Nuclear Instruments and Methods in Physics Research B31 (1988) 146–152
North-Holland, Amsterdam

SEMIEMPIRICAL FORMULATIONS OF SPECTROSCOPIC DATA AND CALCULATIONS

Lorenzo J. CURTIS

Department of Physics and Astronomy, University of Toledo, Toledo OH 43606, USA

The high precision required for spectroscopic classification work has traditionally been achieved through predictive systematizations of observed data and computations by ab initio theoretical methods. Recent advances in the existing experimental data base and in supercomputing capabilities now permit these methods to be extended to new regimes. Through combined parametric expositions of data and computations, large scale trends in isoelectronic, isoionic, isonuclear, and homologous sequences, Rydberg series, etc., have emerged that permit predictions which are more reliable than could be achieved by either ab initio or semiempirical methods separately. Applications of this approach to term splittings, which are particularly sensitive to the inner portion of the wave function, are presented.

1. Introduction

Recent technical developments have placed great computational capabilities at the disposal of atomic spectroscopists, and altered some of the traditional boundaries between experimental and theoretical research. The availability of large scale atomic structure computer codes that are flexible, transportable, and user friendly, coupled with convenient network access to supercomputer facilities has made possible new approaches to atomic research. It is now possible for a researcher to perform ab initio calculations that are custom tailored to optimize the predictive accuracy of a specific interaction being studied experimentally. However, experimental spectroscopic accuracies are very demanding (often to parts in 10^6 or better), and exceed the capabilities of even the most sophisticated ab initio methods when applied to complex atomic systems. Semiempirical systematization methods [1] provide predictions of spectroscopic precision, but require the existence of a substantial base of observed data. The use of laser and tokamak produced plasma, fast ion beam, and astrophysical light sources has greatly expanded the available data base, and it is now possible to select subsets within large blocks of atomic data so as to control the relative strengths of the various interactions within the data sample, and thus probe a specific property. However, for the study of systems for which no adequate data base presently exists, ab initio computations are the only predictive source. We have therefore sought to develop systematic formulations which conjoin observations and computations on a very large scale, to utilize the predictive advantages of both approaches.

In high precision studies, it is usually helpful to reformulate the description in terms of quantities that amplify subtle differences, and semiempirical trends are usually displayed in a parametrically reduced mapping space. This can be achieved, e.g. by forcing many-body interactions to reside in an empirical parameter embedded in a simple independent particle model (as in quantum defect and screening parameter formulations). A suitably parametrized spectral feature can then be examined along an isoelectronic, isonuclear, or homologous sequence, or over a Rydberg series. The evolution of the feature while a single quantity (such as nuclear charge, degree of ionization, number of valence electrons, principal or angular momentum quantum number, etc) is progressively modified can reveal sensitive and subtle regularities, or sudden departures from regularity, that would otherwise go unnoticed. This approach makes possible new evaluation criteria based on agreement between large scale experimental and theoretical trends, rather than isolated specific cases. For example, a theoretical model that predicts an erroneous isoelectronic trend is likely to cross the experimental data at some degree of ionicity yielding local apparent agreement, whereas an alternative theoretical model that reproduces the isoelectronic trend with a constant discrepancy agrees nowhere, but can be empirically corrected to yield highly precise predictions.

Confrontations between empirical trends and ab initio calculations in complex atoms are particularly interesting when quantities sensitive to the inner core portion of the wave function are considered. Spectroscopic measurements of the small energy separations between the individual levels within a spectral term are often of much higher precision than those of gross energies measured relative to the ground state or the ionization limit. Conversely, most theoretical approaches seek wave functions that optimize the prediction of the gross energy (arising primarily from the $1/r$ central Coulomb

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interaction), and treat interactions that fall off more steeply with r perturbatively. Consequently, some of the most precisely measured spectroscopic data in highly ionized atomic systems are very sensitive to the charge distribution of the inner core region, where standard theoretical wave functions are the least well specified. It is therefore not surprising that systematic studies of term splittings (magnetic fine structure and electrostatic direct and exchange electron-electron energies in the LS picture) show regularities, linearities, and discontinuities that are not predicted by ab initio theories.

