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PARITY VIOLATION INDUCED BY WEAK NEUTRAL CURRENTS IN ATOMIC PHYSICS. PART II

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Résumé. — La première partie de ce papier décrit l'évaluation de l'amplitude dipolaire électrique pour les transitions S-S à un photon d'atomes alcalins, induite sous l'effet du potentiel électron-noyau, à courte portée, violant la parité, qui est associé aux courants faibles neutres. Deux méthodes sont présentées en détail : la première nécessite une sommation explicite sur les contributions des états P mélangés aux états S et utilise les informations les meilleures concernant les amplitudes dipolaires électriques S-P. La seconde méthode, mathématiquement plus élégante, évite toute sommation explicite sur les états P à l'aide de techniques de fonction de Green ; si l'on néglige quelques corrections spin-orbite, elle conduit à une formule simple contenant des intégrales de Coulomb tabulées dans la littérature et les défauts quantiques interpolés pour les ondes S et P. La seconde partie est consacrée à une description de moyens possibles permettant la détection de la violation de la parité dans les transitions radiatives S-S avec une brève discussion de processus physiques qui pourraient être une source de difficultés expérimentales. La dernière partie consiste en une analyse théorique de l'influence d'un champ électrique statique sur les transitions radiatives S-S. L'évaluation de l'amplitude du dipôle électrique induit dans le cas du césium indique qu'il y aura compétition avec l'amplitude du dipôle magnétique pour des champs électriques supérieurs à 10 V/cm. Un effet d'interférence entre ces 2 amplitudes donne lieu à une polarisation électronique dans l'état final pouvant atteindre jusqu'à 64 % dans un cas typique. La mesure de cet effet assez particulier aura l'intérêt de fournir le signe de l'amplitude du dipôle magnétique. De plus, la violation de la parité peut se manifester par une dépendance de cette polarisation électronique sur l'état de polarisation du photon incident.

Abstract. — The first part of this paper gives a detailed account of the evaluation of the electric dipole amplitude induced in alkali one-photon S-S transitions, by the parity violating electron-nucleus short range potential $V_{p.v.}$ associated with the weak neutral currents. Two methods are presented : the first involves an explicit sum over the contributions of the P-states admixed with the S-states and incorporates the best information available on S-P electric dipole amplitudes. The second method, mathematically more elegant, avoids with the help of Green's function techniques any explicit sum over the P states, and, provided that some spin-orbit corrections are neglected, leads to a fairly simple formula involving Coulomb integrals tabulated in the literature and the interpolated quantum defects for S and P waves. The second part is devoted to a description of possible ways to detect parity violation induced in radiative S-S transitions, with a brief discussion of physical processes which could be a source of experimental difficulty. The last section of the paper deals with a theoretical analysis of the influence of a static electric field on the radiative S-S transitions. An evaluation of the induced electric dipole amplitude in the case of cesium indicates that it will compete with the magnetic dipole amplitude for electric fields larger than 10 V/cm. An interference effect between these two amplitudes gives rise to an electronic polarization in the final atomic state proportional to the vector product of the static electric field by the photon momentum which, in a typical case, could be as large as 64 % ; the measurement of this interesting and rather peculiar effect will lead to a determination of the sign of the magnetic dipole amplitude. Moreover parity violation could manifest itself by a dependence of this electron polarization on the state of circular polarization of the incident photon.

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Introduction. — In previous publications [1, 2], the authors have shown that the weak neutral currents, which have been recently detected in high energy neutrino scattering on nuclei [3], may, under well defined conditions, give rise to observable effects in atomic physics. The theories of weak interactions featuring neutral currents predict the existence of a short range electron-nucleus potential which, in general, will violate the invariance under space reflexion. This parity violating interaction mixes atomic states of opposite parities. The usual parity selection rules in atomic transitions are no longer strictly valid and mixed electric and magnetic dipole become possible. In such transitions, the photons emitted by an initially unpolarized atom will have on the average a small circular polarization. This will clearly indicate that the two possible orientations of space are not equivalent. In ordinary allowed transitions, this effect is far too small to be observed but in forbidden magnetic dipole transitions like the 6 S-7 S transition in Cesium a circular dichroism of the order of 10^{-4} is predicted.

In reference [2], the authors have developed a general method to compute the matrix element of the parity violating potential $V_{p.v.}$ between single particle s and p states. The final formula is remarkably simple and could be considered as a generalization of the Fermi-Segre formula which is rather successful in predicting the hyperfine splittings of alkali atoms. This result was used to give an order of magnitude estimate of the parity violating effects in magnetic dipole transitions, and to predict their general trend with atomic number : an approximate Z^3 law which favours obviously heavy atoms.

In this paper, we would like to present a detailed account of the evaluation of the electric dipole amplitude induced in S-S transitions by the parity violating electron-nucleus potential. Some of the results were given in reference [2], but a detailed justification was lacking. We shall follow two methods. The first method consists in a straightforward application of the first order perturbation theory. The sum over the P states admixed with the S states involved in the transition is performed explicitly using the best possible information available on the electric dipole S-P amplitude and the matrix element of $V_{p.v.}$ obtained in reference [2]. In order to make the method more practical, a summation over a finite number of P states should be sufficient to obtain an accurate result. We have been able to convince ourselves that it is indeed the case, but a direct justification is quite laborious. The second method, mathematically more involved, uses Green's function technique in order to avoid an explicit summation over the P states. In a first step, one finds an expression which would be very convenient for refined numerical computations. Moreover, if one ignores some spin-orbit effects and makes a mild assumption on the ion-core potential, one can go

further and after some rather technical steps given in Appendix, one arrives at a simple closed formula. In order to get numbers out of it, one only needs to know the interpolated quantum defects for S and P waves. This remarkable feature of the result is due to a cancellation of the contributions involving the internal part of the atomic wave functions. This method although less exact, since it neglects some effects which can be easily incorporated in the first method, is very useful for deriving a rapid estimate involving an error not exceeding 20 %. Within the same set of hypothesis the results agree almost perfectly with those obtained with the first method, keeping only the contribution of the four nearest intermediate P states.

In the next section (2), we give a rather detailed analysis of the possible ways to detect a parity violation in S-S transitions of alkali atoms. Three types of experiments are suggested and a particular attention is paid to hyperfine structure effects. We give a brief discussion of the most troublesome processes which can simulate or mask the effects we would like to observe (influence of a static field, collision induced transitions). Although they certainly represent a source of experimental complications, they do not seem to present unsurmountable difficulties.

Section 3 is devoted to a theoretical analysis of the influence of a static electric field on S-S transitions. Although it cannot simulate a genuine parity violation, it could in principle induce an electric dipole amplitude which will dominate the magnetic dipole. It is found that in the case of the 6 S-7 S transition of Cs, an electric field, kept below the level of one volt/cm, has a negligible effect on the transition. On the other hand, an electric static field is not always a nuisance and in some cases it could be a very valuable tool. We have shown that, through an interference between the magnetic dipole amplitude and the electric dipole amplitude induced by the static field E_0 , an electronic polarization along $\mathbf{k} \wedge \mathbf{E}_0$ (\mathbf{k} being the photon momentum) is produced in the final state. Since the induced electric dipole amplitude can be computed quite reliably, the observation of this polarization will lead to a determination of the M_1 amplitude. In particular, the sign of M_1 could be obtained within some well defined phase convention. The maximum electronic polarization is predicted independently of any particular hypothesis on the atomic wave function and is found to be as large as 64 % in a typical case.

If the S-S transition is induced by a beam of photons having a given circular polarization $\xi = \pm 1$, parity violation will manifest itself by the observation of an electronic polarization of the form $\xi \mathbf{k} \wedge \mathbf{E}_0$, associated with an interference between the electric dipole amplitudes induced, respectively, by the electric static field and the electron-nucleus parity violating potential.

This effect could constitute an interesting alternative to the experiments discussed in section 2.

We would like to emphasize that the experimental investigation of radiative S-S transitions induced by a static electric field, which bears some resemblance with the recently observed two photons S-S transitions [4], is by itself of great interest, independently of the question of parity violation in atomic physics.

