

## A new method for the calculation of Sommerfeld screening parameter $\sigma_1$ in x-ray spectra

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**Abstract.** The paper describes a new method for the calculation of the Sommerfeld screening parameter  $\sigma_1$ . It requires neither the knowledge of the energy separations of spin doublet levels nor is it based on the application of the Hertz law. The only data required for the calculation are the experimental energy values of the level concerned for the series of elements belonging to the same subshell in which the element in the question is situated. As an illustration the values of  $\sigma_1$  are calculated for the  $L_1$ ,  $L_2$  and  $L_3$  levels for elements belonging to the  $4f$  subshell and these are found to be in excellent agreement with those published earlier by Gokhale and Misra. The method brings out the constancy of  $\sigma_1(L_2L_3) - \sigma_1(L_1)$  in a natural way and may thus be regarded as providing theoretical explanation of the Hertz law.

**Keywords.** Screening parameters; spin doublets; irregular doublets; subshell; energy values; Hertz law.

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### 1. Introduction

Sommerfeld [1] in his pioneering work allowed for the screening of nuclear charge by other electrons in the atom by introducing two screening parameters  $\sigma_1$  and  $\sigma_2$  in the series expansion of his well-known relativistic energy equation and obtained the now classic expression

$$E(n, l, j) = -\frac{mc^2}{2} \left[ \frac{\alpha^2(Z - \sigma_1)^2}{n^2} + \frac{\alpha^4(Z - \sigma_2)^4}{n^4} \left( \frac{n}{j + 1/2} - \frac{3}{4} \right) + \dots \right], \quad (1)$$

where  $m$  is the mass of the electron,  $c$  is the velocity of light,  $\alpha$  is the fine structure constant,  $Z$  is the atomic number,  $n$  is the principal quantum number,  $j$  is the total angular momentum quantum number and  $E$  is the energy of the level under consideration. The screening parameter  $\sigma_1$  is identified as accounting for the screening effect of electrons situated in orbits both external and internal to the one under consideration, while the parameter  $\sigma_2$  is interpreted as representing the screening effect of only those electrons which are situated

in orbits internal to the one under consideration. Sommerfeld [1] has shown how the value of  $\sigma_2$  for a spin doublet of levels may be calculated from their experimentally observed energy separation. A knowledge of  $\sigma_2$  and the experimental energy value  $E(n, l, j)$  then allows one to calculate the values of  $\sigma_1$  for these levels by the use of eq. (1). It is found that for a  $(n, l)$  shell  $\sigma_1$  is larger than  $\sigma_2$  and that  $\sigma_1$  increases with  $Z$  while  $\sigma_2$  is independent of  $Z$ . At this stage it may be remarked that the introduction of two screening parameters in (1) appears to be rather arbitrary and some authors [2–5] have tried to introduce a single screening parameter to account for the screening of the nuclear charge by all the other electrons in the atom. However Sommerfeld [1] has given a convincing argument for introducing two screening parameters. According to Sommerfeld the difference  $\sigma_1 - \sigma_2$  is to be ascribed to the effect of outer electronic shells, within which the motion of the electron under consideration occurs. The fact that  $\sigma_1$  increases with  $Z$  is then simply explained by the circumstance that as  $Z$  increases, more and more electronic shells are added on the outside. In fact Sommerfeld has shown that if the electronic shell under consideration is approximated by a uniformly charged spherical shell of radius  $a$  and like wise an outer shell  $i$  containing  $z_i$  electrons is assumed to have the radius  $\rho_i$  the following relation holds between the screening parameters  $\sigma_1$  and  $\sigma_2$  :

$$\sigma_1 = \sigma_2 + a \sum_i \frac{z_i}{\rho_i},$$

where the summation is taken over all the shells  $i$  which are external to the shell under consideration.