There is additional motivation for the study of these term splittings in low lying configurations in highly ionized atoms, because M1 and E2 transitions within and among these levels increase sharply with nuclear charge, are isolated in wavelength, and provide a useful diagnostic tool for the analysis of high temperature astrophysical and laboratory plasmas.

A number of expositions will be presented below that systematically juxtapose observed fine structure data with ab initio calculations so as to elucidate the dynamics of the inner core, and provide predictions that are more reliable than could be achieved by either ab initio or semiempirical methods separately. Data are taken from published or soon to be published sources, and source references or bibliographic compilations are provided. Theoretical calculations were performed for all cases considered here using the multiconfiguration Dirac–Fock code (MCDF) of Grant and coworkers [2, 3], and were carried out via network on the Cray X-MP machine at the National MFE Computer Center in Livermore CA.

2. Screening parameter reductions

Quantities sensitive to the inner portion of the wave function are often well described by a screening parameter formulation, which corresponds to a charge-scaling of the radial coordinate of a hydrogenlike wave function. (The quantum defect approach, which corresponds to a phase shift in the radial coordinate of a hydrogenic wave function, is well suited to the computation of quantities sensitive to the external portion of the wave function, but describes the inner core poorly.) The basic screening parameter approach has long been applied to spectroscopic data [1], but modern developments have made it possible to generalize and extend its usage. The approach involves a one-to-one remapping of the measured intervals into equivalent parameters that characterize the deviation of a complex atom from a corresponding single electron system. If the number of free parameters selected for the mapping equals the number of independent intervals there is no loss of generality or imposition of modeling assumptions, and the only effect of the mapping is to provide quantities that are more regular, slowly varying, and phenomenologically revealing than the raw measurements.

Although simple, the mapping proceeds through several conceptual levels. First the measured intervals are reduced to a theoretically motivated set of equivalent quantities that are likely to be dominated by a single interaction with a specific charge scaling (eg, spin–orbit energy, direct or exchange Slater energy, etc). Second, these quantities are replaced by the effective central charge that would produce the same value in one electron system. Third, the screening parameter S (the difference between the true nuclear charge Z and the effective central charge Z_s) is studied isoelectronically, and has been found to be highly regular as a function of the reciprocal effective central charge, often well represented by the linear relationship

$$S = a + b/(Z - S). \tag{1}$$

Finally, homologous, isonuclear, and Rydberg comparisons can be made among the isolectronic systematizations, and multidimensional trends and regularities identified. Although ab initio theory neither explains nor generally predicts these regularities, empirical successes justify their use on utilitarian grounds.

3. Rydberg series comparisons for fine structure splittings in the Cu sequence

The empirical expression used here to parametrically reduce fine structure separations utilized the best available expression for the fine structure in a hydrogenlike atom, and included a high order Sommerfeld expansion [4] of the Dirac energy, an analytic representation [5] of quantum electrodynamic electronic self-energy corrections, corrections for nuclear motion, including higher order corrections for the relativistic nonseparability of the reduced mass [6–10], and an analytic expression approximating corrections for nuclear penetration [11]. The effects of these various inclusions will be discussed in more detail below. The parametric quantity S for an atom of nuclear charge Z is the amount by which the central charge of a corresponding hydrogenlike system must be diminished to match the measured fine structure.