1. Evaluation of the electric dipole amplitude induced by the parity violating electron-nucleus weak potential.

— We would like to present here the main steps and the results of an evaluation of the electric dipole matrix element induced between states of the same parity by the weak parity violating electron-nucleus potential, $V_{p.v.}^{e.N.}$, with a special attention to the $S_{1/2}$ - $S_{1/2}$ transitions in cesium. Our theoretical analysis will be performed in the framework of the single particle model which gives a good description of the one valence electron states of concern to us. We shall use first order perturbation theory together to the matrix element $\langle n' p_{1/2} | V_{p.v.} | n s_{1/2} \rangle$ obtained in reference [2]. The electric dipole matrix element between perturbed S states reads :

$$\langle \widetilde{n' S}_{1/2} | d_z | \widetilde{n S}_{1/2} \rangle = \sum_{n''} \times$$

$$\times \left\{ \frac{\langle n' S | d_z | n'' P \rangle \langle n'' P | V_{p.v.} | n S \rangle}{E_n - E_{n''}} + \frac{\langle n' S | V_{p.v.} | n'' P \rangle \langle n'' P | d_z | n S \rangle}{E_{n''} - E_n} \right\}. \quad (1)$$

To evaluate the above expression, we shall follow two methods. In the method I, the summation over n'' is performed explicitly using the best information available on the electric dipole amplitudes $\langle n' S | d_z | n'' P \rangle$. If this method is to be practical, a finite number of intermediate states should dominate the final result. The main difficulty in the method is to convince oneself that it is indeed the case.

The method II is more ambitious. One avoids the explicit summation using Green's function technique. But, in order to obtain a close formula, one has to neglect the effect of spin-orbit coupling on the electric dipole matrix elements. The final expression is remarkably simple. It requires only the knowledge of the interpolated quantum defects for S and P states and involves Coulomb functions integrals tabulated in the literature.

1.1 METHOD I. — If one inserts in the above expression the matrix element $\langle n s_{1/2} | V_{p.v.} | n' p_{1/2} \rangle$ given by eq. (29) of reference [2], one arrives at the following expression for the z-component of the electric dipole operator taken between perturbed S states :

$$\langle \widetilde{n'^2 S}_{1/2} | d_z | \widetilde{n^2 S}_{1/2} \rangle = \frac{i(G_F m_e^2 c) Z^2 \alpha^2}{2 \pi \sqrt{2} \hbar^3} Q_w(Z, N) K_r \times \left\{ \sum_{n''} \frac{\langle n'^2 P_{1/2} | d_z | n^2 S_{1/2} \rangle (\epsilon_{n'} \epsilon_{n''})^{3/4} (1 + \delta_0(\epsilon_{n'})) (1 + \delta_1(\epsilon_{n''}))}{\epsilon_{n'} - \epsilon_{n''}} - \sum_{n''} \frac{\langle n'^2 S_{1/2} | d_z | n''^2 P_{1/2} \rangle (\epsilon_n \epsilon_{n''})^{3/4} (1 + \delta_0(\epsilon_n)) (1 + \delta_1(\epsilon_{n''}))}{\epsilon_n - \epsilon_{n''}} \right\}. \quad (2)$$

The sum over n'' should run over the discrete as well as the continuous spectrum. In the discrete part $\epsilon_n, \epsilon_{n'}, \epsilon_{n''}$ stand for the binding energies of the states $| n^2 S_{1/2} \rangle, | n'^2 S_{1/2} \rangle, | n''^2 P_{1/2} \rangle$ in atomic units.

Expressions for $\delta_0(\epsilon)$ and $\delta_1(\epsilon)$, valid when $\epsilon \ll 1$ and $Z \gg 1$, were derived in reference [2] :

$$\left. \begin{aligned} 1 + \delta_0(\epsilon) &= \left[1 + 2(-\epsilon)^{3/2} \frac{\partial \mu}{\partial \epsilon} \right]^{-1/2} \times \\ &\quad \times (1 + o(\epsilon^2)) \\ 1 + \delta_1(\epsilon) &= \left[1 + 2(-\epsilon)^{3/2} \frac{\partial \mu}{\partial \epsilon} \right]^{-1/2} \times \\ &\quad \times (1 - \zeta + o(\epsilon^2) + o(\zeta^2)) \end{aligned} \right\} \quad (3)$$

with

$$\zeta = \frac{V_e(0)}{m_e c^2 \alpha^2} \frac{1}{Z^2} - \frac{\epsilon}{2 Z^2} \quad (4)$$

$V_e(0)$ being the electrostatic potential of the electronic cloud at the nucleus. $\mu(\epsilon)$ is the interpolated quantum defect. Q_w is a kind of weak charge appearing in the weak electron-nucleus potential discussed in reference [1] :

$$V_{p.v.}^{e.N.} = \frac{Q_w G_F}{4 \sqrt{2} m_e c} (\sigma_e \cdot p_e \delta^3(\mathbf{r}) + \delta^3(\mathbf{r}) \sigma_e \cdot p_e). \quad (5)$$

K_r is a relativistic correction factor given in terms of the nuclear radius R :

$$K_r = \left[\frac{\Gamma(3)}{\Gamma(2 \sqrt{1 - (Z\alpha)^2} + 1)} \left(\frac{2 ZR}{a_0} \right) (\sqrt{1 - (Z\alpha)^2} - 1) \right]^2.$$

A first estimation of the electric dipole transition amplitude has been performed following the method

of Bates and Damgaard [5]. These authors use the fact that for states of low binding energies, the electric dipole matrix elements receive contribution mainly from the outer part of the atomic wave function (radial distances r larger than the radius of the ion core r_c). Assuming that the core potential for $r > r_c$ is purely Coulombic, the external wave functions properly normalized can be written in terms of hypergeometric functions. We have used here the wave functions given by formula (A. 10) of reference [2] which differ from those of Bates and Damgaard by the factor $(-1)^{n+l+1} \left[1 + 2(-\epsilon)^{3/2} \frac{\partial \mu}{\partial \epsilon} \right]^{-1/2}$. In

table I, we have collected the values obtained in this manner for $n = 6$, $n' = 7, 8$ and $n'' = 6, 7, 8, 9$. They are affected with the index (c). These values have been corrected for the effect of spin-orbit coupling using first order perturbation [6]. The corrected values are listed in table I with the index (d).

There exists in the literature more refined computations of oscillator strengths in cesium, from which one can extract the modulus of the electric dipole matrix element. Stone [7] used a numerical potential constructed in order to reproduce 40 energy levels of cesium. The spin orbit coupling corrections are automatically included. The values obtained by Stone affected with index (a) are in good agreement with the values given by Bates and Damgaard when the matrix element modulus is $\gtrsim ea_0$, which means that there is no large compensation in the integrand giving the matrix element. The agreement becomes poorer for small matrix elements which are more

affected by a small modification of the wave function.

In the calculations of Norcross [8] appearing under the index (b), the effect of the core polarization neglected in the two previous calculations is included in a semi-empirical way. The effect of this correction is a reduction of the magnitude of the matrix element of the order of 7 % for the more important terms. We shall not give here a complete discussion of the rather complex experimental situation, and only say that there is fair agreement between the calculated electric dipole matrix elements and the measured oscillator strengths in the cases which are important for the evaluation of expression (1).

1.1.1 *The $6S_{1/2} \rightarrow 7S_{1/2}$ transition of cesium.* — In order to perform the evaluation of the matrix element $\langle \widetilde{7S}_{1/2} | d_z | \widetilde{6S}_{1/2} \rangle$ we have used the absolute values given by Stone with the signs given by Bates and Damgaard. This prescription seems justified since the modulus appears to be in fair agreement for the dominant terms. If in the dubious cases where the two amplitudes differ by a factor two, one would assume that a sign reversal has also occurred, the final result would only suffer a modification of the order of 10 %. If one uses the numbers listed in table I under the indices (a), one arrives at the expression :

$$\langle \widetilde{7S}_{1/2} | d_z | \widetilde{6S}_{1/2} \rangle = i 1.12 ea_0 \mathcal{F}(Z, N), \quad (7)$$

where the dimensionless quantity $\mathcal{F}(Z, N)$ is defined as :

$$\mathcal{F}(Z, N) = \frac{G_F}{\sqrt{2}} \frac{m_e^2 c}{\hbar^3} \frac{(Z\alpha)^2}{2\pi} Q_w(Z, N) K_r. \quad (8)$$

TABLE I

Electric-dipole matrix elements for cesium in atomic units ea_0 . Values affected with indices (a) and (b) are deduced from the oscillator strengths computed by Stone [7] and by Norcross [8]. Values (c) are computed by the method of Bates and Damgaard [5] with modification of the normalization factor as given in the text, and values (d) by correcting them from spin-orbit interaction through first-order perturbation theory.

n	$\langle 6S_{1/2} d_z nP_{1/2} \rangle$	$\langle 7S_{1/2} d_z nP_{1/2} \rangle$	$\langle 8S_{1/2} d_z nP_{1/2} \rangle$
6	1.97 (a)	- 1.59 (a)	- 0.411 (a)
	1.83 (b)		
	2.04 (c)	- 1.82 (c)	- 0.411 (c)
	2.04 (d)	- 1.73 (d)	- 0.413 (d)
7	0.120 (a)	4.35 (a)	- 3.57 (a)
	0.11 (b)		
	0.23 (c)	4.21 (c)	- 3.98 (c)
	0.19 (d)	4.25 (d)	- 3.81 (d)
8	0.0368 (a)	0.28 (a)	
	0.030 (b)		
	0.097 (c)	0.47 (c)	7.27 (c)
	0.078 (d)	0.34 (d)	
9	0.0169 (a)	0.086 (a)	
	0.013 (b)		
	0.039 (c)	0.17 (c)	0.80 (c)
	0.026 (d)	0.13 (d)	0.68 (d)

In the *Weinberg* model [9], $Q_w(Z, N)$ is given by

$$Q_w = Z(1 - 4 \sin^2 \theta_w) - N.$$

Taking $\sin^2 \theta = 0.35$, one finds :

$$\begin{aligned} \langle \widetilde{7S}_{1/2} | d_z | \widetilde{6S}_{1/2} \rangle &= -i 1.7 ea_0 10^{-11} \\ &= -i 0.47 \frac{\mu_B}{c} 10^{-8}. \end{aligned} \quad (9)$$

We would like to discuss the corrections to the above result coming from three different sources :

a) Contribution to the sum $\sum_{n''}$ associated with bound states $n'' \geq 10$.

