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M.Sc. (Physics) Sem-IV
X-ray emission

Use of Spin Doublet Formula in X-ray spectra:

The distinct levels cause the appearance in the X-ray spectrum of lines whose wavelength separation is approximately independent of atomic number. In K and L groups, the lines showing this effect are listed in Table 1.

Tabl 1: Spin doublets in the K and L series

K series

Lines		Levels	
α_1	α_2	L_{II}	L_{III}
β_1	β_2	M_{II}	M_{III}

L Series

l.	η	L_{II}	L_{III}
α_2	β_1	L_{II}	L_{III}
β_6	γ_5	L_{II}	L_{III}
⋮	⋮	⋮	
α_1	α_2	M_{IV}	M_V
γ_2	γ_1	N_{II}	N_{III}
β_{45}	β_2	N_{IV}	N_V

ogether with the levels concerned in their emission which display the fetures characteristics of eqn (1) as given

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$$\Delta \nu = \frac{R\alpha^2 (Z-\sigma_2)^4}{n^3 \, l(l+1)} \quad \text{———} \quad (1)$$

where σ_2 is the screening constant,

However, the constant wave-length difference of the $K\alpha_1$ & $K\alpha_2$ lines, whose wave-number difference is that of the levels L_{II}, L_{III}.

The approximate constancy in the wavelength ~~of~~ separation of two levels ~~two lines~~ whose wavenumber difference is that of ~~whose separation is given by the spin doublet formula~~ can be roughly accounted for as follows:

The wavenumber difference in question follows the approximate ~~eqn~~ eq^n (1), or

$$\frac{\Delta \nu}{R} \sim (Z-\sigma_2)^4$$

But by Moseley's laws which also applies to absorption limit,

$$\frac{\nu}{R} \sim (Z-\sigma_1)^3$$

By differentiation of the relation $\nu = \lambda^{-1}$, we find

$$|\Delta \lambda| = \frac{1}{\nu^2} \Delta \nu,$$

and assuming that $\sigma_1 = \sigma_2$ its results shows that $\Delta\lambda$ ~~is~~ is independent of Z, atleast in the higher atomic number ranges, Therefore, we have to describe the application of the accurate formula of which eq^n (1) is an approximation, to the L_{II} L_{III} separation.

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It is most noticeable fact that this formula, including all the terms in higher power of α^2, was developed by Sommerfeld on the basis of the older relativistic quantum theory, without wave mechanics

For $j = l + \frac{1}{2}$

$$E(n, L, j) = -Rhc\left[\frac{(Z-\sigma_1)^2}{n^2} + \frac{\alpha^2 (Z-\sigma_2)^4}{n^4}\left\{\frac{n}{l+1} - \frac{3}{4}\right\}\right.$$

$$+ \frac{\alpha^4 (Z-\sigma_2)^6}{n^6}\left\{\frac{1}{4}\left(\frac{n}{l+1}\right)^3 + \frac{3}{4}\left(\frac{n}{l+1}\right)^3 - \frac{3}{2}\left(\frac{n}{l+1}\right) + \frac{5}{8}\right\}$$

$$+ \frac{\alpha^6 (Z-\sigma_2)^8}{n^8}\left\{\frac{1}{8}\left(\frac{n}{l+1}\right)^5 + \frac{3}{8}\left(\frac{n}{l+1}\right)^4 + \frac{1}{8}\left(\frac{n}{l+1}\right)^3\right.$$

$$\left.\left. - \frac{15}{8}\left(\frac{n}{l+1}\right)^2 + \frac{15}{8}\left(\frac{n}{l+1}\right) - \frac{35}{64}\right\} + \cdots\right] \qquad (2)$$

Similarly for $j = l - \frac{1}{2}$,

$$E(n, L, j) = -Rhc\left[\frac{(Z-\sigma_1)^2}{n^2} + \frac{\alpha^2 (Z-\sigma_2)^4}{n^4}\left\{\frac{n}{l} - \frac{3}{4}\right\}\right.$$

$$+ \frac{\alpha^4 (Z-\sigma_2)^6}{n^6}\left\{\frac{1}{4}\left(\frac{n}{l}\right)^3 + \frac{3}{4}\left(\frac{n}{l}\right)^2 - \frac{3}{2}\left(\frac{n}{l}\right) + \frac{5}{8}\right\}$$

$$+ \frac{\alpha^6 (Z-\sigma_2)^8}{n^9}\left\{\frac{1}{8}\left(\frac{n}{l}\right)^5 + \frac{3}{8}\left(\frac{n}{l}\right)^4 + \frac{1}{8}\left(\frac{n}{l}\right)^3 - \frac{15}{8}\left(\frac{n}{l}\right)^2\right.$$

$$\left.\left. + \frac{15}{8}\left(\frac{n}{l}\right) - \frac{35}{64}\right\} + \cdots\right] \qquad (3)$$

In applying eqn (2) & (3) to the separation of the $L_{II}L_{III}$ doublet, we consider that eqn (2) is to be used for L_{III} with the values $n=2$, $l=1$, $j=\frac{3}{2}$ and that eqn (3) may be applied to L_{II} when the values $n=2$, $l=1$ and $j=\frac{1}{2}$ are inserted.

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using these values, and solving for $\frac{\Delta \nu}{R}$, we obtain

$$\frac{\Delta \nu}{R} = \frac{\alpha^2 (Z-\sigma_2)^4}{2^4}\left[1 + \frac{5}{2}\frac{\alpha^2}{2^2}(Z-\sigma_2)^2 + \frac{53}{8}\frac{\alpha^4}{2^4}(Z-\sigma_2)^4 + \cdots\right] \quad (4)$$

Now Sommerfeld shows that eqn (4) may be solved for $(Z-\sigma_2)$ in an approximation manner that provides the results:

$$(Z-\sigma_2)^2 = \left(\frac{4}{\alpha}\sqrt{\frac{\Delta \nu}{R}} - 5\frac{\Delta \nu}{R}\right)\left(1 + \frac{19}{3^2}\alpha^2 \frac{\Delta \nu}{R}\right) \quad (5)$$

If this formula is applicable to the separation of L_{II} L_{III} we expect that σ_2 will remain constant

It is observed that the variations of σ_2 about the average value of $\sigma_2 = 3.487$ are entirely random in this range. So, the separation of other pairs of levels in the X-ray term can be calculated from the spin doublet formula to obtain the separation of these levels, and the screening constants deduced for them.

Concluded