An example of the application of the screening parameter formulation to the fine structure of the $n\mathrm{p}\ ^2\mathrm{P}$ and $n\mathrm{d}\ ^2\mathrm{D}$ states of the Cu isoelectronic sequence is shown in fig. 1. The symbols represent the observed data [12–15] for $n = 4$–7, and the solid lines are MCDF calculations (where available, the MCDF calculations of Cheng and Kim [16] and Cheng and Wagner [11] were examined and found to be consistent with our own calculations). Dashed lines trace specific charge states in the isoelectronic sequence among the Rydberg series. These Cu data comprise the most comprehensive iso-

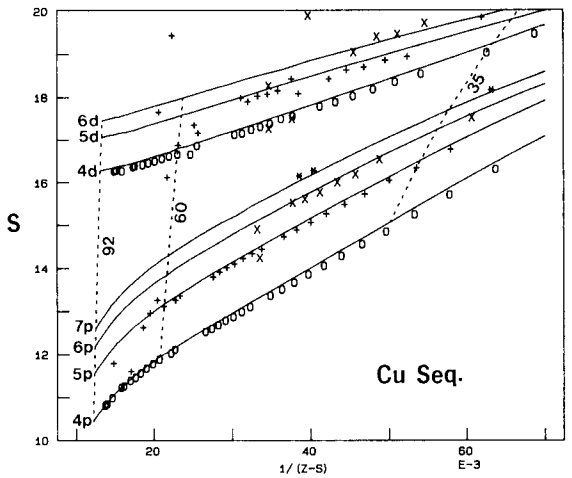

Fig. 1. Fine structure separations followed both isoelectronically and along Rydberg series for the np and nd terms in the Cu sequence, reduced to a plot of the effective screening parameter S vs the reciprocal screened charge $1/(Z-S)$. Measured data are designated for the various principal quantum numbers by the symbols: (○) $n=4$; (+) $n=5$; (×) $n=6$; and (*) $n=7$. The solid curves indicate MCDF calculations, and dashed curves trace the elements Br ($Z=35$), Nd ($Z=60$) and U ($Z=92$) along the Rydberg series.

electronic data base presently available, and extend through as many 55 stages of ionization. (Comparison of fig. 1 with a similar plot presented at the 1980 BFS Conference [17] indicates the large increase in the available data base over that time.)

Although the agreement between theory and experiment is superficially good (to within a few percent) and seems to improve with increasing Z, there is a clear tendency for the theoretical results to overestimate the screening at low Z, and it is not clear whether the apparent agreement at high Z indicates convergence or only a crossing of the trends. Although it is not clearly evident from the plot, least squares fits to these quantities reveal that the observed data have a degree of linearity on this plot that is not present in the MCDF calculations. When studied as a function of the reciprocal screened charge, the screening parameters for the observed data exhibit (to within experimental uncertainties, which are small) a linear dependence for the ^{2}D states for all Z and for the ^{2}P states for $Z \leq 60$ (or, equivalently, up to ionization state +31). For $Z > 60$ there is a sudden departure from linearity. If magnified, this discontinuity is quite sharp, and suggests a possible redistribution of charge in the inner core. The MCDF calculations exhibit a gentle curvature with no linear region and no discontinuity in slope. Semiclassical models suggest a number of mechanisms [18] that could produce such a charge redistribution within the core, but no satisfactory theoretical explanation presently exists.

As described above, many small corrections have been included in the hydrogenlike fitting function. The motivation for this was empirical, based on the finding that the inclusion of additional corrections led to an improvement of the linearity of the plot in the $Z < 60$ region. This suggests the interesting possibility that the linearity criterion (albeit ad hoc) might provide insights into the validity of small corrections to ab initio theory. For example, the model adopted here uses Lamb shift corrections that are screened in the same way as the fine structure. Unscreened Lamb shifts have sometimes been used in ab initio calculations for complex atoms, but Johnson, Blundell and Sapirstein [19] have recently shown that use of the unscreened Lamb shift in the Li iselectronic sequence introduces substantial discrepancies with experiment. The effect of the Lamb shift on the $p_{1/2}$ states is particularly interesting. The hydrogenlike $2p_{1/2}$ Lamb shift is negative for low Z, but changes sign at $Z = 50$ and exceeds that of the $2p_{3/2}$ for $Z > 88$ [20]. For higher n, extrapolations [5] indicate that the zero crossing occurs at lower Z and the $2p_{3/2}$ crossing occurs at higher Z. These crossings cause estimates of the isoelectronic variation of the Lamb shift to be very sensitive to the assumed screening. As another example, Cheng and Wagner [11] have recently used measurements [14] of the spectra of Cu-like and Zn-like ions of elements in the range $Z = 79$–92 to test quantum electrodynamic corrections, and found that corrections for the finite size of the nucleus are also necessary. We have used these results (supplemented by our own MCDF calculations over a wider range of Z) to develop an approximation formula for the dependence of the relative size of the nuclear penetration corrections to the 4p fine structure in the Cu sequence, expressed as a function of the empirical screened charge Z_s, and obtained the empirical relation

