Addendum: Systematics of moments of dipole oscillator-strength distributions for atoms in the first and second row

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The values of $S(1)$ and $L(1)$, i.e., quantities related to straggling of particles, given by Dehmer, Inokuti, and Saxon [Phys. Rev. A 12, 102 (1975)], are inaccurate within the Hartree-Slater model used in that work. Those values are too large by as much as several percent because of an overestimation of contributions from high excitation energies. Revised values of $S(1)$ and $L(1)$, accurate to about 1%, are presented and discussed in greater detail. They are now in closer agreement with other values of N, O, Ne, and Ar found in the literature. All the other $S(\mu)$ and $L(\mu)$ values given by Dehmer, Inokuti, and Saxon remain unchanged.

Dehmer, Inokuti, and Saxon[1] calculated the moments

$$S(\mu)=\int\left(\frac{E}{R}\right)^{\mu}\frac{df}{dE}\,dE \tag{1}$$

of the oscillator-strength distribution df/dE over excitation energy E throughout the entire (discrete and continuous) spectrum for atoms He through Ar by the use of the Hartree-Slater (HS) model, R being the Rydberg energy. The same work also included calculation of

$$L(\mu)=\int\left(\frac{E}{R}\right)^{\mu}\ln\left(\frac{E}{R}\right)\frac{df}{dE}\,dE\,. \tag{2}$$

The actual computation of df/dE obviously must stop at a cutoff value E_C of excitation energy E. Dehmer, Inokuti, and Saxon[1] chose E_C at (200–600)R above the K-shell threshold for all the atoms treated, and used an extrapolation formula

$$\frac{df}{dE}=CE^{-B}\,, \tag{3}$$

where B and C are positive constants determined from the last two df/dE values, i.e., at E_C and below. As stated near the end of Sec. II of Ref. 1, this procedure led to the fulfillment of the criterion that the Thomas-Kuhn-Reiche sum rule $S(0)=Z$ (i.e., the number of atomic electrons) be satisfied to one tenth of a percent, for every subshell. Thus, the procedure is entirely appropriate for the accurate evaluation of $S(\mu)$ and $L(\mu)$ for $\mu \leq 0$.

Nevertheless, the same procedure is now recognized to be unsatisfactory for the evaluation of $S(1)$ and $L(1)$. Because of the additional E factor in the integrand, it is necessary to use a much greater value of E_C. Therefore, we have extended the same calculations. Results of the new work are shown in Table I, which supersedes the entries in the rightmost columns of Tables I and II of Ref. 1. The quantities $S(1)$ and $L(1)$ are important in the theory[2] of straggling of fast charged particles. In this context, results are often presented in terms of the mean excitation energy I_1 for straggling, defined by[2,3]

$$\ln(I_1/R)=L(1)/S(1). \tag{4}$$

Table I includes values of I_1 measured in eV.

We chose a series of E_C values up to about 2×10^4 R above the ionization threshold for every important subshell (see below). The B values in Eq. (3) then came out within 0.5 or less of the exponent $l+3.5$ of the asymptotic df/dE behavior,[4] where l is the orbital-angular-momentum quantum number of the initial state. The region $E>E_C$ now contributes only a few percent to $S(1)$ or $L(1)$. Furthermore,

TABLE I. Values of $S(1)$, $L(1)$, and I_1 for all neutral atoms through Ar. The format $A(B)$ means $A\times10^B$. Values for atomic hydrogen ($Z=1$) are taken from Ref. 3. Some of the last digits appear as subscripts when their significance is uncertain.

Z	$S(1)$	$L(1)$	I_1 (eV)
1	1.333	7.612 (–1)	2.408 (1)
2	7.71	1.37 (1)	8.01 (1)
3	2.10 (1)	5.51 (1)	1.88 (2)
4	4.06 (1)	1.28 (2)	3.18 (2)
5	6.70 (1)	2.39 (2)	4.82 (2)
6	1.00 (2)	3.84 (2)	6.33 (2)
7	1.40 (2)	5.76 (2)	8.33 (2)
8	1.89 (2)	8.14 (2)	1.01 (3)
9	2.44 (2)	1.09 (3)	1.19 (3)
10	3.09 (2)	1.43 (3)	1.39 (3)
11	3.83 (2)	1.83 (3)	1.62 (3)
12	4.67 (2)	2.30 (3)	1.87 (3)
13	5.60 (2)	2.83 (3)	2.13 (3)
14	6.61 (2)	3.43 (3)	2.44 (3)
15	7.73 (2)	4.09 (3)	2.7_3 (3)
16	8.94 (2)	4.83 (3)	3.0_3 (3)
17	1.02_5 (3)	5.64 (3)	3.3_5 (3)
18	1.16 (3)	6.53 (3)	3.6_6 (3)

