STUDIES ON X-RAY SCREENING PARAMETERS: A REVIEW

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Abstract:

In the previous review paper by the author, researches on Sommerfeld's screening parameters right from their inception to mid-seventies were analyzed. A great deal of work has been done in this field after this period. It is pertinent to take account of all these works as the complete and reliable data on screening parameters plays a significant role in the study of x-ray satellites. Moreover, screening parameters give important information about the reliability or otherwise of the energy value data used for their calculation. In fact, these parameters have become an important tool in the analysis of formalism being used in developing a specific theory about spectral analysis. Some authors have theoretically resolved the spin doublet levels and obtained energy values of individual levels making use of Sommerfeld's screening parameters and Sommerfeld - Dirac relativistic energy expression. In this review paper, researches on screening parameters not only for the spin doublets but for $S_{1/2}$ and K levels are also covered.

Keywords: screening parameters, spin doublets, σ_1 *and* σ_2 , $S_{1/2}$ and K levels, X-ray spectra, screening doublets, irregular doublets.

1.INTRODUCTION

Sommerfeld [1], in his pioneering work on analyzing the fine structure of spectral lines extended the epoch-making theory announced by Bohr [2] for the hydrogen atom and introduced two screening parameters σ_1 *and* σ_2 . The review paper by the author [3] gives an account of studies made on screening parameters, mainly those introduced by Sommerfeld, right from the time of their inception to the work done during early seventies. After this specific period extensive work has been done by researchers to get precise values of theoretical as well as the experimental electron spectroscopic energy values, making the resulting values of Sommerfeld screening parameters σ_1 *and* σ_2 more reliable. This review paper gives an account of work done on the Sommerfeld screening parameters after the researches covered in the previous review paper.

2. EXTENSION OF WORK ON SOMMERFELD'S SCREENING PARAMETERS FOR THE SPIN DOUBLETS

Burr and Carson [4] calculated the screening parameter σ_2 for the doublets L_2L_3 (Z=13 to 103), M_2M_3 (Z=31 to 103), M_4M_5 (Z=35,37-53,55-103), N_2N_3 (Z=35,37, 47, 55-60, 62-103), N_4N_5(Z=55, 56, 70-84, 88, 90-95), N_6N_7 (74, 77-83, 90-92), O_2O_3 (55,56, 72-83,88,90,92,94) O_4O_5 (81-83,90,92-95). These authors have used the experimental energy values of Bearden and Burr [5]. Padalia [6] had also made use of the energy values of Bearden and Burr but used the same method of Sommerfeld approximation for the energy value expression. The significance of the work done by Burr and Carson lies in the fact that they made use of the relativistic energy expression in its closed form thereby ruling out the error in results caused due to approximations and series truncation.

Burr and Carson replaced the atomic number Z by (Z- σ_2) in the Sommerfeld-Dirac relativistic energy expression and obtained two equations by inserting the appropriate values of n and j for the two members of a given spin doublet. The difference between these two terms gives the energy level separation between doublet members as a function of σ_2 . Such a value of σ_2 is searched which yields the energy level separation known from the data of Bearden and Burr. Some interesting observations were highlighted by these authors in the analysis part of their work:

1. The values of σ_2 obtained by them (Burr and Carson) differ markedly from those reported by Padalia. This disagreement increases sharply for higher values of Z.
2. Parameter σ_2 for a spin doublet is definitely a function of Z contrary to the earlier observation by Sommerfeld.

3. The inner shell filling is clearly indicated in the values of σ_2 for the spin doublets. By studying σ_2 values for spin doublets L_2L_3 and M_4M_5, it was found that σ_2 values decrease until the subshell is half full and then rise again.
4. The σ_2 values are unusually low for a certain range of atomic numbers for the doublet L_2L_3. These σ_2 values were based on the theoretical energy values reported by Bearden and Burr. Burr and Carson have commented that the anomality in σ_2 values is a clear indication of erroneous energy level separation data used for the calculation. As the experimental data for the energy level separation was not available for these specific cases so the authors emphasized that better level separation could be calculated by extrapolating the σ_2 against Z data.

In the process of pointing out the anomalous energy level separation, Burr and Carson calculated and suggested the new values for L_2L_3 spin doublet separation for transuranium elements. These authors have described the utility of the study of screening parameter σ_2 in getting information about the energy levels for the elements for which energy data is either not available or showing anomality in values. But this method of using σ_2 for completing the energy value data is limited in application as it can be used only for the spin doublets. Gokhale and Misra [7] compiled the data reported by Burr and Carson and gave the mean value of inner screening parameter σ_2 for various spin doublets. These values are given below along with the values reported by Sommerfeld.

