Emissive zones of complex atomic configurations in highly ionized atoms

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(Received 2 August 1982)

The radiative properties of very complex atomic configurations in highly ionized species can be determined easily by means of statistical moments, computed *ab initio* from relativistic radial orbitals. A case of current interest, the spectrum of Gd XII, is studied as an example. The locations and the widths of the zones of the upper configurations responsible for the bulk of the spontaneous emission are determined formally and numerically. The fact that these zones may sometimes lie well above the center of gravity of the configuration can be interpreted by considering the relevant $G^1(nl,n'l-1)$ Slater integral and its angular coefficients. Moreover, it is shown that two transition arrays involving the same upper configuration may actually originate from disconnected zones of the latter. A linear relationship is established formally between the coefficients of $G^1(nl,n'l-1)$ and the J-file sums of Condon and Shortley. This gives us the opportunity to evaluate the sum of the line strengths of all the transitions originating from a given upper level and, therefore, a method for checking oscillator-strength angular calculations.

I. INTRODUCTION

An ever-increasing number of far-ultraviolet and x-ray emission spectra of various ionic species are currently being recorded as part of the continuing investigation of high-temperature plasmas. These spectra often show, together with some individual ionic lines, broad-band-type patterns which can be identified as unresolved transition arrays (UTA) between two atomic configurations, or superpositions of them. *Ab initio* methods for obtaining the radial orbitals and a statistical model yielding simple angular coefficients open the way to global interpretations of such UTA.[1,2]

Among the most complex of these spectra, one finds those of the lanthanide ions in laser-produced plasmas, obtained by O'Sullivan and Carroll.[3] Recently, these authors published other lanthanide spectra in the range 70—130 Å, generated by laser shots at pure metal instead of compound targets.[4] They also gave a qualitative interpretation of the observed complex patterns, which they attribute to $4d$-$4f$ transitions between configurations with a varying number of $4f$ and $5p$ electrons. In the present work, we aim at checking quantitatively this interpretation, using previously published methods. This is done in Sec. II. In Sec. III, the general case of l^{N+1}-$l^N l'$ is studied. We determine which of the levels of $l^N l'$ are responsible for the bulk of the emitted intensity. The corresponding range of energy is called, in the following, a zone of preferential transition probability or, equivalently, an emissive zone. The peculiar location of this zone in some cases can be put into relation with the values of the J-file sums (of the strengths) defined by Condon and Shortley.[5] A linear relationship is established in Sec. IV between these J-file sums and the angular coefficients of some $G^1(nl,n'l')$ Slater energy integrals.

II. Gd XII SPECTRUM

The spectra presented by Carroll and O'Sullivan[4] for the lanthanides in the wavelength region 70—130 Å are attributed to spontaneous emission by highly ionized species, with ionization stages between 8 and 16. For these ions, the lowest configurations contain an open $4f$ subshell, as shown in Table I of Ref. 4. The authors also discuss at length the fact that the $4f$ and $5p$ binding energies are very close for such ions. As an example, they give in Fig. 6 of Ref. 4 a schematic representation of the relevant part of the spectrum of Gd XII with lower configurations of the type $4d^{10}4f^M5p^{M'}$ ($M+M'=5$; $M'=0$ through 5) and higher configurations of the type $4d^9 4f^N 5p^{N'}$ ($N+N'=6$; $N'=0$ through 5).

We first present, in Fig. 1, a quantitative description of the same portion of the Gd XII spectrum, calculated by the relativistic parametric-potential code RELAC.[6] The relativistic wave functions are determined in the central-field approximation. The cen-

TABLE I. *Ab initio* results for 11 transition arrays in the spectrum of Gd XII. The σ quantities are, successively, the standard deviations of the wave-number distributions of the upper-configuration states, of the lower-configuration states, of the transitions (weighted by their strengths), and of the upper-configuration states (weighted by their total emissive strengths). For the δE shift, see the text. The three lowest lines contain the mean wave number of the array, its mean wavelength, and its FWHM.

