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Relativistic effects on transition probabilities in the Mg isoelectronic sequence

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The dipole oscillator strengths (f) for some transitions within the ground complex of the magnesium isoelectronic sequence up to nobelium ($Z = 102$) are calculated using the relativistic wave functions obtained by the parametric-potential method. The length and velocity formulations are used for the transition operator. For the resonance lines, the trend along the sequence differs strongly from the predictions of the *nonrelativistic* Z-dependent theory of many-electron atoms. This behavior is explained in the framework of the *relativistic* Z-dependent theory, which introduces a double power-series expansion in Z^{-1} (for correlation) and $Z^2\alpha^2$ (for relativistic effects). The f value for the first resonance transition increases for low values of Z, as the departure from the Russell-Saunders coupling becomes more important, and decreases at high values of Z owing to the contraction of the orbitals toward the nucleus. The f value for the second resonance transition does not fall off for large Z, since the frequency of the transition increases approximately as Z^4 for high values of Z, owing to the relativistic corrections (spin-orbit, Darwin, and p^4 terms). The length and velocity formulations are discussed, with particular emphasis on how relativistic contributions to the transition energies or to the transition matrix elements occur. Corrections coming from the finite size of the nucleus, the Breit interaction, and the Lamb shift are introduced; although they are significant, they do not alter the general shape of the curves giving the Z dependence of the f values. On the contrary, retardation effects remain unimportant over the entire range of Z.

I. INTRODUCTION

With the increasing interest in controlled thermonuclear reactions, it becomes necessary to study the dipole oscillator strengths (f) for the resonance transitions of highly ionized atoms, in order to estimate the energy loss through impurity ions in the plasma. For the lower stages of ionization (< 15), the systematic trends of the f values along an isoelectronic sequence have been studied in great detail.[1,2] For higher stages of ionization where no experimental data are available, the theoretical studies are mostly based on a perturbation expansion of the nonrelativistic many-electron Hamiltonian in inverse powers of the nuclear charge Z.[3] In this model, for transitions without change in the principal quantum number of the excited electron, the f value for high values of Z decreases as Z^{-1}.

Recently several authors have obtained a very different Z dependence, pointing out that relativistic effects cannot be neglected. Sinanoǧlu and Luken[4] introduced semiempirically the spin-orbit interaction to study oscillator strengths within the shell $n=2$ of the boron sequence. Weiss[5] carried out intermediate coupling calculations with the low-Z Pauli approximation.[6] More recently, Younger and Weiss[7] evaluated in the hydrogenic approximation, the magnitude of the relativistic corrections to the dipole transition matrix element expressed in the length form. Lastly Kim and Desclaux[8] studied the resonance transitions of Li- and Be-like ions in the relativistic Hartree-Fock approximation; they showed that for highly charged ions of the Be I sequence the results deviate strongly from the predictions of the nonrelativistic Z-expansion method.

In this paper we point out that a similar Z dependence can be obtained for the resonance lines of the magnesium isoelectronic sequence, in the framework of the relativistic parametric-potential method.[9] We show that such behavior can be analyzed by means of the relativistic Z-dependent theory of Layzer and Bahcall,[10] which introduces a double power-series expansion in Z^{-1} and $Z^2\alpha^2$ ($\alpha \simeq \frac{1}{137}$ is the fine-structure constant). Corrections arising from the finite size of the nucleus, and from radiative corrections (Breit interaction and Lamb shift) are studied, but they do not alter the main features of the Z dependence. The oscillator strengths are calculated with the length and velocity formulations of the electric dipole operator. We show that the distinction between the contributions of the relativistic effects either on the energy or on the transition operator is somewhat arbitrary, on account of the equivalence between the length and the velocity formulations. Moreover the length formulation is scarcely modified by the relativistic effects; on the contrary, in the velocity formulation relativistic effects cannot be neglected.

II. RELATIVISTIC CALCULATION OF ATOMIC ENERGY LEVELS

A. Z dependence of the relativistic Hamiltonian for a many-electron atom

The relativistic study of one- and two-electron atoms has been extensively reviewed by Bethe and Salpeter.[6] Layzer and Bahcall[10] extended the nonrelativistic Z-expansion formalism to include relativistic effects up to quantities comparable in magnitude with the Lamb shift. Doyle[11] calculated energy levels for atoms with up to ten electrons in the first two shells, using unscreened relativistic hydrogenlike wave functions. We recall here only the main results.

In the central-field approximation the wave function for a relativistic state can be written as

$$|nljm) = \begin{bmatrix} [G_{nlj}(r)/r]\,|ljm\rangle \\ \\ i[F_{nlj}(r)/r]\,|\bar{l}jm\rangle \end{bmatrix}, \quad \text{where } \bar{l} = 2j - l\,. \tag{1}$$

The small component F_{nlj} is of the order of $Z\alpha$ compared with the large component G_{nlj}, which reduces to R_{nl} in the nonrelativistic limit. For an atom of nuclear charge Z, the unit of length a_0/Z is chosen, where a_0 is the Bohr radius. The radial wave functions (G_{nlj}/r and $F_{nlj}/rZ\alpha$) and the corresponding eigenvalue ϵ_{nlj} can be written as an expansion in powers of $\chi = Z^2\alpha^2$.[11] In the particular case of the Coulomb potential $-Z/r$, the coefficients of the expansion do not depend upon Z.

As in the nonrelativistic case the electrostatic interaction Q between the electrons is of the order of Z^{-1} compared with the Dirac Hamiltonians ($H^0 = \Sigma_i h_i$) of the electrons moving in the potential of the nucleus. If Q is treated as a perturbation of H^0, the matrix elements of Q can be expanded in powers of Z^{-1}; the leading term, which is proportional to Z, corresponds to the electrostatic interaction between states belonging to the same complex.[3]

The Breit interaction B is a relativistic correction to the electrostatic interaction between the electrons. Layzer and Bahcall[10] have shown that the most often used form of the Breit interaction obtained for $\chi \ll 1$ is accurate over the entire range of Z, up to quantities of higher order than the Lamb shift. The leading term of B is of order χ compared with Q.

Finally relativistic energies can be written as a double-power-series expansion in Z^{-1} and χ (in atomic units)

$$\begin{aligned} E(\gamma J) &= Z^2 \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} A_{pq}(\gamma J)(Z^2\alpha^2)^p Z^{-q} \\ &= A_{00}Z^2 + A_{01}Z + A_{02} + A_{10}Z^4\alpha^2 + A_{11}Z^3\alpha^2 + \cdots\,. \end{aligned} \tag{2}$$

In the hydrogenlike approximation A_{00} is the same for all the states of a given complex: $A_{00} = -\sum 1/2n^2$; A_{01} corresponds to the nonrelativistic electrostatic interaction among states belonging to the same complex, and A_{11} introduces relativistic two-body interactions coming from Q and B (orbit-orbit, spin-spin, spin-other-orbit, ...) within the complex. The coefficient A_{02} can be obtained by a first-order calculation of the extracomplex configuration interaction arising from the nonrelativistic electrostatic interaction. Relativistic one-electron operators (spin-orbit, Darwin, and mass-correction terms) are introduced by means of A_{10}; for a pure hydrogen type j-j state, A_{01} depends upon the n and j values of the orbitals, but not upon l.

