Sommerfeld Screening Parameters for the L & M Levels in X -Ray Spectra

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Abstract— In Sommerfeld relativistic two body energy equation, two screening parameters and are introduced. Values of and are obtained by various authors using different levels. The current method is superior to previous methods because it doesn't require more than one level to find the value of screening parameters and I have used this method to obtain screening parameters for L1, L23, M1, M23, M45 levels using single level i.e. no reference from a level is taken in calculation of screening parameters of another level.

Key words: Sommerfeld, X -Ray Spectra

I. INTRODUCTION

Ever since the beginning of X-ray spectroscopy the theoretical calculation x-ray term values (inner electron binding energies) has been of great interest. In his pioneering work Sommerfeld (1934) introduced two screening parameters σ_1 (the total screening parameter) and σ_2 (the internal screening parameter) in the series expansion of his well-known two-body relativistic energy equation and obtained the now classic expression:

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

In this expression *m* is the mass of the electron, c is the velocity of light, α is the fine structure constant, Z is the atomic number, j is the total angular momentum quantum number and E is the energy of the level under consideration.

Sommerfeld (1934) and Wentzel calculated σ_1 and σ_2 of different levels using equation (1). Later, Gokhale and Misra (1978) presented equation 1 in finite form thus eliminating the truncation errors arising as result of series expansion. They also calculated σ_1 and σ_2 for spin doublets as well as for single or $S_{1/2}$ levels (L1, M1, N1 levels). In this method, I took the truncated expression given by Gokhale and Misra and re calculated the values of the screening parameters.

II. METHOD

A. Calculation of σ_2

The method is essentially the same as that originally indicated by Sommerfeld and Wentzel (1921). However, here I take that equation in closed form as suggested by Gokhale and Misra (1978), to avoid series truncation errors. I give below a brief discussion of the method used.
Sommerfeld's energy expression in closed form is:

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

Where the symbols have the same meanings as in equation (1). In the above expression, the energy values v/R are taken from theoretical energy values of Huang et al (1976) for free atom. I observed that for first element of each level, σ_1 varies so slowly with the variation in σ_2 such that $d\sigma_1/d\sigma_2$ can be taken as zero. So, for first element of each level, I draw curve of σ_1 versus σ_2 (using equation 2) and fitted the obtained curve to the polynomial of order 2. Then I found $d\sigma_1/d\sigma_2$ from the curve, equate it to zero and obtain the value of σ_2 (As σ_2 does not change much with z). This should be noted that screen doublets are taken as single level.

B. Calculation of σ_1

Using above obtained value of σ_2 throughout for that level, one can easily obtain the value of total screening (σ_1) for different Z of that level by putting value of z and v/R in equation 2.

Z	L-1	L-2	L-3	M-1	M-2	M-3	M-4	M-5
3								
4	2.46779							
5	3.07289	3.46946						
6	3.69316	4.3308						
7	4.32754	5.1422	5.07413					
8	4.95378	5.9683	5.9207					
9	5.58668	6.7952	6.77064					
10	6.20346	7.6127	7.61289					
11	6.41334	7.7286	7.72893	9.20836				
12	6.65677	7.9398	7.94016	9.91685				
13	6.88565	8.1315	8.14214	10.4087	11.0916			
14	7.13618	8.3584	8.37998	10.9567	11.8838			