It might appear simplistic to use a hydrogen like picture for more complex atoms with the nuclear charge modified by suitably introduced screening parameters, particularly in view of the recent theoretical advances which take into account, amongst others, the relativistic and correlation effects [6]. However, as pointed by Misra *et al* [7] there certainly are some approximations inherent in these calculations as well as some hitherto unknown systematic effects which are responsible for the differences between the theoretical and experimental electron binding energy values. One must also remember that these theoretical studies relate to free atoms and that though there is very good agreement between their results and experiment in the case of simple atoms (that is atoms with closed shells or with one electron outside a closed shell), such is not the case for complicated atoms. The greatest difficulty however is faced by theory when it comes to evaluating solid state effects. On the other hand the experimental results obtained by x-ray spectroscopists are invariably obtained from solid targets. We therefore believe that the calculation of the Sommerfeld screening parameters still has its own merits and relevance since the starting point for these calculations are the experimental energy values obtained by the x-ray spectroscopists, so that the systematic unknown effects and effects of approximations mentioned above are automatically taken care of.

A lot of work has been done on the computation of the Sommerfeld screening parameters  $\sigma_1$  and  $\sigma_2$  [1,8–17]. Gokhale and Misra [18] reported the results of their calculation of the values of  $\sigma_1$  for a large number of spin doublet levels in various atomic number ranges. For their calculations they used the energy values given by Bearden and Burr [19] which were the most recent available at that time and the values of  $\sigma_2$  reported by Burr and Carson [17] which were free from series truncation errors.

Gokhale and Misra [18] in their calculation of screening parameter  $\sigma_1$  eliminated the possible series of truncation errors by the use of the Sommerfeld energy expression in

closed form. They also extended their calculation of  $\sigma_1$  for  $S_{1/2}$  levels [20]. However, such methods cannot be used for the calculation of  $\sigma_1$  and  $\sigma_2$  for  $S_{1/2}$  levels which do not form a spin doublet with any other level. For this purpose, they used the method indicated by Sommerfeld and Wentzel [10] which is based on the use of Hertz's law [21] of irregular doublets in x-ray spectra.

Since the calculation of screening parameters  $\sigma_1$  and  $\sigma_2$  requires a knowledge of the relevant spin doublet separations, it was not possible to compute the values of  $\sigma_1$  and  $\sigma_2$  in those cases where the Bearden and Burr [19] compilation gives only the unresolved energy value for the spin doublet. A new method for obviating this difficulty was developed by Misra *et al* [7]. Inserting the values of  $\sigma_1$  and  $\sigma_2$  obtained by this method in the Sommerfeld formula, individual energy values for the two members of such spin doublets were calculated and found to be in very good agreement with the resolved energy values which are obtained in the mean time by experiment [22].

All the methods described above for the calculation of the screening parameters require as a starting point either the knowledge of individual energy values of the components of the spin doublet or, in the case of  $S_{1/2}$  levels, use of the Hertz law [21] for irregular doublets. It would obviously be desirable to have a method which does not require the above mentioned data as a starting point. The object of the present paper is to describe a method devised by us for this purpose.

## 2. Method

The method requires a knowledge of only the energy values for the level under consideration for different atomic numbers in a given subshell. After suitable rearrangement, the Sommerfeld relativistic equation (1), when expressed in Rydbergs, becomes

$$\left(\frac{\nu}{R}\right)_z = \frac{(Z - \sigma_1)^2}{n^2} - \frac{(Z - \sigma_2)^2}{n^2} + \frac{2}{\alpha^2} \left[ 1 - \left( 1 + \frac{\alpha^2 (Z - \sigma_2)^2}{\left\{ n - (j + \frac{1}{2}) + \left[ (j + \frac{1}{2})^2 - \alpha^2 (Z - \sigma_2)^2 \right]^{1/2} \right\}^2} \right)^{-1/2} \right]. \quad (2)$$

Compressing the second and the third terms on the right hand side into a single term, one obtains

$$\left(\frac{\nu}{R}\right)_z = \frac{(Z - \sigma_1)^2}{n^2} + f(\sigma_2, n, j, Z). \quad (3)$$

