Atomic oscillator-strength distributions in spectral series of the lithium isoelectronic sequence*

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We describe a new type of analysis yielding the oscillator-strength distributions in several spectral series throughout the lithium isoelectronic sequence. Individual oscillator strengths have been critically evaluated and tied together by requiring that they fulfill simultaneously four basic spectroscopic constraints: (a) regularities for individual transitions along the isoelectronic sequence, (b) regularities for the transitions of a spectral series, (c) compliance with the requirement of continuity across the spectral series limit, and (d) adherence to f sum rules. With only slight modifications, the best available data fulfill closely all four requirements. The final set of f-value data—which are tabulated and partly presented in illustrations—possess, therefore, a very high degree of internal consistency and reliability. Relativistic corrections for very highly charged Li-like ions are also considered.

I. INTRODUCTION

The body of atomic oscillator strengths (f values) for lighter elements has in recent years increased to a level where searches for interrelations of data have become possible and where the data may thus be tested with respect to their fit into predicted regularities. Several kinds of systematic trends have been derived from general principles of atomic theory,¹ and two trends have proved to be especially useful: (a) regularities for individual transitions along isoelectronic sequences, and (b) regularities for transitions of a spectral series.

Such trends have now been firmly established from available experimental and theoretical data for many important transitions of first-, second-, and third-row elements.²⁻⁴ However, these trends have remained as individual cases, unrelated to each other. Regularity studies do not have to end at this point; they may be carried further by interrelating individual systematic trends, so that more general patterns may emerge for the various spectral series along an isoelectronic sequence, and the oscillator-strength distributions in complete spectral series become apparent. For the lithium sequence, the oscillator-strength material has become so plentiful that such a generalized regularity study appeared to be feasible and promising. In this paper we want to describe our approach and present the important results.

We have combined in this investigation the familiar isoelectronic-sequence trends for given individual transitions with the spectral series regularities and with such general constraints on oscillator strengths as the Wigner-Kirkwood f sum rule and the condition of a smooth transition from the discrete line spectrum to the continuum. We could thus obtain for some prominent spectral series a complete picture of a smoothly varying oscillator-strength distribution along the isoelectronic sequence. The resultant set of data, of which the main parts are presented here, must be regarded as a highly accurate one since it not only adheres closely to the systematic trends but also fulfills simultaneously the two fundamental constraints mentioned above.

A comprehensive oscillator-strength study of the lithium sequence appears to be especially timely because of the current strong interest in the radiative properties of highly stripped, lithiumlike metal ions such as Fe^{23^+} . These are present as impurities in plasmas generated in Tokamak-type thermonuclear fusion research devices⁵ and appear to be a significant factor in the plasma energy balance by contributing strongly to the radiative energy losses.^{6,7}

II. METHOD

A. f-value regularities and other constraints on the data

To interrelate the individual f values, we have applied four principal constraints on the data, i.e., two types of f-value regularities discussed under (a) and (b) below, (c) the requirement of oscillator-strength continuity between the discrete and continuous spectrum, and (d) the Wigner-Kirkwood f sum rule. These "tools" will be reviewed here to the extent necessary for describing our approach.

(a) The f-value dependence on nuclear charge Z. A general result of conventional perturbation theory is that various atomic properties may be expressed as expansions in powers of the inverse nuclear charge Z. For the oscillator strength specifically, the perturbation expansion is

$$f = f_0 + f_1 / Z + f_2 / Z^2 + \cdots, \qquad (1)$$

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where f_0 is a hydrogenic quantity. For lithiumlike ions, with just one electron outside the closed Kshell, f_0 is simply the exactly known hydrogen fvalue.¹ Therefore the f value is known for the point where 1/Z becomes zero, which is very valuable for establishing the systematic trend towards the large-Z end of the sequence. However, it must be noted that Eq. (1) is the result of an entirely nonrelativistic treatment,¹ and relativistic effects are expected to show up for large Z, e.g., for highly stripped lithiumlike ions. Fortunately, some very recent calculations (to be discussed in Sec. IV) provide good estimates of the extent of the changes in the f values owing to relativistic effects. It will be seen that for most lines of Li-like ions relativistic corrections in the f values remain below 5% until Z reaches about 30, i.e., these effects indeed need be considered only for very highly stripped ions.

(b) Systematic trends of f values within a spectral series. Another type of regularity is found for the behavior of f values within a spectral series.¹ For the case of the hydrogen atom, it was established a long time ago⁸ that any given spectral series decreases with the inverse third power of the principal quantum number n', i.e., that

$$f(n, l - n', l \pm 1) \approx c(n')^{-3}$$
 (2)

This behavior sets in for fairly small principal quantum numbers, normally before the upperstate quantum number n' reaches ten. As is evident from the spectra of lithiumlike ions, the energies of the higher singly excited levels approach hydrogenic behavior rather quickly, so that the fvalues for the higher members of the lithium spectral series are expected to follow the above relation [Eq. (2)] closely, too. However, n'should be replaced by an effective quantum number which takes the quantum defect into account. Thus the essentially one-electron lithiumlike spectra are ideally suited for the application of spectral series regularities.

(c) Connection between the discrete spectrum and the series continuum, and the requirement of continuity at the ionization limit. The (absorption) f value for a discrete transition from a lower atomic state i to an upper state k is given (in atomic units) in terms of wave functions ψ_i and ψ_k and energies E_i and E_k as⁹

$$f_{ik} = \frac{2}{3}g_i^{-1}(E_k - E_i) \left| \langle \psi_i | \sum_{p=1}^N \tilde{\mathbf{r}}_p | \psi_k \rangle \right|^2 , \qquad (3)$$

where g denotes the statistical weight and $\sum_{p=1}^{N} \vec{r}_{p}$ is the sum of the position vectors of the N electrons of the atom. The discrete eigenvalues E_i

and E_k may assume any value below the ionization potential E_{I} . If one introduces the line strength

$$S(i, k) \equiv \left| \langle \psi_i | \sum_{p=1}^{N} \tilde{\mathbf{r}}_p | \psi_k \rangle \right|^2 , \qquad (4)$$

then Eq. (3) becomes

$$f_{ik} = \frac{2}{3}g_i^{-1}(E_k - E_i)S(i, k) .$$
 (5)

Analogously, a differential oscillator strength $df/d\epsilon$ taken with respect to the free electron energy ϵ has been introduced for ionizing transitions, i.e., for transitions from a bound state i into the continuum⁹:

$$\frac{df}{d\epsilon} = \frac{2}{3}g_i^{-1}(E_I + \epsilon - E_i)S(i, \epsilon) , \qquad (6)$$

with $S(i, \epsilon)$ defined as in Eq. (4). $E_I + \epsilon$ is the energy of the upper (i.e., ionized) state with respect to the ground state of the atom or, in general, the next lower ion; the free electron energy ϵ can assume any positive value.