TABLE 2.1 COMPARISON OF AVERAGE σ_2 VALUES

Doublet	Average σ_2 values by Sommerfeld	Average σ_2 values by Gokhale and Misra
L_2L_3	3.5	3.46
M_2M_3	8.5	8.26
M_4M_5	13.0	13.25
N_2N_3	17.0	17.09
N_4N_5	24.4	23.24
N_6N_7	34.0	34.51
O_2O_3		29.73
O_4O_5		39.24

Sommerfeld introduced two screening parameters σ_1 *and* σ_2 in the relativistic energy expression in order to take into account the effect of the presence of other electrons on the nuclear charge. As elaborated above and in the review paper by the same author, a great deal of work has been done to get complete information about inner screening parameter σ_2 . Limited data was available prior to the work of Gokhale and Misra [7],[8]. Variation of $\sigma_1 Vs\ Z$ is available Sommerfeld's work [1]. Gokhale and Misra adopted a method to calculate σ_1 which uses the Sommerfeld – Dirac relativistic energy expression in the compact form thereby avoiding the error caused in results due to truncation of series expansion. The screening parameter σ_1 accounts for the screening of the nuclear charge due to the electrons situated in orbits both internal and external to the one under consideration. Gokhale and Misra calculated σ_1 values using the energy values reported by Bearden and Burr and values of σ_2 reported earlier by Burr and Carson.

The value of screening parameter σ_1 remains the same for both the levels of a spin doublet [9]. Gokhale and Misra used the energy equation in its closed form as given below:

$$\frac{(Z-\sigma_1)^2}{n^2} = \left(\frac{v}{R}\right) + \frac{(Z-\sigma_2)^2}{n^2} - \frac{2}{\propto^2}\left[1 - \left(1 + \frac{\propto^2 (Z-\sigma_2)^2}{\{n-\left(j+\frac{1}{2}\right)+\left[\left(j+\frac{1}{2}\right)^2 - \propto^2 (Z-\sigma_2)^2\right]^{\frac{1}{2}}\}^2}\right)^{-\frac{1}{2}}\right] \quad (1)$$

These authors have reported values of total screening parameter σ_1 for for the doublets L_2L_3 (Z=13 to 103), M_2M_3 (Z=31 to 103), M_4M_5 (Z=35,37-53,55-103), N_2N_3 (Z=35,37, 47, 55-60, 62-103), N_4N_5(Z=55, 56, 68, 70-84, 88, 90-95), N_6N_7 (74, 77-83, 90-92), O_2O_3 (55,56, 72-83,88,90,92,94) O_4O_5 (81-83,90,92-95). Gokhale and Misra compared

their result of σ_1 values with those reported by Sommerfeld and found that σ_1 values obtained by them were slightly higher than those by Sommerfeld. The reason for this difference in values was attributed to the truncation error involved in the calculation by Sommerfeld. It was pointed out by Sommerfeld [1] that σ_1 values increase with Z, this rise is more noticeable in those cases where inner shells start filling or are completed. The same phenomenon was observed by Gokhale and Misra [8]. Some σ_1 values were found to be anomalous by these authors, these anomalies were suspected to be originated from the anomalous values of parameter σ_2. These anomalies in parameter σ_2 values were attributed by Burr and Carson to the errors in energy differences used in their calculation, as discussed in the previous section.

A scrutiny of literature on the screening parameters σ_1 and σ_2 reveals that the results lack completeness as these parameters could not be calculated for various levels in a number of elements due to the non-availability of experimental energy values. Misra, Sah and Gokhale [10], filled these gaps in the values of parameter σ_2 using the theoretical atomic energy values of Huang *et al* [11]. In the work of Huang *et al*, binding energy of various atomic orbitals was calculated using an improved form of Hartree-Fock-Slater formalism. These authors have calculated relaxed orbital energies rather than the frozen orbital energies since it has been shown by Lindgren and Rosen [12] that the former gives results in better agreement with experiment as compared to latter.