The expansion (2) is not unique, since the coefficients A_{pq} depend generally upon $\chi Z = Z^3\alpha^2$. The coefficients A_{pq} are constant only for the special case of a single level γJ in the complex with a given angular momentum J.

The predominant terms of the expansion (2) are different according to the range of Z studied. For low Z values, A_{00}, A_{01}, and A_{02} give rise to the main contributions (Russell-Saunders coupling with extracomplex configuration interactions). On the contrary for high Z values, A_{01} and A_{02} are almost negligible, but the relativistic one- and two-body interactions (A_{10} and A_{11}) are predominant (j-j coupling within a given complex).

B. Relativistic radial wave functions and intermediate coupling

1. *Relativistic radial wave functions*

To compute the relativistic radial wave functions, we use the relativistic parametric-potential method described in a previous paper.[9] We briefly indicate the principal points of this method. The zero-order Hamiltonian for an N-electron atom is the sum over one-electron Dirac Hamiltonians corresponding to the central potential $U(r)$. In the parametric-potential method $U(r)$ is represented by an analytic function depending upon a set of parameters, each parameter describing the distribution of charges in a given shell of the atomic core. For the Mg I isoelectronic sequence three parameters are introduced: two (θ_1 and θ_2) associated with the K and L shells of the core, the third (θ_3) corresponding to the mean potential produced by an electron of principal quantum number

$n=3$.

The following formula is used[9]:

$$U(r)=-(1/r)[I+2g_0(\theta_1 r)+8g_1(\theta_2 r)+g_0(\theta_3 r)]\,,$$

where

$$g_l(\theta_i r)=\frac{1}{2(l+1)^2}\sum_{L=0}^{l}(4L+2)f_L(\varphi_L r)\,,$$
$$\varphi_L=\frac{\theta_i(L+1)}{1-0.03L(L+1)}\,, \tag{3}$$
$$f_L(\varphi_L r)=e^{-\varphi_L r}\sum_{j=0}^{2l+1}\left(1-\frac{j}{2l+2}\right)\frac{(\varphi_L r)^j}{j!}\,.$$

For an atom with N electrons and the nuclear charge Z, $I=Z-N+1$. In this work the optimal potential minimizes the total first-order energy of the ground level $3s^2\,{}^1S_0$ of the spectrum, the first-order Hamiltonian excluding the Breit interaction. The optimal potential being the same for all orbitals within the spectrum studied, it is possible to compute the radial wave functions of excited states by numerically solving systems of two coupled first-order differential equations.

2. *Intermediate coupling*

Multiconfiguration wave functions are used for the ground state and for the excited states. The purpose of this work was to study the Z dependence of the f values for the resonance transitions of the Mg I sequence; consequently, only the interactions within the complex $(n=3)^2$ are introduced, since they are predominant at moderate and high values of Z. In this approximation, the wave function of an even state ($J=0$) or the wave function of an odd state ($J=1$) can be expanded over five relativistic states. The mixing coefficients and the energies are obtained by diagonalizing either the matrix H^0+Q or the matrix H^0+Q+B. The transition energies are equal to the difference between the eigenvalues of the corresponding levels.

We shall show further (Sec. V) that it is possible to introduce in an approximate way corrections arising from the Lamb shift and from the finite size of the nucleus.

III. RELATIVISTIC TREATMENT OF ELECTRIC DIPOLE TRANSITIONS

A. General formulas

The lowest-order term which appears in the study of a transition from the state $|\Psi_{JM})$ to the state $|\Psi_{J'M'})$ through emission or absorption of one photon of momentum $\vec{k}$ and polarization $\vec{e}$ is given by[12]

$$(\Psi_{JM}|\sum_j \vec{\alpha}_j\cdot\vec{e}\,e^{i\vec{k}\cdot\vec{r}_j}|\Psi_{J'M'})=(\Psi_{JM}|\vec{T}_\nabla\cdot\vec{e}|\Psi_{J'M'})\,, \tag{4}$$

where $\vec{\alpha}_j$ is the Dirac vector of the jth electron of the atom, and $\vec{T}_\nabla$ the transition operator expressed in the velocity formulation. When the retardation is negligible, i.e., $e^{i\vec{k}\cdot\vec{r}_j}\simeq 1$, and when the wave functions are the zero-order functions Ψ^0_{JM} and $\Psi^0_{J'M'}$ of a given central potential, associated with the energies E^0_J and $E^0_{J'}$, it is possible to write.

$$i\alpha(\Psi^0_{JM}|\sum_j \vec{r}_j|\Psi^0_{J'M'})(E^0_J-E^0_{J'})$$
$$=(\Psi^0_{JM}|\sum_j \vec{\alpha}_j|\Psi^0_{J'M'})\,. \tag{5}$$

This relation leads to the length formulation of the transition operator $\vec{T}_r=\sum_j \vec{r}_j$.

The absorption oscillator strengths in the velocity and in the length formulation are defined by

$$f_\nabla(\Psi_J\rightarrow\Psi_{J'})=2.7477\times10^9\,\frac{1}{\sigma(2J+1)}\,D^2_\nabla\,,$$
$$f_r(\Psi_J\rightarrow\Psi_{J'})=3.0375\times10^{-6}\,\frac{\sigma}{2J+1}\,D^2_r\,, \tag{6}$$

where σ (in cm^{-1}) is the wave number of the transition and where D^2, the square of the transition matrix element expressed in atomic units, is defined by

$$D^2=\sum_{MM'}(\Psi_{JM}|\vec{T}|\Psi_{J'M'})^2\,.$$

When central-field wave functions are used, D_∇ can be expressed by means of radial integrals such as

$$\int_0^\infty G_{nlj}F_{n'l'j'}\,dr=\langle nlj\,|\overline{n'\,l'j'}\rangle\,. \tag{7}$$

The radial integrals which appear in the expression D_r are

$$\int_0^\infty r(G_{nlj}G_{n'l'j'}+F_{nlj}F_{n'l'j'})\,dr=\langle nlj\,|\,r\,|\,n'l'j'\rangle\,. \tag{8}$$

On account of the types of radial integrals (7) and (8), it is impossible to separate the relativistic contributions to the transition operator coming from either the large components G or the small components F of the radial wave functions.

B. *Z* dependence of the transition matrix element

In this section we restrict the discussion to the transitions $s\rightarrow p$, which appear in the study of the resonance lines of the Mg I sequence. For one-electron wave functions, the matrix elements of the operator $\vec{\alpha}$ are given by

$$(s_{1/2}\|\vec{\alpha}\|p_{3/2}) = -\frac{4i}{\sqrt{3}}\langle p_{3/2}|\bar{s}_{1/2}\rangle = \frac{2}{\alpha\sqrt{3}}(\epsilon_{p_{3/2}} - \epsilon_{s_{1/2}})\langle s_{1/2}|r|p_{3/2}\rangle ,$$
$$(s_{1/2}\|\vec{\alpha}\|p_{1/2}) = i\left(\frac{2}{3}\right)^{1/2}(\langle p_{1/2}|\bar{s}_{1/2}\rangle + 3\langle s_{1/2}|\bar{p}_{1/2}\rangle) = \frac{1}{\alpha}\left(\frac{2}{3}\right)^{1/2}(\epsilon_{p_{1/2}} - \epsilon_{s_{1/2}})\langle s_{1/2}|r|p_{1/2}\rangle . \tag{9}$$

Along an isoelectronic sequence, when hydrogenlike Dirac wave functions are used, it is possible to write

$$\langle nlj|r|n'l'j'\rangle = (A/Z)(1 + B\alpha^2Z^2 + \cdots) \tag{10}$$

where B is related to the contraction of the relativistic orbitals toward the nucleus, with increasing Z. Consequently for one-electron wave functions, D_r varies approximately as Z^{-1}.