Transition	$4d^9 4f^6$ → $4f^5$	$4d^9 4f^5 5p$ → $4f^4 5p$	$4d^9 4f^4 5p^2$ → $4f^3 5p^2$	$4d^9 4f^3 5p^3$ → $4f^2 5p^3$	$4d^9 4f^2 5p^4$ → $4f 5p^4$	$4d^9 4f 5p^5$ → $5p^5$	$4d^9 4f^5 5p$ → $4f^5$	$4d^9 4f^4 5p^2$ → $4f^4 5p$	$4d^9 4f^3 5p^3$ → $4f^3 5p^2$	$4d^9 4f^2 5p^4$ → $4f^2 5p^3$	$4d^9 4f 5p^5$ → $4f 5p^4$
σ_{upper} (cm^{-1})	107 340	109 680	108 840	102 120	88 630	66 490	109 680	108 840	102 120	88 630	66 490
σ_{lower} (cm^{-1})	42 420	51 020	53 830	53 080	46 710	32 320	42 420	51 020	53 830	53 080	46 710
σ_{array} (cm^{-1})	75 560	72 280	66 800	58 480	51 840	22 370	87 740	83 750	76 770	66 380	50 490
δE (cm^{-1})	184 150	207 170	230 190	253 210	276 230	299 250	10 440	8 350	6 260	4 170	2 090
σ_z (cm^{-1})	88 890	88 820	83 910	74 200	63 830	35 450	88 170	111 720	112 030	95 110	63 530
T_{av} (cm^{-1})	1 390 070	1 415 530	1 440 990	1 466 440	1 491 900	1 517 360	1 272 190	1 332 160	1 391 710	1 451 250	1 510 790
λ_{av} (Å)	71.9	70.6	69.4	68.2	67.0	65.9	78.6	75.1	72.8	68.9	66.2
FWHM (Å)	9.2	8.5	7.6	6.4	5.5	2.2	12.8	11.1	9.3	7.4	5.2

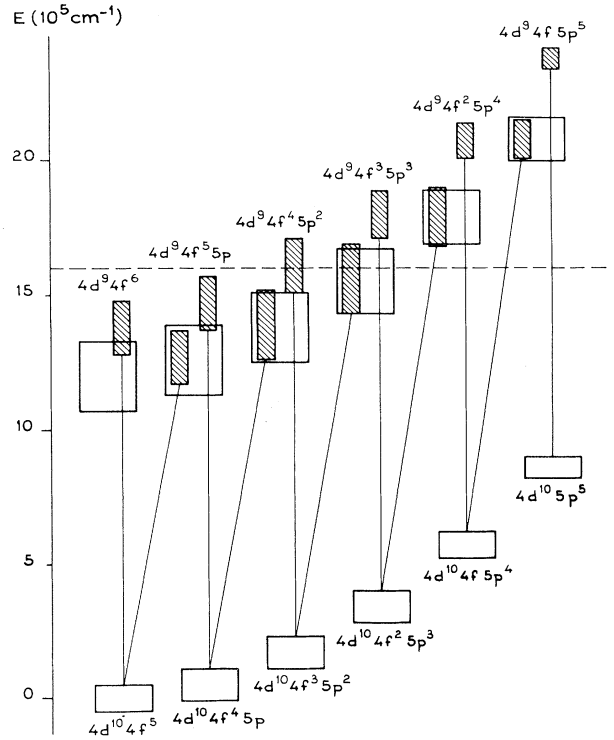

FIG. 1. Low configurations and transition arrays in the spectrum of Gd XII. Each rectangle features a wave-number distribution. Its mean ordinate is the mean wave number; its vertical dimension is equal to 2.355 σ, σ^2 being the variance. The broad rectangles correspond to the configurations and the narrow rectangles to the emissive zones relevant to the "vertical" or "oblique" transitions. The broken horizontal line represents the ionization limit.

tral potential is described by an analytic function depending on a set of parameters which take into account the shell structure of the atom. The parameters are varied in such a way as to minimize the mean total first-order energy (including the contributions of closed shells) of the 24 relativistic configurations associated with the configurations $4d^{10}4f^5$, $4d^{10}5p^5$, $4d^9 4f^6$, and $4d^9 5p^6$, which are the most different configurations occurring in the relevant part of the Gd XII spectrum. When the central potential is determined, nonrelativistic approximations for the energy radial integrals relevant to the Coulomb and spin-orbit interactions are derived.[7,8]

