NOTE ON RELATIVISTIC RÖNTGEN L–DOUBLETS AND THE "SCREENING CONSTANT."

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ABSTRACT.

Screening constant in the relativity formula for x-ray L-doublet separations has been computed from the wave-lengths for elements of atomic number 74 to 92, in two ways, (1) using the complete formula, and (2) using only the first three terms (Sommerfeld's formula). The second calculation is found to give values more nearly independent of the atomic number than the complete formula, and is therefore to be preferred. This result is shown to be in agreement with a recent *development of Bohr's correspondence principle*, a suggestion by him that in such a series no term should be included which is smaller than the energy radiated by an electron per revolution, as calculated on the classical theory. The wave-length measurements, however, are not yet accurate enough to decide the question definitely.

IN a recent paper by Sommerfeld and Heisenberg,[1] the problem of the sharpness of spectral lines was considered from the standpoint of Bohr's latest extension of the "Correspondence Principle." According to this idea, expressed in his lectures at Göttingen during the past summer, any quantum calculation which involves energies smaller than the energy lost per revolution by an electron revolving about the nucleus, as calculated on the classical basis, should not be taken into account.

In the above-mentioned paper, the authors investigated the question of how many of the relativity corrections to use in the calculation of the L-doublets, without interfering with this point of view. It was suggested by Professor Sommerfeld that the author seek for some evidence in the heaviest atoms that the calculation of the L-doublets is really spoiled by using more than the number of terms which Bohr's point of view would indicate. This was effected in the following manner.

I. The screening constant.—In the theory of the x-ray L-doublets[2] the wave-number difference of the doublet is expressed completely by the formula

$$\frac{\Delta\nu}{R} = \frac{2}{\alpha^2}\left\{\left[1 + \frac{\alpha^2(Z-s)^2}{(n_2' + \sqrt{K_2{}^2 - \alpha^2(Z-s)^2})^2}\right]^{-1/2} - \left[1 + \frac{\alpha^2(Z-s)^2}{(n_1' + \sqrt{K_1{}^2 - \alpha^2(Z-s)^2})^2}\right]^{-1/2}\right\}, \quad (a)$$

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[1] Sommerfeld and Heisenberg, Zeit. fur Physik, **10**, p. 393, 1922.

[2] Sommerfeld, Atombau und Spektrallinien, p. 605.

where $\alpha = 2\pi e^2/ch$, the constant of fine structure; Z is the atomic number, s is the screening constant, R is the Rydberg constant, and n' and K are the radial and azimuthal quantum numbers, respectively. For the L-doublets, $n_2' = K_2 = 1$, $n_1' = 0$, and $K_1 = 2$, so (a) becomes

$$\frac{\Delta\nu}{R} = \frac{1}{\alpha^2}\left[\sqrt{4 - \alpha^2(Z - s)^2} - \sqrt{2}\sqrt{1 + \sqrt{1 - \alpha^2(Z - s)^2}}\right]. \qquad (b)$$

If we expand (a) into a power series in $\alpha^2(Z - s)^2$, we get, indicating each half of (a) by the symbol (n', K),

$$
\begin{aligned}
(n', K) = (Z - s)^2\Bigg[& \frac{1}{(n' + K)^2} + \frac{\alpha^2(Z - s)^2}{(n' + K)^4}\left\{\frac{1}{4} + \frac{n'}{K}\right\} \\
& + \frac{\alpha^4(Z - s)^4}{(n' + K)^6}\left\{\frac{1}{8} + \frac{3}{4}\frac{n'}{K} + \frac{3}{2}\left(\frac{n'}{K}\right)^2 + \frac{1}{4}\left(\frac{n'}{K}\right)^3\right\} \\
+ \frac{\alpha^6(Z - s)^6}{(n' + K)^8}\Bigg\{ & \frac{5}{64} + \frac{5}{8}\left(\frac{n'}{K}\right) + 2\left(\frac{n'}{K}\right)^2 \\
& + \frac{23}{8}\left(\frac{n'}{K}\right)^3 + \left(\frac{n'}{K}\right)^4 + \frac{1}{8}\left(\frac{n'}{K}\right)^5\Bigg\} \\
+ \frac{\alpha^8(Z - s)^8}{(n' + K)^{10}}\Bigg\{ & \frac{7}{128} + \frac{35}{64}\frac{n'}{K} + \frac{75}{32}\left(\frac{n'}{K}\right)^2 + \frac{345}{64}\left(\frac{n'}{K}\right)^3 \\
& + \frac{105}{16}\left(\frac{n'}{K}\right)^4 + \frac{207}{64}\left(\frac{n'}{K}\right)^5 + \frac{25}{32}\left(\frac{n'}{K}\right)^6 + \frac{5}{64}\left(\frac{n'}{K}\right)^7\Bigg\} + \cdots\Bigg].
\end{aligned}
\qquad (c)
$$