The Z dependence of D_∇ depends simultaneously upon the variations of $\Delta\epsilon = \epsilon_{nlj} - \epsilon_{n'l'j'}$ and $\langle nlj|r|n'l'j'\rangle$.

For $ns \rightarrow n'p$ transitions ($n \neq n'$), the leading term of $\Delta\epsilon$ varies as Z^2, so that D_∇ is proportional to Z, as in the nonrelativistic theory.

For the $ns_{1/2} \rightarrow np_{3/2}$ transition, $\Delta\epsilon$ increases as Z^4 for high values of Z (spin-orbit interaction) so that D_∇ is proportional to Z^3. For the $ns_{1/2} \rightarrow np_{1/2}$ transition $\Delta\epsilon$ varies as Z (nonrelativistic electrostatic interaction within the complex), consequently D_∇ remains approximately constant along the isoelectronic sequence. The different behavior of the intracomplex $ns_{1/2}$-np_j transitions ($j=\frac{1}{2}$ or $j=\frac{3}{2}$) is simply due to the relativistic contributions to the transition frequency.

C. Relativistically allowed decay; length and velocity formulations

Using the effective operator formalism,[13] the transition operator for $s \rightarrow p$ transitions can be written in the equivalent form

$$O^{(1)} = R_{01}w^{(01)1}(s,p) + R_{11}w^{(11)1}(s,p) , \tag{11}$$

where the double-tensor operator has been defined by Feneuille.[14] The R_{11} coefficient, which vanishes in the nonrelativistic limit, corresponds to specific relativistic effects; R_{11} is associated with the relativistically allowed spontaneous decay of the intercombination transitions,[15] ${}^3P_1$-${}^1S_0$ for example. In this section we will show that the magnitude of the ratio R_{11}/R_{01} depends upon the formulation chosen (length or velocity).

The velocity formulation has been already used by one of us[15] with success, to perform calculations of the resonance line ${}^3P_1$-${}^1S_0$ in group-II elements. These calculations showed that the transition probabilities were reduced by a factor of approximately 2, when the relativistically allowed decay (direct part) is added to the indirect part coming from the intermediate coupling.

Recently, Drake[16] using nonrelativistic wave functions has shown that both indirect and direct parts are automatically included, provided that the transition matrix element is expressed in the length formulation. This result is approximately valid when relativistic wave functions and operators are used, as is shown below.

In the Appendix we show that in the length formulation R^r_{11}/R^r_{01} is proportional only to the relative variation of the radial integrals $\langle s_{1/2}|r|p_j\rangle$ ($j=\frac{1}{2}$ or $\frac{3}{2}$) [cf. Eq. (10)]. This value always remains small, even for highly ionized spectra. Moreover, for low values of Z ($\chi \ll 1$), the relative order of magnitude of the relativistically allowed decay, R_{11}/R_{01} is greater in the velocity formulation than in the length formulation, by the quantity $\chi\xi_p/(\sqrt{2}\,\Delta\epsilon)$, which varies as Z^3 for intracomplex transitions ($\chi\xi_p$ is the fine-structure constant of the p electron). For high values of Z R_{11}/R_{01} is almost equal to the hydrogenlike value: $R^r_{11}/R^r_{01} \approx 0$ and $R^\nabla_{11}/R^\nabla_{01} \approx 1/\sqrt{2}$.

In conclusion, when the length formulation is used, the relativistically allowed decay remains almost negligible over the entire range of Z, and the relativistic corrections are almost exclusively introduced by taking into account the shift of the wave functions toward the nucleus. On the contrary, in the velocity formulation the relativistic operator $w^{(11)1}$ cannot be neglected: R^∇_{11} introduces simultaneously the relativistic contraction of the orbitals and contributions coming from the spin-orbit interaction. The length formulation gives more weight to the part of the wave functions which extends far from the nucleus, so that the corresponding matrix element is less sensitive to relativistic effects than in the velocity formulation. On account of the equivalence of the length and velocity forms of the transition matrix element, relativistic effects either on transition frequencies or on radial matrix element are closely related, and the distinction between these is somewhat arbitrary.

D. Choice of the formulation used

The dipole and velocity formulas give different numerical values, when approximate wave functions are used, and it is impossible to know in a pure theoretical way, which expression is the more suitable. Pragmatically, cancellation effects occur in the calculation of the transition matrix element; the numerical value of the transition matrix element is more sensitive to small changes in the wave functions when the cancellation is important. Consequently the more reliable results are undoubtedly those for which the cancellation effects are the least. Moreover, when retardation effects cannot be neglected, the velocity formulation enables one to introduce them in a simple way.

In this work we use both formulations to study the f values of the resonance lines of the Mg I sequence. The difference between the results gives an indication on the magnitude of the contributions coming from the extracomplex correlation effects, which are neglected in our treatment.

IV. RESULTS

The method described above has been used for computing the f values for all $J=0\rightarrow J'=1$ transitions within the $(n=3)^2$ complex of the Mg I isoelectronic sequence. We study in great details the resonance lines. In our notations, the ground state is s_0, the lowest $J'=1$ level is p_1', and the second $J'=1$ level is p_1''. Neglecting configuration interactions, the state s_0 belongs to the $3s^2$ configuration. For the first ions of the sequence, deviations from LS coupling are almost negligible, and the levels p_1' and p_1'' correspond respectively to the $3s3p\,^3P_1$ and $3s3p\,^1P_1$ states. As Z increases, the coupling gradually changes into the j-j coupling scheme, for which p_1' and p_1'' become identical to the $(3s_{1/2}3p_{1/2})J'=1$ and $(3s_{1/2}3p_{3/2})J'=1$ states. The transition energies for s_0-p_1' and s_0-p_1'' are denoted by σ' and σ'', and the corresponding f values by f' and f''.

In Fig. 1, f' and f'' are plotted vs Z; the f values are obtained to the first-order approximation, neglecting the Breit interaction and using either the velocity formula or the length formula. The curves are very similar to those obtained for the Be I sequence by Kim and Desclaux[8] using relativistic Hartree-Fock wave functions. The values of f' remain always smaller than those of f'' (notice the different scales), and for $Z>50$ both f values deviate appreciably from the results extrapolated from the lighter ions of the sequence using the qualitative predictions of the nonrelativistic Z-dependent theory.[2] Indeed the f' curve presents a broad flat maximum, and the f'' curve a significant minimum. These results are not at all surprising and can be predicted in the relativistic Z-dependent theory (Sec. II and III), as shown below.