In Fig. 1, each broad rectangle features the position and width of a configuration, in the sense that its average ordinate is the mean wave number of the configuration-state distribution, and that its vertical dimension is the full width at half maximum (FWHM)

$$2(2\ln 2)^{1/2}\sigma = 2.355\sigma$$

of the same distribution, the variance being denoted σ^2. Each rectangle would contain about 76% of the states, in the assumption that the distribution is really Gaussian. The corresponding values of σ are presented for the upper and lower configurations of the arrays in the first two lines of Table I. They have been obtained by introducing the values of the nonrelativistic Slater and spin-orbit integrals in the formulas of Ref. 1. It can be said, in supplement to these numbers, that (i) for the lower configurations, the spin-orbit constant ζ_{5p} contributes appreciably to σ_{lower}, as it is apparent in the $5p^5$ case, for which it brings the only contribution; and (ii) for the upper configurations, the major contributions to σ_{upper} come from the $(4d,4f)$ Slater integrals, as proven by its approximate proportionality to $[N(14-N)]^{1/2}$ (N being the number of $4f$ electrons).

In a second step, we have calculated the mean wave numbers and the widths of the relevant transition arrays, using formulas of Refs. 1 and 2. Two sets of arrays occur, corresponding to the $4d$-$4f$ and $4d$-$5p$ transitions, respectively. The third and fourth lines of Table I contain the numerical results, namely, the quantities σ_{array} and δE; σ^2_{array} is the variance of the array, and δE is the weighted average wave number of the array minus the difference between the average wave numbers of the two configurations [Ref. 1, Eq. (14)]. Evidence for the quantity $\delta E(l^N l' \rightarrow l^{N+1})$ has been presented through explicit calculations by Cowan[9] in 1968. It has been shown later[1] that it is proportional to N; this is apparent for both sets of arrays, after it is recalled that complementary arrays $4d^{10}nl^N$-$4d^9nl^{N+1}$ and nl^{4l-N+2}-$4dnl^{4l-N+1}$ ($nl=4f$ or $5p$) give identical results. The explicit formulas for δE are listed in Table II as numerical applications of Eq. (14) of Ref. 1. Because the $F^k(l,l')$ and $G^k(l,l')$ integrals have generally the same order of magnitude, the predominant positive coefficient of $G^1(l,l')$ ensures that δE is normally positive. The fact that δE is very large for the array of the $4d$-$4f$ type and small for the $4d$-$5p$ type reflects the fact that

$$G^1(4f,4d) \gg G^1(4d,5p) .$$

This is due to the overlap of the $4d$ and $4f$ orbitals being much larger than that of $4d$ and $5p$.

The σ_{array} values in Table I are calculated more easily by considering the complementary arrays, namely, $4f^m5p^n$-$4d\,4f^{m-1}5p^n$ and $4f^m5p^n$-$4d\,4f^m5p^{n-1}$, which are of the type studied in Sec. II B of Ref. 2. For both sets, the $(4d,4f)$ Slater integrals bring the largest contributions, although for the first set the $4f$ subshell is "active," whereas it is "passive" for the second set. In the three lowest lines of Table I, the average wave numbers T_{av} of the arrays, their average wavelengths λ_{av}, and their FWHM are shown. In the cases of the $4d$-$4f$ arrays, the comparison of δE (line 4) with T_{av} (line 6) shows the importance of the δE shift, as it changes λ_{av} by 15% or more.

All the arrays strongly overlap, as do also the lower and upper configurations in Fig. 1. The latter fact raises the question: Is it valid to apply the RELAC *ab initio* code and the angular results for the various σ and δE quantities as if the configurations were pure and isolated? The answer depends on the magnitude of the Slater integrals relevant to the mixing between the configurations. These integrals are

$$R^k(4f4f,4f5p) ,$$

$$R^k(4f5p,5p5p) ,$$

$$R^k(4f4d,5p4d) ,$$

and

$$R^k(4f4d,4d5p)$$

with appropriate values of k. Upon inspection of

TABLE II. Numerical formulas for the δE shift in the l^{N+1}-$l^N l'$ transition array. See text and Ref. 1, Eq. (14). For example, the formulas for f^{N+1}-$f^N d$ and d^{N+1}-$d^N f$ only differ by the value of $4l+1$.