The method of expansion (and the first three terms) is indicated in "Atombau und Spektrallinien," p. 582. For the L-doublet, $\Delta\nu/R$ then reduces to [3]

$$
\frac{\Delta\nu}{R} = \frac{\alpha^2}{2^4}(Z - s)^4\Bigg\{1 + \frac{5}{2}\frac{\alpha^2}{2^2}Z - s)^2 + \frac{53}{8}\frac{\alpha^4}{2^4}(Z - s)^4 \\
+ \frac{303}{16}\frac{\alpha^6}{2^6}(Z - s)^6 + \cdots\Bigg\}. \qquad (d)
$$

If we take the first three terms of this series, and solve for $(Z - s)^2$, we get

$$(Z - s)^2 = \left(\frac{2^2}{\alpha}\sqrt{\frac{\Delta\nu}{R}} - 5\frac{\Delta\nu}{R}\right)\left(1 + \frac{19}{32}\alpha^2\frac{\Delta\nu}{R}\right). \qquad (e)$$

The "screening constant" s is rather an empirical than a theoretical constant and must be determined from experimental data for $\Delta\nu/R$. It expresses the screening effect of the electrons in the K-shell and the remaining electrons in the L-shell, on an electron tumbling into the L-shell. That is, $(Z - s)$ tells us how much of the total nuclear charge is effective in radiation. For all of the heavier elements, the L-shell is

[3] Page, Bull. Nat. Res. Council, **2**, p. 380, gets 831/32 for the coefficient of the fourth term. This seems to be due to an error in computation.

complete, and since the electrons in the other shells, the M, N, O shells, etc., are far away, and have little or no influence in determining s, we should expect s to be a constant for all of the heavier elements.

The question then arises, shall we use the complete formula (b), or the formula (e), in determining s? Bohr's development of the "Correspondence Principle" would tell us that we should use as many terms in the expansion (d) as will give us energy differences greater than the radiation damping. Duane and Patterson[1] have concluded from their calculations that it would be necessary to use five or six terms in the expansion in order to get a value of s giving $\Delta \nu/R$ within the limits of experimental error. This would be practically equivalent to using the complete formula (b) instead of Sommerfeld's formula (e).

In order to see which formula would give us the result anticipated, namely, a constant value of s throughout the system of elements, two sets of calculations were made, one using the complete formula (b), the other using (e). The results are shown below:

Atomic No.	Element.	$\Delta \nu/R$.	s_b from (b).	s_e from (e).	$\Delta s = (s_e - s_b)$ $\times 10^3$.
74	W	98.54	3.500	3.508	8
76	Os	111.08	3.566	3.574	8
77	Ir	118.64	3.486	3.494	8
78	Pt	125.92	3.496	3.507	11
79	Au	133.80	3.479	3.492	13
81	Tl	150.49	3.481	3.497	16
82	Pb	160.02	3.424	3.441	17
83	Bi	169.73	3.402	3.419	17
90	Th	250.86	3.390	3.428	38
92	Ur	278.73	3.435	3.486	51

Due to the smallness of the difference in (b), it was necessary to use seven-place logarithms in the calculations of s given in the fourth column. The calculations thus made gave an accuracy of about two units in the last decimal place.

The values of $\Delta \nu/R$ are taken from the precision measurements of Coster[2] for the sharpest of the L-doublets, $\beta_1 - \alpha_2$.