Misra, Sah and Gokhale [10] used the method described by Burr and Carson [4] employing Sommerfeld-Dirac relativistic energy expression in its closed form. These authors have reported parameter σ_2 for spin doublets L_2L_3 (Z=10-12, 21-29, 39-47, 57-71,96-103), M_2M_3 (Z=18-32, 39-47, 57-71, 85-87, 96-103), M_4M_5 (Z=24-36 ,39-47, 54, 57-71,91,96,97,103), N_2N_3 (Z=36,38-103), N_4N_5(Z=42-54, 57-67, 69, 70, 72-79, 84-87, 89, 91-103), N_6N_7 (63-80, 83-89, 91-103), O_2O_3 (52-54,57-89, 91-103), O_4O_5 (76-80,83-89,91-103), O_6O_7 (95-103), P_2P_3 (83-103). In the analysis of results of their work, these authors found that σ_2 values reported by them smoothly fit in the gaps of data provided by Burr and Carson. It is also observed that the unusual scattering in σ_2 Vs Z curves drawn by Burr and Carson has been removed when these σ_2 values were recalculated by them. As it was earlier observed by Burr and Carson that the σ_2 Vs Z curves show a dip in the regions of inner shell filling, the same trend is observed in the curves drawn by Misra, Sah and Gokhale. The striking difference is that the dip in the curves drawn by Misra, Sah and Gokhale is more prominent. These authors explained the comparatively larger dips in their σ_2 values due to the fact that the values reported by Burr and Carson are based on the experimental data obtained with solid targets whereas their results were based on theoretically calculated energy values for free atoms.

But this discrepancy turns out to be anomaly for the doublet M_2M_3 in the atomic number range Z=21-29 where the electrons are filling an inner shell (3d). The dip in the σ_2 Vs Z curve becomes so large that σ_2 values become negative for Z=22-25. The dip in σ_2 values in the inner shell filling region was explained by Burr and Carson as resulting due to the fact that when the shell which is being filled is inner to the one under consideration then the spacing between the spin doublet levels would be strongly influenced. In this connection, it is to be pointed out that Nefedov [13] has attributed the hump in the L_2L_3 separation as a function of Z in the region ($21 \leq Z \leq 30$) to exchange interaction between the 2p hole and the electron in the incompletely filled 3d shell. However, the dip in σ_2 values reported by Misra, Sah and Gokhale protruding to negative values is physically untenable and the authors suspected the neglect of some important factor in the energy values of Huang *et al*. But in general, the satisfactory agreement between the σ_2 values calculated from energy values of Huang *et al* and those calculated from Bearden and Burr energy value compilation leads to the conclusion that the energy level separation obtained from energy values of Huang *et al* are quite reliable for the atomic number range where the inner shells are not being filled up.

3. METHOD FOR CALCULATING SOMMERFELD'S SCREENING PARAMETERS FOR EXPERIMENTALLY UNRESOLVED SPIN DOUBLETS

Bearden and Burr [5] reported the values of experimentally observed spin doublet separations for different spin doublets for a large number of elements, thereby making it possible to compute σ_2 values using a method which needs the doublet separation. The method was used to calculate σ_2 and subsequently σ_1 values by several authors as discussed above. But these calculations do not cover the entire range of elements and levels due to the nonavailability of experimental doublet separation. Though the σ_2 values for such elements were

calculated by Misra, Sah and Gokhale [10] using theoretically calculated energy values of Huang *et al*. As discussed above, the σ_2 values for certain ranges of atomic numbers were found anomalous in nature indicating the neglect of some important factor in the calculation of energy values reported by Huang *et al*.

To complete the data of σ_1 and σ_2 values based on reliable energy values, Misra, Sah and Gokhale [21] devised a new method for calculating screening parameters σ_1 and σ_2 using the experimental energy values of the experimentally unresolved doublet members. The results were reported for the following cases:

L_2L_3 (Z=5-16), M_2M_3 (Z=17-30), M_4M_5 (Z=21-34 ,36, 54), N_2N_3 (Z=33, 34, 36, 38-46, 48-54,61), N_4N_5(Z=41,42, 44-53,57-67,69), N_6N_7 (58-60, 62, 64-73,75, 76, 88), O_2O_3 (49-53, 57-60,62-71, 91), O_4O_5 (73-75, 77-80, 84,88,91).

The anomaly of negative σ_2 values as obtained by Misra, Sah and Gokhale [10] using theoretically calculated energy values of Huang *et al* for the doublet M_2M_3 in the atomic number range $22 \leq Z \leq 25$ does not occur with the σ_2 values obtained by them when they [21] recalculated this parameter using the new method employing the experimentally unresolved energy values reported by Bearden and Burr. Furthermore, the excessively large dips in σ_2 Vs Z curves in the inner shell filling regions which resulted from the calculation based on theoretical energy values are not observed.

Misra, Sah and Gokhale [21], calculated the energy of individual levels which could not be resolved experimentally, substituting the σ_1 and σ_2 values obtained by this new method in the Sommerfeld energy formula. Fuggle and Martensson [22] have published a tabulation of core level binding energies, as measured by electron spectrometers in different laboratories in which the M_2M_3, M_4M_5, N_2N_3, N_4N_5 and N_6N_7 subshell binding energies have been successfully resolved. When the energy values given by Fuggle and Martensson, were compared with the theoretically calculated resolved energy values reported by Misra, Sah and Gokhale they were found to agree much better with them than with the theoretical energy values of Huang *et al*.