$$\frac{\text{nuclear penetration}}{\text{fs}} = -1.06\times10^{-6}\left[1-2.1(\alpha Z_s)^4\right]\exp(11.1\alpha Z_s). \quad (2)$$

Eq. (2) was then utilized in the semiempirical data reduction. Another consideration is the treatment of the relativistic nonseparability of the reduced mass, and its specific application to J-dependent fine structure. A diversity of approaches yielding different suggested corrections can be found in the published literature [e.g., 6–10] and the correct specification of mass dependent factors appears to be an open question that semiempirical studies can address.

A number of these questions have been examined in a study summarized in table 1, which tested the use of linearity as a criterion for the inclusion of various small

Table 1
Values for χ^2/degree-of-freedom obtained by fitting reduced experimental 4p fs splittings for the Cu sequence ($35 \leq Z \leq 56$) to eq. (1), using various models for QED and nuclear penetration corrections in the semiempirical data reduction. Weights were obtained from quoted experimental uncertainties, and there were 15 experimental points and 2 fitting parameters.

Quantum electrodynamic corrections	χ^2	
	Without nuclear penetration	With nuclear penetration
Anomalous moment ($g-2$) only	0.856	0.837
Unscreened hydrogenlike Lamb shift	0.937	0.915
Hydrogenlike Lamb shift, same screening as fs	0.729	0.714

interaction terms in the semiempirical data reduction. Using measured data for the 4p fine structure of the Cu isoelectronic sequence for 15 points in the region $35 \leq Z \leq 56$, weighted least squares adjustments of the parameters a and b in eq. (1) were made to screening parameter reductions using several models for QED and nuclear penetration corrections. Weights were obtained from the quoted experimental uncertainties. QED corrections were made in three alternative ways: one included only the anomalous magnetic moment correction, $g-2$; a second included the full hydrogenlike Lamb shift with no screening; and a third included the full hydrogenlike Lamb shift but used the same screening as the fine structure. Each fit was also performed with and without the nuclear penetration corrections of eq. (2). Table 1 presents the value of χ^2 per degree-of-freedom. It indicates that, compared to the $g-2$ model, inclusion of the fine-structure-screened Lamb shift improved the fit, whereas the inclusion of the unscreened Lamb shift worsened it. Inclusion of the nuclear penetration corrections improved the fits slightly in all cases.

Since the validity of eq. (1) is grounded only on empirical evidence, it would be premature to draw conclusions from table 1 concerning ab initio theory, but this does indicate that semiempirical interpolations can be sharpened by improving the hydrogenlike reduction formula, and it can be presumed that this will also be true for states of higher n. For the linear regions, the fits to the observed data are sufficiently well determined to permit extrapolations of the slope and intercept to higher members of the p and d Rydberg series, and comprehensive predictions were made earlier [15] that have been confirmed for $Z \leq 60$ by subsequent measurements. For the region $Z > 60$, we have also sought ways to combine the theoretical calculations with the Cu data to make predictions in other isoelectronic sequences, which are described in the next section.