β) Contribution associated with the continuous spectrum of the one particle p states $|P_{1/2} \epsilon\rangle$.

γ) Contribution associated with auto-ionizing states belonging to the configuration $|np_{1/2}^{-1} 6s_{1/2} 7s_{1/2}\rangle$ with $n \leq 5$.

In order to estimate the contribution $9 < n'' \leq 12$, we have still used the values of Stone. The contribution associated with $n'' > 12$ has been treated with the continuum. To obtain an estimation of the continuum, we have taken the transition matrix elements obtained by Burgess and Seaton [10] through an extension, to the continuum part of the p state spectrum, of the method of Bates and Damgaard. The spin-orbit correction, although small in absolute value, becomes comparable to the full electric dipole amplitude. The contribution involving the dipole matrix element $\langle 6S_{1/2} | d_z | P_{1/2} \epsilon \rangle$ has also been estimated using the results of Norcross [8] and Weisheit [11]. Although the two types of calculation give results which in detail may differ considerably, the order of magnitude of the final results are not very different. The conclusion we have reached is that the contribution of discrete states with $n'' > 9$, together with the continuum part of the one particle spectrum, is not likely to exceed 5 % of that of the lower lying states.

The contribution of the autoionizing states requires a special treatment, since it involves the matrix element $V_{p.v.}$ between 6S, or 7S, wave function and deeply bound one-particle p state associated with the hole. For such state, the approximate expressions (25) and (26) of reference [2] are no longer reliable. Let us consider a typical contribution :

$$A = \frac{\langle 7S_{1/2} | d_z | \alpha \rangle \langle \alpha | V_{p.v.} | 6S_{1/2} \rangle}{E_{6S_{1/2}} - E_\alpha}$$

where the autoionizing state $|\alpha\rangle$ is associated to the particle-hole configuration $6s_{1/2} 7s_{1/2} (np_{1/2})^{-1}$ with $2 \leq n \leq 5$. In the Hartree-Fock approximation one has :

$$\begin{aligned} E_{6S_{1/2}} - E_\alpha &= E_{6S_{1/2}} - (E_{6S_{1/2}} + E_{7S_{1/2}} - E_{np_{1/2}}) = \\ &= E_{np_{1/2}} - E_{7S_{1/2}}. \end{aligned}$$

Using the particle-hole formalism [12], one can express the products

$$\langle 7S_{1/2} | d_z | \alpha \rangle \langle \alpha | V_{p.v.} | 6S_{1/2} \rangle$$

in terms of one-particle states matrix elements, and arrive at the final expression :

$$A = \frac{\langle 7S_{1/2} | V_{p.v.} | np_{1/2} \rangle \langle np_{1/2} | d_z | 6S_{1/2} \rangle}{E_{7S_{1/2}} - E_{np_{1/2}}}$$

$$2 \leq n \leq 5.$$

Using the wave function given by C. Froese Fisher [13], we computed for $n = 5$ the ratio r of A to the corresponding expression involving the valence state $6p_{1/2}$. We found $r \sim 2 \times 10^{-2}$. For $n < 5$, similar estimates give much smaller results ($< 10^{-3}$).

In conclusion, it appears quite legitimate to neglect the corrections α , β , γ) in the evaluation of the electric dipole amplitude. In the next section, we shall present a different method of evaluating the electric dipole amplitude between states perturbed by $V_{p.v.}$ which will provide us with a further justification.

1.1.2 The $6S_{1/2} \rightarrow 8S_{1/2}$ transition of cesium. —

The matrix element of the electric dipole operator between the perturbed $6^2S_{1/2}$ and $8^2S_{1/2}$ states of Cs has also been performed, using the numbers listed in table I with the index (a) when they are available, and with the index (d) otherwise.

One finds :

$$\langle \widetilde{8S}_{1/2} | d_z | \widetilde{6S}_{1/2} \rangle = 0.43 ica_0 \mathcal{F}(Z, N), \quad (10)$$

and in the framework of the *Weinberg* model with $\sin^2 \theta_w = 0.35$:

$$\langle \widetilde{8S}_{1/2} | d_z | \widetilde{6S}_{1/2} \rangle = -i 0.65 \times 10^{-11} ea_0.$$

1.1.3 The $6P_{1/2} \rightarrow 7P_{1/2}$ transition of thallium. —

In reference [2], we have noted that the analysis performed with $nS \rightarrow n'S$ transitions in alkali states can be extended to $nP_{1/2} \rightarrow n'P_{1/2}$ transitions in gallium or thallium. We have performed an evaluation of the electric dipole amplitude $\langle 6P_{1/2} | d_z | 7P_{1/2} \rangle$ using a formula similar to (1). We have included in the calculation nS states with $n = 7, 8, 9$. We have not found any detailed calculations of the oscillator strengths. When data are available, we have taken the electric dipole amplitude $\langle 6P_{1/2} | d_z | nS_{1/2} \rangle$ from experiment [14], with the sign given by Bates and Damgaard. When no data exist we have used Bates and Damgaard matrix elements with spin-orbit corrections obtained from first order perturbation theory. The numbers used in this computation are given in table II. The matrix element of the electric dipole between the perturbed $6P_{1/2}$ and $7P_{1/2}$ states in thallium is found to be :

$$\langle \widetilde{7P}_{1/2} | d_z | \widetilde{6P}_{1/2} \rangle = -0.49 ica_0 \mathcal{F}(Z, N) \quad (11)$$

and in the framework of the Weinberg model :

$$\langle \widetilde{7P}_{1/2} | d_z | \widetilde{6P}_{1/2} \rangle = i 0.78 \times 10^{-10} e a_0.$$

The neglect of intermediate states involving the excitation of 6s electrons can be shown to introduce an incertitude of the order of 20 %.

TABLE II

Electric-dipole matrix elements for thallium in atomic units ea_0 . Index (a) affects the values deduced from experimental data [14], index (b) the values calculated by the method of Bates and Damgaard [5] with modification of the normalization factor as given in the text and values (c) are obtained by correcting them from spin-orbit interaction through first order perturbation theory.

n	$\langle 6P_{1/2} d_z nS_{1/2} \rangle$	$\langle 7P_{1/2} d_z nS_{1/2} \rangle$
—	—	—
	— 0.742 (a)	
7	— 0.734 (b)	2.42 (b)
	— 0.62 (c)	2.45 (c)
	— 0.223 (a)	
8	— 0.187 (b)	— 2.79 (b)
	— 0.192 (c)	— 2.78 (c)
	— 0.125 (a)	
9	— 0.093 (b)	— 0.48 (b)
	— 0.129 (c)	— 0.48 (c)

It is instructive to compare the electric dipole amplitude, induced by the weak neutral currents, for thallium and cesium, in the framework of the Weinberg model with $\sin^2 \theta_w = 0.35$:

$$\frac{\langle \widetilde{7P}_{1/2} | d_z | \widetilde{6P}_{1/2} \rangle_{\text{Tl}}}{\langle \widetilde{7S}_{1/2} | d_z | \widetilde{6S}_{1/2} \rangle_{\text{Cs}}} = \frac{-0.49 \mathcal{F}(Z=81, N=124)}{1.12 \mathcal{F}(Z=55, N=78)} \simeq -4.6.$$

1.2 METHOD II. — Although we have been able to convince ourselves that the dipole matrix element given by the formula (1) is dominated by the contribution of the intermediate P states which have energies close to those of the S states involved, this was achieved at the price of an appreciable numerical work. It would be of great interest to have a method which avoids the explicit summation over intermediate states.