15	7.40149	8.6184	8.63514	11.543	12.6292	12.5563		
16	7.67648	8.8928	8.90434	12.1188	13.4012	13.3536		
17	7.96112	9.1802	9.18632	12.7152	14.1307	14.111		
18	8.24952	9.4733	9.47375	13.3308	14.8904	14.8991		
19	8.40596	9.61578	9.61616	13.5314	15.0387	15.0488		
20	8.56842	9.76842	9.76872	13.7935	15.2838	15.2958		
21	8.83225	10.0291	10.0347	14.3875	15.8517	15.9461	18.8253	
22	9.10517	10.2999	10.3113	15.0037	16.4493	16.6279	19.6639	
23	9.38502	10.5784	10.5959	15.64	17.0653	17.329	20.5333	
24	9.74324	10.9443	10.9623	16.5339	18.0089	18.299	22.1412	22.11
25	9.95677	11.1552	11.1756	16.9266	18.398	18.6941	22.3043	22.4
26	10.2470	11.452	11.4686	17.5746	19.1142	19.3557	23.2053	23.285
27	10.5395	11.7516	11.764	18.2374	19.8479	20.034	24.1435	24.207
28	10.835	12.0545	12.0624	18.8929	20.5724	20.7014	25.0535	25.0987
29	11.2023	12.436	12.435	19.8267	21.6518	21.6645	26.867	26.8727
30	11.43	12.6653	12.6639	20.2299	22.0521	22.0641	26.9385	26.9445
31	11.6388	12.8738	12.8725	20.5745	22.375	22.394	26.9845	26.9989
32	11.8423	13.077	13.076	20.9162	22.6985	22.7263	27.1277	27.1486
33	12.0432	13.2787	13.2769	21.264	23.0407	23.0657	27.3463	27.3636
34	12.2436	13.4802	13.4774	21.6199	23.3954	23.4168	27.6131	27.7277
35	12.4394	13.6773	13.6733	21.9755	23.7515	23.769	27.8996	27.9119
36	12.6346	13.8741	13.8687	22.3348	24.1134	24.1265	28.2072	28.2175
37	12.7841	14.0229	14.0166	22.5338	24.2925	24.3059	28.2582	28.2689
38	12.9322	14.1705	14.1633	22.741	24.4846	24.4986	28.351	28.3622
39	13.0998	14.3382	14.3308	23.031	24.7699	24.8428	28.5819	28.6007
40	13.2716	14.5104	14.5028	23.3381	25.0751	25.093	28.8456	28.873
41	13.467	14.7067	14.6996	23.7362	25.4801	25.5013	29.2412	29.2831
42	13.6419	14.8831	14.8746	24.0686	25.8156	25.8368	29.5556	29.5947
43	13.8184	15.0614	15.0515	24.4081	26.1593	26.1805	29.8835	29.9192
44	13.9963	15.2414	15.2298	24.756	26.5125	26.5336	30.2256	30.2573
45	14.1743	15.4216	15.4083	25.1066	26.8688	26.8897	30.5725	30.6006
46	14.3769	15.6276	15.6118	25.5443	27.3205	27.3402	31.0425	31.0601
47	14.5338	15.786	15.7689	25.8259	27.6017	27.6221	31.2974	31.3155
48	14.6881	15.9419	15.9233	26.1017	27.8773	27.8983	31.5482	31.5669
49	14.835	16.09	16.0701	26.356	28.1285	28.1512	31.7726	31.7921
50	14.9793	16.2354	16.2142	26.6043	28.3735	28.3981	31.9925	32.013
51	15.1232	16.3808	16.358	26.8545	28.6221	28.6472	32.2183	32.2392
52	15.2665	16.5256	16.501	27.1053	28.8717	28.8973	32.4475	32.4686
53	15.4095	16.6703	16.6439	27.3576	29.1235	29.1494	32.681	32.7025
54	15.5519	16.8144	16.7861	27.6101	29.3758	29.4021	32.9167	32.9385
55	15.672	16.9357	16.9055	27.7927	29.5537	29.581	33.0676	33.0897
56	15.7923	17.0571	17.0251	27.9785	29.7355	29.764	33.2253	33.2478
57	15.922	17.1883	17.1545	28.1972	29.9525	29.9825	33.4246	33.4485
58	16.1143	17.3827	17.3473	28.6502	30.4134	30.4513	33.8965	33.933
59	16.2783	17.5486	17.5115	28.9971	30.7637	30.8069	34.2452	34.2894
60	16.4445	17.7166	17.6778	29.3511	31.1214	31.1701	34.6023	34.6546
61	16.6121	17.8862	17.8457	29.7102	31.4842	31.5387	34.9652	35.0259
62	16.7817	18.0568	18.0145	30.0726	31.8503	31.9109	35.3319	35.4012
63	16.9491	18.2271	18.183	30.4335	32.2184	32.2795	35.704	35.7698
64	17.0929	18.3725	18.3266	30.7041	32.4895	32.5543	35.9667	36.0368
65	17.29	18.572	18.5243	31.1683	32.9684	33.0304	36.4642	36.5221
66	17.4619	18.7459	18.6963	31.5396	33.3475	33.4099	36.849	36.9026
67	17.6345	18.9206	18.869	31.9128	33.7287	33.7916	37.2364	37.2853
68	17.8081	19.0963	19.0428	32.2889	34.1127	34.1762	37.627	37.6712
69	17.9828	19.2732	19.2178	32.6675	34.4994	34.5636	38.0208	38.06
70	18.1586	19.4508	19.3935	33.0488	34.8888	34.9539	38.4178	38.4519
71	18.3097	19.6038	19.5444	33.3423	35.1848	35.2531	38.7109	38.7654
72	18.4612	19.757	19.6956	33.6353	35.4802	35.552	39.004	39.0395