The use of integer f values for the discrete spectrum and differential *f* values for the continuous spectrum becomes evident when directly observable quantities, such as spectral absorption or emission coefficients, are considered. For example, the absorption coefficient per atom (or the absorption cross section) α_{ν} at a given frequency ν is related to the differential f value $df/d\epsilon$ as follows¹⁰ (SI units):

$$\alpha_{\nu} = \frac{1}{4\pi\epsilon_0} \frac{\pi e^2 h}{m_e c} \frac{df}{d\epsilon} = \frac{1}{4\pi\epsilon_0} \frac{\pi e^2}{m_e c} \frac{df}{d\nu} . \tag{7}$$

For discrete transitions, α_{ν} peaks sharply around the line frequency ν_0 , so that Eq. (7) can be readily integrated to determine the total absorption coefficient (per atom):

$$A_{\nu_0} = \int_0^\infty \alpha_\nu \, d\nu = \frac{1}{4\pi\epsilon_0} \, \frac{\pi e^2 f}{m_e c} \,. \tag{8}$$

It is this quantity A_{ν_0} —multiplied with the lower-state atom density $N_{n,l}$ and the length of the absorbing layer-that is directly observable experimentally and may thus be applied to the determination of discrete f values. For the continuous spectrum, on the other hand, only the quantity $\alpha_{\nu} d\nu$, i.e., a band of continuum of width $d\nu$, can be directly observed. (Actually, in many instances a sum $\sum_{i} \alpha_{i,\nu} d\nu$ is observed. The summation arises because of the very extended spectral range of the continua, which often causes an overlap of different series continua from the various atomic states i. Also, the bremsstrahlung continuum has to be included in the summation.)

Although Eq. (8) holds true for the entire spec-

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trum, it thus becomes difficult, if not impossible, to carry out the integration of the absorption coefficient for a particular series continuum, and it is also of much less interest. One may therefore consider the discrete f values for the lines, where the integration is meaningful and desirable, as special cases of the differential f values for the continuum. Since Eqs. (5) and (6) may be formally unified into a more general relation which covers the entire energy range, there should be a smooth connection at the ionization limit, where the energy ranges of the two equations overlap.

Several authors have discussed the physical significance of a smooth transition from the discrete spectrum to the continuum. For example, in the early 1920's, Sommerfeld¹¹ explained this behavior in terms of the correspondence principle. He stated that physically there is no sharp distinction between a transition to a high quantum state and a transition to infinity (i.e., a photoionizing transition).

The motion of the electron in a bound state can be represented by a Fourier series, with the inclusion of more and more terms as the ionization limit is approached. Beyond this limit it is no longer sufficient to use a Fourier series; the Fourier integral is necessary for the representation of the motion.

Continuity of $df/d\epsilon$ across the ionization limit has, in fact, been shown to exist for hydrogen, for which exact wave functions are known (see, e.g., Marr and Creek¹²). Marr and Creek also reviewed the situation for the principal series of the alkalies and concluded that the assumption of continuity is indeed justified within the experimental accuracy.

Turning now to the task of connecting the discrete spectrum and the continuum, one must consider that in order to compare the f values for the lines with the differential oscillator strengths $df/d\epsilon$ for bound-free transitions, the discrete f values must also be given (or better, distributed) per unit energy range. For a discrete transition within a spectral series, the oscillator strength is a function of the effective principal quantum number n'_{eff} of the upper state $(n'_{eff} = n' - \mu_{n'})$, where $\mu_{n'}$ is the quantum defect^{9,13}). Since for any two adjacent members of the series $\Delta n'_{eff} \approx 1$, the f value may be considered to be distributed over a range of approximately $\Delta n'_{eff} = 1$ (for which there is a corresponding range of energies $\Delta \epsilon$). Thus to a small increment dn'_{eff} corresponds a portion df of the total oscillator strength f for the transition, or

$$df = f \, dn'_{\rm eff} \quad . \tag{9}$$

Integrating this expression, one obtains

$$f = \int df = \int_{\Delta \epsilon} \left(\frac{df}{d\epsilon} \right) d\epsilon = \int_{\Delta \epsilon} f\left(\frac{dn'_{\text{eff}}}{d\epsilon} \right) d\epsilon , \quad (10)$$

where ϵ is the energy (in rydberg units) of the upper state with respect to the appropriate ionization limit. For discrete transitions, $df/d\epsilon$ is therefore represented by the quantity $f(dn'_{\text{eff}}/d\epsilon)$. ϵ is given by

$$\epsilon = -(Z - N + 1)^2 / (n'_{\text{eff}})^2 = -Z_c^2 / (n'_{\text{eff}})^2 , \qquad (11)$$

where Z is the nuclear charge, N is the number of electrons before ionization (N=3 for the lithium isoelectronic sequence), and $Z_c \equiv Z - N + 1$ is the core charge. One obtains by differentiation

$$\frac{d\epsilon}{dn'_{\text{eff}}} = \frac{2Z_c^2}{(n'_{\text{eff}})^3}$$
(12)

and

$$\frac{df}{d\epsilon_{\text{discrete}}} = \frac{f \, d \, n_{\text{eff}}'}{d\epsilon} = \frac{(n_{\text{eff}}')^3 f}{2Z_c^2} \,. \tag{13}$$

[It should be noted here that Eq. (13) is strictly true only when the quantum defect is constant within a spectral series. However, for ions of the lithium sequence the quantum defect is essentially constant for high quantum numbers n', and it is in this region of the discrete spectrum that the concept of a differential oscillator strength is most meaningful.]

For a given spectral series, therefore, one plots (i) the quantity $(n'_{\rm eff})^3 f/(2Z_c^2)$ vs $\epsilon = -Z_c^2/(n'_{\rm eff})^2$ for the discrete transitions and (ii) $df/d\epsilon$ vs ϵ for the bound-free transitions, in order to obtain an overall picture of the oscillator-strength distribution.

(d) f sum rules. Of the various f sum rules, the partial sum rule by Wigner¹⁴ and Kirkwood¹⁴ appears to be the most useful one for our purposes since it is concerned only with the transitions of a given spectral series. The rule states that for one-electron systems the f sum of a spectral series $nl + l \pm 1$ (including its continuum and all downward transitions, as well as the virtual transitions into occupied states) is

$$\sum f = \frac{1}{3} \frac{(l+1)(2l+3)}{2l+1} \text{ for } n, l \to l+1 , \qquad (14)$$

or

$$\sum f = -\frac{1}{3} \frac{l(2l-1)}{2l+1} \quad \text{for } n, \ l \to l-1 \ . \tag{15}$$

For the most common series this rule yields the following numerical values:

$$\begin{split} ns - p + 1, \quad np - s + -\frac{1}{9}, \quad np - d + \frac{10}{9}, \\ nd - p + -\frac{2}{5}, \quad nd - f + \frac{7}{5}. \end{split}$$

For lithiumlike atomic systems, where only the

radiating electron is outside the closed $1s^2$ shell, the one-electron model is a very close approximation. Thus the sum rule is expected to be fulfilled to within a few percent.

B. Cross correlations

The above-described analytical tools have been applied to obtain a set of "best" data from the extensive numerical *f*-value material available for the lithium sequence. As the first step, the compiled material on the Li sequence has been critically evaluated, and the selected data have been used to determine empirically the 1/Z-dependence for the oscillator strengths of a large number of transitions. All selected f values have then been subjected—in this order—to (a) the isoelectronic sequence trends, (b) the spectral series regularities, (c) the condition of f-value continuity for the transition from lines to continuum, and (d) the partial f sum rule. A redundancy is generated by the application of the f sum rule insofar as the fsums may also be derived from the data after the first three constraints are applied. If the agreement obtained is not sufficiently close, the numerical data may be modified to obtain the best fit with the theoretical f sums.