Let us write the dipole matrix element between the S states perturbed by the parity violating potential $V_{\text{p.v.}}$ as :

$$\begin{aligned} E_{1z} &= \langle \widetilde{n'S} | d_z | \widetilde{nS} \rangle = \\ &= \langle n'S | d_z \frac{1}{\varepsilon_n - H_1} V_{\text{p.v.}} | nS \rangle \\ &+ \langle n'S | V_{\text{p.v.}} \frac{1}{\varepsilon_{n'} - H_1} d_z | nS \rangle. \end{aligned} \quad (12)$$

H_1 is the one-particle hamiltonian for the states of

angular momentum l . If one introduces the state $\widetilde{\psi}(\varepsilon, \varepsilon_n)$ with angular momentum $l = 1$ defined as :

$$|\widetilde{\psi}(\varepsilon, \varepsilon_n)\rangle = \left(\frac{1}{\varepsilon - H_1} \right) d_z | nS \rangle, \quad (13)$$

one obtains immediately the following expression for E_{1z} :

$$\begin{aligned} E_{1z} &= \langle \widetilde{\psi}(\varepsilon_n, \varepsilon_n) | V_{\text{p.v.}} | nS \rangle + \\ &+ \langle n'S | V_{\text{p.v.}} | \widetilde{\psi}(\varepsilon_n, \varepsilon_n) \rangle. \end{aligned} \quad (14)$$

We can associate a radial wave function $\bar{u}_1(\varepsilon, \varepsilon_n, \rho)$ with the state $|\widetilde{\psi}(\varepsilon, \varepsilon_n)\rangle$, and in the Appendix, \bar{u} is shown to obey the inhomogeneous differential equation :

$$\left(\frac{d^2}{d\rho^2} - \frac{2}{\rho^2} + v(\rho) + \varepsilon \right) \bar{u}_1(\varepsilon, \varepsilon_n, \rho) = \rho u_{n_0}(\rho), \quad (15)$$

$v(\rho)$ is the ion core potential written in atomic units, which reduces to $2/\rho$ when $\rho > \rho_c$ (ρ_c is the core radius). u_{n_0} is the radial wave function associated with the S bound state of reduced energy ε_n . Performing now the angular integration appearing in the expression (14), one arrives at the following expression of E_{1z} :

$$\begin{aligned} E_{1z} &= \langle \widetilde{n'S}_{1/2} | d_z | \widetilde{nS}_{1/2} \rangle \\ &= i \frac{ea_0}{8\pi} \frac{G_F m_e^2 c}{\sqrt{2} \hbar^3} \alpha^2 \times \\ &\times Q_w \left\{ \frac{u_{n_0}(\rho)}{\rho} \Big|_{\rho=0} \frac{\bar{u}_1(\varepsilon_n, \varepsilon_n, \rho)}{\rho^2} \Big|_{\rho=0} \right. \\ &\left. - \frac{u_{n_0}(\rho)}{\rho} \Big|_{\rho=0} \frac{\bar{u}_1(\varepsilon_n, \varepsilon_n, \rho)}{\rho^2} \Big|_{\rho=0} \right\}, \end{aligned} \quad (16)$$

where ε_n and $\varepsilon_{n'}$ are the reduced energies of $nS_{1/2}$ and $n'S_{1/2}$, respectively.

The above formula is certainly the most convenient for refined numerical computations, if one has at one's disposal accurate S wave functions. The radial wave function $\bar{u}_1(\varepsilon, \varepsilon_n, \rho)$ can be obtained by a numerical integration of the inhomogeneous differential eq. (15) ⁽¹⁾. We shall use it here to derive an approximate expression for E_{1z} , which becomes exact for large effective quantum numbers ν_n and $\nu_{n'}$, and more precisely in the limit : $\nu_n \rightarrow \infty$, $\nu_{n'} \rightarrow \infty$ with $\nu_n - \nu_{n'}$ fixed.

A detailed derivation is given in Appendix I. Here we shall only sketch the main steps. One introduces the two solutions $\mathcal{U}_i(\varepsilon, \rho)$ and $\mathcal{V}_i(\varepsilon, \rho)$ of the homogeneous differential equation :

$$\left(\frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} + v(\rho) + \varepsilon \right) u_i(\varepsilon, \rho) = 0, \quad (17)$$

⁽¹⁾ Such a method has been devised by R. M. Sternheimer [15] in numerical computation of electric polarizabilities of alkali atoms.

which satisfies the following conditions :

$$\lim_{\rho \rightarrow 0} \frac{\mathcal{U}_l(\varepsilon, \rho)}{\rho^{l+1}} = 1, \quad \lim_{\rho \rightarrow \infty} \mathcal{U}_l(\varepsilon, \rho) = 0$$

and

$$\mathcal{U}_l(\varepsilon, \rho) \frac{\partial}{\partial \rho} \mathcal{U}_l(\varepsilon, \rho) - \frac{\partial}{\partial \rho} \mathcal{U}_l(\varepsilon, \rho) \mathcal{U}_l(\varepsilon, \rho) = 1.$$

Note $\mathcal{U}_l(\varepsilon, \rho)$ exists only if $\varepsilon \neq \varepsilon_{nl}$, ε_{nl} being a bound state energy associated with an orbital angular momentum l .

In the appendix, these functions are used to construct the Green's function associated with the differential eq. (17). Knowing the Green's function, one can solve immediately the inhomogeneous eq. (15). One obtains in this way the following expression of the electric dipole amplitude :

$$E_{1z} = iea_0 \frac{G_F m_e^2 c}{8 \pi \sqrt{2} \hbar^3} \alpha^2 Q_W \frac{u_{n_0}(\rho)}{\rho} \Big|_{\rho=0} \frac{u_{n_0}(\rho)}{\rho} \Big|_{\rho=0} \times [I(\varepsilon_n, \varepsilon_{n'}) - I(\varepsilon_{n'}, \varepsilon_n)], \quad (18)$$

with

$$I(\varepsilon, \varepsilon') = \int_0^\rho \mathcal{U}_1(\varepsilon, \rho) \mathcal{U}_0(\varepsilon', \rho) \rho \, d\rho. \quad (19)$$

In the Appendix, it is argued that the difference $I(\varepsilon_n, \varepsilon_{n'}) - I(\varepsilon_{n'}, \varepsilon_n)$ is dominated by the contributions from the external region $\rho > \rho_c$ (ρ_c is the ion core radius), due to a cancellation between the internal region contributions ($0 < \rho < \rho_c$) in the limit of small ε_n and $\varepsilon_{n'}$. Using the quantum defect theory and the results of reference [2], the difference

$$I(\varepsilon_n, \varepsilon_{n'}) - I(\varepsilon_{n'}, \varepsilon_n)$$

can then be expressed in terms of the Coulomb integrals tabulated by Bates and Damgaard [5]. The relative error introduced in this way is found to be of the order of $v_n^{-7} = (-\varepsilon_n)^{7/2}$, an error which is smaller than those already introduced in the calculation. Let us quote the final result giving the electric dipole amplitude between the perturbed S states :

$$\begin{aligned} \langle \widetilde{n'} S_{1/2} | d_z | \widetilde{n} S_{1/2} \rangle &\approx iea_0 \frac{G_F m_e^2 c}{12 \sqrt{2} \hbar^3} (Z\alpha)^2 \times \\ &\times Q_W (1 + \Delta(\varepsilon_n, \varepsilon_{n'})) K_r(R, Z) (-1)^{n+n'+1} \\ &\times \left\{ \frac{I^{B,D}(\varepsilon_n, \varepsilon_{n'})}{\sin \pi(\mu_1(\varepsilon_n) - \mu_0(\varepsilon_n))} \right. \\ &\left. - \frac{I^{B,D}(\varepsilon_{n'}, \varepsilon_n)}{\sin \pi(\mu_1(\varepsilon_{n'}) - \mu_0(\varepsilon_{n'}))} \right\}. \quad (20) \end{aligned}$$

The Bates and Damgaard integrals $I^{B,D}(\varepsilon_n, \varepsilon_{n'})$ are given by :

$$I^{B,D}(\varepsilon, \varepsilon') = \int_0^\infty u_1^{B,D}(\varepsilon, \rho) u_0^{B,D}(\varepsilon', \rho) \rho \, d\rho, \quad (21)$$

with :

$$\begin{aligned} u_l^{B,D}(\varepsilon, \rho) &= \\ &= [v^2 \Gamma(v-l) \Gamma(v+l+1)]^{-1/2} W_{v,l+1/2} \left(\frac{2\rho}{v} \right) \\ &\left(\varepsilon = -\frac{1}{v^2} \right). \end{aligned}$$