Transitions	δE
$p \rightleftarrows s$	$\frac{N}{4l+1}[\frac{1}{2}G^1(p,s)]$
$d \rightleftarrows p$	$\frac{N}{4l+1}[-\frac{1}{5}F^2(d,p)+\frac{19}{15}G^1(d,p)-\frac{3}{70}G^3(d,p)]$
$f \rightleftarrows d$	$\frac{N}{4l+1}[-\frac{8}{35}F^2(f,d)-\frac{2}{21}F^4(f,d)+\frac{137}{70}G^1(f,d)$ $-\frac{2}{105}G^3(f,d)-\frac{5}{231}G^5(f,d)]$

their relative magnitudes and those of the "diagonal" integrals which are much larger, it can be inferred that configuration mixing, although possibly responsible for strong local level mixing, should not spoil appreciably the pure-configuration variances mentioned above.

III. EMISSIVE ZONES

In their schematic representation of the low configurations of Gd XII, Carroll and O'Sullivan (Ref. 4, Fig. 6) also indicate the expected location of those levels of each upper configuration which radiate strongly towards the lower configurations. They infer this qualitative result from lists of f values calculated by Sugar[10] for a series of $4d$-$4f$ absorption spectra from the ground levels of triply ionized lanthanides. Actually, these ground levels are of no particular interest in the present problem, so a different approach must be chosen.

For that purpose, it is necessary to compute a weighted average of the energies of the upper states, the weight being for each state n the sum of the intensities (or, more simply, of the strengths S_{mn}) of the transitions which start from that state (a *state* means, in the following, an *atomic wave function* in intermediate coupling, not a *level*). This average can be written, in the l^{N+1}-$l^N l'$ case, as

$$q(l^N l') = \sum_{mn} E_n S_{mn} / \sum_{mn} S_{mn} \ , \tag{1}$$

where E_n is the energy of the upper state n and where the sums run over all the states m and n of the lower and upper configurations. If the analogous average were computed for the energies E_m of the lower states, the result would be

$$q(l^{N+1}) = E_{\mathrm{av}}(l^{N+1}) \ ,$$

the simple average of the energies of the states of l^{N+1}; this comes from the fact that $\sum_n S_{nm}$ is here a quantity independent of m, according to the well-known J-file sum rule of Condon and Shortley,[5] valid in the l^N configurations (the dependence on n of $\sum_m S_{mn}$ is studied in Sec. IV). Now, it is evident that

$$q(l^N l') - q(l^{N+1}) = T_{\mathrm{av}}(l^N l' \rightarrow l^{N+1}) \ , \tag{2}$$

the weighted average energy (or wave number) of the transition array. From the definition of the δE quantity (see Sec. II), it is found that

$$q(l^N l') = E_{\mathrm{av}}(l^N l') + \delta E(l^N l' \rightarrow l^{N+1}) \ . \tag{3}$$

This simple result means that the emissive states of $l^N l'$ are located, on the average, at δE above the center of gravity of the configuration. It is not changed if a passive open subshell λ^ν is added to both l^{N+1} and $l^N l'$.

It is also interesting to know how wide this zone of $l^N l'$ is. For that purpose, it is possible to evaluate the variance

$$\sigma_z^2 = \left(\sum_{mn} E_n^2 S_{mn} / \sum_{mn} S_{mn}\right) - \left(\sum_{mn} E_n S_{mn} / \sum_{mn} S_{mn}\right)^2 \ , \tag{4}$$

where the subscript z stands for "emissive zone." The result is easily obtained, because σ_z^2 is that part of

$$\sigma_{\mathrm{array}}^2 = \left[\sum_{mn} (E_n - E_m)^2 S_{mn} / \sum_{mn} S_{mn}\right] - \left[\sum_{mn} (E_n - E_m) S_{mn} / \sum_{mn} S_{mn}\right]^2 \tag{5}$$

which contains only Slater and spin-orbit integrals of the $l^N l'$ configuration. This means taking into account, in Table II of Ref. 1, only the parts with the N-dependent coefficients denoted y, v, and w, plus the second, third, and sixth parts of H_7.

