Fine-structure intervals for the lowest P terms in the Cu, Zn, Ga, and Br isoelectronic sequences for $Z \leq 92$

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Theoretical and semiempirical predictions of fine-structure intervals for the lowest P terms in the Cu, Zn, Ga, and Br sequences are presented for all ions with $Z \leq 92$. Through the use of screening parameter reductions of both the existing data base and the *ab initio* multiconfiguration Dirac-Fock computations reported herein, a new empirical decomposition has been discovered that permits measurements for the Cu sequence to be combined with theoretical computations to make precise predictions for the Zn, Ga, and Br sequences. These predictions are of higher precision than could be obtained solely by *ab initio* methods, and extend to much higher Z than semiempirical extrapolations alone would permit. These results provide insights into the interaction of the active and core electrons, and test a method that is applicable to many other systems.

I. INTRODUCTION

Forbidden transitions between low-lying fine-structure levels in highly ionized atoms provide a useful diagnostic tool for the analysis of high-temperature astrophysical and laboratory plasmas. $M1$ and $E2$ transitions between these levels become relatively stronger with increasing nuclear charge, and provide a source of intense radiative emission lines in an isolated and conveniently detectable wavelength region. These transitions are also useful for radiative absorption studies if the lower level is heavily populated due to its stability or metastability. Thus the $ns^2np \, ^2P$ ground terms in the B, Al, and Ga sequences, the $ns^2np^5 \, ^2P$ ground terms in the F, Cl, and Br sequences, and the $nsnp \, ^3P$ excited terms (with metastable $J=0$ levels) in the Be, Mg, and Zn sequences are important systems for consideration.

Spectroscopic identification of impurity lines requires a very accurate knowledge of the transition wavelengths. The requirements (often to within parts in 10^5 or better) can exceed the precision attainable with available *ab initio* theoretical methods, and the use of semiempirical methods involving predictive interpolations and extrapolations of the existing data base are often necessary. Screening parametrizations[1] can yield the requisite accuracies, but they require the existence of a substantial data base within the specific isoelectronic sequence under consideration. An exposition is presented here of a new method that utilizes information in a data-rich isoelectronic sequence, together with *ab initio* calculations of a secondary quantity, to make predictions of fine structures in data-poor isoelectronic sequences.

Recently many new experimental measurements have become available and comprehensive sets of theoretical calculations have been performed for transitions in the sequences described above with $n=2$ and 3, which have been comprehensively summarized in Ref. 2. Linearized screening parametrizations have been used[3–6] to study the homologous systems with $n=4$ to moderately high stages of ionization, but there were indications that the linearization could not be extended beyond 30 stages of ionization.[7] Recent new measurements[8–15] now permit these studies of the $n=4$ sequences to be extended to a new high-charge regime, and precision observations for the Cu isoelectronic sequence are now available through 55 stages of ionization.

Studies of systematic trends in the computations and in the empirical data base have revealed an independence and separability of components of the effective screening that are associated with the closed-shell and open-shell portions of the core. A semiempirical procedure then permits experimental results for the Cu sequence to be combined with theoretical results to make reliable predictions for the Zn, Ga, and Br sequences for $Z \leq 92$. These predictions are expected to be much more accurate than *ab initio* computations, and can be extended to higher Z values than standard semiempirical extrapolations.

II. SYSTEMS SELECTED FOR STUDY

The fine-structure intervals considered herein can be designated by their nominal LS designations as follows:

Cu sequence,

$$4p(^2P_{1/2}-^2P_{3/2}) \; ;$$

Zn sequence,

$$4s4p(^3P_0-^3P_2) \; ;$$

Ga sequence,

$$4s^24p(^2P_{1/2}-^2P_{3/2}) \; ;$$

Br sequence,

$$4s^24p^5(^2P_{3/2}-^2P_{1/2}) \; .$$

For both the Ga and Br sequences the lower level corresponds to the ground state, and for the Zn sequence the lower level is metastable since its only energetically allowed decay is absolutely forbidden by the $J=0 \nrightarrow J=0$ selection rule. Sequences such as these that contain a