4. SOMMERFELD SCREENING PARAMETERS FOR $S_{1/2}$ LEVELS IN X-RAY SPECTRA

The methods described for the calculation of Sommerfeld screening parameters are applicable for the energy levels forming spin doublets. Screening parameters σ_1 and σ_2 for $S_{1/2}$ levels (L_1, M_1, N_1 etc.) cannot be calculated using these methods. Pairs of levels like L_1L_2, M_1M_2, M_3M_4, N_1N_2, N_3N_4 etc. are called irregular doublets or screening doublets. Two members of a screening doublet have the same value of the principal quantum number n and total angular momentum quantum number j but different values of the azimuthal quantum number l.

Hertz [14] observed that if $\sqrt{(\upsilon/R)}$ measured by him for the L_1 and L_2 levels for 55 Cs to 60 Nd and those measured by Duane and Patterson [15] for 74 W to 92 U were plotted against Z, the resulting curves for the two levels were parallel. This observation is famous by his name as Hertz's law for the irregular doublets. In X-ray spectra, the levels forming the screening doublets get separated because of different screening of nuclear charge experienced by the electrons situated in these levels. Sommerfeld and Wentzel [16] and Wentzel [17], in the process of analyzing the behavior of levels forming the irregular doublets introduced the 'reduced term' defined as:

$$\left(\frac{\upsilon}{R}\right)red. = \left(\frac{\upsilon}{R}\right)exp - \left[\frac{\propto^2 (Z-\sigma_2)^4}{n^4}\left(\frac{n}{j+\frac{1}{2}} - \frac{3}{4}\right)\right] = \frac{(Z-\sigma_1)^2}{n^2} \qquad (2)$$

The value of $\left(\frac{\upsilon}{R}\right)red.$is the same for both the levels of a spin doublet, but if reduction process is applied to the members of a screening doublet and the difference of the square roots of the reduced terms is taken, a constant term independent of Z is obtained. This leads to the conclusion that difference of the values of the screening parameter σ_1 for the levels of the screening doublet is a constant and the σ_1 Vs Z curves for them are exactly parallel.

This observation led Sommerfeld and Wentzel [16] and Wentzel [17] to devise a method for calculating σ_1 values for $S_{1/2}$ levels and reported the values of σ_1 and σ_2 for levels L_1, M_1 and N_1. But the main drawback of the method used by them is the truncation error that is caused in the results due to the use of the Sommerfeld- Dirac relativistic energy formula in the expanded form and truncating it after the term Z^8. Gokhale and Misra [8] recalculated the values of

σ_1 *and* σ_2 for levels L_1, M_1 and N_1. Taking the Sommerfeld- Dirac relativistic energy formula in its closed form. The energy values used by these authors are those reported by Bearden and Burr [5].

5. SCREENING PARAMETER FOR THE K-LEVEL

Sommerfeld [1] in his work on the screening parameters has shown a broken line as a result for σ_1 values for the K level. He, presumably put $\sigma_2 = 0$ in the series expansion of the relativistic energy formula retaining only the terms up to Z^6 and calculated σ_1 values. Blokhin [18] without giving any justification states: "For the K level, total screening parameter $\sigma_1 = 0.3$ and it hardly depends on Z and the value of inner screening $\sigma_2 = 0$ for all Z".

Misra, Singh and Gokhale [19] systematized the work on σ_1 values for the K level in an elaborate way. They substituted the energy values reported by Bearden and Burr and $\sigma_2 = 0$ in Sommerfeld's energy equation and calculated σ_1 for the K level for all the elements of the periodic table. These authors have confirmed the observation of Sommerfeld that σ_1 is an increasing function of Z for K level. It was also found in this work that the energy values reported by Liberman *et al* [20] that were used for the calculation of σ_1 values for $Z > 95$ (except Z= 97) are giving σ_1 values that do not fit in the regular nature of σ_1 Vs Z curve for the K level. Misra, Singh and Gokhale recalculated these σ_1 values by using the relaxed-orbital relativistic Hartree-Fock-Slater energy values reported by Huang *et al*. The σ_1 values so obtained were found to fit much better in σ_1 Vs Z curve.

5. CONCLUSION

This review paper gives a detailed account of different significant works on Sommerfeld's screening parameters. In addition, their use in analyzing the energy values used for their calculation is also mentioned. Some new methods to calculate not only the screening parameters but also the resolved energy values for spin doublet levels have been highlighted.

6. REFERENCES

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