In the same manner, for the array $l^{N+1}\lambda^\nu \ldots$-$l^N l' \lambda^\nu \ldots$, σ_z^2 comprises the parts of $\sigma_{\mathrm{array}}^2$ given in Ref. 2 which contain only energy integrals of the upper configuration. The numerical values of σ_z for the 11 arrays relevant to the case of Gd XII (Fig. 1) are given in the fifth line of Table I. It can be noticed that, although σ_z^2 is a part of $\sigma_{\mathrm{array}}^2$, it is larger in all the cases studied. This is not surprising since many contributions to $\sigma_{\mathrm{array}}^2$ have a negative value.

A schematic representation of the location and of the widths of the emissive zones is given in Fig. 1, in the shape of narrow hatched rectangles of vertical dimension 2.355 σ_z. Five among the six upper configurations give rise to two different arrays. For each of them, two hatched rectangles are drawn, the left one for the $4d$-$5p$ transition and the right one for $4d$-$4f$. Two remarkable phenomena appear, which are discussed below.

(i) The location of the emissive zone in a given upper configuration strongly depends on the transition considered; this is directly linked with the different magnitudes of δE for the two sets of arrays (fourth line of Table I) (see Sec. II).

(ii) The emissive zone, for the $4d$-$4f$ transitions, may even lie well above the bulk of the state distribution.

IV. METASTABILITY AND THE G^1 COEFFICIENTS

To understand more deeply the peculiar location of the emissive zones for the $4d$-$4f$ transition (six

upper hatched rectangles on Fig. 1), it is interesting to study the dependence of the J-file sum of Condon and Shortley (Ref. 5, p. 279) on the quantum numbers, in the configurations where it is not simply proportional to $2J+1$. Let us recall that a J-file sum is the sum of the strengths of all the transitions connecting a given J level with the states of the other configuration.

The prototype of the configurations mentioned above is $l^N l'$ in the l^{N+1}-$l^N l'$ array. The basic sum to be computed in this case is

$$\sum_m S_{mn} = \sum_m ((l^N l')n \mid \vec{D} \mid l^{N+1} m) \times (l^{N+1} m \mid \vec{D} \mid (l^N l')n) , \quad (6)$$

where $\vec{D} = -e\sum_i \vec{r}_i$ is the usual dipole operator. In the second-quantization formalism (see Judd[11]), the $\vec{D}$ operators in the sum can be written, respectively,

$$\sum_{\alpha\beta} b_\alpha^\dagger (\alpha \mid \vec{d} \mid \beta) a_\beta$$

and

$$\sum_{\gamma\delta} a_\gamma^\dagger (\gamma \mid \vec{d} \mid \delta) b_\delta ,$$

where $a, a^\dagger$ ($b, b^\dagger$) annihilate and create states of a single l (l') electron. The resulting product can be transformed by using

$$b_\alpha^\dagger a_\beta a_\gamma^\dagger b_\delta = b_\alpha^\dagger b_\delta \delta(\beta,\gamma) + b_\alpha^\dagger a_\gamma^\dagger b_\delta a_\beta . \quad (7)$$

In this expansion, the first term is a one-electron operator acting on the l' electron, and the second term, when combined with the monoelectronic elements of $\vec{d}$, is a multiple of the bielectronic operator $\sum_{i>j}(C_i^{(1)} C_j^{(1)})$ acting on an l,l' pair, which also occurs in the expansion of the electrostatic operator $\sum_{i>j} e^2/r_{ij}$. The final result therefore is not surprising: the sum $\sum_m S_{mn}$ of Eq. (6) is equal to

$$k((l^N l')n \rightarrow l^{N+1}) = [l_> /(2l'+1) + C(G^1;n)](I_{ll'})^2 , \quad (8)$$

where $l_>$ is the larger of l and l', $C(G^1;n)$ is the coefficient of the $G^1(l,l')$ Slater integral in the electrostatic energy of the state n, and

$$I_{ll'} = e\int_0^\infty R_l(r) r R_{l'}(r) dr$$

is the usual dipolar radial integral. The corresponding J-file sum can then be written as

$$k((l^N l')\alpha J \rightarrow l^{N+1}) = (2J+1)[l_> /(2l'+1) + C(G^1;\alpha J)](I_{ll'})^2 . \quad (9)$$