A. Transition energies

In Fig. 2, $\ln\sigma'$ and $\ln\sigma''$ are plotted vs Z. For Z greater than 20 (extracomplex correlations almost negligible) the Z dependences of the energies σ' and σ'' are different. Indeed σ' grows very slowly over the entire range of Z, approximately as $Z^{1.6}$; for low values of Z, σ'' varies as $Z^{1.8}$ but increases more rapidly ($\sim Z^4$) for high values of Z. The Z dependence of the energy can be obtained from the relation (2); in this expansion the coefficients A_{pq} are not unique, since Z appears simultaneously in the powers series (Z^{-1} and χ) and in A_{pq}, in accordance with the fact that

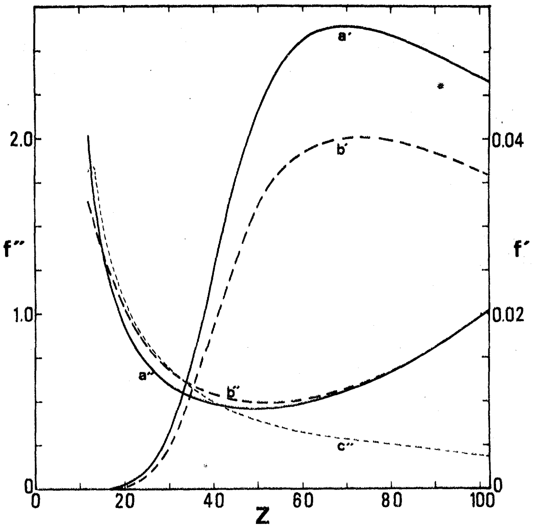

FIG. 1. Z dependence of the f values for the resonance lines of the Mg I sequence. a' (f_r) and b' (f_∇) correspond to the $s_0\rightarrow p_1'$ transition (scale on right); a'' (f_r), b'' (f_∇), and c'' (nonrelativistic, Ref. 2) correspond to the $s_0\rightarrow p_1''$ transition (scale on left).

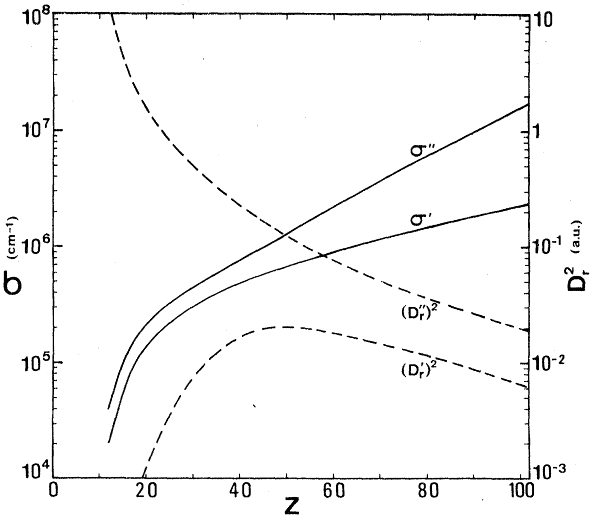

FIG. 2. Z dependence of the transition energies σ and of the transition matrix element $(D_r)^2$ for the resonance lines. Prime corresponds to the $s_0\rightarrow p_1'$ transition and double prime to the $s_0\rightarrow p_1''$ transition.

correlation and relativistic effects are strongly connected. Nevertheless for a given range of Z expression (2) gives the gross feature of the Z dependence. We denote by $\Delta A'_{pq}$ the difference between the coefficients A_{pq} obtained in the study of the energy levels s_0 and p'_1 in a screened hydrogenlike approximation, and by $\Delta A''_{pq}$ the same for levels s_0 and p''_1.

The energy σ', which corresponds to a transition $\Delta n = \Delta j = 0$, vanishes if the correlation effects are negligible (hydrogenlike approximation). If only the configuration interactions within the complex $(n=3)^2$ are introduced $\Delta A'_{00} \approx \Delta A'_{10} \approx \Delta A'_{02} \approx 0$, so that it is possible to write

$$\sigma' \approx \Delta A'_{01} Z + \Delta A'_{11} Z^3 \alpha^2 .$$

In Fig. 3, σ'/Z is plotted vs Z^2 (σ' is obtained by the relativistic parametric-potential method). This curve shows that for intermediate values of Z, the departure from the hydrogenlike behavior is negligible. For high values of Z, σ'/Z increases more rapidly than Z^2, because the term $\Delta A'_{10} Z^4 \alpha^2$ arising from the one-electron relativistic operators cannot be neglected. Furthermore, the central potential introduces partially extracomplex correlation effects; the leading term, which does not depend upon Z, can explain the deviation from the straight line for low values of Z.

The Z dependence of σ'' is more complicated, and can be written as

$$\sigma'' \approx \Delta A''_{01} Z + \Delta A''_{10} Z^4 \alpha^2 + \Delta A''_{11} Z^3 \alpha^2 + \cdots .$$

For low values of Z, the term $\Delta A''_{01} Z$ (intracomplex interactions) is predominant; on the contrary for high values of Z, σ'' increases approximately as Z^4.

B. Transition matrix elements

Two phenomena occur simultaneously in the evaluation of the transition matrix elements: first, the intermediate coupling and the configuration mixing, and second the effects coming from the radial integrals.

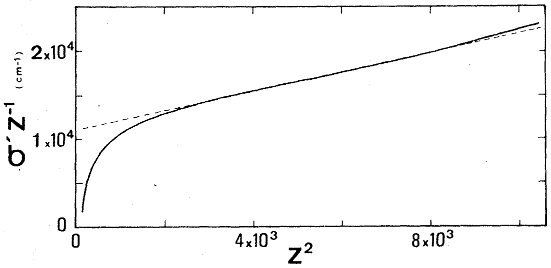

FIG. 3. Z dependence of the transition energy σ' of the $s_0 \rightarrow p'_1$ transition. $\sigma' Z^{-1}$ is plotted vs Z^2. The dashed curve points out that, in first approximation, $\sigma' Z^{-1}$ varies linearly with Z^2.

1. Intermediate coupling

Examples of the configuration-mixing coefficients for the levels s_0, p'_1, and p''_1 are given in Table I. For low values of Z, configuration interactions between the LS terms ^1S of the configurations $3s^2$, $3p^2$, and $3d^2$ are not negligible. As Z increases, the weight of the $(3p_{3/2})^2$ state falls rapidly, but the weight of the $(3p_{1/2})^2$ state decreases very slowly, inasmuch as the difference between the energies of the $3s_{1/2}$ and $3p_{1/2}$ orbitals remains small. For the p'_1 and p''_1 levels, the coupling in the low-Z region is close to the LS coupling limit within a sp configuration, and for p''_1 configuration interactions are not negligible. As Z increases, configuration mixing decreases and the coupling shifts towards the j-j coupling limit. For Z greater than 60, intermediate coupling and configuration interactions are almost negligible.

2. Radial integrals

The Z dependence of the radial integrals occurring in the length and velocity formulas is plotted vs Z in Fig. 4. In the length formulation the integrals $\langle 3s_{1/2} | r | 3p_j \rangle$ ($j = \frac{1}{2}$ or $\frac{3}{2}$) are nearly equal. For example, for U^{+80} the numerical values are 0.1378 and 0.1290 for $j = \frac{3}{2}$ and $j = \frac{1}{2}$, respectively.

In the nonrelativistic limit the moduli of the three integrals which occur in the velocity formulation [see Eq. (9)] are equal. The moduli of the two integrals, which appear in the study of the $3s_{1/2} \rightarrow 3p_{1/2}$ transition, remain equal to one another

TABLE I. Configuration mixing coefficients for the s_0, p'_1 and p''_1 levels of the Mg I isoelectronic sequence.