$\mu_l(\varepsilon)$ is the interpolated quantum defect associated with the bound states of orbital angular momentum l (²); the correcting term $\Delta(\varepsilon_n, \varepsilon_{n'})$ is given by :

$$\begin{aligned} 1 + \Delta(\varepsilon_n, \varepsilon_{n'}) &= \left(1 + \frac{\partial \mu_0}{\partial v} \Big|_{\varepsilon_n} \right)^{-1/2} \times \\ &\times \left(1 + \frac{\partial \mu_0}{\partial v} \Big|_{\varepsilon_{n'}} \right)^{-1/2} (1 - \zeta) \\ &+ O(\varepsilon_n^2) + O(\varepsilon_{n'}^2) + O(\zeta^2), \quad (22) \end{aligned}$$

with

$$\zeta \approx 1.8 Z^{-2/3}.$$

In this formula, the effects of spin-orbit couplings, not contained in the relativistic correction factor $K_r(R, Z)$, have been neglected : spin-orbit splittings in the energy denominators, spin-orbit corrections to the electric dipole amplitude $\langle nS | d_z | n'P \rangle$; and all the corrections associated with the ion core polarizability are also ignored. Within these limitations, this formula is certainly extremely useful to get a rapid estimate of electric dipole amplitudes induced by parity violation, since it only requires the knowledge of the interpolated quantum defects for s and p waves, i.e. the energy spectrum.

It is instructive to compare the results obtained using this formula with those of the previous sections. The electric dipole amplitudes $6S_{1/2} \rightarrow 7S_{1/2}$ and $6S_{1/2} \rightarrow 8S_{1/2}$ in Cs are found to be :

$$\langle \widetilde{7S} | d_z | \widetilde{6S} \rangle = i 0.93 ea_0 \mathcal{F}(Z, N), \quad (23)$$

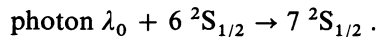
$$\langle \widetilde{8S} | d_z | \widetilde{6S} \rangle = i 0.40 ea_0 \mathcal{F}(Z, N). \quad (24)$$

These numbers are in fairly good agreement with those of the previous sections (1.12 and 0.43 respectively). If in the sum upon the intermediate nP states with $6 \leq n \leq 9$, one uses energy denominators where the spin-orbit splittings have been subtracted away, and Bates and Damgaard electric dipole amplitudes with no spin-orbit corrections, the agreement between the two methods becomes almost perfect : the numbers coincide within 1 %. This internal consistency shows that the sum upon intermediate states is indeed dominated by the P states with nearest energies.

2. Possible ways of detecting parity violation in the cesium $6S_{1/2} \rightarrow 7S_{1/2}$ radiative transition. — In a previous publication [2], we have given a discussion of

(²) Interpolation formulae for alkali can be found in reference [16].

the mechanisms which can give rise to non vanishing magnetic dipole transitions between S states in alkali atoms. Although it appears rather difficult to give any precise predictions, we concluded that the modulus of the magnetic dipole transition, expressed in unit of Bohr magneton, is likely to lie in the range 10^{-5} - 10^{-4} in the case of the cesium $6^2S_{1/2}$ - $7^2S_{1/2}$ transition. It is certainly of great interest to find an experimental procedure which could yield the modulus of the magnetic dipole amplitude and its sign, within some well defined phase convention. It is of course out of question to detect the spontaneous one-photon radiative decay of the $7^2S_{1/2}$ level to the ground state, the branching ratio with respect to allowed modes being extremely small (of order 10^{-13}). On the other hand, it appears possible, using the intense photon beam produced by tunable dye-lasers, to excite the transition starting from the ground state $6^2S_{1/2}$ with a reasonable probability. The simplest method, in principle therefore, is to measure the excitation cross-section :



The $7^2S_{1/2}$ final state is detected through the observation of the radiation associated with the $7S$ - $6P$ transitions. With an incident photon beam having a frequency bandwidth $\Delta\omega$ smaller than the Doppler width Γ_D , the maximum cross-section at the resonance frequency $\omega_0/2\pi = \hbar^{-1}(E_{7S} - E_{6S})$ is given in terms of the magnetic dipole amplitude

$$M_{1z} = \frac{1}{c} \langle 7^2S_{1/2} | \mu_z | 6^2S_{1/2} \rangle$$

by the following expression :

$$\sigma_{\max}^{\text{ex}}(6S \rightarrow 7S) = \frac{1}{4\sqrt{2}\pi} g(F, F') \frac{\Gamma_{M_1}}{\Gamma_D} \lambda_0^2, \quad (25)$$

Γ_D is the Doppler width ⁽³⁾

$$\Gamma_D = \omega_0 \sqrt{\frac{kT}{Mc^2}},$$

with M the mass of the Cs atom and T the absolute temperature. Γ_{M_1} is the rate associated with the spontaneous $7S \xrightarrow{M_1} 6S$ transition

$$\Gamma_{M_1} = \frac{4\omega_0^3}{(4\pi\epsilon_0)c^3\hbar} |M_{1z}|^2,$$

$g(F, F')$ is a numerical factor which takes into account the hyperfine quantum numbers of the initial and final states. For a nuclear spin I , $F = I \pm \frac{1}{2}$ and

$$g\left(I - \frac{1}{2}, I + \frac{1}{2}\right) = g\left(I + \frac{1}{2}, I - \frac{1}{2}\right) = \frac{4I(I+1)}{3(2I+1)^2}, \quad (26)$$

$$g(F, F) = \frac{2}{3} \frac{F(F+1)(2F+1)}{(2I+1)^3}.$$

⁽³⁾ Note that our definition of the Doppler width differs from the one conventionally used in spectroscopy.

If we take $|M_{1z}| = 10^{-4} \mu_B/c$, we find :

$$\Gamma_{M_1} = 0.50 \times 10^{-5} \text{ s}^{-1}.$$

For $T = 550$ K, the evaluation of Γ_D gives :

$$\Gamma_D = 2.16 \times 10^9 \text{ s}^{-1}.$$

With these numbers, for $I = \frac{7}{2}$, $F = I - \frac{1}{2} = 3$, and $F' = I + \frac{1}{2} = 4$, the numerical value obtained for the maximum cross-section is :

$$\sigma_{\max}^{\text{ex}} = 2.3 \times 10^{-25} \text{ cm}^2. \quad (27)$$

It can be noted that it is smaller than the cross-section for elastic scattering by one order of magnitude, which explains why it is important to detect the effects under interest at a different frequency.

With an incident beam of photons of 3×10^{17} quanta per second, corresponding to a power of 0.1 W, the yield of fluorescent photons associated with the $7S_{1/2} \rightarrow 6P_{3/2}$ and $7S_{1/2} \rightarrow 6P_{1/2}$ transitions is given versus the Cs vapour pressure p and the length of the illuminated column by :

$$N_f = 3.4 \times 10^9 \left(\frac{273}{T}\right)^{3/2} (p \text{ torr})(l \text{ cm}) \text{ photons/s.} \quad (28)$$

The measurement of $\sigma_{\max}^{\text{ex}}$ can yield the modulus of $|M_{1z}|$, but not the sign which has to be known if one wants to arrive at a complete determination of the electric-dipole amplitude induced by parity violation, from an eventual measurement of P_c . In order to determine the sign of M_{1z} , we shall consider a different technique which involves an interference with the electric dipole amplitude induced by an external electric field. We discuss this effect in the next chapter. We would like to discuss here different ways of detecting parity-violation in the forbidden radiative transition $6S_{1/2} \rightarrow 7S_{1/2}$.

2.1 TYPE 1 EXPERIMENT. — An ensemble of unpolarized cesium atoms is illuminated alternatively by a beam of right and left circularly polarized photons. Parity violation would manifest itself by the existence of a difference between the cross-sections relative to right and left polarized photons $\sigma_{R,L}$. One can define an asymmetry

$$A = \frac{\sigma_R - \sigma_L}{\sigma_R + \sigma_L},$$

which is clearly equal to the circular polarization P_c of the light emitted in the spontaneous emission $7S_{1/2} \rightarrow 6S_{1/2}$, and as shown in ref. [2] (eq. (38)), P_c satisfies the following relation ⁽⁴⁾ :

$$P_c = \frac{2I_m E_1 M_1^*}{|E_1|^2 + |M_1|^2} \simeq 2 \frac{I_m \langle \widetilde{6S}_{1/2} | d_z | \widetilde{7S}_{1/2} \rangle}{\left\langle 6S_{1/2} \left| \frac{\mu_z}{c} \right| 7S_{1/2} \right\rangle}. \quad (29)$$

⁽⁴⁾ The electric dipole amplitude induced by parity violation being pure-imaginary, one has to remind that :

$$\langle \widetilde{6S}_{1/2} | d_z | \widetilde{7S}_{1/2} \rangle = - \langle \widetilde{7S}_{1/2} | d_z | \widetilde{6S}_{1/2} \rangle.$$

Assuming the same total intensity as before of right (or left) polarized photons, one should observe a difference between the number of fluorescent photons when the incident beam polarization is changed from right to left. With $|M_{1z}| = 10^{-4} \mu_B/c$ and

$$\begin{aligned} \mathcal{N}_f^R &\approx \mathcal{N}_f^L \approx \mathcal{N}_f : \\ \mathcal{N}_f^R - \mathcal{N}_f^L &= 6.4 \times 10^5 \left(\frac{273}{T}\right)^{3/2} \times \\ &\times (p \text{ torr}) (l \text{ cm}) \text{ photons/s.} \end{aligned} \quad (30)$$

Note that if the magnetic dipole matrix element has been overestimated by a factor 3, $\mathcal{N}_f^R + \mathcal{N}_f^L$ is reduced by a factor 9 and $\mathcal{N}_f^R - \mathcal{N}_f^L$ by a factor 3.