Of course, k cannot be negative. But it can be zero (for some states in extreme coupling schemes), in which case the state is metastable as regards the $l' \rightarrow l$ transition. Conversely, all such metastable states (in Russell-Saunders coupling, whole terms) correspond to the same value of the G^1 coefficient. Many such cases can be found in the electrostatic matrices for the $d^N p$ configurations.[12] For example, in pure Russell-Saunders coupling, 180 among the 270 states of $d^8 p$ are metastable with respect to the $p \rightarrow d$ transition. An extreme case is that of the $l^{4l+1} l'$ configuration, in which only the ^1P term, with 3 states, combines radiatively with $l^{4l+2}\,^1S$, whereas the $[(4l+2)(4l'+2)-3]$ other states are metastable with respect to the $l' \rightarrow l$ transition. This agrees with the well-known behavior of the $G^k(l,l')$ coefficients in the $l^{4l+1} l'$ configurations (Ref. 5, pp. 298 and 299). For example, if $G^1(f,d)$ was the only nonzero energy integral in $d^9 f$, the standard deviation σ_{upper} of that configuration would be less than $0.3G^1$ and the δE quantity about $2G^1$. The array $4d^{10}5p^5$-$4d^9 4f 5p^5$, on the extreme right of Fig. 1, is close to that situation because the $4d$-$4f$ interaction is by far the predominant interaction.

It can be noticed that the ratio $\delta E/\sigma_{\text{upper}}$ increases with N in the l^{N+1}-$l^N l'$ series, because δE is proportional to N, whereas the (l,l') part of σ^2_{upper} has a parabolic $N(4l-N+2)$ dependence on N.

Along the same lines as above, the J-file sum for a level αJ of the upper configuration in the $l^{N+1} l'^{N'-1}$-$l^N l'^{N'}$ array is found to be equal to

$$k((l^N l'^{N'})\alpha J \rightarrow l^{N+1} l'^{N'-1}) = (2J+1)[N' l_> /(2l'+1) + C(G^1;\alpha J)](I_{ll'})^2 . \quad (10)$$

The factor $(2J+1)$ is to be replaced by $(2S+1)(2L+1)$ when the sum is computed for a whole (S,L) term in pure Russell-Saunders coupling. These results are unchanged if a passive subshell λ^ν is added to both configurations.

If configuration mixing affects, for example, the upper configuration, the J-file sum still depends in the same way on the coefficient(s) $C(G^1;\alpha J)$, but each associated N'-dependent term in Eq. (10) has to be multiplied by the relevant percentage of the level αJ for the corresponding configuration.

The formal expression for the J-file sum in Eq. (10) can be used for checking extensive angular calculations for electric dipole strengths in any pure or

intermediate coupling. Very simple checks of this kind can be made by comparing Table 3[9] of Condon and Shortley (Ref. 5, p. 251) or Tables I—III of Ufford and Miller[13] with Appendix 21 of Slater.[12] It can also be noticed that the sum rule in Eq. (A6) of Starace[14] is the particular case $N'=4l'+2$ of Eq. (10).

Equation (10) can be summed over αJ to yield the total strength of the array. The result, which is evidently the same whichever configuration is above the other, is

$$K=\sum_n k((l^N l'^{N'})n\rightarrow l^{N+1}l'^{N'-1}) =2l_> \begin{bmatrix} 4l+1 \\ N \end{bmatrix} \begin{bmatrix} 4l'+1 \\ N'-1 \end{bmatrix} (I_{ll'})^2 , \quad (11)$$

a formula in agreement with Eq. 31.67 of Sobelman[15] and with Eq. 14.92 of Cowan.[16] If a passive open subshell λ^ν is added to both combining configurations, K is to be muliplied by

$$\begin{bmatrix} 4\lambda+2 \\ \nu \end{bmatrix}$$

(Ref. 16, Eq. 14.93).

V. CONCLUSION

The first part of the present work, i.e., the quantitative prediction of the locations and widths of low configurations and their transition arrays in a highly ionized atom has been achieved through the combined use of an *ab initio* relativistic computer code and of statistical properties already formally available. In the second part, the zones of the upper configurations which undergo strong transitions towards the lower configurations have been determined in location and width. In the configurations which give rise to two arrays, the emissive zone is not the same for both arrays. For the $4d$-$4f$ arrays, this zone lies well above the main part of the upper configuration, a fact which is linked with the J-file sums and with the coefficients and value of the $G^1(4f,4d)$ integral.