For a number of spectral series and ions in the lithium sequence, the data were so incomplete that no redundancy could be achieved. In these cases the f sum rule was applied to provide the missing contribution (for example, the contribution of the continuum transitions).

C. Data assembly and evaluation

Results of studies on systematic trends for a number of prominent transitions of the lithium sequence have already been reported.² Additional, more recently published material has been studied here and has confirmed these regularities, except for slight modifications in some cases. Furthermore, some additional trends have been established.

Most of the *f*-value data for the discrete transitions have been obtained from quantum-mechanical calculations and lifetime experiments.¹⁵ The critical evaluation of the literature data has been carried out according to the scheme discussed in detail in Sec. C of the general introduction of Ref. 16. In essence, the critical factors in each method have been analyzed.

The most advanced theoretical data are from calculations based on multiconfigurational wave functions.¹⁷⁻²⁰ Other theoretical methods include the self-consistent field (Hartree-Fock) approximation,^{17,21-25} pseudopotential approaches,²⁶⁻³⁴ the nuclear charge expansion method^{18,19,35-37} (which is expected to be especially accurate for the higher-charged ions), and the well-known Coulomb approximation,³⁸ which is particularly suited for the essentially one-electron system encountered in the lithium sequence.

The majority of the experimental data has been obtained by the beam-foil technique in the form of lifetimes of excited atomic states.³⁹⁻⁷¹ Lifetimes for neutral lithium have also been measured with the delayed-coincidence technique⁷² and the method of zero-field level crossing⁷³ (also known as the Hanle-effect technique).

The results of anomalous dispersion (hook) measurements⁷⁴ have also been utilized for the determination of f values for the principal series of neutral lithium. But since the f values are only on a relative scale, they have been normalized to the f value calculated for the resonance transition by Weiss.¹⁷

Lifetime results often cannot be readily converted into *f*-value data. In SI units, the lifetime τ_k of an excited atomic state *k* is related to the *f* value f_{ik} for a transition $i \rightarrow k$ by²

$$\tau_{k} = \left(2\pi e^{2} (m_{e} c \epsilon_{0})^{-1} g_{k}^{-1} \sum_{i} (g_{i} \lambda_{ik}^{-2} f_{ik})\right)^{-1}, \quad (16)$$

where λ is the wavelength and the sum must be taken over all lower states *i* which radiatively combine with *k*. Thus if the sum contains two or more significant terms, lifetime data can be converted into *f* values only if the relative *f* values for these transitions — the "branching ratios"— are known from some other method.

For the continuous spectrum of neutral lithium, the measurement of the photoionization cross section σ by Hudson and Carter⁷⁵ is used to determine the differential oscillator-strength distribution as a function of the kinetic energy ϵ of the ejected electron. In SI units, the relation between σ and $df/d\epsilon$ is as follows¹²:

$$\frac{df}{d\epsilon} = 4\pi\epsilon_0 \frac{m_e c}{\pi e^2 h} \sigma , \qquad (17)$$

where ϵ is the kinetic energy in joules. For $df/d\epsilon$ in Ry⁻¹, one obtains numerically $df/d\epsilon = 0.124 \times 10^{22} \sigma (m^{-2} \text{ Ry}^{-1})$.

The data of McDowell and Chang,⁷⁶ who use Hartree-Fock wave functions which include polarization and correlation effects, have been used in the determination of the continuum contribution to the f sum for the principal series of BeII through Ne VIII.

To obtain the total continuum contribution, we had to resort to extrapolations beyond the cutoff energy for which the results are given in each case. We made use of the asymptotic dependence of $df/d\epsilon$ on E for high energies, where $df/d\epsilon$ falls off as $E^{-7/2}$ (see, for example, Fano and Cooper⁷⁷); $E = h\nu = E_I + \epsilon - E_i$ is the photon energy of the photoionizing transition, as defined in Eq. (6).

III. RESULTS

A. Principal series 2s-np and corresponding continuum

Throughout the lithium sequence, the *f*-value material for discrete transitions of the principal series 2s - n'p, as well as for the corresponding bound-free transitions, is so abundant that an extensive analysis of this series has been undertaken. For the first three discrete transitions of the series (2s-2p, 2s-3p, and 2s-4p), where a large amount of data is available for many ions. the 1/Z-dependence of the f value is presented graphically in Figs. 1-3. The curves presented are final results of this study, i.e., they have been subjected to all of the constraints discussed earlier. They thus reflect not only the initial critical evaluation-which includes such factors as possible cascading effects in the beam-foil data-but also the interrelation with the 2s-n'p series data for each ion and the connection with the continuous spectrum. Only minor adjustments in the f values were required to have the final data consistent within a few percent with all four constraints.

The quite drastic change from 2s-2p to 2s-3pand 2s-4p can be explained in terms of a complex interplay of factors such as polarization and relaxation, which have a very significant effect on the overlap of the wave functions of the initial and final states. For transitions to 4p and higher states of the series, however, these factors play a very limited role, and the form of the oscillator-strength distribution along the sequence for 2s-5p and higher transitions is practically indentical to that shown in Fig. 3 for the 2s-4p transition. The magnitude of the f value decreases with increasing principal quantum number of the upper state; this is a consequence of the decrease in the overlap of the wave functions, which is more than enough to offset the slight increase in the energy of the transition.

In order to examine the spectral series behavior for a particular ion, the *f* values for the discrete transitions were first converted to a smooth curve of $df/d\epsilon$ (i.e., to differential oscillator strengths) as a function of energy according to Eq. (13). To this was added the continuum distribution of $df/d\epsilon$, with the constraint of continuity at the boundary between discrete lines and

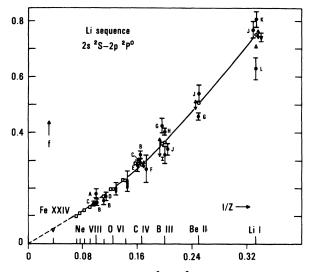


FIG. 1. f value for the $2s^2S-2p^2P^o$ multiplet of the Li sequence vs 1/Z. The data sources are (a) theory: \bigcirc Weiss,¹⁷ SCF with configuration interaction; \Box Onello et al.,¹⁸ Z expansion method; \triangle Hameed et al.,³³ SCF with core polarization; ∇ Chapman,²¹ SCF; \ddagger other theoretical methods combined^{22-24, 26-32, 38} (SCF, pseudopotential approximation, Coulomb approximation); (b) experiment: • beam-foil data from (A) Buchet et al.,⁵³ (B) Berkner et al.,⁴⁵ (C) Knystautas et al.,⁶³ (D) Barrette et al.,⁴³ (E) Martinson and Bickel,⁶⁵ (F) Poulizac et al.,⁷⁰ (G) Bromander,⁵⁰ (H) Roberts and Head,⁷¹ (I) Martinson et al.,⁶⁶ (J) Andersen et al.,³⁹ (K) Bickel et al.,⁴⁹ (L) Buchet et al.⁵⁴; combined beam foil results-for Nv: Berkner et al., 45 Bickel et al., 48 Desesquelles, 57 Berry et al.,⁴⁶ Barrette et al.,⁴³ Dufay et al.,⁵⁸ Buchet et al.,⁵⁵ Dumont,⁵⁹ Kernahan et al.⁶²; -for Ovi: Berkner et al.,⁴⁵ Martinson et al.,⁶⁴ Buchet et al.,⁵³ Pinnington et al.,⁶⁷ Kynstautas et al.⁶³; ∇ Hanle effect, Brog et al.⁷³ The error bars on the experimental points represent the authors' uncertainty estimates. To preserve clarity, experimental or theoretical results have been combined when they agree closely.