73	18.612	19.9097	19.8462	33.9251	35.7724	35.8479	39.294	39.3304
74	18.7634	20.0629	19.9974	34.2156	36.0653	36.1448	39.5454	39.6227
75	18.9133	20.2146	20.1467	34.4998	36.3519	36.7354	39.8709	39.9078
76	19.0633	20.3667	20.2963	34.7838	36.6383	36.726	40.1568	40.1932
77	19.2303	20.5358	20.4628	35.1187	36.9777	37.0698	40.502	40.5364
78	19.3733	20.6806	20.6052	35.3785	37.239	37.3361	40.7614	40.7955
79	19.5244	20.8336	20.7556	35.6618	37.5249	37.6273	41.0486	41.0818
80	19.6654	20.9763	20.8958	35.9133	37.7775	37.8856	41.3	41.3313
81	19.8028	21.1149	21.032	36.1521	38.0163	38.131	41.5373	41.5694
82	19.9396	21.2529	21.1675	36.3878	38.2521	38.3738	41.772	41.8036
83	20.0749	21.3895	21.3016	36.6186	38.483	38.6118	41.8833	42.0329
84	20.2102	21.526	21.4356	36.8481	38.7125	38.8491	42.2317	42.2617
85	20.3451	21.6619	21.569	37.075	38.9393	39.0843	42.4592	42.4882
86	20.481	21.7979	21.7025	37.3523	39.1653	39.3193	42.6866	42.7147
87	20.6061	21.9234	21.8255	37.4963	39.3582	39.5219	42.8794	42.9063
88	20.7315	22.0488	21.9486	37.6902	39.5503	39.7245	43.0723	43.0981
89	20.861	22.1782	22.0757	37.8945	39.7529	39.9387	43.2777	43.3025
90	20.9919	22.3084	22.2037	38.1012	39.9578	40.1558	43.4864	43.5101
91	21.145	22.4611	22.3545	38.3789	40.2353	40.4483	43.7737	43.7982
92	21.2908	22.6049	22.4963	38.6269	40.4814	40.7097	44.0285	44.0531
93	21.437	22.75	22.6396	38.8774	40.7304	40.9753	44.2877	44.3123
94	21.5965	22.9067	22.7946	39.1641	41.0152	41.2785	44.5862	44.6116
95	21.7452	23.053	22.9394	39.4156	41.265	41.5464	44.8494	44.8726
96	21.8859	23.1898	23.0746	39.6359	41.4812	41.7824	45.0778	45.1
97	22.0488	23.3488	23.2324	39.925	41.7687	42.0907	45.3849	45.4031
98	22.1932	23.4979	23.3803	40.1814	42.0211	42.3656	45.6556	45.6709
99	22.3598	23.6479	23.5292	40.4388	42.2738	42.6425	45.9285	45.9408
100	22.5184	23.799	23.6793	40.6979	42.5274	42.9221	46.2043	46.2133
101	22.6783	23.9508	23.8306	40.9574	42.7811	43.204	46.4824	46.488
102	22.8398	24.1033	23.9828	41.2169	43.0339	43.4872	46.7619	46.7638
103	22.993	24.2447	24.1237	41.4404	43.2473	43.7332	47.0014	47.0006
104	23.1479	24.3867	24.2655	41.6591	43.4596	43.9805	47.2421	47.2385
105	23.3067	24.5292	24.4078	41.8867	43.6694	44.2279	47.4829	47.4764
106	23.467	24.6721	24.5509	42.109	43.8769	44.4759	47.7244	47.7148

Table 1: Values of σ_1 For Different Levels

III. Discussion and Comparison with Earlier Results

It should be realised that the energy values used in this paper are for free atoms, not that obtained from the solid targets.