TABLE I. Fine-structure separations for the $4p\ ^2P$, $4s4p\ ^3P(J=2-0)$, $4s^24p\ ^2P$, and $4s^24p^5\ ^2P$ terms in the Cu, Zn, Ga, and Br isoelectronic sequences, using semiempirical (SE) and Dirac-Fock (DF) methods. The SE predictions incorporate both experimental data and differential DF computations into the determination, and are expected to be more accurate than the DF calculations alone. Experimentally observed values are indicated by a source footnote in the SE column. Bibliographies of source references given for a, Cu in Ref. 3; b, Zn in Ref. 4; d, Ga in Ref. 5; f, Br in Ref. 6. Recent original sources are as follows. Cu: i, Reader et al. in Ref. 9; j, Reader and Luther in Ref. 8; k, Seely et al. in Ref. 10. Zn: c, Isberg and Litzén in Ref. 11; e, Joshi and van Kleef in Ref. 12; g, Trigueiros et al. in Ref. 13. Ga: h, Reader et al. in Ref. 15.

Z	Ion	Cu sequence Q	Cu SE	Cu DF	Zn sequence Q	Zn SE	Zn DF	Ga sequence Q	Ga SE	Ga DF	Br sequence Q	Br SE	Br DF
29	Cu	0+	248[a]	164									
30	Zn	1+	874[a]	731	0+	579[b]	500						
31	Ga	2+	1718[a]	1546	1+	1382[c]	1273	0+	826[d]	399			
32	Ge	3+	2788[a]	2595	2+	2405[b]	2280	1+	1767[d]	1478			
33	As	4+	4110[a]	3891	3+	3680[b]	3531	2+	2940[d]	2686			
34	Se	5+	5698[a]	5455	4+	5211[e]	5045	3+	4376[d]	4123			
35	Br	6+	7580[a]	7312	5+	7031[e]	6846	4+	6089[d]	5831	0+	3685[f]	3666
36	Kr	7+	9779[a]	9488	6+	9163[g]	8962	5+	8108[d]	7841	1+	5370[f]	5368
37	Rb	8+	12335[a]	12015	7+	11591	11422	6+	10467[h]	10185	2+	7375[f]	7388
38	Sr	9+	15269[a]	14924	8+	14431	14257	7+	13198[h]	12894	3+	9728[f]	9758
39	Y	10+	18622[a]	18249	9+	17681	17501	8+	16322[h]	16003	4+	12460[f]	12509
40	Zr	11+	22425[a]	22024	10+	21379	21189	9+	19884[h]	19546	5+	15607[f]	15675
41	Nb	12+	26720[a]	26288	11+	25560	25359	10+	23928[h]	23560	6+	19191[f]	19290
42	Mo	13+	31547[a]	31079	12+	30264	30048	11+	28467[h]	28083	7+	23274[f]	23391
43	Tc	14+	36953	36437	13+	35530	35298	12+	33563	33156	8+	27868	28018
44	Ru	15+	42953[j]	42406	14+	41400	41150	13+	39240[h]	38821	9+	33055[f]	33211
45	Rh	16+	49538[j]	49031	15+	47918	47650	14+	45567[h]	45122	10+	38800[f]	39012
46	Pd	17+	56963[j]	56357	16+	55128	54844	15+	52572[h]	52104	11+	45180[f]	45467
47	Ag	18+	65067[j]	64434	17+	63079	62779	16+	60320[h]	59817	12+	52340	52622
48	Cd	19+	74012[j]	73313	18+	71819	71508	17+	68855[h]	68311	13+	60202	60526
49	In	20+	83774[j]	83045	19+	81398	81081	18+	78161[h]	77636	14+	68857	69231
50	Sn	21+	94430[j]	93688	20+	91871	91555	19+	88356	87850	15+	78358	78789
51	Sb	22+	106150	105297	21+	103292	102987	20+	99492	99007	16+	88757	89256
52	Te	23+	118807	117934	22+	115719	115437	21+	111614	111169	17+	100111	100690
53	I	24+	132541	131661	23+	129211	128966	22+	124783	124396	18+	112477	113151
54	Xe	25+	147415	146543	24+	143831	143640	23+	139057	138753	19+	125915	126704
55	Cs	26+	163495	162647	25+	159642	159526	24+	154501	154308	20+	140487	141412
56	Ba	27+	180910[j]	180045	26+	176711	176694	25+	171181	171130	21+	156260	157345
57	La	28+	200270[j]	198810	27+	195764	195219	26+	190397	189292	22+	174049	174574
58	Ce	29+	220575	219019	28+	215751	215176	27+	210049	208871	23+	192613	193173
59	Pr	30+	242017	240751	29+	236871	236644	28+	230826	229945	24+	212271	213219
60	Nd	31+	265110[j]	264090	30+	259623	259707	29+	253218	252596	25+	233488	234793
61	Pm	32+	290079	289122	31+	284234	284451	30+	277452	276912	26+	256473	257979
62	Sm	33+	316900[j]	315936	32+	310681	310964	31+	303503	302979	27+	281219	282864
63	Eu	34+	345727	344628	33+	339112	339342	32+	331525	330893	28+	307864	309540
64	Gd	35+	376570[j]	375294	34+	369547	369681	33+	361529	360749	29+	336423	338100
65	Tb	36+	409435	408036	35+	401984	402082	34+	393520	392649	30+	366910	368644
66	Dy	37+	444490[j]	442960	36+	436599	436652	35+	427670	426697	31+	399486	401275