continuum. Figures 4 and 5 are illustrations of the 2s-p series for LiI and C IV, respectively. The energy values on the abscissa are in rydberg units, with the ionization energy of the 2s state as the point of origin. Evidently, for 2s-4p and the higher transitions, the distribution of oscillator strengths along the series follows a very regular pattern. While the shapes of the curves for Li I and C IV are guite different, the redistribution of oscillator strengths that occurs among the first few transitions of the 2s-n'pseries from the neutral atom to the ionized species takes place in an orderly, gradual fashion. For C IV and the more highly ionized members of the lithium sequence, the form of the oscillator strength distribution has become essentially "stabilized," and only a scaling of the magnitude of $df/d\epsilon$ takes place for successive ions.

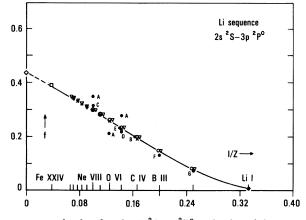


FIG. 2. f value for the $2s^2S-3p$ ² P^o multiplet of the Li sequence vs 1/Z. The data sources are (a) theory: \bigcirc Weiss, ¹⁷ SCF; \times Onello, ¹⁹ Z expansion method; \bigtriangledown Zapol' *et al.*, ²⁹ pseudopotential calculation; \Box Chapman, ²¹ SCF; \diamond hydrogenic f value; (b) experiment: \bullet beam-foil data from (A) Buchet *et al.*, ⁵³ (B) Buchet-Poulizac and Buchet, ⁵⁶ (C) Barrette and Drouin, ⁴¹ (D) Heroux, ⁶⁰ (E) Buchet and Buchet-Poulizac, ⁵² (F) Martinson *et al.*, ⁶⁶ (G) Hontzeas *et al.*, ⁶¹; * Filippov, ⁷⁴ hook method (relative value, normalized to f(2s-2p) from Weiss¹⁷). No error bars are given for the beam-foil data, since for the conversion from lifetimes to f values the (small) contribution of the 3s-3p transition, which has been obtained from other sources, must be considered.

For the first eight ions of the Li sequence, literature data are available which permit the construction of the dependence of the differential oscillator strength on energy for the bound-free region of the spectrum near the ionization threshold. By the use of extrapolation techniques for higher energies, as noted earlier, and by applying the constraint of continuity across the ionization limit, the total continuum contribution could be established. These results were then added to the total line contribution in each case to establish the total f sum for the series. The agreement with the Wigner-Kirkwood partial f sum rule $\left[\sum f(2s-p)=1\right]$ has been found to be quite good, with deviations from the predicted value not exceeding 6%. Since this sum rule is rigorously applicable only to a one-electron system, the true $f \min \max$ indeed differ slightly from the value predicted by the sum rule as a result of electron correlation effects. However, the difference is not expected to be more than a few percent for the low-Z ions of the sequence.

For Na IX through Ni XXVI, no continuum data are available in the literature. Thus for these ions our analysis has been reversed; i.e., the Wigner-Kirkwood sum rule has been applied to predict the continuum contributions by setting the total f sum equal to 1.

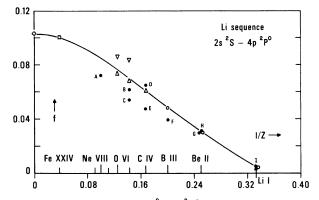


FIG. 3. f value for the $2s^2S-4p^2P^0$ multiplet of the Li sequence vs 1/Z. The data sources are (a) theory: \bigcirc Moitra and Mukherjee,²² SCF: \triangle Warner,³¹ scaled Thomas-Fermi calculation; $X \\ Kelly, Z^5 \\ SCF-Slater approximation; \Box Doschek$ *et al.*, 20 SCF with configurationinteraction: \Diamond hydrogenic f value. (b) experiment: \bullet beam-foil data from (A) Barrette and Drouin,⁴¹ (B) Buchet and Buchet-Poulizac,⁵² (C) Heroux,⁶⁰ (D) Buchet-Poulizac and Buchet,⁵⁶ (E) Martinson and Bickel,⁶⁵ (F) Martinson et al.,⁶⁶ (G) Hontzeas et al.,⁶¹ (H) Andersen et al.,⁴⁰ (I) Buchet et al.⁵⁴; \blacktriangle Filippov,⁷⁴ hook method (relative value, normalized to f(2s-2p) from Weiss¹⁷). No error bars are given for the beam-foil data, since for the conversion from lifetimes to f values the contributions of the 3s-4p, 4s-4p, and 3d-4p transitions, which have been obtained from other sources, must be considered.

The final data resulting from the analysis for the 2s-p series throughout the lithium isoelectronic sequence up to Ni XXVI are presented in Table I. Results are presented for the discrete transitions 2s-2p through 2s-7p, and in addition, partial sums for all remaining boundbound transitions $\sum_{n'=8}^{\infty} f(2s-n'p)$ of the series are given, as well as total line sums. It should be emphasized again that these are selected, critically evaluated data for this principal series which have subsequently been examined—and, if necessary, modified—with respect to their fit into isoelectronic sequence trends and spectral series behavior and checked (when possible) against f sum rules.

The oscillator-strength distribution along the lithium sequence for the 2s-p series is illustrated in Fig. 6; cumulative sums are formed from the data of Table I for all ions of the sequence up through Ni XXVI, and the nonrelativistic hydrogenic sums are accumulated at the left-hand side of the graph. It can be seen from the illustration that the (nonrelativistic) f values for the high-Z ions smoothly approach the nonrelativistic hydrogenic values. The oscillator strength for the resonance transition (2s-2p) declines rapidly along the sequence and tends to zero for infinite

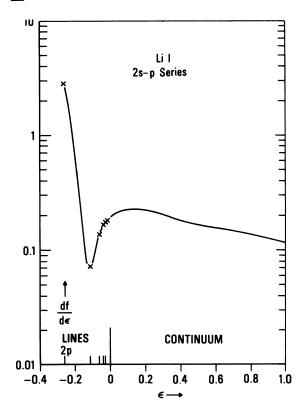


FIG. 4. Semilogarithmic plot of $df/d\epsilon$ vs ϵ for the 2s-p series of neutral lithium, based on the best available data. These have been slightly modified to comply with the requirement of continuity at $\epsilon = 0$ and to produce the best fit with the systematic trends.

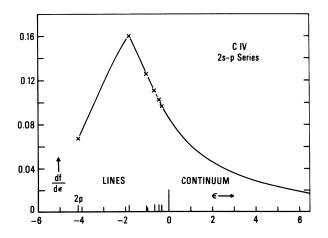


FIG. 5. Dependence of $df/d\epsilon$ on ϵ for the 2s-p series of C iv, based on the best available data. These have been slightly modified to comply with the requirement of continuity at $\epsilon = 0$ and to produce the best fit with the systematic trends.