The variations of s_e about an average value 3.492[3] are probably due to the variations in the experimental values for $\Delta \nu/R$. It would have been better to use a weighted average from all the L-doublets for the computations. But the sixth column shows that the values of s_b are more nearly independent of Z than the values of s_e.

II. **Relation of correspondence principle to expansion of** $\Delta \nu/R$.—Let

[1] Duane and Patterson, Proc. Nat. Acad. Sci., 6, p. 516, 1920.

[2] Coster, Zeits. f. Phys., vol. 6, p. 190, 1921.

[3] Cf. Sommerfeld, l. c., p. 611.

us now see whether formula (*e*) is in agreement with the correspondence principle. This would mean that the fourth term of the energy difference in Eq. (*d*) must be smaller than the difference in the energy radiated per revolution in the two L-orbits, calculated according to classical theory. The energy thus calculated is

$$U = \frac{2}{3}\frac{e^2}{c^3}\int_0^\tau \dot{v}^2 dt, \tag{1}$$

where τ is the time of one revolution. For an ellipse, we may write $r = a(1 - \epsilon \cos u)$. Because of constant sectorial velocity,

$$(p/m)dt = xdy - ydx = a^2\sqrt{1 - \epsilon^2}\,(1 - \epsilon \cos u)du.$$

Now since $m\dot{v} = e^2(Z - s)/r^2$,

$$\dot{v}^2 dt = \frac{e^4(Z - s)^2}{a^4(1 - \epsilon \cos u)^4 m^2}\cdot a^2\sqrt{1 - \epsilon^2}\,(1 - \epsilon \cos u)\frac{m}{p}du,$$

and Eq. (1) becomes

$$U = \frac{2}{3}\frac{e^6(Z - s)^2\sqrt{1 - \epsilon^2}}{a^2 p c^3 m}\int_0^{2\pi}\frac{du}{(1 - \epsilon \cos u)^3}, \tag{2}$$

where u is the eccentric anomaly and p is the angular momentum, which remains constant throughout the revolution. The integral is most easily evaluated by complex methods,[1]

$$\int_0^{2\pi}\frac{du}{(a + \epsilon \cos u)^3} = \frac{1}{2}\frac{d^2}{da^2}\int_0^{2\pi}\frac{du}{(a + \epsilon \cos u)}$$
$$= \frac{1}{2}\frac{d^2}{da^2}\left[\frac{2\pi}{\sqrt{a^2 - \epsilon^2}}\right] = \pi\left[-\frac{2a^2 + \epsilon^2}{(a^2 - \epsilon^2)^{5/2}}\right].$$

Putting $a = 1$, and $f = 1 + \epsilon^2/2 = \frac{1}{2}[3 - K^2/(n' + K)^2]$,

$$U = \frac{8\pi}{3}\alpha^3 R(Z - s)^4 h\frac{f}{K^5}. \tag{3}$$

(This is only the first term of a rapidly converging series, since m has been considered a constant in the integration.)

The energy difference between the two L-orbits is therefore [2]

$$U_1 - U_2 = (8\pi/3)\alpha^3 R(Z - s)^4 h(f_1/K_1^5 - f_2/K_2^5)$$
$$= (8\pi/3)\alpha^3 R(Z - s)^4 h(1.375 - .031), \tag{4}$$

and the ratio of the fourth term to $(U_1 - U_2)$ is

$$(h\Delta\nu)_4/(U_1 - U_2) = 3.38 \times 10^{-14}(Z - s)^6. \tag{5}$$

[1] See Sommerfeld, Atombau und Spektrallinien, Zusatz 6, p. 666.

[2] This result is given in the article by Sommerfeld and Heisenberg, loc. cit.

Hence, even for $(Z - s) = 100$, the fourth term is only a little more than 3 per cent of the energy radiated per revolution calculated according to classical theory, while the third term in the expansion is of the same order of magnitude, for the range of atomic numbers considered.

A simple calculation shows that if we neglect the fourth term for atomic numbers below 90, we should neglect the third term for atomic numbers below 50 and the second term for atomic numbers below 20. These calculations agree fairly well with the results given in the article by Sommerfeld and Heisenberg.

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