}$$

$$(R_{1a})_{G_L\to G_{L-1}} = K\Big\{-\frac{i}{2k+1}\frac{(k-L+1)(k-L+2)}{2L-1}F(k-L+3;2k+2;\,-2)\Big\}, \tag{28}$$

where $k = |\kappa|$, $\psi(Z)$ denotes the first polygamma function and

$$K = 2^{k-L+\frac{3}{2}}i^{L-1}\pi\left(\frac{2}{\alpha Z}\right)^L\frac{1}{\sqrt{\omega}}\frac{(k-L)!}{(2k)!}\frac{(2L)!}{L!}.$$

From the relation

$$F(a;c;x) = F(a-1;c;x)+\frac{x}{c}F(a;c+1;x),$$

we see that the coefficients of $\frac{1}{2}i\alpha Z$ in R_5 and R_{1a} are both zero. The other relations between contiguous confluent hypergeometric functions [7]) enable us to write

$$(R_5)_{k=L} = K_1[F_1+(\tfrac{1}{2}\alpha Z)^2\{(L+\tfrac{1}{2}+T_1)F_1-L\}], \tag{29}$$

$$(R_5)_{k=L+1} = \frac{1}{(L+1)(2L+1)} K_1 \left[F_{11}+(\tfrac{1}{2}\alpha Z)^2 \left\{\left(\frac{3-2L}{2(2L-1)}+T_2\right) F_{11} + \frac{2}{2L+3} F_{12}\right\}\right], \quad (30)$$

$$(R_{1a})_{k=L} = \frac{2}{\alpha Z}\frac{1}{2L+1} K_1 \left[F_3+(\tfrac{1}{2}\alpha Z)^2 \left\{-\frac{2(L-1)}{2L-1} F_5 + \left(-\tfrac{3}{2}-\frac{2(2L-1)}{L(2L+1)} + T_1\right) F_3\right\}\right], \quad (31)$$

$$(R_{1a})_{k=L+1} = \frac{2}{\alpha Z}\frac{2}{(L+1)(2L+1)(2L+3)} K_1 \left[F_{12}+(\tfrac{1}{2}\alpha Z)^2 \left\{\left(L(L-1)-\tfrac{15}{2} - \frac{2L-1}{(L+1)(2L+3)} + \frac{3(5L-2)}{2L-1} + T_2\right) F_{12} - \frac{3(L-1)}{2L-1} F_9\right\}\right], \quad (32)$$

$$i(R_3)_{k=L} = \tfrac{1}{2}\alpha Z \frac{1}{2L-1} K_1 F_2, \quad (33)$$

$$i(R_3)_{k=L+1} = \tfrac{1}{2}\alpha Z \frac{2}{(2L-1)(L+1)(2L+1)} K_1 F_6, \quad (34)$$

$$i(R_{1a})_{\substack{G_L\to G_{L-1}\\ k=L}} = \frac{2}{(2L-1)(2L+1)} K_1 F_5, \quad (35a)$$

$$i(R_{1a})_{\substack{G_L\to G_{L-1}\\ k=L+1}} = \frac{6}{(L+1)(2L+1)(2L-1)(2L+3)} K_1 F_9, \quad (35b)$$

where

$$T_1 = 2\{\psi(3)-\tfrac{1}{2}(L+1)(\ln 2+\psi(1))\},$$

$$T_2 = 2\left\{\psi(3)-\frac{L+2}{L+1}(\ln 2+\psi(2))\right\},$$

$$K_1 = (K)_{k=L} = 2^{\frac{1}{2}} i^{L-1}\pi \left(\frac{2}{\alpha Z}\right)^L \frac{1}{\sqrt{\omega}}\frac{1}{L!}.$$

The confluent hypergeometric functions involved are

$F_1 = F(1; 2L+1; -2)$, $F_2 = F(2; 2L+1; -2)$, $F_3 = F(2; 2L+2; -2)$,
$F_5 = F(3; 2L+2; -2)$, $F_6 = F(3; 2L+3; -2)$, $F_9 = F(4; 2L+4; -2)$,
$F_{11} = F(2; 2L+3; -2)$, $F_{12} = F(3; 2L+4; -2)$, $F = F(1; 2L+2; -2)$.