The energy separation  $\Delta(\nu/R) = |(\nu/R)_{Z'} - (\nu/R)_Z|$  for a given level for two atomic numbers  $Z$  and  $Z' = Z \pm r$  will be

$$\Delta\left(\frac{\nu}{R}\right) = \left| \frac{(Z' - \sigma'_1)^2}{n^2} - \frac{(Z - \sigma_1)^2}{n^2} \right| + \Delta f(Z, Z'), \quad (4)$$

where  $\Delta f(Z, Z') = |f(\sigma'_2, n, j, Z') - f(\sigma_2, n, j, Z)|$ , and  $\sigma'_1$  has been written for  $\sigma_1(Z')$  and similarly  $\sigma'_2$  for  $\sigma_2(Z')$ . In (4), the value of  $\Delta(\nu/R)$  can be calculated from experimental energy values in eV adopted by Bearden and Burr [19], so that the unknown quantities

in expression (4) are  $\sigma_1, \sigma'_1$  and  $\sigma'_2$  which is equal to  $\sigma_2$  since in a first approximation, the value of inner screening parameter  $\sigma_2$  is almost independent of  $Z$  [1,17,20]. Writing  $\Delta\sigma_1(Z, Z') = |\sigma_1(Z') - \sigma_1(Z)| = \Delta\sigma_1(Z', Z)$  for the magnitude of the difference between  $\sigma_1$  of the atomic number  $Z$  concerned and  $\sigma'_1$  of another atomic number  $Z' = Z \pm r$ , the screening parameter  $\sigma'_1$  in (4) may be expressed as

$$\sigma_1(Z') = \sigma_1(Z) \pm \Delta\sigma_1(Z, Z'), \tag{5}$$

where the upper sign is taken for  $Z' > Z$  and the lower one for  $Z' < Z$ .

In (5),  $\Delta\sigma_1(Z, Z')$  will be obtained by summing up the  $\Delta\sigma_1(Z, Z \pm r)$  values from  $r = 1$  to  $r = |Z' - Z|$ , so that we finally obtain

$$\begin{aligned} \Delta\sigma_1(Z, Z') = & \Delta\sigma_1(Z, Z \pm 1) + \Delta\sigma_1(Z \pm 1, Z \pm 2) + \dots \\ & + \Delta\sigma_1[Z \pm (r - 1), Z \pm r]. \end{aligned} \tag{6}$$

Thus, if the values of  $\Delta\sigma_1(Z, Z')$  and  $\Delta f(Z, Z')$  are known, it becomes possible to calculate the value of  $\sigma_1(Z)$  by the use of (4).

We now describe the method of calculation of the quantities  $\Delta\sigma_1(Z, Z')$  and  $\Delta f(Z, Z')$  taking as an example the  $L_1$  level for  $57 \leq Z \leq 71$ .

### 2.1 Calculation of $\Delta\sigma_1(Z, Z')$

A trial value of  $\sigma_2$  is given on the right hand side of the Sommerfeld relativistic equation (2) and the corresponding  $\sigma_1$  is calculated for different atomic numbers ( $57 \leq Z \leq 71$ ) by adopting term values for the  $L_1$  level given by Bearden and Burr [19]. This process is continued for various assumed values of  $\sigma_2$  at intervals of 0.1 in the range  $\sigma_2 = 2.0$  to 3.0. The values of  $\Delta\sigma_1(Z, Z + 1)$  for  $57 \leq Z \leq 71$ , so obtained are tabulated in table 1. A perusal of these values shows that  $\Delta\sigma_1(Z, Z + 1)$  is almost independent of the assumed  $\sigma_2$  for any consecutive pair of atomic numbers. It can therefore be concluded that whatever be the true values of  $\sigma_2$  for a sub-shell, the values of  $\Delta\sigma_1(Z, Z + 1)$  remain the same so that one can justifiably take the average of these values as the true value of  $\Delta\sigma_1(Z, Z + 1)$ . Thus if value of  $\sigma_1$  for an element is known, the value of  $\sigma_1$  for any other element  $Z'$  can be obtained by the use of eqs (5) and (6).