If an analogous question was asked about the zones of the *lower* configurations which combine strongly with the upper configurations, the answer would be easily given. Because the J-file sum rule applies to each of the lower configurations studied, the sum $\sum_n S_{mn}$ is independent of m, and

$$q(\text{lower})=\sum_{mn} E_m S_{mn} / \sum_{mn} S_{mn}$$

is identical to the simple average E_{av} (lower); therefore the "absorbant zones" have the same locations and widths as the lower configurations themselves. The same is true for both configurations in the arrays of the type $l^N l'$-$l^N l''$.

The situation about the J-file sum rules can now be summarized.

(i) For an electric dipole jump between two pure configurations, $l''l^N\ldots\rightarrow l'l^N\ldots$, the strength of the J file (i.e., the sum of the strengths of all the lines departing from—or ending in—a given αJ level) is proportional to $2J+1$.

(ii) For an electric dipole jump between two pure configurations,

$$l^N l'^{N'} l''^{N''}\ldots\rightarrow l^{N+1}l'^{N'-1}l''^{N''}\ldots ,$$

when all the formal energies of a group of levels contain the exchange Slater integral $G^1(l,l')$ with the same coefficient (possibly, zero), the strengths of the J files referring to these levels are proportional to $2J+1$.

(iii) For the same jump as in (ii), when the coefficient of $G^1(ll')$, denoted $C(G^1;\alpha J)$, has not the same value for all the considered J levels, the strengths of the J files are a linear function of $C(G^1;\alpha J)$; this linear function is, for the initial levels αJ of the array $l^N l'^{N'} l''^{N''}\ldots\rightarrow l^{N+1}l'^{N'-1}l''^{N''}\ldots$,

$$k([l^N l'^{N'} l''^{N''}\cdots)\alpha J\rightarrow l^{N+1}l'^{N'-1}l''^{N''}\cdots)=(2J+1)[N'l_>/(2l'+1)+C(G^1;\alpha J)](I_{ll'})^2 , \quad (12)$$

where $l_>$ is the larger of l and l'. The result given in (ii) is evidently a particular case of Eq. (12).

Equation (12) gives the answer to the problems raised by Starace (Ref. 14, p. 1783) and by Sobelman (Ref. 15, p. 315).

Concerning the case of Gd XII studied in Sec. II as a prototype, other important results are significant.

(i) The transition radial integral

$$I_{4d4f}=e\int_0^\infty R_{4d}(r)rR_{4f}(r)dr$$

is about 2.5 times larger than I_{4d5p} in the present *ab initio* evaluation.

(ii) The sum of the angular parts of all the strengths of a given array shows a marked decrease from the left to the right sides of Fig. 1; it is, for example, equal to 7722 for $4d^{10}4f^5$-$4d^9 4f^6$ and 280 for $4d^{10}4f\,5p^4$-$4d^9 4f\,5p^5$.

(iii) The ionization limit, which is represented on Fig. 1 by a broken horizontal line, brings in another reason for the arrays on the right side of the same figure not to contribute appreciably to the spectrum.

(iv) Other sets of arrays, for example,

$$4d^{10}5s\,4f^{M}5p^{M'}-4d^{9}5s\,4f^{M+1}5p^{M'}\ ,$$

correspond to lower (and upper) configurations in the same ranges of energy as those in Fig. 1 and should be considered.

(v) The ratio of the intensities of two arrays originating from the same upper configuration may not be equal to the ratio of their total line strengths, since the emissive zones may be partially disconnected and differently populated, according to the plasma conditions. However, this does not contradict the fact that the ratio of the total intensities of two transition arrays arising on the same lower configuration can yield information on the populations of the upper configurations, as claimed in Refs. 1 and 2.

Whereas facts (i)—(iii) would result in a simplification of the Gd XII spectrum, the occurrence of other sets of arrays [see (iv)] would make it more complex. Moreover, neighboring ions like Gd XI, Gd XIII, etc., are also present in the emitting plasma. Consequently, much more work would be needed for interpreting the broad, rather structureless pattern which has been published for gadolinium by Carroll and O'Sullivan.[4]

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