TABLE I. (*Continued.*)

Z	Ion	Q	Cu sequence SE	Cu sequence DF	Q	Zn sequence SE	Zn sequence DF	Q	Ga sequence SE	Ga sequence DF	Q	Br sequence SE	Br sequence DF
67	Ho	38 +	481 925	480 176	37 +	473 565	473 499	36 +	464 159	463 003	32 +	434 327	436 099
68	Er	39 +	521 720[j]	519 799	38 +	512 880	512 738	37 +	502 977	501 681	33 +	471 423	473 228
69	Tm	40 +	563 823	561 953	39 +	554 491	554 494	38 +	544 071	542 853	34 +	510 733	512 782
70	Yb	41 +	608 510[j]	606 757	40 +	598 658	598 884	39 +	587 707	586 639	35 +	552 507	554 878
71	Lu	42 +	656 181	654 344	41 +	645 798	646 043	40 +	634 291	633 169	36 +	597 138	599 645
72	Hf	43 +	706 782	704 850	42 +	695 842	696 103	41 +	683 762	682 579	37 +	644 567	647 214
73	Ta	44 +	760 000[j]	758 416	43 +	748 487	749 209	42 +	735 813	735 010	38 +	694 518	697 724
74	W	45 +	815 800[j]	815 191	44 +	803 701	805 506	43 +	790 426	790 607	39 +	746 954	751 318
75	Re	46 +	875 502	875 330	45 +	862 795	865 150	44 +	848 881	849 526	40 +	803 122	808 148
76	Os	47 +	939 296	938 992	46 +	925 945	928 300	45 +	911 365	911 925	41 +	863 194	868 369
77	Ir	48 +	1 007 141	1 006 348	47 +	993 127	995 126	46 +	977 848	977 972	42 +	927 151	932 146
78	Pt	49 +	1 078 995	1 077 574	48 +	1 064 284	1 065 805	47 +	1 048 292	1 047 843	43 +	994 952	999 651
79	Au	50 +	1 154 812[k]	1 152 854	49 +	1 139 384	1 140 519	48 +	1 122 650	1 121 721	44 +	1 066 563	1 071 064
80	Hg	51 +	1 235 101	1 232 379	50 +	1 218 933	1 219 459	49 +	1 201 423	1 199 794	45 +	1 142 475	1 146 570
81	Tl	52 +	1 319 890	1 316 351	51 +	1 302 969	1 302 828	50 +	1 284 648	1 282 264	46 +	1 222 711	1 226 366
82	Pb	53 +	1 408 405[k]	1 404 984	52 +	1 390 708	1 390 838	51 +	1 371 570	1 369 342	47 +	1 306 565	1 310 659
83	Bi	54 +	1 500 481[k]	1 498 498	53 +	1 481 986	1 483 709	52 +	1 462 002	1 461 248	48 +	1 393 859	1 399 666
84	Po	55 +	1 597 953	1 597 127	54 +	1 578 650	1 581 675	53 +	1 557 795	1 558 212	49 +	1 486 357	1 493 612
85	At	56 +	1 701 090	1 701 119	55 +	1 680 945	1 684 984	54 +	1 659 166	1 660 484	50 +	1 584 300	1 592 741
86	Rn	57 +	1 810 156	1 810 682	56 +	1 789 124	1 793 842	55 +	1 766 400	1 768 264	51 +	1 687 945	1 697 254
87	Fr	58 +	1 925 433	1 926 183	57 +	1 903 508	1 908 618	56 +	1 879 786	1 881 923	52 +	1 797 577	1 807 508
88	Ra	59 +	2 047 214	2 047 776	58 +	2 024 350	2 029 463	57 +	1 999 595	2 001 609	53 +	1 913 470	1 923 655
89	Ac	60 +	2 175 808	2 175 860	59 +	2 151 985	2 156 778	58 +	2 126 144	2 127 721	54 +	2 035 946	2 046 083
90	Th	61 +	2 311 538	2 310 693	60 +	2 286 707	2 290 819	59 +	2 259 754	2 260 514	55 +	2 165 282	2 175 043
91	Pa	62 +	2 454 744	2 452 643	61 +	2 428 885	2 431 954	60 +	2 400 747	2 400 353	56 +	2 301 846	2 310 892
92	U	63 +	2 605 781	2 601 988	62 +	2 578 859	2 580 462	61 +	2 549 505	2 547 513	57 +	2 445 956	2 453 905