### 2.2 Calculation of $\Delta f(Z, Z')$

From eqs (2) and (3) one obtains

$$\begin{aligned} f(\sigma_2, n, j, Z) = & \frac{2}{\alpha^2} \left[ 1 - \left( 1 + \frac{\alpha^2 (Z - \sigma_2)^2}{\left\{ n - (j + \frac{1}{2}) + \left[ (j + \frac{1}{2})^2 - \alpha^2 (Z - \sigma_2)^2 \right]^{1/2} \right\}^2} \right)^{-1/2} \right] - \frac{(Z - \sigma_2)^2}{n^2}. \end{aligned} \tag{7}$$

**Table 1.** Values of  $\Delta\sigma_1(Z, Z + 1)$  for the  $L_1$  level.

$Z, Z + 1$	$\sigma_2$											$\langle \Delta\sigma_1(Z, Z + 1) \rangle_{AV}^*$
	2.0	2.1	2.2	2.3	2.4	2.5	2.6	2.7	2.8	2.9	3.0	
57, 58	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.15	0.1511
58, 59	0.17	0.17	0.17	0.17	0.17	0.17	0.16	0.16	0.16	0.16	0.16	0.1651
59, 60	0.18	0.18	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.1729
60, 61	0.17	0.17	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.16	0.1625
61, 62	0.17	0.17	0.17	0.17	0.17	0.17	0.16	0.16	0.16	0.16	0.16	0.1646
62, 63	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.1702
63, 64	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.1690
64, 65	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.16	0.16	0.16	0.1670
65, 66	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.17	0.17	0.17	0.17	0.1759
66, 67	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.1691
67, 68	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.1691
68, 69	0.18	0.18	0.18	0.18	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.1734
69, 70	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.18	0.1809
70, 70	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.1690

\*In calculating these averages the individual values of  $\Delta\sigma_1(Z, Z + 1)$  up to four figures of decimals were used since it was found that values of  $\sigma_1(Z)$  calculated by the use of (4) are very sensitive to small variations in the value of  $\Delta\sigma_1$ .

**Table 2.** Values of  $\Delta f(Z, Z + 1)$  for the  $L_1$  level.

$Z, Z + 1$	$\sigma_2$											$\langle \Delta f(Z, Z + 1) \rangle_{AV}^*$
	2.0	2.1	2.2	2.3	2.4	2.5	2.6	2.7	2.8	2.9	3.0	
57, 58	3.3	3.3	3.2	3.2	3.2	3.2	3.2	3.1	3.1	3.1	3.1	3.18
58, 59	3.5	3.5	3.4	3.4	3.4	3.4	3.4	3.3	3.3	3.3	3.3	3.37
59, 60	3.7	3.7	3.6	3.6	3.6	3.6	3.6	3.5	3.5	3.5	3.5	3.57
60, 61	3.9	3.9	3.9	3.8	3.8	3.8	3.8	3.7	3.7	3.7	3.7	3.79
61, 62	4.1	4.1	4.1	4.1	4.0	4.0	4.0	4.0	3.9	3.9	3.9	4.01
62, 63	4.4	4.3	4.3	4.3	4.3	4.2	4.2	4.2	4.2	4.1	4.1	4.24
63, 64	4.6	4.6	4.6	4.5	4.5	4.5	4.5	4.4	4.4	4.4	4.4	4.49
64, 65	4.9	4.9	4.8	4.9	4.8	4.7	4.7	4.8	4.7	4.6	4.6	4.74
65, 66	5.1	5.1	5.1	5.1	5.0	5.0	5.0	5.0	4.9	4.9	4.9	5.00
66, 67	5.4	5.4	5.4	5.3	5.3	5.3	5.3	5.2	5.2	5.2	5.1	5.28
67, 68	5.7	5.7	5.7	5.6	5.6	5.6	5.5	5.5	5.5	5.5	5.4	5.57
68, 69	6.0	6.0	6.0	5.9	5.9	5.9	5.9	5.8	5.8	5.8	5.7	5.87
69, 70	6.4	6.3	6.3	6.3	6.2	6.2	6.2	6.1	6.1	6.1	6.0	6.19
70, 71	6.7	6.7	6.6	6.6	6.6	6.5	6.5	6.5	6.4	6.4	6.4	6.52

\*In calculating these averages the individual values of  $\Delta f(Z, Z + 1)$  up to two figures of decimals were used for the reasons similar to those stated in the footnote of table 1.