Thus at threshold the ICC's for both an electric and a magnetic multipole on the

K shell are given, to order $\alpha^2 Z^2$, by

$$\beta_L^{(1)} = T\left(\frac{2}{\alpha Z}\right)^2 \frac{1}{(L+1)(2L+1)^2} F_3^2 \left\{1+\frac{\alpha^2 Z^2}{2F_3}\left[-\frac{L(3L^2-6L+1)}{(L+1)(2L-1)}\right.\right.$$
$$+\frac{(L+1)^2}{2L+1}(F-F_3)\left(\frac{3-2L}{2(2L-1)}+\frac{(4L+3)(L-2)}{(L+1)^2(2L-1)}+T_2\right)$$
$$-\frac{(L+1)^2}{2L+1}\left(F-\frac{L+2}{L+1}F_3\right)\left(L^2-L+\tfrac{7}{2}-\frac{2L-1}{(L+1)(2L+3)}-\frac{8L}{2L-1}+T_2\right)$$
$$\left.+\frac{L}{2L+1}F_3\left(-\tfrac{3}{2}-\frac{6L-1}{L(2L+1)}-\frac{(L-1)}{L(L+1)}-\frac{L(2L+3)(L-3)}{(L+1)(2L-1)}+T_1\right\}, \tag{36}$$

$$\beta_L^{(0)} = \frac{T}{2L+1} L_1\left[1+\frac{\alpha^2 Z^2}{2}\left\{\left(1-\frac{L^2(L+1)}{L_1}\right)\left(\left(L^2-\tfrac{3}{2}-\frac{2L-1}{(L+1)(2L+3)}+T_2\right)\right.\right.\right.$$
$$\left.+\frac{F-F_1}{(L+1)-(L+2)F}\left(2-L^2-\frac{4}{(L+1)(2L+3)}\right)\right)$$
$$+\frac{(L+1)L^2}{L_1}\left(\left[-\tfrac{1}{2}+\frac{L-1}{L}+\frac{L-1}{(L+1)(2L+1)}+T_1\right]\right.$$
$$\left.\left.\left.+\frac{1}{L(2L+1)}F_3\left[2+L+\frac{1}{L}-\frac{L(L-1)(2L+3)}{(L+1)(2L-1)}-\frac{4}{L(2L+1)}\right]\right)\right\}\right], \tag{37}$$

where

$$T = 16\pi\alpha\left(\frac{2}{\alpha Z}\right)^{2L}\left(\frac{1}{L!}\right)^2,$$

and

$$L_1 = L\{(L+1)-(L+2)F\}^2+(L+1)L^2$$
$$= L\left\{\frac{F(2;\,2L+4;\,-2)}{(L+1)(2L+3)}\right\}^2+(L+1)L^2.$$

We notice that the coefficient of αZ is zero. To lowest order the corresponding formulas are

$$\beta_{L,0}^{(1)} = T\left(\frac{2}{\alpha Z}\right)^2 \frac{L}{L+1}\left\{\frac{F(2;\,2L+2;\,-2)}{2L+1}\right\}^2, \tag{38}$$

$$\beta_{L,0}^{(0)} = \frac{T}{2L+1}\{[(L+1)-(L+2)F(1;\,2L+2;\,-2)]^2+(L+1)L^2\}$$
$$= \frac{L(L+2)}{(L+1)(2L+1)}(\tfrac{1}{2}\alpha Z)^4 \beta_{L+1,0}^{(1)}+T\frac{L^2(L+1)}{2L+1}. \tag{39}$$

Eqs. (38) and (39) are in agreement with the results obtained by Drell [1]) and by

Dancoff and Morrison [2]) respectively. Drell erroneously considered $\beta^{(1)}_{L,0}$ to vanish at threshold and thus neglected the first term in eq. (39); however, it does turn out that this term is in fact much smaller than the second term.

Finally, we may write

$$\beta^{(\lambda)}_{L} = \beta^{(\lambda)}_{L,0}(1+C^{(\lambda)}_{L}\alpha^2Z^2), \tag{40}$$

where the values of $C^{(\lambda)}_{L}$ are given in table 1. This formula enables us to compile numerical values for the ICC's which we present in table 2. These results are compared graphically in fig. 1 with the results of Spinrad.