closed-shell inner core and one, two, three, or seven out-of-shell electrons are particularly well suited to semiempirical specification. Here the lowest configuration possessing nonzero fine structure contains a single spectral term, and the separations between the levels of maximum and minimum J are prescribed (in the single-configuration intermediate-coupling picture) by $3\zeta/2$, where ζ is the spin-orbit energy. This is not the case for the four, five, and six out-of-shell electron configurations, and separations within and between the various spectral terms must be considered to extract ζ from the electrostatic energy contributions that also connect them.

Since each of the intervals given above corresponds to a physically interpretable quantity ζ, they can usefully be compared both along and among these sequences. Moreover, the isoelectronic data base for the Cu sequence is presently the most extensive in existence, and the spin-orbit interactions that occur within its closed-shell nickel-like core differ from those in the Zn, Ga, and Br sequences only by the presence of $n=4$ electrons.

III. EXPERIMENTAL DATA BASE

Data compilations that included detailed source references for the desired intervals in these four sequences have been published relatively recently,[3-6] and only those primary source references that have appeared subsequent to these compilations will be cited here. Primary source references not directly cited here can be found in Ref. 3 for Cu-like Ge-Mo, in Ref. 4 for Zn-like ions, in Ref. 5 for Ga-like Ga-Kr, and in Ref. 6 for Br-like ions. For the Zn sequence, not all of the source references cited in Ref. 4 are included in Table I. Here the measurements for $Z=40-42$ are questionable since they lie substantially off isoelectronic and isonuclear trends, and are currently the object of a reinvestigation.[14] The primary source references are extended for the Cu sequence by Refs. 8–10, for the Zn sequence by Refs. 11–13, and for the Ga sequence by Ref. 15. The observed fine-structure intervals are listed among the semiempirical predictions in the columns headed SE in Table I, and can be identified by the presence of a footnote to the primary or secondary source reference.