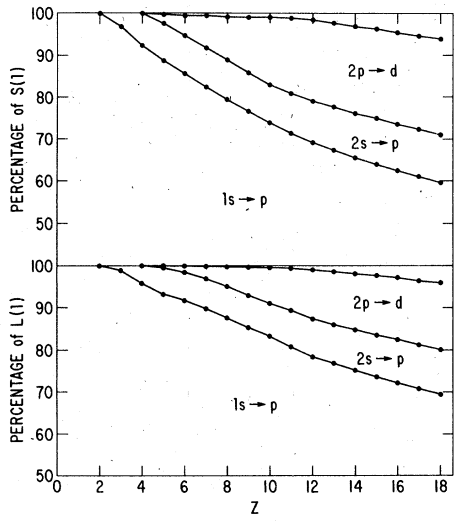

FIG. 1. Contributions to $S(1)$ and $L(1)$ from different subshells, expressed in percentage, for all neutral atoms through Ar. The upper half refers to $S(1)$ and the lower half to $L(1)$. Note that the zero of the vertical axis is suppressed in each case. The portion below the lowest curve represents the contributions from the $1s \rightarrow p$ transitions. The next portion, between the lowest two curves, represents the contributions from $2s \rightarrow p$ transitions. The third portion represents the contributions from the $2p \rightarrow d$ transitions. The uppermost portion represents contributions from the other transitions.

we have examined the trends of shellwise contributions $S_{nl}(1)$ and $L_{nl}(1)$ as E_C is successively increased. We can estimate a limiting value of $S_{nl}(1)$ or $L_{nl}(1)$ by analyzing the results as a function of the variable $l + 3.5 - B$ or I_{nl}/E_C in the neighborhood of zero, where I_{nl} is the ionization threshold for the nl subshell. [More specifically, when one plots the shellwise contribution against the variable $\xi = (l + 3.5 - B)^2/(2 - B)^2$, one finds a behavior very close to a straight line, which permits a reliable extrapolation to $\xi = 0$. The denominator $(2 - B)^2$ qualitatively accounts for the divergence that should occur at $B = 2$ for any l, according to Eq. (3). The use of squares in the definition of ξ is based on experience and not on rigorous mathematics.] In this way, we conclude that the values in Table I should be accurate to about 1% or better.

The magnitudes of shellwise contributions should be noted here. As to $S(1)$ of Ne, for instance, the $1s$-p transitions contribute 74%, the $2s$-p transitions 9%, the $2p$-d transitions 16%, and the $2p$-s transitions 1%. For $L(1)$ of Ne, the $1s$-p transitions account for 83%, and the other transitions correspondingly less. The overall trends of the shellwise contributions are shown in Fig. 1. The overwhelming importance of the $1s$-p transitions is clearly attributable to their high threshold energies. The major contributions from the $2p$-d transitions occur because of their large oscillator strength in the moderately high continuum and of up to six electrons in the $2p$ subshell. (Indeed, the $2p$-d contributions increase gradually as one goes from B to C, N and so on up to Ne.) Our findings on the shellwise contributions are in general accord with the Hartree-Fock results on rare gases by Bell, Bish, and Gill.[5] They also should provide a guide for reliable estimates of $S(1)$ and $L(1)$ for molecules as well, because dominant contributions come from innermost shells, which are little affected by the molecular binding.

Because the dominant contributions arise from the K shell, which is insensitive to outer-shell filling, $S(1)$ and $L(1)$ increase monotonically with the atomic number Z as the df/dE shifts to higher excitation energies. In particular, $S(1)$ behaves as $Z^{7/3}$, as already noted in Ref. 1. Cummings[6] also presented a similar but more precise Z dependence (i.e., $Z^{2.24}$) of $S(1)$ values computed from the Hartree-Fock model. The Z dependence of $L(1)$ is approximately proportional to $Z^{2.7}$. The I_1 value consequently is roughly proportional to $Z^{1.8}$.

The revised values of $S(1)$ and $L(1)$ for Ne and Ar show improved agreement with literature values (cf. Table VI of Ref. 1). Further comparison has been made with other sources[5-8]: Our values for Ne and Ar are within one percent of the results of Bell, Bish, and Gill.[5] Also, our values for O and N agree just as well with the results of Zeiss, Meath, McDonald, and Dawson.[7] Furthermore, the close agreement of our $S(1)$ value with accurate configuration-mixing calculations[8] for Ne is especially rewarding. Although our method of calculation is based on the single-electron model, our results for $S(1)$ and $L(1)$ for other atoms are likely to be quite reliable because these quantities are dominated by K-shell properties which are little influenced by electron-correlation effects.

Finally, we may add that the study of $S(\mu)$ and $L(\mu)$ for $-6 \leq \mu \leq 1$ has been extended to all neutral atoms with $19 \leq Z \leq 38$. Results of this work are now being prepared for publication.

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