Z, but this loss of f value is essentially recovered by the next two transitions of the series. In fact, the first partial f sum, f(2s-2p)+f(2s-3p), nearly approaches a constant value for ions with $Z \ge 10$. The total line contribution to the f sum, and thus the ratios of the line sum to the continuum, also remains nearly constant beyond C IV. Thus this single illustration contains, in very compact form, all of the essential f-value data on the principal series for all Li-like ions. However, as noted earlier, no account is as yet taken of any relativistic effects. As seen on the far left-hand side of the graph and discussed later, the f-value distribution for very-high-Z ions will be appreciably changed by the inclusion of relativistic effects.

B. Other spectral series

A considerable amount of literature is available regarding transitions of the 2p-d and 2p-sseries, so that an analysis similar to that described for the principal series could be undertaken for these series as well. The same constraints have been applied, but the situation has become more complex. For example, for the principal series, the photoionization cross section data (as a function of energy) could be simply converted to the quantity $df/d\epsilon$ by the use of a proportionality constant, since the 2s electron can jump only to orbital p states. However, a 2pelectron can undergo transitions to both s and dstates, so that the photoionization cross section of the 2p electron includes implicitly a summation of the cross sections for ionization to continuum states of both s and d symmetry. To utilize the total-cross-section data, one needs to know the values of the corresponding radial integrals for 2p-s and 2p-d transitions in order to subdivide this total contribution into its constituent components. Fortunately, Leibowitz²⁷ performed calculations of "partial" cross sections (i.e., 2p-s, 2p-d, etc.) for many photoionizing transitions of CIV, so that for this ion the continuum contribution to the total f sum can be determined for nearly any transition of interest.

A further difference and complication arises in the application of the sum rule. For the 2s-pseries no downward transitions had to be considered, but for the 2p electron it is necessary to include the contributions of both the 2p-2stransition and the virtual transition into the 1sstate, since both these transitions are possible in a one-electron model. Since an emission process would take place in such cases, the quantity that must be incorporated into the f sum is an oscillator strength f_{ki} for emission. This emission f value is related to the absorption f value

2s-3p transitions,	for transitions of the		
ic sequence. For the $2s-2p$ and	n. (b) (Nonrelativistic) f sums		
ie principal transitions of the $2s-n'p$ series of the Li isoelectronic sequence. For the $2s-2p$ and $2s-3p$ transitions,	ef. 82) and relativistic and nonrelativistic multiplet data are given. (b) (Nonrelativistic) f sums for transitions of the		
incipal transitions of the $2s-n$	2) and relativistic and nonrelat	ice.	
TABLE I. (a) Oscillator strengths for the pri	eted relativistic line f values (from Ref. 82	s-p series of the lithium isoelectronic sequen	
TABLE I. (a)	elected relativi	is-p series of t	

					(a)								
Ion	Nuclear charge Z	Multiplet nonrelativistic re	2s-2p .et relativistic	Lines relativistic $s_{1/2} - p_{3/2} = s_{1/2} - p_{1/2}$	lativistic <i>s</i> _{1/2} - <i>p</i> _{1/2}	Multiplet nonrelativistic re	2s-3p let relativistic	Lines re <i>s</i> _{1/2} - <i>þ</i> _{3/2}	Lines relativistic $\frac{1}{2}p_{3/2} = \frac{s_{1/2}-p_{1/2}}{s_{1/2}}$	Nonrel: 2s-4p	Nonrelativistic multiplet values 2s-4p 2s-5p 2s-6p 2s-7p	multiplet 2s-6p	values 2s-7p
Liı	с, -	0.753		0.502	0.251	0.0055		0.0036	0.0018	0.0045	0.0027	0.0017	0.0011
Be II B III	50 4	0.366				0.151				0.0486	0.0130 0.0241	0.0129	0.0078
C IV	9	0.286				0.197				0.0610	0.0290	0.0156	0.0092
N V	7	0.235		ratio of	n of	0.233		rat	ratio of	0.0696	0.0322	0.0170	0.0102
O VI	œ	0.199	~	2:1 is	is	0.257		2:	2:1 is	0.0766	0.0343	0.0181	0.0107
F vii	9 0	0.176		maintained	ained	0.277	_	main	maintained	0.0814	0.0358	0.0194	0.0112
Ne VIII Na IV	21	0.138				0.304				0.088	0.0373	0.0197	0.0116
MgX	12	0.125				0.316				0.089	0.0379	0.0200	0.0118
Aľxi	13	0.115				0.324				0.092	0.0384	0.0202	0.0119
Si XII	14	0.106	_			0.333				0.094	0.0388	0.0204	0.0120
P XIII	15	0.098				0.340				0.095	0.0391	0.0205	0.0121
S XIV	16	0.092				0.345				0.095	0.0394	0.0207	0.0122
Cl xv	17	0.080	0.005	0.050	200.0	0.350				0.096	0.0397	0.0208	0.0122
	10	100.0	0.065	860.0	070.0	000.0	١			1.60.0	0.0398	0.0200	0.0199
K XVII	00	0.073				0.363				0.008	0.0400	01010	0.0199
Ca AVIII Se XIX	21	0.069				0.367				0.098	0.040	0.0211	0.0124
Tixx	22	0.065	0.073	0.051	0.021	0.370	0.368	0.243	0.125	0.099	0.040	0.0211	0.0124
Λ ΧΧΙ	23	0.062				0.372				0.099	0.040	0.0212	0.0124
Cr xxII	24	0.059				0.375				0.10	0.040	0.0212	0.0124
Mn XXIII	25	0.056				0.377				0.10	0.040	0.0212	0.0125
Fe XXIV	26	0.053				0.379				0.10	0.040	0.0212	0.0125
Co XXV	1.7	160.0				0.361				0.100	0.040	0.0213	0710.0
Ni XXVI	78	0.050	0.064	0.048	0.017	0.383	0.375	0.246	0.129	0.101	0.040	0.0213	0.0125
•													
• •	•												
	42	0.033	0 068	0.056	0 011	0 403	0 374	0 240	0.134	0 102	0.041	0.0214	0.0126
•										104.0			
•	•												
	•												
Μ ΓΧΧΙΙ	74	0.018	0.136	0.129	0.0069	0.418	0.319	0.183	0.136	0.102	0.041	0.0215	0.0126
•	•												
	•												
•	•												