TABLE 1

Values of $C_L{}^{(\lambda)}$

λ	$L=1$	$L=2$	$L=3$	$L=4$	$L=5$
0	0.620	0.874	0.938	0.968	0.986
1	−0.601	−1.163	−1.760	−2.165	−2.860

TABLE 2

Threshold values of internal conversion coefficients for the K shell deduced from the $\beta_L{}^{(\lambda)} = \beta^{(\lambda)}_{L,0}(1+C_L{}^{(\lambda)}\alpha^2Z^2)$

ω(mc^2 units)	Z	$\beta_1{}^{(1)}$	$\beta_2{}^{(1)}$	$\beta_3{}^{(1)}$	$\beta_4{}^{(1)}$	$\beta_5{}^{(1)}$
0.0026664	10	1.903(3)	3.094(5)	1.985(7)	7.174(8)	1.693(10)
0.0107085	20	1.201(2)	4.902(3)	7.867(4)	7.116(5)	4.200(6)
0.024259	30	2.412(1)	4.401(3)	3.145(3)	1.265(4)	3.320(4)
0.043553	40	7.803(0)	8.073(1)	3.254(2)	7.363(2)	1.088(3)
0.068947	50	3.287(0)	2.199(1)	5.688(1)	8.252(1)	7.807(1)
0.100957	60	1.755(0)	7.709(0)	1.388(1)	1.399(1)	9.203(0)
0.140322	70	9.181(−1)	3.215(0)	4.265(0)	3.166(0)	1.530(0)
0.188113	80	5.608(−1)	1.525(0)	1.554(0)	8.814(−1)	3.276(−1)

ω(mc^2 units)	Z	$\beta_1{}^{(0)}$	$\beta_2{}^{(0)}$	$\beta_3{}^{(0)}$	$\beta_4{}^{(0)}$	$\beta_5{}^{(0)}$
0.002664	10	1.834(2)	1.235(5)	2.201(7)	1.782(9)	8.184(10)
0.0107085	20	4.540(1)	7.568(3)	3.342(5)	6.715(6)	7.619(7)
0.024259	30	1.985(1)	1.447(3)	2.791(4)	2.461(5)	1.214(6)
0.043553	40	1.091(1)	4.372(2)	4.609(3)	2 243(4)	5.988(4)
0.068947	50	6.771(0)	1.679(2)	1.088(3)	3.284(3)	5.266(3)
0.100957	60	4.532(0)	7.446(1)	3.156(2)	6.277(2)	6.210(2)
0.140322	70	3.165(0)	3.606(1)	1.022(2)	1.360(2)	7.470(1)
0.188113	80	2.286(0)	1.831(1)	3.390(1)	2.841(1)	1.934(0)

Figures in parentheses indicate the power of 10 by which the number must be multiplied.

3. Screening and Nuclear Size Deffects

The effect of screening on the bound electron can be examined analytically in the non-relativistic limit by approximating the screened Coulomb potential by the Hulthén potential [9])

$$V(r) = \frac{Ze\lambda e^{-\lambda r}}{1-e^{-\lambda r}}, \tag{41}$$

where [10])

$$\lambda \approx 0.23\mu. \tag{42}$$

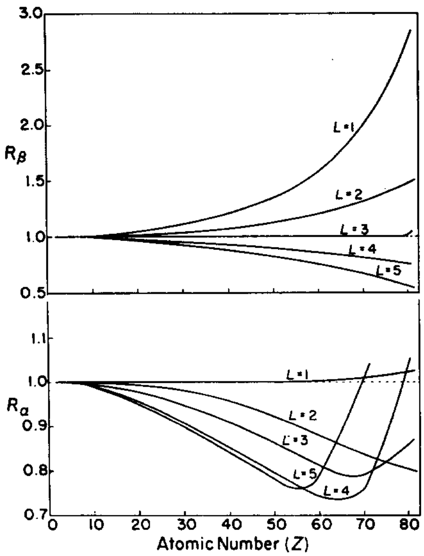

Fig. 1. Ratio of numerical results of Spinrad for the internal conversion coefficients at threshold to the analytical results, where R_α and R_β refer to electric and magnetic transitions respectively, $R_{\alpha,\beta} = \beta_L^{1,0}(\text{numerical})/\beta_L^{1,0}(\text{analytical})$.