A. $\Delta\ \sigma_1$ *values*

The results available to me on the calculation of σ_1 and σ_2 are those due to Sommerfeld and Wentzel (1921) , Sommerfeld (1934) and Gokhale and Misra (1978).A comparison of their values of $\Delta\ \sigma_1$ with those found in present in given work in Table 2.

It will be seen from table 2 that my values of $\Delta\ \sigma_1$ agree fairly close with those of the earlier workers.

Doublet	Sommerfeld and Wentzel (1921)	Sommerfeld (1934)	Gokhale & Misra (1978)	Present work
L_1-$L_{2,3}$	1.21	1.14	1.20	1.22
M_1-$M_{2,3}$	1.72	1.71	1.74	1.75

Table 2: Values of $\Delta\ \sigma_1$ for irregular doublets

B. σ_1 *values*

Examination of Table 1 shows that values of σ_1 are in agreement with the observations made by Gokhale and Misra (1977,1978). But my values are more precise and are up to four decimal places.

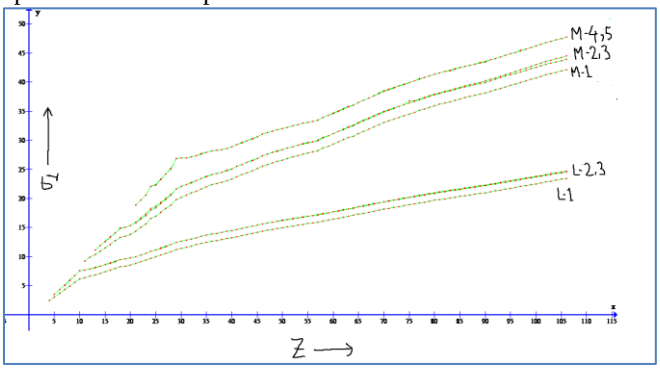

Figure: Plot of Total Screening (σ_1) For Different Levels Vs. Z

C. σ_2 *values*

This comparison shows that for L-1 level, my value is in agreement with the value suggested by Gokhale and Misra (1978). For L-2 /L-3 level, my value of σ_2 approaches the value found by Burr and Carson (1974). For M-1 level, my value of σ_2 is slightly greater than that of Gokhale and Misra . For M-2/M-3 levels, my value of σ_2 is greater than that of Burr and Carson. Following the same trend, in M-4/M-5 levels; my values of σ_2 are greater than σ_2 values of Burr and Carson.

This increase in my value of σ_2 as compared to other workers is easily understood. As with increase in Z, the σ_1 versus σ_2 gradient increases and in turn gives higher value of σ_2.

Level	Sommerfeld (1934)	Various authors	Present work
L_1	2.0	2.52(Gokhale & Misra)	2.5
$L_{2,3}$	3.5	3.46(Burr & Carson)	3.3
M_1	6.8	6.87(Gokhale & Misra)	7.5
$M_{2,3}$	8.5	8.26(Burr & Carson)	8.8
$M_{4,5}$	13.0	13.25(Burr & Carson)	14.35

Table 3: Comparison of average σ_2 values

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REFERENCES

[1] Bearden J A and Burr A F, *Rev. Mod. Phys. 39 125-42*
[2] Gokhale B G and Misra U D, 1977 *J. Phys. B At. Mol. Phys. 3599-607.*
[3] Gokhale B G and Misra U D, 1978 *J. Phys. B At. Mol. Phys. 11 2077-86*
[4] Sommerfeld A 1934 *Atomic Structure and Spectral Lines 5th German edn, transl.* H L Brose (New York: Dutton)
[5] Sommerfeld A and Intzel G *Phys. 1921 Z. Phys. 7 86-92*