IV. DIRAC-FOCK COMPUTATIONS

Single-and multiple-configuration Dirac-Fock (MCDF) computations were performed for the lowest P states in the Cu, Zn, Ga, and Br isoelectronic sequences. The calculations were carried out by network using the National Magnetic Fusion Computer Center CRAY X-MP E computer, with supportive calculations using the NAS 6650 and VAX 765 computers at the University of Toledo. The code used was an improved version[16] of the program MCDF developed by Grant and co-workers.[17] Computations were made using a number of different options in the code and for various configuration inclusions, and were selected on the basis of agreement with experimental observations in the region of moderate to high Z. Perturbative corrections were included to account for the finite size of the nucleus and the Breit interaction, as well as vacuum polarization, electron self-energy, and other quantum electrodynamic effects. The results, selected as described below, are presented in Table I in the columns labeled DF.

Although the Cu (Ref. 18) and Zn (Ref. 19) sequences have been studied previously by MCDF methods for selected values of Z, these calculations were repeated here so that the results could be compared for all values of Z using the same identical code. For the Cu and Zn sequences, the results quoted in Table I are single-configuration $4p$ and $4s4p$ calculations. In the case of the Ga sequence the single-configuration $4s^24p$ calculations agreed well with experiment at low Z, but inclusion of $4p^3$ and $4s4p^2$ seemed to improve the agreement at higher Z (at the expense of lower-Z agreement). Thus for the Ga sequence the results presented in Table I included these three configurations and utilized the MCDF-EAL (extended average level) option of the program.[17] The role of the inclusion of configurations of both parities for the homologous B isoelectronic sequence is discussed in Ref. 20. For the B sequence, Huang et al.[21] observed that an MCDF calculation of the fine structure can acquire a nonphysical gross structure residue, if inconsistent choices of configurations are used that lead to different nonrelativistic correlation energies for the two fine-structure levels. It has been asserted by Das et al.[20] that this problem is an artifact of the MCDF-OL (optimized level) approach, and should not affect the MCDF-EAL calculations performed here. For the Br sequence, the single-configuration $4s^24p^5$ calculations also agreed well at low Z, but the inclusion of the $4s4p^6$ configuration improved the agreement at higher Z (again, at the expense of low-Z agreement) and the two-configuration MCDF-EAL computation is reported in Table I. The role of the inclusion of configurations of both parities has been discussed for the homologous F isoelectronic sequence in Ref. 22.

V. SCREENING PARAMETER FORMULATION

In comprehensive studies of fine-structure splittings in a wide variety of multiple-electron systems,[1] it has been found that the isoelectronic behavior of the spin-orbit energy ζ can usually be mapped into a linearly varying parameter through a data reduction using a screened hydrogenic expression. The procedure introduces no free parameters, and merely converts the fine-structure splitting into the effective central charge that would yield the same splitting in a single-electron atom. Despite its simplicity, the isoelectronic behavior of the resulting screening parameter is usually very regular and slowly varying, which permits high-precision interpolative and extrapolative predictions and manifestly reveals misclassifications. The procedure consists of converting the measured intervals $3\zeta/2$ into equivalent screening parameters through a Sommerfeld expansion of the screened Dirac energy, given for a $4p$ term by

$$3\zeta/2 = R\alpha^2(Z-S)^4$$

$$\times \left[1 + \sum_i C_i \alpha^{2i}(Z-S)^{2i} + \cdots \right]\bigg/128 . \quad (1)$$

Here R is the reduced-mass-corrected Rydberg constant,

α is the fine-structure constant, Z is the nuclear charge, and S denotes the empirical screening parameter that Eq. (1) serves to define. To adequately describe the Dirac energy to very high Z, it is necessary to include a substantial number of higher-order terms in the Sommerfeld expansion (the C_i coefficients are tabulated to 18th order in αZ in Ref. 23). It has been noted empirically that the isoelectronic regularity of S is improved if detailed quantum electrodynamic corrections (functionally formulated in Ref. 24) are included in Eq. (1) (represented by the ellipsis), with the Z dependences also replaced by $Z-S$.