2.2 TYPE 2 EXPERIMENT. — Here we suppose that one has succeeded in polarizing a gaseous target of cesium with a pressure, say of one torr. With the recent developments in optics, this does not seem to be an impossible task. If one illuminates this target with a linearly polarized light beam having the correct frequency to induce the forbidden $6S_{1/2} \rightarrow 7S_{1/2}$ transition, one should observe, if parity is violated, a linear dependence of the cross-section on the cosine of the angle θ between the polarization of the cesium vapour and the momentum of the incident photons. If one forgets about hyperfine interaction the backward-forward asymmetry is simply given by :

$$\mathcal{A} = \frac{\sigma(\theta = \pi) - \sigma(\theta = 0)}{\sigma(\theta = \pi) + \sigma(\theta = 0)} = P_e \langle \sigma_z \rangle, \quad (31)$$

$\langle \sigma_z \rangle$ being the electronic polarization of the target.

When including the hyperfine interaction, if the target is assumed completely polarized (in the sense that $|\langle \mathbf{F} \rangle| = |\langle \mathbf{S} \rangle + \langle \mathbf{I} \rangle|$ has reached its maximum value $I + \frac{1}{2}$), the above formula remains valid both for the transitions $F = I + \frac{1}{2} \rightarrow F' = I + \frac{1}{2}$ and $F = I + \frac{1}{2} \rightarrow F' = I - \frac{1}{2}$.

2.3 TYPE 3 EXPERIMENT. — As in the preceding case, this type of experiment involves the measurement of a correlation between the electronic polarization and the photon momentum, but this time in the final state. We propose to look for a small electronic polarization in the final state, the incident beam being linearly polarized. For obvious symmetry reasons, the polarization should be directed along the beam. If one ignores hyperfine structure effects, the polarization defined as $P_e = 2 \langle S_z \rangle$ is equal to P_c . The correction factor associated with the hyperfine interaction can be easily worked out :

$$\begin{aligned} P_e &= \gamma(F, F') P_c \quad \text{for the } F \rightarrow F' \text{ transition} \\ \text{if } F &= F', \\ \gamma \left(I + \frac{1}{2}, I + \frac{1}{2} \right) &= -\gamma \left(I - \frac{1}{2}, I - \frac{1}{2} \right) = \frac{1}{2I + 1}, \\ \text{if } F &\neq F', \\ \gamma(F, F') &= \frac{2F'(F' + 1)}{(2I + 1)^2}. \end{aligned} \quad (32)$$

For $I = \frac{7}{2}$, the value relevant for the natural Cs isotope, one thus obtains for the $F = 3 \rightarrow F' = 4$ transition :

$$P_e = \frac{5}{8} P_c.$$

One can still consider another type of experiment for detecting parity violation but since it involves the interference of the electric dipole induced by parity-violation with the electric dipole induced by an external electric field, we shall discuss this effect at the end of the next chapter.

The practical realization of these experiments raises evidently numerous technical difficulties. A detailed discussion of the possible means to overcome them has not its place in this theoretical paper. Instead of going into a description of possible experimental arrangements, we would rather discuss the physical processes which may simulate the effects we are looking for.

As we have already pointed out [2], an external electric field, although it mixes states of different parity, does not give rise to any circular polarization in spontaneous transition of unpolarized atoms. With the same line of reasoning based on symmetry considerations, one can show that a static or a quasi-static magnetic field can induce effects similar to that to be searched in the types of experiments suggested previously. As a result of thermal effects, the atoms are slightly polarized along the direction of the field, but the Boltzmann factor $\mu_B B_0/kT$ being of the order of 10^{-7} for $B_0 = 1 \text{ G}$, this can be neglected. More important effects are associated with the existence of the hyperfine interaction $a\mathbf{S} \cdot \mathbf{I}$.

Let us consider an ensemble of atoms in a given hyperfine state such that

$$\langle F_z \rangle = \langle I_z \rangle = \langle S_z \rangle = 0.$$

If a static magnetic field is applied adiabatically along the z direction, $\langle F_z \rangle$ remains zero, but $\langle S_z \rangle$ (and $\langle I_z \rangle$) acquire a non zero value of the order of $\mu_B B_0/a$. Furthermore, even with an unpolarized initial state, the transition probabilities are not invariant through a reflexion by a plane containing the z -axis. It is then not surprising to find that the asymmetry $A = \frac{\sigma_R - \sigma_L}{\sigma_R + \sigma_L}$ is non zero even if parity is not violated. For instance, in the case of the transition between the hyperfine levels $F = I - \frac{1}{2} = 3 \rightarrow F' = I + \frac{1}{2} = 4$, one finds that :

$$A \simeq 6.5 \times 10^{-4} B_0 (\text{G}).$$

In the type 1 experiment, no magnetic field is needed and to maintain the residual fields below the level, say of 10^{-2} G , does not seem to raise a too severe problem. In the type 2 and 3 experiments, a magnetic field of the order of one gauss may be helpful in the design of the experiment, but it can be chosen perpendicular to the incident beam, so one has to worry only about a misalignment of the apparatus giving rise to a small component along the light beam. In any case,

it will be possible to study the effect of a reversal of the sense of propagation of the incident light, all the rest of the apparatus being kept fixed. The ratio between the asymmetry associated with a magnetic field and the asymmetry induced by a parity violating interaction should reverse its sign.

As a final remark, we would like to rise the problem of the *background* processes which do not lead to any circular polarization but can mask the parity violating effects. For instance, if the type 1 experiment is performed in presence of a static electric field, the asymmetry A is reduced by a factor $\Gamma_{M_1}/(\Gamma_{M_1} + \Gamma_E)$, where Γ_E is the transition rate induced by the electric field. The influence of a static electric field will be discussed thoroughly in the next section. We shall find that if the static field is kept below the level of 1 V/cm, $\Gamma_E \ll \Gamma_{M_1}$ in the case of the 6 S \rightarrow 7 S transition of Cs, provided the transition magnetic moment is of the order of $10^{-4} \mu_B/c$.

Another source of *background* are the processes associated with atomic collisions. During a collision, the wave functions of the two atoms are distorted and an electric dipole transition between the perturbed atomic levels becomes allowed. The collision states of two cesium atoms can be classified with the help of the molecular terms of the diatomic molecule Cs_2^2 . For two incoming atoms in 6 S states, one has the two terms $^1\Sigma_g^+$ and $^3\Sigma_u^+$ while the outgoing 6 S-7 S states could give rise to the four terms $^1\Sigma_g^+$, $^3\Sigma_u^+$, $^1\Sigma_u^+$, $^3\Sigma_g^+$, the first two terms being associated with the symmetric combination $|6\text{ S}, 7\text{ S}\rangle + |7\text{ S}, 6\text{ S}\rangle$, the two others with the antisymmetric combination

$$|6\text{ S}, 7\text{ S}\rangle - |7\text{ S}, 6\text{ S}\rangle.$$

The following electric dipole transitions are allowed :

$$\text{photon } (\lambda_0) + ^1\Sigma_g^+ (6\text{ S}, 6\text{ S}) \rightarrow ^1\Sigma_u^+ (6\text{ S}, 7\text{ S}),$$

$$\text{photon } (\lambda_0) + ^3\Sigma_u^+ (6\text{ S}, 6\text{ S}) \rightarrow ^3\Sigma_g^+ (6\text{ S}, 7\text{ S}).$$

A complete discussion of the above process is clearly outside the scope of the present paper and will be the subject of a separate publication. We shall only say here that the frequency spectrum associated with collision induced transition is very broad; a simple argument based on the fourth uncertainty principle shows that its width is at least one hundred times larger than the Doppler width typical of the direct radiative transition, so that the line associated with the latter will appear as a peak sticking out from a broad background. Since the interference between the collision induced and direct transition amplitudes averages to zero, the signal due to the forbidden magnetic transitions could — in principle — be extracted unambiguously.