4. Isonuclear comparisons of fine structures of $ns^x np^y$ P terms

The Cu sequence is basically a single electron spectrum, and is expected to be reasonably well described by theoretical calculations. We have therefore addressed the question of whether the extensive measurements made for and the regularities revealed in the Cu sequence can be exploited to yield precise predictions in more complex and less reliably calculable systems. We have sought to utilize the data for the 4p fine structure in the Cu sequence to specify the fine structures of the lowest lying P states in the Zn, Ga, Ge, Se and Br sequences. The dominant configurations for these systems consist of a closed $n=3$ shell nickel core, with various numbers of additional 4s and 4p valence electrons. Fig. 2 shows a combined screening parameter study of the fine structures of the lowest P terms in the Cu (4p), Zn (4s4p), Ga($4s^2 4p$), Ge ($4s^2 4p^2$), Se ($4s^2 4p^4$) and Br ($4s^2 4p^5$) isoelectronic sequences, where the dominant assumed configurations are given in parentheses. (The As sequence with its half-filled 4p shell is of less practical use and was omitted.) The various intervals were rewritten as (or, for the Ge and Se sequences, reduced to) spin–orbit parameters.

The circles represent experimental observations (Cu [12–15], Zn [21–24], Ga [25,26], Ge[27], Se [27–29], Br [30]), the solid curves denote our MCDF calculations, and the dashed lines trace isonuclear comparisons. The

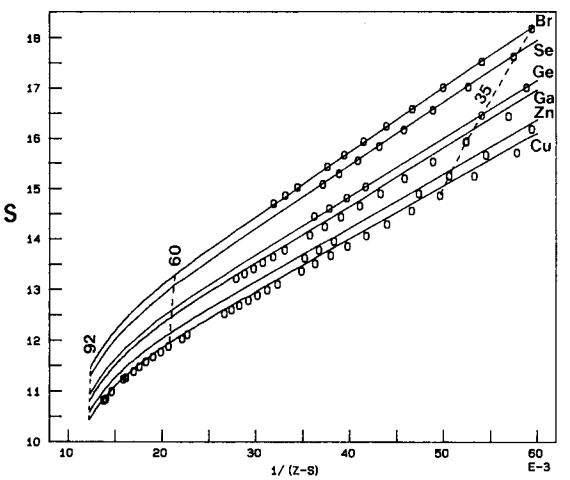

Fig. 2. Fine structure separations followed along both isoelectronic and isonuclear sequences for the $4s^x 4p^y\ ^{1,3}P$ terms in the Cu, Zn, Ga, Ge, Se and Br sequences, reduced to a plot of the screening parameter S versus the reciprocal screened charge $1/(Z-S)$. The circles denote experimental measurements, the solid lines trace the MCDF calculations, and the dashed lines connect the isonuclear ions Cl ($Z=17$), Nd ($Z=60$) and U ($Z=92$) across the sequences.

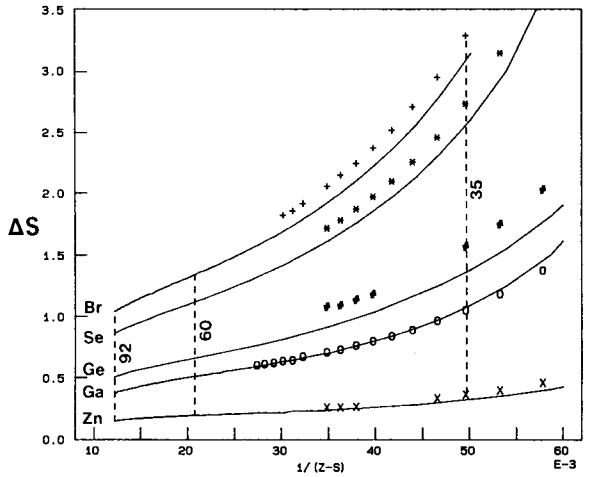

Fig. 3. Subtracted element-by-element differences between the screening parameter in either the Zn, Ga, Ge, Se or Br sequence and the corresponding quantity in the Cu sequence. The experimental values are denoted by : (×) Zn sequence; (○) Ga sequence; (#) Ge sequence; (*) Se sequence, and (+) Br sequence. The solid lines trace the MCDF calculations, and the dashed lines connect isonuclear ions of Cl ($Z = 17$), Nd ($Z = 60$) and U ($Z = 92$) across the sequences.