This potential gives rise to a wave equation which can be solved exactly. We find that

$$\psi_K \approx \frac{\mu^{\frac{3}{2}}}{\pi^{\frac{1}{2}}} \sqrt{1-\left(\frac{1}{75.7}\right)^2} e^{-\mu r}\left\{1+\frac{\mu^2 r^2}{466}+O(\mu^4 r^4)\right\}. \tag{43}$$

The differences between the ICC's obtained by using the latter wave equation and those obtained by using the non-relativistic Coulomb wave function $\psi_K = (\mu^{\frac{3}{2}}/\pi^{\frac{1}{2}}) e^{-\mu r}$ can be obtained readily by evaluating the radial integrals, designated by I and I_s, which arise in the respective cases. To the order required

$$I = \int_0^\infty e^{-\frac{1}{4}x^2} x^{-2L+1} J_{2k}(x) dx = 2^{k-3L+2} \frac{\Gamma(k-L+1)}{\Gamma(2k+1)} F(k-L+1; 2k+1; -2), \tag{44}$$

$$I_s = \sqrt{1-\left(\frac{1}{75.7}\right)^2} I + \Delta I, \tag{45}$$

and

$$\Delta I = \tfrac{1}{466}(\tfrac{1}{8})^2 \int_0^\infty e^{-\frac{1}{4}x^2} x^{-2L+5} J_{2k}(x)\mathrm{d}x$$
$$= \tfrac{1}{466} 2^{k-3L+2} \frac{\Gamma(k-L+3)}{\Gamma(2k+1)} F(k-L+3;\, 2k+1;\, -2)$$
$$= \tfrac{1}{466}(k-L+2)(k-L+1) \frac{F(k+L-1;\, 2k+1;\, -2)}{F(k-L+1;\, 2k+1;\, -2)} I. \tag{46}$$

Thus we are able to show that

$$(I_s)_{\max} \leqq (1+\tfrac{1}{80})I. \tag{47}$$

This in turn leads to the conclusion that the ICC's obtained by using a Hulthén potential differ by less than 1% from those obtained in the pure Coulomb case. Physically, this is what we expect because screening should have very little effect on K shell electrons.

The main effect of screening consists of a considerable lowering of the threshold energy from its unscreened value [11]). Thus qualitatively screening effects may be accounted for by replacing Z by $Z_{\mathrm{eff}} < Z$. This would result in an increase in the ICC's.

To examine the effects of finite nuclear size, we note that for the true wave function we have $r\psi \to 0$ as $r \to 0$ in contrast to the Dirac wave function which is singular at the origin. Thus the contribution to the radial integrals from a sphere of radius R around $r = 0$ should be small. We neglect this small contribution and also subtract out the comparatively large contribution we have actually included because of the fact that we did use Dirac wave functions.

From our evaluation of the radial integrals, we see that the calculation of the lowest order contribution involves essentially the evaluation of the two integrals

$$B \equiv \int_0^\infty e^{-\frac{1}{4}x^2} x^{-2L+1} J_{2\gamma}(x)\mathrm{d}x, \tag{48}$$

and

$$D \equiv \int_0^\infty e^{-\frac{1}{4}x^2} x^{-2L+2} J_{2\gamma+1}(x)\mathrm{d}x. \tag{49}$$

Let $B = B_{\mathrm{C}} + \Delta B$ and $D = D_{\mathrm{C}} + \Delta D$, where

$$\Delta B = \int_0^{x_m} e^{-\frac{1}{4}x^2} x^{-2L+1} J_{2\gamma}(x)\mathrm{d}x, \tag{50}$$

$$\Delta D = \int_0^{x_m} e^{-\frac{1}{4}x^2} x^{-2L+2} J_{2\gamma+1}(x)\mathrm{d}x, \tag{51}$$

and

$$x_m = \sqrt{8\mu R} = C\sqrt{\alpha Z}; \tag{52}$$

C is a constant which, for $R = 1.2\, A^{\frac{1}{3}}$ fm, is equal to $0.1577\, A^{\frac{1}{6}}$.

Using the series expansion for the Bessel function, evaluating the integrals and retaining only lowest order terms in αZ, we find that

$$\begin{aligned}(\Delta B)_{k=L} &= C_1 \frac{2^{-2(L-1)}}{(2L)!}\alpha Z,\\ (\Delta B)_{k=L+1} &= O(\alpha^2 Z^2),\\ (\Delta D)_{k=L} &= O(\alpha^2 Z^2),\\ (\Delta D)_{k=L+1} &= O(\alpha^3 Z^3),\end{aligned} \tag{53}$$

where

$$C_1 = 3.1079 \times 10^{-3} A^{\frac{1}{3}}.$$

Thus we are able to estimate the effect of the finite size of the nucleus on the lowest order contributions to the ICC's. We deduce that

$$(\beta_{L,0}^{(0)})_{\text{finite size}} = \left(1 - \frac{L+1}{L} C_1 \alpha Z\right) \beta_{L,0}^{(0)}, \tag{54}$$

$$(\beta_{L,0}^{(1)})_{\text{finite size}} = (1 - C_2 \alpha^2 Z^2) \beta_{L,0}^{(1)}. \tag{55}$$