The alkali dimers could also be a source of difficulties since this kind of experiment will have to be performed at relatively high vapor pressure. However, there is no known strong absorption band of Cs_2^2 molecules [17] in the wavelength range corresponding

to the 6 S-7 S excitation. As in the case of collisions, we believe that, if the frequency resolution of the excitation and detection apparatus is good enough, the effect associated with molecules could be subtracted away. Recent experimental results on the excitation of the Cs 6 S-7 S transition in presence of a weak electric field seems to support this conclusion [18].

3. Influence of a static electric field on $n\text{S}-n'\text{S}$ transitions.

3.1 ELECTRIC DIPOLE AMPLITUDE INDUCED BY AN EXTERNAL STATIC ELECTRIC FIELD. — A static electric field mixes states of different parity. As a consequence electric dipole radiative transitions between S states become possible when an atom described by a parity conserving hamiltonian is under the action of a static electric field. As already pointed out [1, 2], this effect can easily be distinguished from a genuine parity violation.

We shall introduce an effective dipole operator \mathbf{D}_{eff} , the matrix elements of which are given in terms of the external static field by the following expression :

$$\begin{aligned} \langle n' \text{S}_{1/2} | \mathbf{D}_{\text{eff}} | n\text{S}_{1/2} \rangle = & \\ = \langle n' \text{S}_{1/2} | \mathbf{d} \cdot \mathbf{E}_0 G(E'_n) \mathbf{d} | n\text{S}_{1/2} \rangle + & \\ + \langle n' \text{S}_{1/2} | \mathbf{d} G(E_n) \mathbf{d} \cdot \mathbf{E}_0 | n\text{S}_{1/2} \rangle, & \quad (33) \end{aligned}$$

where \mathbf{d} is the ordinary electric dipole operator of the atom and $G(E) = (E - H)^{-1}$, H being the unperturbed atomic hamiltonian.

The effective dipole operator \mathbf{D}_{eff} can be obtained by a contraction with the vector E_{0j} of the second rank tensor operator $\mathbf{T}_{ij} = d_i G(E_n) d_j + d_j G(E'_n) d_i$:

$$D_{\text{eff},i} = \mathbf{T}_{ij} E_{0j}.$$

Since we are interested in the matrix element of \mathbf{T}_{ij} between two states of angular momentum $\frac{1}{2}$, only the irreducible parts of \mathbf{T}_{ij} , $\mathbf{T}_{ij}^{(0)} = \frac{1}{3} T_{kk} \delta_{ij}$ and

$$\mathbf{T}_{ij}^{(1)} = \frac{1}{2}(\mathbf{T}_{ij} - \mathbf{T}_{ji}),$$

transforming respectively as an angular momentum 0 and 1, contribute. The Wigner-Eckart theorem tells us that acting in the spin space, $\mathbf{T}_{ij}^{(0)}$ is proportional to the unit matrix and $\varepsilon_{ijk} \mathbf{T}_{ij}^{(1)}$ to the Pauli matrix σ_k . Note that, if in H we neglect the spin-orbit coupling, \mathbf{T}_{ij} commutes with the three components of the spin so that $T^{(1)}$ is identically zero.

If σ and σ' stand for the spin components of the $n\text{S}_{1/2}$ and $n'\text{S}_{1/2}$ states, the above considerations imply the following decomposition :

$$\begin{aligned} \langle n' \text{S}_{1/2} \sigma' | \mathbf{D}_{\text{eff}} | n\text{S}_{1/2} \sigma \rangle = & \alpha_{n'n} \mathbf{E}_0 \delta_{\sigma',\sigma} + \\ + i\beta_{n'n} (\boldsymbol{\sigma} \wedge \mathbf{E}_0)_{\sigma',\sigma}. & \quad (34) \end{aligned}$$

Let us first investigate the implication of time reversal invariance. With a suitable phase convention, the time reversal operator T is given by (see for instance [19]) :

$$T = \Pi_x \otimes \sigma_y^{(n)} K,$$

where the product Π_α runs over the electrons of the atom and K is the complex conjugation operator.

If H is even under time reflexion, \mathbf{D}_{eff} is also even :

$$T^{-1} \mathbf{D}_{\text{eff}} T = \mathbf{D}_{\text{eff}} .$$

One immediately obtains the following identity :

$$\begin{aligned} \alpha_{n',n} \delta_{\sigma',\sigma} + i\beta_{n',n}(\boldsymbol{\sigma} \wedge \mathbf{E}_0)_{\sigma',\sigma} = \\ = \alpha_{n',n}^* \delta_{\sigma',\sigma} - i\beta_{n',n}^*(\boldsymbol{\sigma}_y(\boldsymbol{\sigma} \wedge \mathbf{E}_0)^* \boldsymbol{\sigma}_y)_{\sigma',\sigma} . \end{aligned}$$

From which it follows that $\alpha_{n',n}$ and $\beta_{n',n}$ are both real. Hermiticity of the dipole operator implies :

$$\alpha_{n'n} = \alpha_{n'n} \quad \text{and} \quad \beta_{n'n} = -\beta_{nn'} . \quad (35)$$

In order to obtain expressions of $\alpha_{n'n}$ and $\beta_{n'n}$ in terms of the matrix element of d_z , it is convenient to consider particular spin and electric field configurations.

If we choose $\sigma = \sigma'$ and \mathbf{E}_0 along the z -axis, and consider the z -component of \mathbf{D}_{eff} :

$$\begin{aligned} \alpha_{n'n} = \langle n' S_{1/2} \sigma | d_z(G(E_n) + \\ + G(E_{n'})) d_z | n S_{1/2} \sigma \rangle . \quad (36) \end{aligned}$$

To find $\beta_{n'n}$, we take $\sigma' = -\sigma$ and \mathbf{E}_0 along the x -axis :

$$\begin{aligned} \beta_{n'n} = \frac{1}{2} \sum_{\sigma} \{ i(\sigma_y)_{\sigma,-\sigma} \times \\ \times \langle n' S_{1/2} -\sigma | d_x(G(E_n') - G(E_n)) d_z | n S_{1/2} \sigma \rangle \} ; \quad (37) \end{aligned}$$

we have used the fact that $\beta_{n'n}$ is associated with the antisymmetric part of the tensor \mathbf{T}_{ij} .

Let us give the explicit expression for $\alpha_{n',n}$ and $\beta_{n',n}$ in terms of the radial integrals :

$$\langle \rho \rangle_n^{n'j} = \int_0^\infty u_{n_0}(\rho) u_{n'1j}(\rho) \rho \, d\rho \quad (38)$$

with $l = 1, j = \frac{3}{2}, \frac{1}{2}$.

Besides the reality of $\alpha_{n'n}$ and $\beta_{n'n}$, one would like to verify that $\beta \equiv 0$ when $\langle \rho \rangle_n^{n'1/2} = \langle \rho \rangle_n^{n'3/2}$, and when the spin-orbit splitting in the energy denominators is neglected :

$$\begin{aligned} \alpha_{n'n} = + \frac{2}{9} a_0^3 \sum_{n''} \{ \langle \rho \rangle_n^{n''1/2} \langle \rho \rangle_n^{n''1/2} \times \\ \times [(\varepsilon_n - \varepsilon_{n''1/2})^{-1} + (\varepsilon_{n'} - \varepsilon_{n''1/2})^{-1}] \\ + 2 \langle \rho \rangle_n^{n''3/2} \langle \rho \rangle_n^{n''3/2} \\ \times [(\varepsilon_n - \varepsilon_{n''3/2})^{-1} + (\varepsilon_{n'} - \varepsilon_{n''3/2})^{-1}] \} \quad (39) \end{aligned}$$

$$\begin{aligned} \beta_{n'n} = \frac{2}{9} a_0^3 \sum_{n''} \{ \langle \rho \rangle_n^{n''1/2} \langle \rho \rangle_n^{n''1/2} \times \\ \times [(\varepsilon_{n'} - \varepsilon_{n''1/2})^{-1} - (\varepsilon_n - \varepsilon_{n''1/2})^{-1}] \\ - \langle \rho \rangle_n^{n''3/2} \langle \rho \rangle_n^{n''3/2} \\ \times [(\varepsilon_{n'} - \varepsilon_{n''3/2})^{-1} - (\varepsilon_n - \varepsilon_{n''3/2})^{-1}] \} \quad (40) \end{aligned}$$

$\varepsilon_n, \varepsilon_{n''1/2}$ and $\varepsilon_{n''3/2}$ being respectively the reduced energy of the $nS, n''P_{1/2}$ and $n''P_{3/2}$ states. It is seen on formula (40) that $\beta_{n'n} \equiv 0$ if spin-orbit coupling is neglected.