		Ar^{+6} $Z=18$	Te^{+40} 52	U^{+80} 92
s_0	$(3s_{1/2})^2$	0.9818	0.9936	0.9971
	$(3p_{1/2})^2$	0.1097	0.0866	0.0737
	$(3p_{3/2})^2$	0.1521	0.0704	0.0190
	$(3d_{3/2})^2$	−0.0184	−0.0111	−0.0051
	$(3d_{5/2})^2$	−0.0227	−0.0142	−0.0063
p'_1[a]	$3s_{1/2}3p_{1/2}$	0.8249	0.9813	0.9993
	$3s_{1/2}3p_{3/2}$	0.5606	0.1851	0.0310
	$3d_{3/2}3p_{1/2}$	−0.0318	−0.0412	−0.0198
	$3d_{3/2}3p_{3/2}$	−0.0538	−0.0323	−0.0100
	$3d_{5/2}3p_{3/2}$	0.0371	−0.0097	−0.0057
p''_1[a]	$3s_{1/2}3p_{1/2}$	−0.5500	−0.1805	−0.0298
	$3s_{1/2}3p_{3/2}$	0.8104	0.9781	0.9980
	$3d_{3/2}3p_{1/2}$	0.1167	0.0646	0.0500
	$3d_{3/2}3p_{3/2}$	0.0509	0.0119	0.0026
	$3d_{5/2}3p_{3/2}$	0.1567	0.0805	0.0263

[a] Coefficients of $3s_{1/2}3p_{1/2}$ and $3s_{1/2}3p_{3/2}$ in the LS coupling limit: 0.816, 0.577.

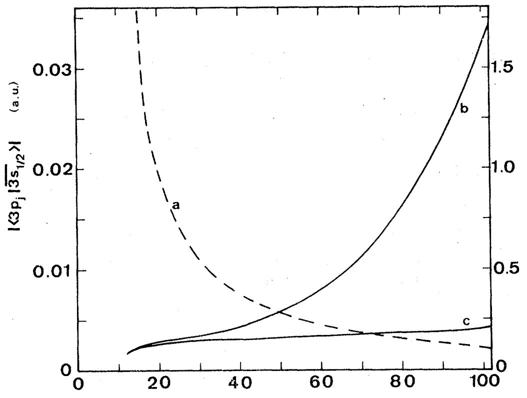

FIG. 4. Z dependence of the transition radial integrals. a corresponds to $|\langle 3s_{1/2}|r|3p_j\rangle|$ with $j=\frac{1}{2}$ or $\frac{3}{2}$ (scale on right), b corresponds to $|\langle 3p_{3/2}|\overline{3s_{1/2}}\rangle|$ (left axis), and c corresponds to $|\langle 3p_{1/2}|\overline{3s_{1/2}}\rangle| \simeq |\langle 3s_{1/2}|\overline{3p_{1/2}}\rangle|$ (left axis).

along the isoelectronic sequence (the relative variation is smaller than 10^{-4}) and are nearly independent on Z. On the contrary, for the $3s_{1/2} \rightarrow 3p_{3/2}$ transition the radial integral grows as Z increases and varies as Z^3 for high values of Z. These results are in agreement with the arguments of Sec. III B.

The different behavior of the $3s_{1/2}$-$3p_j$ transitions can be explained by the shifts of the wave functions towards the nucleus. In a previous paper,[17] it has been shown that even for nonhydrogenlike spectra, the shift depends approximately on j, and not on l; consequently the $\langle 3s_{1/2}|3p_{1/2}\rangle$, $\langle 3p_{1/2}|\overline{3s_{1/2}}\rangle$, and $\langle 3s_{1/2}|r|3p_{1/2}\rangle$ radial matrix elements for the $3s_{1/2} \rightarrow 3p_{1/2}$ transition are nearly independent of the relativistic effects, since both orbitals contract by roughly the same ratio. On the contrary, the cancellation effects which occur in the calculation of the radial matrix element corresponding to the $3s_{1/2} \rightarrow 3p_{3/2}$ transition disappear at high values of Z, and the integral increases. This contraction is a purely relativistic effect[17] which cannot be reproduced in a nonrelativistic approach, except if relativistic and correlation effects (extracomplex and core polarization effects) are simultaneously introduced.

3. *Transition matrix elements* D_r^2

In Fig. 2 we report the variations of $\ln D_r^2$ vs Z, for the s_0-p_1' and s_0-p_1'' transitions. $(D_r'')^2$ decreases approximately as $Z^{-2.7}$ over the entire range of Z. For low values of Z, $(D_r')^2$ increases as Z^5; this result arises from the spin-orbit mixing of the ${}^3P_1$ and ${}^1P_1$ states. For high values of Z, $(D_r')^2$ decreases as $Z^{-2.2}$; this variation corresponds to the Z^{-1} variation of $\langle|r|\rangle$, increased by the relativistic contraction of the relativistic orbitals. For high values of Z, $(D_r')^2$ and $(D_r'')^2$ become of the same order of magnitude.

C. *f* values

1. *Results*

In the length formulation, the f value is proportional to the product $\sigma \times D_r^2$ [Eq. (5)]. From Fig. 2 it is apparent that f'' decreases for low values of Z; for high values of Z, the contribution of the spin-orbit interaction of the $3p$ electron ($\approx Z^4$), which occurs in σ'', is predominant so that f'' increases with Z.

For low values of Z, f' increases since σ' and $(D_r')^2$ increase simultaneously, respectively on account of the intracomplex configuration interactions and of the intermediate coupling effects. For high values of Z, the contraction of the orbitals toward the nucleus is the more important phenomenon, so that f' decreases slowly.

For high values of Z, though both transitions are allowed in j-j coupling, f' remains smaller than f''. Indeed σ' is always smaller than σ'', and $(D_r')^2$ smaller than $(D_r'')^2$. For example for U^{+80}, the ratio f''/f' is equal to 17.

2. *Length and velocity formulations*

For the s_0-p_1'' transition, the calculated values until Z equals roughly 50 are in rather good agreement with earlier published results,[2] although extracomplex correlation effects are neglected in our treatment. The deviation between the numerical values obtained in the length or velocity formulations does not exceed 10%. For example for Ar^{+6} the f value increases by a factor 8.8%, when the length formulation is used; for U^{+80}, the corresponding change is equal to 0.5%.

The energy of the s_0-p_1' transition does not vanish, only because of correlation and relativistic effects, whereas the levels s_0 and p_1'' are nondegenerate in the relativistic hydrogenlike approximation. Consequently, large cancellations occur in the calculation of the energy difference σ', which is very sensitive to the correlation effects. For example for U^{+80}, $\sigma''/\sigma' \approx 5.5$. Therefore the discrepancy between f_r and f_∇ is greater for f' than for f''. Moreover for large values of Z, when the velocity formulation is used, very large cancellations appear in the evaluation of the radial part of the transition matrix element—for example, in the j-j coupling limit for U^{+80}, $(D_\nabla''/D_\nabla')^2 \approx 79$. Lastly, for high values of Z, the velocity formulation is more sensitive to small changes in the intermediate coupling than the length formulation. For example for U^{+80}, with the intermediate coupling, $(D_\nabla''/D_\nabla')^2 \approx 125$; this value is to be compared with the value obtained in j-j coupling. For U^{+80}

the discrepancy between f_r' and f_∇' is equal to 26%, but for all the reasons given above, the results obtained with the length formulation seem to be more reliable, since the cancellations are weaker in this case.