The empirical linearization of the data is accomplished by plotting the screening parameter S versus the reciprocal screened charge $1/(Z-S)$. If a few ions near the neutral end of the sequence (where mixing with excited core configurations becomes significant) are excluded, this plot is usually very nearly linear for over 20 stages of ionization.[1,3-6] In such cases, the system can be precisely described by the two parameters a and b, obtained by their weighted least-squares adjustment to the reduced data in the fitting equation

$$S = a + b/(Z-S) . \tag{2}$$

As will be shown below, this linearity seems to break down abruptly at about 30 stages of ionization. Classical models have been considered[7] that suggest a relativistic restructuring of the inner core occurs in the vicinity $Z=60$, which could explain this behavior. As a test of the conjecture that the break in slope is a result of effects within the inner core, we have tested a model in which the screening parameters for the various charge states of a given atom are decomposed into two parts, corresponding to the closed- and open-shell portions of the core:

$$S = S_0 + \Delta S . \tag{3}$$

For the sequences considered here, S_0 is associated with the closed nickel-like core and is assumed to be the same for all four sequences, and ΔS is associated with the passive $n=4$ electrons, is zero for the Cu sequence, and differs among the Zn, Ga, and Br sequences.

VI. RESULTS

The isoelectronic behavior of both the data base and the Dirac-Fock calculations is displayed through a reduction to S, plotted versus $1/(Z-S)$, in Fig. 1. Circles indicate the measured data, solid lines denote the calculations, and dashed lines trace the charge states of Br $(Z=35)$ and Nd $(Z=60)$ through the various sequences. Several trends can be noted. There is a definite tendency for the Dirac-Fock calculations to overestimate the screening (underestimate the splitting) for the Cu, Zn, and Ga sequences, and this tendency decreases with increasing Z. For the Br sequence (which is an inverted structure arising from hole rather than electron states), the Dirac-Fock calculations underestimate the screening, and this also decreases with increasing Z. In the region between $Z=35$ and $Z=60$ the experimental points form nearly straight lines on this plot, although the Dirac-Fock calculations contain small curvatures. For $Z>60$, the theoretical values for S drop sharply for all four sequences, as do the experimental
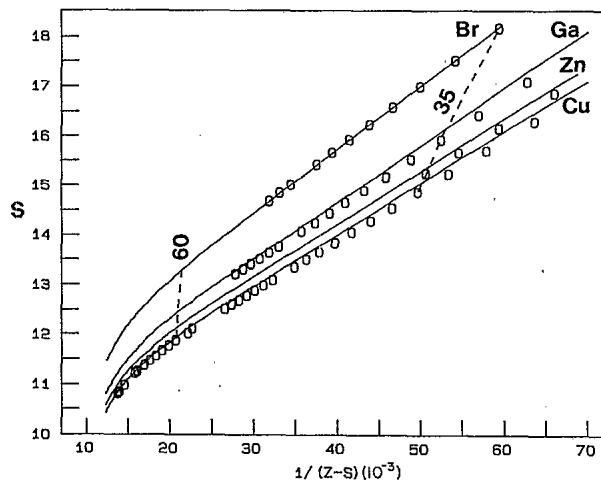

FIG. 1. Fine-structure separations for the Cu, Zn, Ga, and Br sequences, reduced to a screening parameter plot of S vs $1/(Z-S)$ using Eq. (1). The circles denote experimental measurements, the solid lines trace the Dirac-Fock calculations, and the dashed lines connect the ions of Br $(Z=35)$ and of Nd $(Z=60)$ across the sequences.

values for the Cu sequence.