When the trial values of  $\sigma_2$  (from 2.0 to 3.0) at an interval of 0.1 are substituted in the above expression, eleven values of  $f(\sigma_2, n, j, Z)$  are obtained for the atomic number  $Z$ . When the same process is repeated for the atomic number  $Z + 1$  and the difference between the values corresponding to a given assumed value of  $\sigma_2$  is taken, one obtains  $\Delta f(Z, Z + 1)$ . The value of this quantity for different assumed values of  $\sigma_2$  are tabulated in table 2 for the atomic number range 57 to 71. A perusal of these values shows that

**Table 3.** Values of  $\sigma_1(Z)$  for the levels  $L_1, L_2$  and  $L_3$  calculated with different values of  $Z'$ .

Z	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	$\langle\sigma_1\rangle_{AV}$
57 $L_1$	-	16.00	15.99	15.97	15.99	15.99	15.99	15.99	15.99	16.04	16.04	16.01	16.03	16.03	16.02	16.01
57 $L_2$	-	17.21	17.20	17.20	17.20	17.20	17.20	17.20	17.20	17.20	17.20	17.20	17.20	17.20	17.20	17.20
57 $L_3$	-	17.20	17.19	17.19	17.20	17.20	17.20	17.20	17.20	17.20	17.20	17.20	17.20	17.20	17.20	17.20
58 $L_1$	16.15	-	16.13	16.13	16.13	16.14	16.14	16.14	16.14	16.14	16.14	16.17	16.14	16.13	16.20	16.14
58 $L_2$	17.35	-	17.34	17.35	17.35	17.35	17.35	17.35	17.35	17.35	17.35	17.35	17.35	17.35	17.36	17.35
58 $L_3$	17.34	-	17.34	17.34	17.34	17.34	17.34	17.35	17.35	17.35	17.35	17.38	17.37	17.37	17.37	17.35
59 $L_1$	16.31	16.30	-	16.29	16.30	16.31	16.30	16.31	16.30	16.31	16.30	16.30	16.30	16.30	16.30	16.30
59 $L_2$	17.51	17.51	-	17.52	17.52	17.52	17.52	17.51	17.52	17.52	17.52	17.52	17.52	17.52	17.52	17.52
59 $L_3$	17.51	17.51	-	17.50	17.51	17.51	17.51	17.51	17.51	17.51	17.51	17.51	17.51	17.51	17.51	17.51
60 $L_1$	16.47	16.47	16.46	-	16.48	16.49	16.48	16.48	16.48	16.48	16.48	16.48	16.47	16.47	16.47	16.48
60 $L_2$	17.69	17.69	17.70	-	17.69	17.69	17.69	17.68	17.69	17.69	17.69	17.69	17.69	17.69	17.69	17.69
60 $L_3$	17.68	17.68	17.68	-	17.69	17.69	17.69	17.69	17.69	17.69	17.69	17.69	17.69	17.69	17.69	17.69
61 $L_1$	16.64	16.63	16.63	16.64	-	16.66	16.65	16.65	16.64	16.64	16.64	16.67	16.64	16.64	16.64	16.64
61 $L_2$	17.85	17.85	17.86	17.85	-	17.87	17.86	17.85	17.85	17.85	17.85	17.86	17.86	17.86	17.86	17.86
61 $L_3$	17.85	17.85	17.85	17.86	-	17.85	17.85	17.85	17.85	17.85	17.85	17.85	17.85	17.85	17.85	17.85
62 $L_1$	16.81	16.81	16.81	16.82	16.83	-	16.80	16.80	16.80	16.80	16.80	16.80	16.80	16.80	16.80	16.80
62 $L_2$	18.02	18.02	18.02	18.02	18.03	-	18.02	18.01	18.02	18.01	18.02	18.02	18.02	18.02	18.02	18.02
62 $L_3$	18.01	18.01	18.01	18.02	18.01	-	18.02	18.02	18.02	18.02	18.02	18.02	18.02	18.02	18.01	18.02
63 $L_1$	16.98	16.97	16.98	16.98	16.98	16.97	-	16.98	16.97	16.97	16.97	16.97	16.97	16.97	16.97	16.97
63 $L_2$	18.19	18.19	18.19	18.19	18.19	18.19	-	18.16	18.18	18.19	18.19	18.19	18.19	18.19	18.19	18.19
63 $L_3$	18.18	18.18	18.18	18.19	18.18	18.19	-	18.19	18.18	18.19	18.19	18.19	18.18	18.18	18.26	18.19
64 $L_1$	17.14	17.14	17.14	17.15	17.14	17.15	17.14	-	17.13	17.13	17.13	17.13	17.13	17.13	17.14	17.14
64 $L_2$	18.36	18.36	18.36	18.35	18.35	18.35	18.35	-	18.37	18.37	18.37	18.36	18.36	18.37	18.37	18.36
64 $L_3$	18.34	18.35	18.35	18.36	18.36	18.36	18.36	-	18.34	18.35	18.35	18.35	18.35	18.35	18.35	18.35

contd.....