For low values of Z the discrepancy between f_r' and f_∇' is large (+47% for Ar^{+6}), but in this case the f_∇' results seem to be more relevant. Indeed the f_r' results are more sensitive to a small change in the intermediate coupling and very large cancellation effects occur in the evaluation of the relativistically allowed decay of a pure ${}^3P_1$ state, when the length formulation is used.

D. Comparison with other works

Figure 5 shows the results obtained for the transitions $3p^2\,{}^3P_0 \rightarrow 3s3p\,{}^3P_1$ [or $(3p_{1/2})^2 J=0 \rightarrow (3s_{1/2}3p_{1/2})J'=1$ using the *j-j* coupling notations]. In this case the f value always decreases with Z.

Figure 6 presents the Z dependence of the f value for the transition $3p^2\,{}^1S_0 \rightarrow 3s3p\,{}^1P_1$ [$(3p_{3/2})^2 J=0$ -$(3s_{1/2}3p_{3/2})J'=1$]. The curve is very similar to that obtained for f''.

In both cases we compare our results with the f values deduced from the multiplet f values published by Smith and Wiese.[2] The agreement is satisfactory until $Z=50$.

The reliability of our results can be tested by comparing them with previous experimental and theoretical data. No experimental data are available for ions heavier than Ar^{+6}. Except the f values obtained by Crossley and Dalgarno[18] using the Z-expansion method, all the theoretical studies concern elements lighter than Fe^{+14}. For the f value f' of the spin-forbidden transition, data are only available for Mg I[19,20] and Fe^{+14}.[21,22] In Table II we give some results concerning Mg I, Ar^{+6}, and Fe^{+14}; our theoretical values are obtained by taking into account the Gaunt interaction (Sec. V A) and by using the length and velocity formulations. For Mg I the value f_∇' agrees well with the experimental one, when taking into account the discrepancy of the experimental results. For low values of Z, our results are in good agreement with previous data, specially those compiled by Smith and Wiese,[2] showing that extracomplex correlation effects are almost negligible. For high values of Z, except for the $3s3p\,{}^3P_1$-$3p^2\,{}^3P_0$ transition, the values differ greatly from the results extrapolated from the low stages of ionization using the nonrelativistic Z-dependent theory, showing that relativistic effects on energies and the relativistic contraction of the orbitals toward the nucleus cannot be neglected.

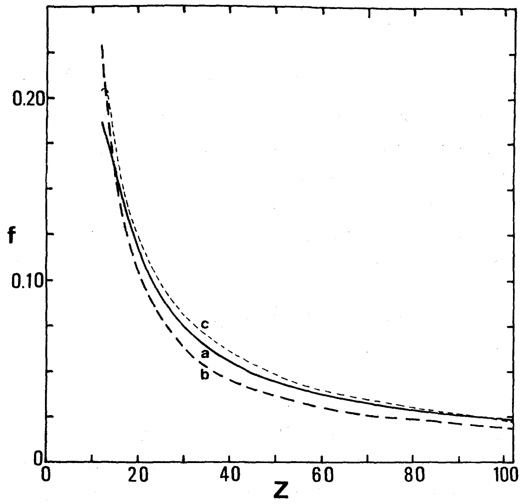

FIG. 5. Z dependence of the f values for the $3s3p\,{}^3P_1 \rightarrow 3p^2\,{}^3P_0$ transition: *a* (f_r), *b* (f_∇), and *c* (nonrelativistic, Ref. 2).

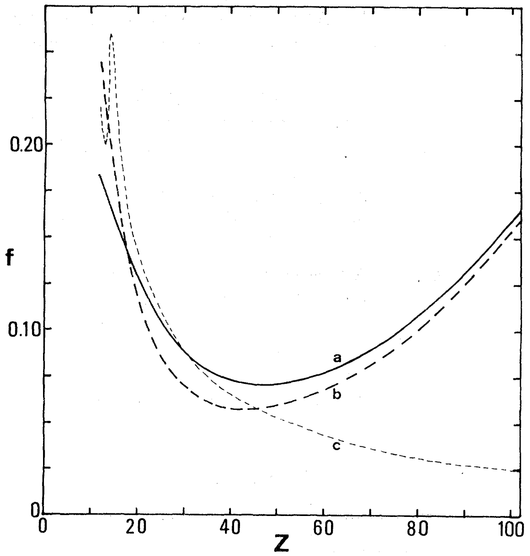

FIG. 6. Z dependence of the f values for the $3s3p\,{}^1P_1 \rightarrow 3p^2\,{}^1S_0$ transition: *a* (f_r), *b* (f_∇), and *c* (nonrelativistic, Ref. 2).

V. DISCUSSION

In the previous section, the computed f values are obtained in the velocity or in the length formulation neglecting retardation effects on the transition operator. As Z increases, these retardation effects become more important, since the wavelength of the transition becomes of the same order of magnitude as the mean radius of the electronic orbitals. The corresponding contribution is easily evaluated by using the expression $\vec{\alpha} e^{i\vec{k}\cdot\vec{r}}$ for the

TABLE II. Comparison of f_∇ and f_r between present and previous results.

			Present work			
	Transitions	λ (Å)	f_∇	f_r	Expt.	Previous theory
Mg I	$3s^2\,{}^1S_0 \rightarrow 3s3p\,{}^3P_1$	4571	0.17×10^{-5}	0.26×10^{-7}	$(0.21\pm0.02)\times10^{-5}$ [a] $(0.39\pm0.04)\times10^{-5}$ [b]	0.4×10^{-5} [c]
	$3s^2\,{}^1S_0 \rightarrow 3s3p\,{}^1P_1$	2852	2.02	1.64		1.81 [c]
	$3s3p\,{}^3P_1 \rightarrow 3p^2\,{}^3P_0$		0.229	0.187		0.204 [c]
Ar^{+6}	$3s^2\,{}^1S_0 \rightarrow 3s3p\,{}^1P_1$	586	1.07	1.17	0.86 ± 0.05 [d]	1.21 [c]
	$3s3p\,{}^3P_1 \rightarrow 3p^2\,{}^3P_0$	641	0.122	0.133	0.10 ± 0.01 [d]	0.14 [c]
Fe^{+14}	$3s^2\,{}^1S_0 \rightarrow 3s3p\,{}^3P_1$	417	0.19×10^{-2}	0.29×10^{-2}		0.228×10^{-2} [e] 0.35×10^{-2} [f]
	$3s^2\,{}^1S_0 \rightarrow 3s3p\,{}^1P_1$	284	0.69	0.79		0.81 [g] 0.75 [e] 0.83 [f]
	$3s3p\,{}^3P_1 \rightarrow 3p^2\,{}^3P_0$	318	0.076	0.088		0.087 [e] 0.10 [f]

[a] Reference 19.
[b] Reference 20.
[c] Reference 23.
[d] Reference 24.
[e] Reference 21.
[f] Reference 22.
[g] Reference 25.

transition operator. Nevertheless we have verified that these effects remain negligible even for large values of Z; for example, in the case of U^{+80} the corresponding contributions to f' and f'' are respectively equal to +0.03 and −0.24%.