G. A. MARTIN AND W. L. WIESE

		TABLE I.	. I. (Continued).		
			(b) f sums		
	Nuclear	$\sum_{n'=8}^{\infty} f(2s-n'p)$	$\sum_{n'=2}^{\infty} f\left(2s-n'p\right)$	$\int_{0}^{\infty} \left(\frac{df}{d\epsilon}\right) d\epsilon$	
Ion	Cuarge Z	(Higher lines)	(All lines)	- 14	Total f sum
Li I		0.003	0.772	0.291	1.063
Bell	9 4	0.012	0.657	0.287	0.944
BIII	o D	0.022	0.632	0.338	0.970
C IV	9	0.026	0.624	0.342	0.966
N V	7	0.028	0.625	0.354	0.979
0 vi	æ	0.028	0.624	0.370	0.994
F VII	6	0.031	0.631	0.346	0.977
Ne viii	10	0.032	0.634	0.343	0.977
Na IX	11	0.032	0.631	0.369	
Mg X	12	0.033	0.633	0.367	
Al XI	13	0.033	0.635	0.365	
Si xII	14	0.033	0.637	0.363	
P XIII	15	0.033	0.638	0.362	
S XIV	16	0.035	0.639	0.361	
Clxv	17	0.035	0.640	0.360	
Ar XVI	18	0.033	0.640	0.360	
K XVII	19	0.034	0.641	0.359	Continuum f sum adjusted to give
Ca XVIII	20	0.034	0.641	0.359	$\sum f_{\text{total}} = 1$
Sc XIX	21	0.035	0.643	0.357	
Ti xx	22	0.035	0.643	0.357	
Λ ΧΧΙ	23	0.034	0.641	0.359	
Cr XXII	24	0.035	0.643	0.357	
Mn XXIII	25	0.035	0.642	0.358	
Fe XXIV	26	0.034	0.640	0.360	
Co xxv	27	0.035	0.641	0.359	
Ni XXVI	28	0.035	0.643	0.357	
	•				
•	•				
•	•				
Mo XL	42				
	•				
	•				
•	•				
W LXXII	14				
•	•				
. .	• •				
Hvdrogenic ion	. (8)	0.0349	0.649	0.351	1.000
	*				

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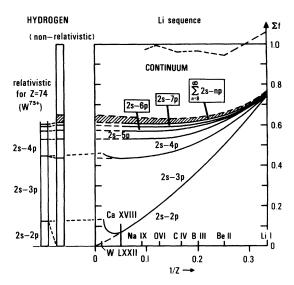


FIG. 6. Oscillator-strength distribution for the 2s-p series of the lithium isoelectronic sequence. The broken line at the top of the figure indicates the actual f sums obtained by summing line and continuum f values. For f(2s-2p) and the first partial sum, f(2s-2p) + f(2s-3p), both the relativistic results of Kim and Desclaux⁸² (solid lines) and the nonrelativistic results taken directly from Figs. 1 and 2 (broken lines) are included for Ca XVIII (Z = 20) through W LXXII (Z = 74).

 f_{ik} by

$$g_i f_{ik} = -g_k f_{ki} , \qquad (18)$$

where g_i and g_k are the statistical weights of the lower and upper states, respectively. The resulting set of data for the 2p-s series, which is given in Table II, includes the 2p-2s and 2p-1s transitions, and their headings have been enclosed in parentheses to indicate this difference. We simply converted the data for $f_{ik}(2s)$ -2p) according to the above formula [Eq. (18)] to obtain $f_{ki}(2p-2s)$. For 2p-1s, it was not possible to utilize this conversion since we did not have any data available for this virtual transition. Nevertheless, we were able to assign f values for this transition in the following way: Beginning with the first upward transition of the series (i.e., 2p-3s) we formed cumulative sums of f values for each ion of the sequence up through NeVIII, using the data of Table II. For each of these partial sums the data were plotted as a function of 1/Z (and are illustrated in Fig. 7), and beyond Ne VIII the curves were extrapolated to the hydrogenic values. Using the cross-section data of Leibowitz²⁷ to determine $df/d\epsilon$ and applying the constraint of continuity at the ionization threshold, we established the continuum f sum for C IV. This value was plotted on the graph in order to determine the total positive part of the f sum for this ion. In addition, the

					f values					f sums		
	Nuclear										$\int_{a}^{\infty} \left(\frac{df}{d} \right)_{A}$	
Ion	charge Z	2 <i>p</i> -3s	2 <i>p</i> -4s	2 p - 5s	2 <i>p</i> -6s	2. <i>p</i> -7s	(2 p - 2s)	(2 <i>p</i> -1 <i>s</i>)	$\sum_{n'=8}^{\infty} f(2p-n's)$ (Higher lines)	$\frac{\sum_{m'=1}^{\infty} f(2p-n's)}{\text{(All lines)}}$	$\int_0 \sqrt{d\epsilon} \int^{a} \epsilon$ (Continuum)	f sum
Liı	°	0.115	0.014	0.0044	0.0021	0.0012	-0.251	-0.025	0.0033	-0.136	0.025	
Be II	4	0.0665	0.010	0.0038	0.0019	0.0011	-0.168	-0.049	0.0029	-0.131	0.020	ļ
BIII	5	0.0470	0.0081	0.0033	0.0017	0.0010	-0.122	-0.070	0.0026	-0.128	0.017	Data
C IV	9	0.0376	0.0069	0.0030	0.0015	0.0009	-0.095	-0.084	0.0023	-0.127	0.016 a	adjusted
NV	7	0.0322	0.0062	0.0028	0.0014	0.0008	-0.078	-0.094	0.0020	-0.127	0.016	to give
0 VI	80	0.0287	0.0056	0.0026	0.0013	0.0007	-0.066	-0.101	0.0019	-0.126	0.015	ZJ total
FVII	6	0.0263	0.0052	0.0024	0.0012	0.0007	-0.059	-0.104	0.0018	-0.125	0.014	= -0.111
Ne viir	10	0.0245	0.0049	0.0023	0.0011	0.0007	-0.052	-0.108	0.0018	-0.125	0.014	
•											•	
•	•											
•	•											
Hydrogenic ion	(∞)	0.0136	0.0030	0.0012	0.0006 0.0004	0.0004	0.000	-0.139	0.0010	-0.119	0.008	-0.111
^a For C IV, the continuum f value of 0.016 is based on a calculation (Ref. 27)	sontinuum	f value of	f 0.016 is l	based on a	calculati	on (Ref. 2	12				2	

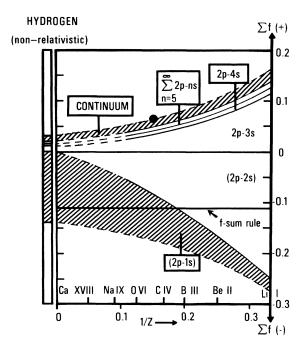


FIG. 7. Oscillator-strength distribution for the 2p-s series of the Li sequence. The continuum f sum for C IV is based on a calculation by Leibowitz.²⁷

continuum contribution for the asymptotic hydrogen point could be used to determine the total positive f sum for $1/Z \rightarrow 0$. With these two points available, and judging by the cumulative buildup of the positive f sums for the 2p-s series, the other continuum f sums could be roughly estimated by interpolation or extrapolation, and these results are included in Table II. We were thus finally able to estimate the f values for the $2p \rightarrow 1s$ (virtual) "emission" transition by assuming that the total f sum for each ion of the lithium sequence is equal to the value of $-\frac{1}{6}$ predicted by the Wigner-Kirkwood sum rule for the 2p-sseries; i.e., for each ion the absolute value of $f_{ki}(2p - 2s)$ was subtracted from the total positive f sum, and in each case the deviation of this difference from $-\frac{1}{6}$ provided an f value for $2p \rightarrow 1s$.