Table 3. Contd...

Z	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	$\langle\sigma_1\rangle_{AV}$
65 $L_1$	17.31	17.31	17.31	17.31	17.31	17.31	17.31	17.30	-	17.29	17.30	17.30	17.30	17.30	17.30	17.31
$L_2$	18.53	18.53	18.53	18.53	18.53	18.52	18.52	18.54	-	18.53	18.54	18.53	18.53	18.53	18.53	18.53
$L_3$	18.52	18.52	18.52	18.52	18.52	18.52	18.52	18.51	-	18.53	18.53	18.53	18.52	18.52	18.52	18.52
66 $L_1$	17.48	17.48	17.47	17.49	17.48	17.48	17.48	17.47	17.47	-	17.49	17.48	17.48	17.48	17.48	17.48
$L_2$	18.70	18.70	18.70	18.70	18.70	18.70	18.70	18.70	18.70	-	18.71	18.70	18.70	18.71	18.71	18.70
$L_3$	18.69	18.69	18.69	18.69	18.69	18.69	18.69	18.69	18.70	-	18.70	18.70	18.70	18.70	18.70	18.69
67 $L_1$	17.70	17.68	17.65	17.65	17.65	17.65	17.65	17.65	17.65	17.66	-	17.65	17.64	17.65	17.65	17.66
$L_2$	18.87	18.87	18.87	18.87	18.87	18.87	18.87	18.88	18.86	18.87	-	18.87	18.87	18.87	18.87	18.87
$L_3$	18.86	18.86	18.86	18.86	18.86	18.87	18.87	18.86	18.87	18.87	-	18.86	18.85	18.85	18.86	18.86
68 $L_1$	17.86	17.82	17.82	17.82	17.82	17.82	17.82	17.82	17.81	17.82	17.81	-	17.81	17.82	17.82	17.82
$L_2$	19.04	19.04	19.04	19.04	19.06	19.05	19.03	19.04	19.04	19.04	19.04	-	19.04	19.04	19.04	19.04
$L_3$	19.03	19.03	19.03	19.03	19.03	19.03	19.09	19.03	19.03	19.03	19.03	-	19.02	19.02	19.02	19.03
69 $L_1$	18.00	17.99	17.99	17.99	17.99	17.99	18.01	17.99	17.99	17.99	17.99	17.99	-	18.00	17.98	18.00
$L_2$	19.21	19.21	19.21	19.21	19.21	19.21	19.21	19.21	19.20	19.22	19.21	19.21	-	19.21	19.21	19.21
$L_3$	19.21	19.25	19.23	19.21	19.21	19.21	19.21	19.20	19.21	19.30	19.20	19.19	-	19.20	19.21	19.22
70 $L_1$	18.21	18.23	18.17	18.18	18.20	18.25	18.17	18.17	18.17	18.17	18.17	18.17	18.18	-	18.18	18.19
$L_2$	19.41	19.40	19.41	19.41	19.41	19.41	19.41	19.42	19.41	19.41	19.41	19.41	19.41	-	19.42	19.41
$L_3$	19.38	19.40	19.38	19.38	19.38	19.38	19.38	19.38	19.38	19.45	19.37	19.37	19.50	-	19.40	19.39
71 $L_1$	18.34	18.34	18.34	18.35	18.34	18.34	18.34	18.34	18.34	18.34	18.34	18.42	18.34	18.30	-	18.35
$L_2$	19.57	19.57	19.57	19.57	19.57	19.57	19.57	19.56	19.58	19.57	19.57	19.57	19.57	19.57	-	19.57
$L_3$	19.56	19.57	19.55	19.56	19.56	19.56	19.63	19.55	19.56	19.61	19.55	19.55	19.56	19.56	-	19.57