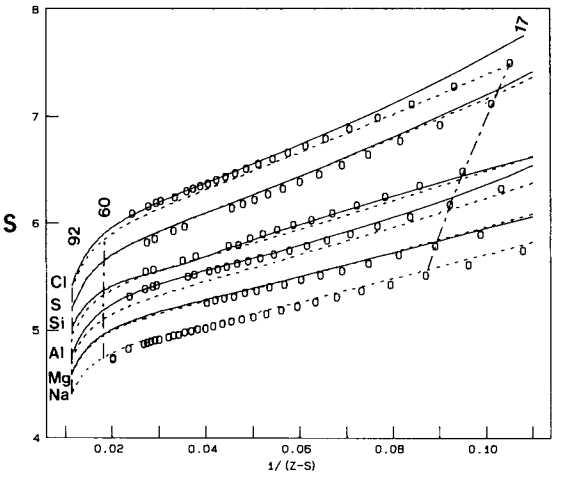

Fig. 4. Fine structure separations followed along both isoelectronic and isonuclear sequences for the $3s^x3p^y\ ^{1,3}P$ terms in the Na, Mg, Al, Si, S and Cl sequences, reduced to plot of the screening parameter S vs the reciprocal screened charge $1/(Z - S)$. The circles denote experimental measurements, the solid lines trace the MCDF calculations, and the dashed lines connect the isonuclear ions of Cl ($Z = 17$), Nd ($Z = 60$) and U ($Z = 92$) across the sequences.

tendency for the MCDF calculations to overestimate the screening is clear for the Cu, Zn and Ga sequences, but there are indications of possible crossings of the theoretical and experimental curves for the Ge, Se, and Br sequences. As can be seen from the plot, the theoretical calculations for all six sequences exhibit a similar downturn in this space for high Z. Since data for $Z > 60$ exist only for the Cu sequence, attempts were made to utilize the Cu data to make predictions for the other five sequences. (Fig. 2 extends an earlier presentation in ref. [31] to include the Ge and Se sequences.)

Fig. 3 presents a plot of the isonuclear difference between the screening parameters for each of the other five sequences and those of the Cu sequence, plotted versus the reciprocal screened charge for the Cu sequence. Although the curves are not linear on this plot, the MCDF results do not show any discontinuity in slope at $Z = 60$. This suggests that the screening parameter for these sequences can be decomposed into a dominant component arising from the closed $n = 3$ core and a smaller component arising from the out-of-shell $n = 4$ electrons. In addition, the observed values for Zn, Ga, Ge, Se and Br indicate that the MCDF calculations tend to underestimate this difference by an amount that is roughly constant for each sequence, permitting them to be empirically corrected. Thus the core component of S can be accurately deduced from measurements in the Cu sequence and the out-of shell component can be theoretically computed from isonuclear differences.

This approach should be applicable to other homologous sequences provided a sufficient base of measured data exists. Figs. 4 and 5 present sets of screening parameter and differential screening plots (homologous to figs. 2 and 3) for the the Na, Mg, Al, Si, S and Cl sequences, which have a filled $n = 2$ Ne-like core. The

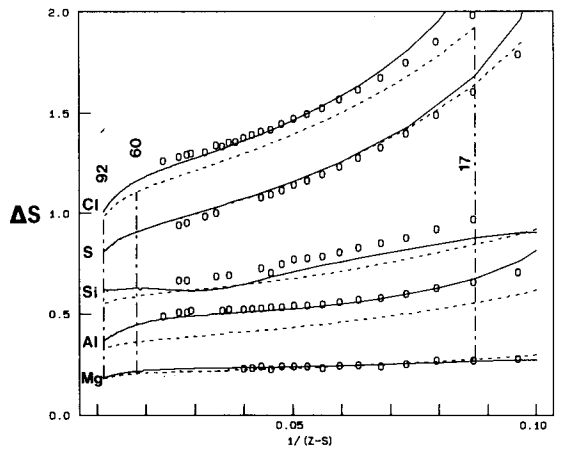

Fig. 5. Subtracted element-by-element differences between the screening parameter in either the Mg, Al, Si, S or Cl sequence and the corresponding quantity in the Na sequence. Circles denote experimental values, dashed lines trace the SCDF calculations, solid lines trace the MCDF calculations, and dot–dashed lines connect the isonuclear ions Br ($Z = 35$), Nd ($Z = 60$) and U ($Z = 92$) across the sequences.