The accuracy of these predicted f values for the virtual $2p \rightarrow 1s$ transition may be checked by the following procedure, which has been made possible by the work of Gabriel.⁷⁸ He calculated transition probabilities and wavelengths in intermediate coupling for all lines of the $1s^22s$ -1s2s2p and $1s^22p$ - $1s2p^2$ transition arrays for the lithiumlike ions O VI, Si XII, Ca XVIII, and Fe XXIV. By using his data for either of these transition arrays, we converted the individual transition probabilities to line strengths, which were in turn summed to find absolute strengths for the transition array as a whole. These could then be modified by the appropriate angular factors (see, for example, Menzel⁷⁹) to obtain absolute strengths for a (single electron) multiplet of the type $2p^2P^o \rightarrow 1s^2S$. Finally, by using the very narrow range of wavelengths given in each case by Gabriel, we were able to convert these multiplet strengths to a correspondingly narrow range of f values for 2p-1s. However, unlike the transition arrays treated by Gabriel, the virtual transition that we are concerned with is a transition into an already filled level, and thus it should be interpreted as a hydrogenlike case, but with screening by two other 1s electrons. Therefore, we considered that the 2pelectron lies outside the inert $1s^2$ core, so that it is screened by two electrons and the effective core charge Z_{eff}^{c} seen by the 2p electron obeys the inequality

$$Z - 2 \leq Z_{\text{eff}}^c \leq Z. \tag{19}$$

If the 2p electron were able to jump down to a 1s orbital without disturbing the $1s^2$ core, again it would experience a screening of the type described above. To provide upper and lower limits on the 1s-2p wavelengths for the abovementioned lithiumlike ions, we used the results of relativistic calculations of Dirac hydrogenic wave functions by Younger and Weiss⁸⁰; for the unscreened case we used the wavelength corresponding to the actual nuclear charge Z, while for the case of total screening by the two core (1s) electrons the wavelength corresponding to a charge of Z-2 was employed. The results are shown in Fig. 8, and it is seen that our earlier predicted f values lie between the results obtained by using Gabriel's wavelengths and the wavelengths of those in which the screening by the core electrons is assumed to be complete. However, in no case did our results deviate from those of Gabriel by more than 17%.

An analogous procedure was followed in analyzing the material for the 2p-d series. The results are presented in Table III, as well as the accompanying Fig. 9. However, there are no downward transitions possible in this case, so that—once the cumulative sums are plotted along the sequence—the continuum data can be derived from the sum rule, which states that the total f sum for each ion is equal to $\frac{10}{9}$. The results of Leibowitz²⁷ have again been used to obtain an actual continuum f sum for C IV, and Fig. 9 demonstrates that the agreement with the sum rule is excellent.

A partial analysis has also been undertaken

 Π . Oscillator strengths (f values) and f sums for transitions of the lithium isoelectronic sequence.

TABLE

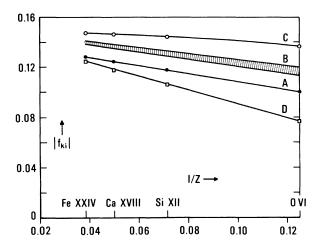


FIG. 8. Absolute value of the (emission) oscillator strength f_{ki} for the virtual $2p \rightarrow 1s$ transition in the Li sequence vs 1/Z. Curve A shows our results derived from the analysis of the oscillator-strength distribution. For curves B, C, and D, Gabriel's results⁷⁸ for the average of $1s^2 2p \rightarrow 1s2p^2$ and $1s^2 2s \rightarrow 1s2s2p$ were used to obtain line strengths for a multiplet of the type $2p^2P^o$ $\rightarrow 1s^2S$, which were converted to *f* values by using (B) the range of Gabriel's calculated wavelengths for lines of $1s^2 2p \rightarrow 1s2p^2$ and $1s^2 2s \rightarrow 1s2s2p$, (C) wavelengths calculated by Younger and Weiss⁸⁰ for a hydrogenic ion of nuclear charge *Z*, and (D) wavelengths calculated by Younger and Weiss for a hydrogenic ion of nuclear charge *Z*-2 (to account for screening by the core electrons).

for higher spectral series in the Li sequence, but the amount of material available is considerably less complete than for the series already discussed. As a result, the accuracy of the data is somewhat poorer. Attempts to construct fsums for these series are hampered by the greater uncertainties in individual f values. This problem is in turn compounded for those series which include downward (emission) transitions (with negative f values). In such a case, the partial compensation of positive and negative contributions to the f sums results in even greater uncertainties in *estimated* partial sums, such as the contributions from the continuum and the virtual transitions. Nevertheless, some valuable consistency checks can be made; e.g., the behavior of f values for individual discrete transitions can be investigated along the isoelectronic sequence for regularity and smoothness, and can similarly be studied for the dependence of $df/d\epsilon$ on ϵ throughout a spectral series for individual ions. Although there are no graphical presentations given here for these higher series, tables of discrete f values have been assembled for several transitions and will be presented elsewhere.⁸¹

				f values				f sums		
	Nuclear						1		$\int \int \frac{df}{df} df$	
Ion	charge Z	2 p -3d	2 <i>p</i> -4 <i>d</i>	2 <i>p</i> -5d	2 <i>p</i> -6d	2 <i>p</i> -7 <i>d</i>	$\sum_{(\text{Higher lines})}^{\infty} f(2p - n'd)$	$\sum_{n'=3}^{\infty} f(2p - n'd)$ (All lines)	$\int_0 \langle d\epsilon \rangle^{ac}$ (Continuum)	Total f sum
Liı	3	0.667	0.125	0.0470	0.0239	0.0135	0.0377	0.914	0.197	
Be II	4	0.652	0.124	0.0477	0.0240	0.0140	0.0376	0.899	0.212	
3 III	5	0.651	0.124	0.0475	0.0235	0.0140	0.0373	0.897	0.214	Continuum
N	9	0.654	0.124	0.0472	0.0234	0.0139	0.0370	0.900	0.211 ^a	J sum
N <	7	0.658	0.124	0.0469	0.0230	0.0136	0.0370	0.903	0.208 /	adjusted
I VI	80	0.662	0.123	0.0466	0.0229	0.0135	0.0367	0.905	0.206	to give
F vii	6	0.666	0.123	0.0464	0.0227	0.0134	0.0356	0.907	0.204	$\sum J t_{\text{total}} = 1.111$
Nevili	10	0.667	0.123	0.0461	0.0226	0.0132	0.0348	0.907	0.204	
	•								ı	
	•									
	•									
Hydrogenic ion	(8)	0.696	0.122	0.0444	0.0216	0.0123	0.0319	0.928	0.183	1.111

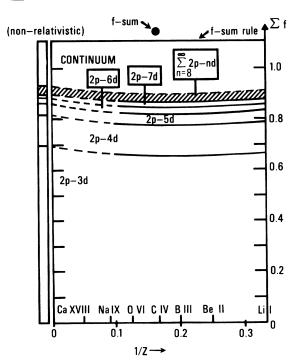


FIG. 9. Oscillator-strength distribution for the 2p-d series of the Li sequence. The continuum f sum for C iv is based on a calculation by Leibowitz.²⁷

IV. RELATIVISTIC CORRECTIONS

Relativistic effects become important for highly charged Li-like ions since the core field, i.e., the net field of the nucleus minus the two inner electrons (Z-2), becomes so strong that the radiating electron acquires relativistic speeds.