Hitherto we have neglected all the radiative corrections to the energy levels; to the lowest order in α the corresponding effects occur in the Breit interaction and in the Lamb shift. Moreover we have assumed that the nucleus is a motionless point charge. In this section we evaluate the importance of these neglected contributions, in order to study the limit of validity of our treatment.

A. Correction for nuclear motion and structure

The corrections for the interaction of the nuclear moment with the electrons are negligible even in the case of the f value f' of the intercombination line of Mg I.[26] The nuclear motion gives rise to a correction to the energy levels which is approximately equal to $-10^{-3}Z^{-1}$ compared to the $A_{00}Z^2$ term; consequently this phenomenon is negligible compared to the correlation effects.

On the contrary, the corrections arising from the finite nuclear size can become significant for high values of Z, since the mean radius of the orbitals decreases as Z^{-1} while the nuclear radius grows as $A^{1/3}$ (A is the atomic-mass number). These corrections are more significant for $s_{1/2}$ and $p_{1/2}$ electrons, whose wave functions do not vanish at the origin, and they increase as $Z^4A^{2/3}$.[6]

We have evaluated the effects due to the finite size of the nucleus by assuming that the nucleus is spherically symmetrical and that the electric charge is uniformly distributed through the nuclear volume. The corresponding contributions to σ, D_∇^2, and f_∇ are given on Table III for the resonance lines of the isotopes ^{130}Te, ^{180}Hf, and ^{238}U. The corrections are greater for f' than for f'', and are significant for high values of Z.

B. Radiative corrections

The radiative corrections arise from the interaction of the electrons with their own virtual radiation field and can be evaluated by perturbation in the framework of quantum electrodynamics.[12] The Breit interaction corresponds to the exchange of a virtual photon between two electrons, and the Lamb shift involves the emission and the absorption of the virtual photon by the same electron.

1. *Breit interaction*

In this work we simplify the calculations by considering the leading term—i.e., the Gaunt operator[27]—corresponding to the unretarded interaction between two Dirac currents. The matrix elements of the Gaunt interaction are evaluated within the complex $(n=3)^2$, and the resulting

TABLE III. Relative magnitude of the correction coming from the finite nuclear size and from the Gaunt interaction (%).

		Finite nuclear size			Gaunt			Finite nuclear size + Gaunt		
		σ	D^2_∇	f_∇	σ	D^2_∇	f_∇	σ	D^2_∇	f_∇
$s_0 \to p_1'$	^{130}Te	−0.15	−0.36	−0.21	1.5	−2.7	−4.2	1.4	−3.1	−4.4
	^{180}Hf	−0.93	−2.4	−1.4	2.8	−1.8	−4.7	1.9	−4.2	−6.2
	^{238}U	−5.4	−13	−8.0	4.3	−1.7	−5.9	−0.92	−15	−14
$s_0 \to p_1''$	^{130}Te	−0.08	−0.17	−0.09	0.23	0.09	−0.14	0.15	−0.08	−0.23
	^{180}Hf	−0.30	−0.62	−0.32	0.15	0.06	−0.09	−0.14	−0.56	−0.42
	^{238}U	−1.1	−2.1	−1.0	−0.01	0.06	0.07	−1.0	−2.0	−0.94

matrix is diagonalized in order to obtain the intermediate coupling and the shifts of the energies. Examples of the corresponding contributions to σ, D^2_∇, and f_∇ are reported on Table III. For f'', the corrections are almost negligible ($<0.2\%$); the contributions on σ' and $(D'_\nabla)^2$ are of opposite sign, so that f' decreases by a 5% factor when the Gaunt interaction is introduced.

Table III gives the total contributions on σ, D^2_∇, and f_∇ coming from the finite nuclear-size effects and from the Gaunt interaction. These corrections to the transition frequencies cancel partially, but they are additive in the case of f'.

2. *Lamb shift*

For heavy atoms, where $Z\alpha$ is not negligible, the Lamb shift cannot yet be accurately calculated. The contributions of the Lamb shift are especially important for s electrons, and they increase in a first approximation as $Z^4\alpha^3$. The order of magnitude of the lowest-order Lamb shift for the $3s_{1/2}\, 3p_{1/2}$, and $3p_{3/2}$ orbitals can be obtained from the hydrogenlike approximation[6] using the screening factor $s = 11$. For the $3s_{1/2}$ orbital the second-order Lamb shift is of the order of $Z^5\alpha^4$,[12] and cancels nearly half of the first-order contribution. The relative contributions of the first- and second-order Lamb shift on the transition energies σ' and σ'' are reported on Table IV. The corrections are almost negligible for σ'', but they are significant for σ'.

All the corrections discussed above are only significant for the resonance transition corresponding to the lowest excited state of highly ionized atoms, since in this case large cancellation effects occur. Nevertheless these corrections are always smaller than the discrepancy between the values obtained by the length or velocity formulation, and they do not modify the shape of the curves giving the dependence on the value of Z of the oscillator strengths.

VI. CONCLUSION

The oscillator strengths for the resonance transitions of the Mg sequence obtained from the parametric-potential method exhibit a behavior similar to that obtained for the Be sequence using relativistic Hartree-Fock wave functions. For higher stages of ionization ($Z > 50$), the qualitative predictions of the nonrelativistic Z-expansion theory are not valid. Indeed the f value for the first resonance transition decreases owing to the relativistic contraction of the orbital toward the nucleus; for the second resonance line the frequency increases as Z^4 for high values of Z, since the spin-orbit interaction is predominant, and consequently the f value increases.

Retardation effects on the transition operator are negligible over the entire range of Z. Corrections arising from the finite nuclear size and from the Lamb shift do not affect significantly the f value for the second resonance line, but their contributions are significant (~15%) for the first resonance line.

The relativistic contributions to the energies or to the transition matrix elements cannot be separated, since they depend upon the formulation chosen—length or velocity. In the length formulation, relativistic contributions to the transition matrix element are not very important and arise

TABLE IV. Relative contributions of the Lamb shift to the transition energies (%). Transition energies calculated by taking into account the corrections due to the Lamb shift: (A) $Z^4\alpha^3$ term; (B) the $Z^5\alpha^4$ term is included in the energy of the $3s_{1/2}$ orbital.

	$s_0 \to p_1'$		$s_0 \to p_1''$	
	A	B	A	B
Te^{+40}	0.19	0.33	0.047	0.177
U^{+80}	−3.03	−1.40	−0.63	−0.35
No^{+90}	−4.76	−2.43	−0.74	−0.43

from the relativistic shift of the wave functions toward the nucleus. In the velocity formulation, additional relativistic contributions proceed from the relativistic corrections to the transition operator; consequently, the relativistically allowed decay is almost negligible when the length formulation is used, but cannot be neglected in the velocity formulation.