**Table 4.** Average values of  $\sigma_1(Z)$  for the levels  $L_1, L_2$  and  $L_3$ .

	Z														
	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71
<i>Present work</i>															
$\sigma_1(L_1)$	16.01	16.14	16.30	16.48	16.64	16.80	16.97	17.14	17.31	17.48	17.66	17.82	18.00	18.19	18.35
$\sigma_1(L_2)$	17.20	17.35	17.52	17.69	17.86	18.02	18.19	18.36	18.53	18.70	18.87	19.04	19.21	19.41	19.57
$\sigma_1(L_3)$	17.20	17.35	17.51	17.69	17.85	18.02	18.19	18.35	18.52	18.69	18.86	19.03	19.22	19.39	19.57
$\langle \sigma_1(L_2 L_3) \rangle_{AV}$	17.200	17.350	17.515	17.690	17.855	18.020	18.190	18.355	18.525	18.695	18.865	19.035	19.215	19.405	19.565
$\sigma_1(L_2 L_3) - \sigma_1(L_1)$	1.190	1.210	1.215	1.210	1.215	1.220	1.220	1.215	1.215	1.215	1.205	1.215	1.215	1.215	1.215
<i>G&amp;M*</i>															
$\sigma_1(L_1)$	15.996	16.143	16.308	16.482	16.647	16.811	16.980	17.148	17.316	17.486	17.657	17.826	18.001	18.175	18.350
$\sigma_1(L_2 L_3)$	17.196	17.343	17.508	17.682	17.847	18.011	18.180	18.348	18.516	18.686	18.857	19.026	19.201	19.375	19.550

\*Gokhale and Misra [18,20].



for any atomic number pair  $(Z, Z + 1)$ , the value of  $\Delta f(Z, Z + 1)$  remains almost the same whatever may be the assumed value of  $\sigma_2$  so that one can assume that  $\Delta f(Z, Z + 1)$  is independent of  $\sigma_2$  for a particular sub-shell. Thus, as was done in the case of  $\Delta\sigma_1(Z, Z')$  discussed above, one can obtain the value of  $\Delta f(Z, Z \pm r)$  through the use of the expression

$$\Delta f(Z, Z') = \Delta f(Z, Z \pm 1) + \Delta f(Z \pm 1, Z \pm 2) + \dots + \Delta f[Z \pm (r - 1), Z \pm r]. \quad (8)$$

### 3. Results and discussion

Results of our calculations of  $\sigma_1$  by the use of the method described in §2 are presented in table 3 for the levels  $L_1, L_2$  and  $L_3$  in the atomic number range  $57 \leq Z \leq 71$ . In this table, we have listed the individual values of  $\sigma_1(Z)$  as obtained by the use of eq. (4), taking different pairs of  $Z$  and  $Z'$  for the calculation, where  $Z' (\neq Z)$  varies from 57 to 71. It is gratifying to note that the value of  $\sigma_1(Z)$  so obtained remains almost the same whatever may be the value of  $Z'$  used for the calculations. We thus conclude that the average of the fourteen values of  $\sigma_1(Z)$  so obtained represents the true value of  $\sigma_1(Z)$ .

It is interesting to compare the values of  $\sigma_1(L_1)$  and  $\sigma_1(L_2L_3)$  with those obtained earlier by Gokhale and Misra [18, 20]. Such a comparison is shown in table 4 which brings out the excellent agreement between the values of the screening constants reported in the present study and those published by Gokhale and Misra. This table also lists the values of  $\sigma_1(L_2L_3) - \sigma_1(L_1)$  as obtained in the present study. It is seen that these values are in very good agreement with the value 1.20 calculated by Gokhale and Misra [20] making use of the Hertz law [21]. It is remarkable that the present study has brought out the constancy of  $\sigma_1(L_2L_3) - \sigma_1(L_1)$  as a function of  $Z$  in a natural way. This may thus be taken as providing a theoretical explanation of the experimental observation which led to the enunciation of the Hertz law [21] for irregular doublets. Of no less interest is the fact that the results of present calculations show the near exact equality of  $\sigma_1$  values for the  $L_2$  and  $L_3$  levels.

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