data base for the Na sequence [32–34] benefits from measurements for its highly ionized members recently made by Reader et al [34]. Recent data source compilations are available for the Mg [35], Al [36], and Cl [36] sequences, and an earlier source compilation [37] is complemented by recent tokamak observations [38–40] for the Si and S sequences.

The effect of configuration interaction on these ab initio calculations is shown here, with single configuration computations (SCDF) indicated by dotted lines and the MCDF computations indicated by solid lines. The MCDF results appear to converge toward (or cross) the experimental trend at higher Z, but are inferior to the SCDF results at low Z. This is clearly a result of the well known "spillover of gross structure" that can occur when a code treats configuration interaction in a slightly different manner for the individual J states [41]. Although the effect is smaller when (as suggested by Hata, Grant and Das [42,43]) the EAL option of the MCDF program is used rather than the OL or EOL options, this is very sensitive to the configurations included, and indicates ambiguities in the MCDF prediction which can be reduced by comparison with experiment on this plot. Another possibility for reducing the discrepancies between theory and experiment revealed by this plot would be the inclusion of the Breit interaction within the self-consistent loop (rather than as a perturbation) in the MCDF calculation. Various workers have tested the effect of this computationally costly modification on the gross structure, and in some instances noticeable shifts in the predicted levels have occurred [44]. The exposition of the fine structure on this sensitive plot would provide an excellent test for this type of calculation.

Fig. 4 indicates that there is again a high Z downturn in the theoretical curves on this plot. However, experimental data are not yet available for sufficiently high Z to determine whether a discontinuity also occurs in these sequences at either $Z = 60$ or at ionization stage $+31$, corresponding to that observed in the Cu sequence. Fig. 5 shows that the high Z downturn is largely contained in the Na computations, and only a small effect appears in the difference between the individual MCDF computed screening parameters and the corresponding values for Na.

For the $nsnp$ configurations (in, eg, Mg, Zn, and Cd sequences), the position of the $J = 1$ component also depends upon the exchange Slater energy G_1. This quantity can be reduced to a screening parameter representation by a similar procedure to that described above, and also has been found to exhibit linear behavior for S as a function of $1/(Z - S)$ [45]. For the ns^2np^2 and the ns^2np^4 configurations (in e.g., the Si, Ge, In, and the S, Se, I sequences), the fine structure also involves the direct Slater energy F_2, which can also be treated in terms of a screening parametrization [1].

5. Conclusions

Through the combined use of ab initio theoretical computations and the semiempirical systematization of measured data, the use of highly precise predictive methods developed to describe term splittings in data-rich systems can be extended into regimes in which little or no data yet exist. In addition, these systematic studies of fine structure in highly ionized complex atoms can provide information on the inner regions of the core where few screening electrons are interposed between the deeply penetrating active electron and the nucleus, and may therefore yield information similar to that obtained in heavy atoms stripped down to one or two electrons. Although the theoretical specification of a highly stripped system is cleaner than that of a deeply penetrating orbital in a partially stripped system, the ease of production and spectroscopic precision attainable with the latter offers promise for the study of certain types of interactions that become important only at high Z.

I am grateful to Professors Bengt Edlén, David Ellis, Indrek Martinson, and to Roger Haar for valuable suggestions, and to Drs. Victor Kaufman, Ulf Litzén, Joseph Reader and Jack Sugar for providing access to new measurements prior to publication. The work was supported by the US Department of Energy, Division of Chemical Sciences, Office of Basic Energy Sciences, under contract number DE AS05 80ER10676.

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