As the nuclear charge increases, the first relativistic effect to become important is that of spin-orbit interaction, which affects the f value both through the line strength as well as the transition energy [see Eq. (3)]. Another relativistic correction which becomes significant only at much higher values of the nuclear charge is the shrinkage of the electron orbits and the accompanying mass increase of the electron, again because of the relativistic speeds. This orbital effect will directly modify the transition integral.

Kim and Desclaux, ⁸² as well as Weiss, ⁸³ have recently studied theoretically the relativistic effects on the energies and f values of several very highly ionized Li-like ions. From Kim and Desclaux's results for the f values, we have constructed Figs. 10 and 11 for the spectral lines of the doublets 2s-2p and 2s-3p. Their results are slightly modified for small Z to connect smoothly to the best critically evaluated data

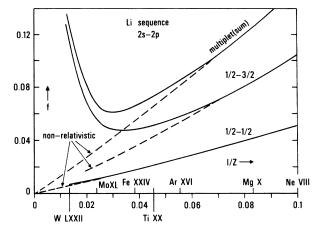


FIG. 10. Relativistic oscillator strengths for the $2s_{1/2}$ - $2p_{1/2}$ and $2s_{1/2}$ - $2p_{3/2}$ transitions for very highly charged Li-like ions. This graph represents the greatly expanded lower-left-hand corner of Fig. 1. The broken lines are the (interpolated) nonrelativistic *f* values, with the multiplet value taken directly from Fig. 1, and the solid lines are based on the relativistic *f* values calculated by Kim and Desclaux.⁸²

there. These graphs are thus essentially the greatly magnified far-left-hand sides of Figs. 1 and 2. The nonrelativistic data presented earlier, i.e., the multiplet (or doublet) values, are again included as the upper broken line. The other two (lower) broken lines represent the non-relativistic f values for the two individual doublet

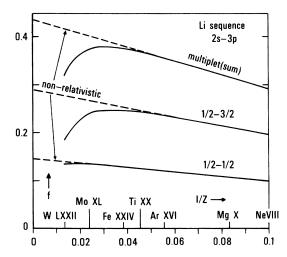


FIG. 11. Relativistic oscillator strengths for the $2s_{1/2}$ - $3p_{1/2}$ and $2s_{1/2}$ - $3p_{3/2}$ transitions for very highly charged Li-like ions. This graph represents the greatly expanded left-hand side of Fig. 2. The broken lines are the (interpolated) nonrelativistic f values, with the multiplet value taken directly from Fig. 2, and the solid lines are based on the relativistic f values calculated by Kim and Desclaux.⁸²

- \	6	41		

State	NV	Ar xvı	Fe xxiv	Kr xxxiv	Mo XL	W lxxii
$2p_{1/2}$ (relativistic)	0.740	2.36	3.62	5.38	6,56	15.80
$2p_{3/2}$ (relativistic)	0.742	2.59	4.79	10.12	15.77	126.1
2p (nonrelativistic)	0.738	2.31	3.44	4.86	5.70	10.19
$3p_{1/2}$ (relativistic)	4.35	38.7	85.5	171.0	237.7	824.7
$3p_{3/2}$ (relativistic)	4.35	38.8	85.8	172.4	240.4	857.6
3p (nonrelativistic)	4.35	38.5 ^a	84.4 ^a	166.8 ^a	229.6	733.3

TABLE IV. Calculated relativistic and nonrelativistic excitation energies (in Ry) for the 2p and 3p states of some Li-like ions (from Refs. 82 and 83).

^a Onello *et al*.,¹⁸ Onello.¹⁹

components, which are always in the ratio of 2:1 for $s_{1/2}-p_{3/2}: s_{1/2}-p_{1/2}$. It is seen that the relativistic f values of the $s_{1/2}$ - $p_{1/2}$ lines deviate very little from the nonrelativistic data, even for the highest point presented, which is 71-timesionized tungsten. Thus the relativistic f value of the $2s_{1/2}$ - $2p_{1/2}$ line still approaches zero in the high-Z limit. The large relativistic corrections occur in the $s_{1/2}$ - $p_{3/2}$ lines, especially for the 2s-2p case, where the f value increases drastically beyond Mo XL. This large increase in the f value is apparently almost entirely owing to a very pronounced increase in the excitation energy E_{k} for the state $2p_{3/2}$, which strongly enlarges the difference $(E_k - E_i)$ in Eq. (3). (E_i) is the ground-state energy and therefore remains zero by definition.) To demonstrate the magnitude of the energy corrections, we have tabulated (Table IV) the results of Kim and Desclaux⁸² (as well as Weiss⁸³), who have calculated the nonrelativistic as well as relativistic energy values. It is seen that the relativistic energy change in the $2p_{3/2}$ level becomes very drastic, while for the $2p_{1/2}$ level the energy still remains close to the nonrelativistic value, up to the ion W LXXII. For the two 2s-3p transitions, the energy changes are -on an absolute scale-again very similar to the conditions for the 2s-2ptransitions. However, since the nonrelativistic energy difference between upper and lower states $(E_k - E_i)$ is much larger for the 2s-3p transitions than for the 2s-2p transitions, the relativistic energy change has only a small overall effect on the f value.

Thus one should generally expect that the largest relativistic effects occur for transitions where the nonrelativistic energy difference $(E_k - E_i)$ is very small, i.e., for transitions in the same shell. This would mean that for the different spectral series presented here the most drastic changes occur in the first lines of those series where the leading lines are $\Delta n = 0$ transitions, while the other lines remain relative-

ly unaffected up to very high values of Z.

The slightly modified data of Kim and Desclaux (to give the best fit for low-Z ions) have also been incorporated into Table I and Fig. 6 to show the overall effect of the relativistic corrections on the oscillator strength distribution. In Fig. 6, where the relativistic changes can be shown only for 2s-2p and the partial sum f(2s-2p) + f(2s-3p), we have also inserted, at the far-left-hand side, the results of relativistic calculations by Younger and Weiss⁸⁰ for a hydrogenic ion of charge Z=74. It is evident that this hydrogenic distribution is very closely approached by the two Li transitions for which data are available, so that one would expect this to happen for the other transitions of this series, too.

V. SUMMARY

Several fundamental spectroscopic requirements have been utilized to perform a generalized analysis of the available line and continuum f values for the lithium isoelectronic sequence. The body of data has thus been tied together in a uniform manner and has been adjusted for greatest consistency. The resultant data adhere closely to regularities and f sum rules and obey the condition of continuity at the transition point from discrete to continous spectrum. Thus the comprehensive sets of data obtained for several spectral series and for a large range of ions along the sequence must be regarded as highly accurate ones. Relativistic effects have been considered for the very highly charged ions and are found to be very similar to those for hydrogenic ions. This study may be considered as a first example of a comprehensive data analysis technique where a large number of original, unrelated f-value data are interrelated and adjusted to fit basic spectroscopic rules and constraints. Additional applications should be possible for other simple (essentially one-electron) atomic systems, such as sodiumlike ions; however,

for isoelectronic sequences of greater complexity it would be impossible to utilize fully and definitively the generalized analysis scheme undertaken in this study, since the one-electron model would no longer apply.

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