By inspection, we see that C_2 is greater than zero and that it increases with decreasing L. We have not evaluated it explicitly because B and D themselves are only the lowest order parts of the exact integrals given by eqs. (13) and (14). By contrast, we did carry out an exact computation of $(\beta_{L,0}^{(0)})_{\text{finite size}}$ because the correction term here is of order αZ and because we know from our previous calculations that, when the radial integrals for a point nucleus are evaluated to order $\alpha^2 Z^2$ times the lowest order term, no terms or order αZ times the lowest order term occur. Since C_1 is a relatively small number, we see that $(\beta_{L,0}^{(0)})_{\text{finite size}}$ and $\beta_{L,0}^{(0)}$ never differ by more than 0.2%. Now Church and Weneser [12]) assert that there is an appreciable difference between the finite-size and point-nucleus wave functions up to a radius of the order of 10 R; if we exclude a region of this radius in the evaluation of our radial integrals, then, since C_1 is proportional to the radius of the excluded region, we find that $(\beta_{L,0}^{(0)})_{\text{finite size}}$ and $\beta_{L,0}^{(0)}$ may differ by up to 2%. This, of course, is still a relatively small difference.

4. Discussion of Results

As already pointed out, the lowest order terms appearing in the analytical expressions for the magnetic and electric ICC's (i.e., $\beta_{L,0}^{(0)}$ and $\beta_{L,0}^{(1)}$) have been obtained by a non-relativistic calculation. Numerical results computed from these expressions were compared to the numerical results of Spinrad. We also saw that these relativistic and non-relativistic computations are in close agreement for low Z but that large differences, which are strongly L dependent, occur for high Z and that if we consider the ratio of the non-relativistic to the relativistic results we find that for the electric

ICC's this ratio varies from 1 to 4, being greater for higher L values, whereas for the magnetic ICC's this ratio varies from 1 to $\frac{1}{5}$, being smaller for higher L values. If we compare our fig. 1 to the corresponding fig. in ref. [3]) we see that our corrections to the non-relativistic results serve to bring the analytical results into closer agreement with the numerical results except in the case of $\beta_4^{(0)}$ and $\beta_5^{(0)}$ where the discrepancies are very small anyway. The strong L dependence of $C_L^{(1)}$ is also in the desired direction; this is not so for the L dependence of $C_L^{(0)}$ but here the L dependence is very much weaker. The remaining deviations are presumably due to the neglect of higher order αZ terms in the analytical results.

Regarding the influence of finite nuclear size, we conclude that the effect is to decrease both the electric and magnetic ICC's relatively to their point nucleus values, the decrease in the electric ICC's being of order $\alpha^2 Z^2$ times the point nucleus values whereas the decrease in the magnetic ICC's is of order αZ times the point nucleus values. Furthermore, we see that the effect is more pronounced for smaller L values. These conclusions are in qualitative agreement with those obtained by Church and Weneser [12]).

We have seen that the effect of screening on the bound electron is negligible in the non-relativistic approximation and that a qualitative examination of the effects of screening on the continuum state electron shows that they should tend to increase the ICC's, a conclusion borne out by the results of Reitz [13]). As already pointed out, the main effect of screening consists of a considerable lowering of the threshold energy from its unscreened value. Thus, in making a comparison between experimental and theoretical values of the ICC's at threshold, it is preferable to classify an element by its ω value rather than by its Z value. Experiments are difficult to perform at threshold and we know in fact only one such published value [14]). This refers to $_{75}\mathrm{Rr}^{187}$ for which [11]) $\omega_{\mathrm{expt.}} = 0.14\ mc^2 = 71.7$ keV. Since we know that the energy of the emitted gamma rays is 72 keV we are thus able to deduce that the energy of the conversion electrons is 0.3 keV. The transition involved is known to be E1 and the corresponding theoretical value of the ICC is 0.67. Experiment gives a value of the order of 2 for the ICC but the extent of possible deviations from this figure is not quoted. Thus we see that the quantitative comparisons between experiment and theory will have to await more extensive experimental investigations.

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