APPENDIX: SPECIFIC RELATIVISTIC EFFECTS IN THE EQUIVALENT OPERATOR FORMALISM FOR $s \to p$ ELECTRIC DIPOLE TRANSITIONS

Using the equivalent operator formalism[13] and central-field relativistic wave functions, it is possible to obtain the following result [see Eq. (11)]:

Length formulation:

$$\begin{aligned} R_{11}^{r} &= \tfrac{2}{9}\sqrt{3}\,(\langle s_{1/2}|r|p_{1/2}\rangle - \langle s_{1/2}|r|p_{3/2}\rangle)\,, \\ R_{01}^{r} &= -\tfrac{1}{9}\sqrt{6}\,(\langle s_{1/2}|r|p_{1/2}\rangle + 2\langle s_{1/2}|r|p_{3/2}\rangle)\,. \end{aligned} \tag{12}$$

Velocity formulation:

$$\begin{aligned} R_{11}^{\nabla} &= (-2i\sqrt{3}/9\alpha)[(\epsilon_{p_{1/2}} - \epsilon_{s_{1/2}})\langle s_{1/2}|r|p_{1/2}\rangle \\ &\quad - (\epsilon_{p_{3/2}} - \epsilon_{s_{1/2}})\langle s_{1/2}|r|p_{3/2}\rangle]\,, \\ R_{01}^{\nabla} &= (i/3\alpha)(\tfrac{2}{3})^{1/2}[(\epsilon_{p_{1/2}} - \epsilon_{s_{1/2}})\langle s_{1/2}|r|p_{1/2}\rangle \\ &\quad + 2(\epsilon_{p_{3/2}} - \epsilon_{s_{1/2}})\langle s_{1/2}|r|p_{3/2}\rangle]\,. \end{aligned} \tag{13}$$

If we introduce to first order in χ, the relativistic corrections on the energies and on the radial matrix elements, we can write

$$\begin{aligned} &\langle s_{1/2}|r|p_j\rangle = \langle r\rangle_{\mathrm{NR}} + \chi\langle \Delta r\rangle_j\,, \\ &\epsilon_{p_j} = \epsilon_p^{\mathrm{NR}} + \chi\epsilon_p^{\mathrm{R}} + \tfrac{1}{2}a_j\chi\xi_p, \quad a_{1/2} = -2, \quad a_{3/2} = +1\,, \\ &\epsilon_{s_{1/2}} = \epsilon_s^{\mathrm{NR}} + \chi\epsilon_s^{\mathrm{R}}\,, \end{aligned} \tag{14}$$

where ϵ^{NR} are the nonrelativistic energies, $\chi\epsilon^{R}$ the contributions of the mass and Darwin terms, and $\chi\xi_p$ the fine-structure constant of the p electron; $\langle r\rangle_{\mathrm{NR}}$ is the nonrelativistic integral, and $\langle \Delta r\rangle$ is related to the relativistic contraction toward the nucleus. With these notations, we obtain

$$\begin{aligned} R_{11}^{r} &= \tfrac{2}{9}\sqrt{3}\,\chi\,(\langle \Delta r\rangle_{1/2} - \langle \Delta r\rangle_{3/2})\,, \\ R_{01}^{r} &= -\tfrac{1}{9}\sqrt{6}\,[3\langle r\rangle_{\mathrm{NR}} + \chi(\langle \Delta r\rangle_{1/2} + 2\langle \Delta r\rangle_{3/2})]\,. \end{aligned} \tag{15}$$

For transitions such that the zero-order energies ϵ_p^{NR} and ϵ_s^{NR} are different, the relativistic corrections to the equivalent transition operator in the velocity form are given, to the first order in χ, by

$$\begin{aligned} R_{11}^{\nabla} &= (-2i\sqrt{3}/9\alpha)\chi\{(\epsilon_p^{\mathrm{NR}} - \epsilon_s^{\mathrm{NR}})(\langle \Delta r\rangle_{1/2} - \langle \Delta r\rangle_{3/2}) - \tfrac{3}{2}\xi_p\langle r\rangle_{\mathrm{NR}}\}\,, \\ R_{01}^{\nabla} &= (i\sqrt{6}/9\alpha)\{3(\epsilon_p^{\mathrm{NR}} - \epsilon_s^{\mathrm{NR}})\langle r\rangle_{\mathrm{NR}} + \chi[3(\epsilon_p^{R} - \epsilon_s^{R})\langle r\rangle_{\mathrm{NR}} + (\epsilon_p^{\mathrm{NR}} - \epsilon_s^{\mathrm{NR}})(\langle \Delta r\rangle_{1/2} + 2\langle \Delta r\rangle_{3/2})]\}\,. \end{aligned} \tag{16}$$

In the length formulation, only the relativistic contraction of the orbitals occurs. On the contrary, in the velocity formulation both the relativistic effects on energies and on wave functions appear simultaneously.

The relative contribution of the specific relativistic effects is given by

$$\begin{aligned} &\frac{R_{11}^{r}}{R_{01}^{r}} = -\frac{\sqrt{2}}{3}\,\chi\frac{\delta\langle \Delta r\rangle}{\langle r\rangle_{\mathrm{NR}}}\,, \\ &\text{where} \\ &\delta\langle \Delta r\rangle = \langle \Delta r\rangle_{1/2} - \langle \Delta r\rangle_{3/2}\,, \\ &\frac{R_{11}^{\nabla}}{R_{01}^{\nabla}} = \frac{R_{11}^{r}}{R_{01}^{r}} + \frac{\chi}{\sqrt{2}}\,\frac{\xi_p}{\epsilon_p^{\mathrm{NR}} - \epsilon_s^{\mathrm{NR}}}\,. \end{aligned} \tag{17}$$

It is obvious that in the velocity formulation, the spin-orbit interaction of the p electron increases the value of the ratio R_{11}/R_{01}.

In the hydrogenlike approximation, it is possible to show that for the $3s \to 3p$ transitions, the ratio $R_{11}^{\nabla}/R_{01}^{\nabla}$ can be expressed as

$$\begin{aligned} \frac{R_{11}^{\nabla}}{R_{01}^{\nabla}} &= \frac{1}{\sqrt{2}}\left(\frac{1 - \frac{2}{3}\chi\,\delta\langle \Delta r\rangle/\langle r\rangle_{\mathrm{NR}}}{1 - \frac{1}{3}\chi\,\delta\langle \Delta r\rangle/\langle r\rangle_{\mathrm{NR}}}\right) \\ &\approx \frac{1}{\sqrt{2}}\left(1 - \frac{\chi}{3}\,\frac{\delta\langle \Delta r\rangle}{\langle r\rangle_{\mathrm{NR}}}\right) \approx \frac{1}{\sqrt{2}}\,. \end{aligned} \tag{18}$$

Using the relativistic parametric-potential method, we have obtained for Ar^{+6} the following numerical values. $R_{11}^{\nabla}/R_{01}^{\nabla} = 1.10 \times 10^{-2}$, $R_{11}^{r}/R_{01}^{r} = 6.85 \times 10^{-4}$, and $\chi\xi_p/(\sqrt{2}\,\Delta\epsilon) = 1.04 \times 10^{-2}$ which are in good agreement with the relations (17). For U^{+80}, the numerical values are $R_{11}^{\nabla}/R_{01}^{\nabla} = 0.55$ and $R_{11}^{r}/R_{01}^{r} = 0.031$, which can be compared with the hydrogenlike values for U^{+92}: $R_{11}^{\nabla}/R_{01}^{\nabla} = 0.71$ and $R_{11}^{r}/R_{01}^{r} = 0.028$.

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