Although data extending to and beyond $Z=60$ exist only for the Cu sequence, the theoretical calculations for all four sequences are very similar in shape (although displaced from each other) in the region $Z>60$. If the downturn in S beyond $Z=60$ has its origin deep within the inner core, then the Cu sequence, which has only inner-core screening, should specify this behavior for all four sequences considered here. To test this, the screening parameter S_0 for the Cu sequence was subtracted from the corresponding quantity S for each of the other three
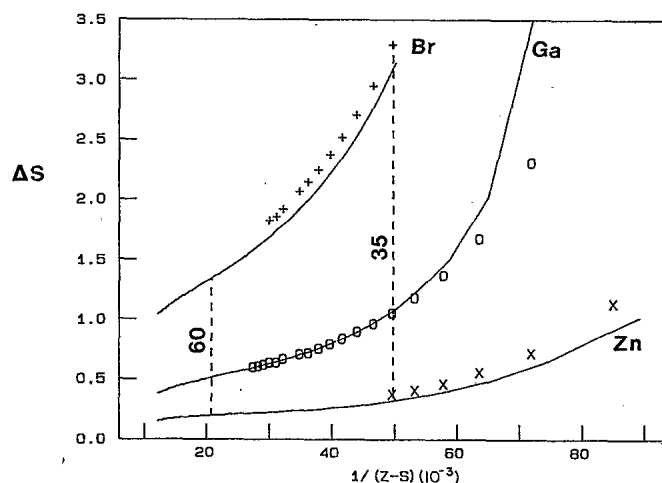

FIG. 2. Subtracted element-by-element differences between the screening parameter in either the Zn, Ga, or Br sequence and the corresponding quantity in the Cu sequence. The experimental values are denoted by $\times$, Zn sequence; O, Ga sequence; and $+$, Br sequence. The solid lines trace the Dirac-Fock calculations, and the dashed lines connect ions of Br $(Z=35)$ and Nd $(Z=60)$ across the sequences.

sequences to form ΔS in Eq. (3), using both the experimental and the theoretical values. The results are presented in Fig. 2, plotted versus the reciprocal screened charge for the Cu sequence. Although these plots are not linear, there are useful features. The drop off beyond $Z=60$ is no longer present, indicating that no part of it arises from the screening by $n=4$ electrons, and suggesting that a reliable extrapolation can be made to $Z=92$. Further, the experimental and theoretical ΔS curves are very similar in shape, and can be brought into almost exact agreement if the Dirac-Fock differences are multiplied by the empirical factors 1.25 for the Zn sequence, 1.03 for the Ga sequence, and 1.08 for the Br sequence.

The semiempirical interpolations and extrapolations presented in the columns labeled SE in Table I were obtained by exploitation of features displayed in Figs. 1 and 2. For $Z \leq 56$, the linearity of the plot in Fig. 1 was utilized, and a linear fit to Eq. (2) was used to interpolate and extrapolate. For $57 \leq Z \leq 92$, two types of corrections were necessary. First, S_0 as obtained from the Cu data was interpolated using a quadratic polynomial in the quantity $1/(Z-S_0)$, and extrapolated similarly from $Z=83$ to $Z=92$ using the theoretical value at $Z=92$. The predicted values for ΔS were computed from the theoretical differences, corrected by the factors 1.25, 1.03, and 1.08 as described above, and added to the values for S_0. The values of S so obtained were used in Eq. (1) to compute the appropriate fine structures for each sequence. Except for cases where experimental values exist, these semiempirical values are reported in Table I in the columns labeled SE.

VII. CONCLUSIONS

The methods presented here permit reliable extrapolations of fine-structure splittings in the Zn, Ga, and Br isoelectronic sequences through more than 40 stages of ionization. The accuracy of these predictions is subject to experimental verification, but the trends in Figs. 1 and 2 suggest that this may approach the precision of the available measurements in the Cu sequence. The method should be applicable to extrapolative predictions in other similar sets of isoelectronic sequences, and the separability of the closed- and open-shell screening effects revealed here suggests possible improvements in the *ab initio* formulation.

ACKNOWLEDGMENTS

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