$\alpha_{n',n}$ and $\beta_{n',n}$ have been computed using electric dipole amplitudes obtained through a procedure similar to that described in section 1 : the modulus of the electric dipole matrix element is taken from the oscillator strengths computation of Stone [7] and the sign is assumed to be the one given by the Bates and Damgaard method with the phase-convention of reference [2]. Let us quote the result for the $7S \rightarrow 6S$ transition in cesium :

$$\begin{aligned} \alpha_{7,6} = \alpha_{6,7} = -305 a_0^3 \\ \beta_{7,6} = -\beta_{6,7} = 45 a_0^3 . \quad (41) \end{aligned}$$

One finds that $\beta_{n'n}$ is roughly 7 times smaller than $\alpha_{n'n}$, this is the order of magnitude expected. The electric field induced spin-independent $7S \rightarrow 6S$ amplitude is given in unit of μ_B/c as :

$$E_1 \approx 1.62 \times 10^{-5} \frac{\mu_B}{c} E_0 \text{ (V/cm)} . \quad (42)$$

For a field of the order of 10 V/cm, the induced electric dipole transition is of the same order of magnitude as our estimated magnetic dipole amplitude.

It is also worthwhile to note that the effects discussed in this section are closely related to the two photons S-S transition which has been observed recently [4]. The electric dipole transition under the influence of a static field can be considered as a two-photon process involving a real transverse photon and a virtual longitudinal photon associated with the instantaneous Coulomb interaction between the atomic electron and the static charge sources of the static electric field.

Let us briefly discuss the selection rules for electric dipole transitions induced by an electric static field between the hyperfine levels of two S states. When the spin-orbit coupling is negligible, the effective dipole operator acts like a scalar on atomic wave functions. It is clear that only transitions with $\Delta F = 0$ are allowed. For heavy alkali atoms like cesium the spin-orbit corrections cannot be ignored. The effective interaction with the radiation field contains both a scalar and a vectorial part. With unpolarized light, one should observe two strong lines associated with $\Delta F = 0$ transitions and two weaker ones associated with $\Delta F = \pm 1$ transitions. The same lines pattern is expected in two photons S-S transitions. However, due to the antisymmetry properties of the operator $\mathbf{T}_{ij}^{(1)}$, the $\Delta F = \pm 1$ lines will be present only if the two photons have different frequencies ω_1, ω_2 and different polarizations $\boldsymbol{\varepsilon}_1$ and $\boldsymbol{\varepsilon}_2$, the transition amplitude being of the form

$$\boldsymbol{\varepsilon}_1 \wedge \boldsymbol{\varepsilon}_2 \cdot (\mathbf{T}(\omega_1, \omega_2) - \mathbf{T}(\omega_2, \omega_1)) .$$

In the two photons experiment without Doppler broadening where $\omega_1 = \omega_2$ and $\varepsilon_1 = \varepsilon_2$, no $\Delta F = \pm 1$ should be observed even in the presence of a strong spin-orbit coupling.

As an illustration, let us derive the ratio of the intensity of the two types of lines in the case of the $6S \rightarrow 7S$ transition induced in atomic cesium by a static field \mathbf{E}_0 . Let us assume that \mathbf{E}_0 is perpendicular to the photon-momentum and makes an angle θ with the electric field carried by the incident photon.

We define $\mathfrak{P}(F_+, F_-)$ as the probabilities of the transitions $F_+ \rightarrow F_- (F_{\pm} = I \pm \frac{1}{2}, I$ is the nuclear spin) normalized in such a way that their sum is equal to one. We have also assumed that in the initial state the different hyperfine levels are equally populated :

$$\mathfrak{P}(F_+ \rightarrow F_+) = \frac{I+1}{2I+1} \frac{\alpha^2 \cos^2 \theta}{\alpha^2 \cos^2 \theta + \beta^2 \sin^2 \theta} + \frac{(2I+3)(I+1)}{3(2I+1)^2} \frac{\beta^2 \sin^2 \theta}{\alpha^2 \cos^2 \theta + \beta^2 \sin^2 \theta},$$

$$\mathfrak{P}(F_- \rightarrow F_-) = \frac{I}{2I+1} \frac{\alpha^2 \cos^2 \theta}{\alpha^2 \cos^2 \theta + \beta^2 \sin^2 \theta} + \frac{(2I-1)I}{3(2I+1)^2} \frac{\beta^2 \sin^2 \theta}{\alpha^2 \cos^2 \theta + \beta^2 \sin^2 \theta},$$

$$\mathfrak{P}(F_+ \rightarrow F_-) = \mathfrak{P}(F_- \rightarrow F_+) = \frac{4I(I+1)}{3(2I+1)^2} \frac{\beta^2 \sin^2 \theta}{\alpha^2 \cos^2 \theta + \beta^2 \sin^2 \theta}.$$

Taking $I = \frac{7}{2}$, $\alpha/\beta \approx -305/45$, one finds for instance :

$$\frac{\mathfrak{P}(F=4, F=3)}{\mathfrak{P}(F=3, F=3)} \approx \frac{3}{4} \frac{\beta^2}{\alpha^2} \operatorname{tg}^2 \theta \approx 0.016 \operatorname{tg}^2 \theta \quad \left(\theta \neq \frac{\pi}{2} \right).$$

Although the effects discussed here are somewhat outside our main line of interest, they clearly deserve a careful experimental investigation.

3.2 INTERFERENCE EFFECTS BETWEEN THE MAGNETIC DIPOLE AMPLITUDE AND THE ELECTRIC DIPOLE AMPLITUDE INDUCED BY AN EXTERNAL STATIC ELECTRIC FIELD. — We shall consider a situation in which the transition amplitude induced by a static field is of the same order of magnitude as M_{1z} . For an incident photon in a state of plane polarization described by the unit vector ε , the $nS \rightarrow n'S$ amplitude can be obtained from the effective transition matrix \mathcal{T} acting only on spin variables :

$$\mathcal{T} = (\alpha \mathbf{E}_0 \uparrow + i\beta \boldsymbol{\sigma} \wedge \mathbf{E}_0 + M_{1z} \boldsymbol{\sigma} \wedge \hat{k}) \cdot \varepsilon; \quad (43)$$

α and β are given by expressions (39) and (40) (the indices n and n' have been dropped); \hat{k} is the unit vector along the photon momentum \mathbf{k} , \uparrow is the unit two by two matrix. We shall limit ourselves to transitions between the same hyperfine state $\Delta F = 0$. It is only for such transitions that an interference of

the type $\alpha E_0 M_{1z}$ can be observed. In the transition matrix \mathcal{T} , the spin operator $\boldsymbol{\sigma}$ is to be replaced by $2g_F \mathbf{F}$ where :

$$g_{F \pm 1/2} = \pm \frac{1}{2I+1}.$$

In order to simplify the analysis, let us consider the particular case with the electric field \mathbf{E}_0 parallel to the polarization vector of the incident photon : $\mathbf{E}_0 = \varepsilon E_0$ and assume that the initial state is unpolarized. The density matrix ρ_f of the final spin state is then given by :

$$\rho_f \propto \frac{\mathcal{T} \mathcal{T}^\dagger}{(2F+1)}.$$

The excitation cross-section is proportional to $\operatorname{Tr}(\mathcal{T} \mathcal{T}^\dagger)$:

$$\sigma_{\max}^{\text{ex}} \propto \alpha^2 E_0^2 + \frac{4}{3} \frac{F(F+1)}{(2I+1)^2} |M_{1z}|^2. \quad (44)$$

In order to account for the effect of the electric static field, one has to perform in formula (25) the following replacement :

$$\Gamma_{M_1} \rightarrow \Gamma_{M_1} \left(1 + \frac{3}{4} \frac{(2I+1)^2}{F(F+1)} \frac{\alpha^2 E_0^2}{|M_{1z}|^2} \right).$$

The study of the variation of the excitation cross-section versus E_0^2 , will lead to a determination of the ratio :

$$\frac{|M_{1z}|^2}{\alpha^2 E_0^2}.$$

With the same static electric field configuration ($\mathbf{E}_0 = E_0 \varepsilon$), it is easily seen that the final atomic state is polarized along $\hat{k} \wedge \mathbf{E}_0$ (this result is expected from symmetry consideration, since the vector $\mathbf{k} \wedge \mathbf{E}_0$ has the transformation properties under space and time reflexion of angular momentum) :

$$\begin{aligned} \langle \mathbf{F} \rangle &= \frac{\operatorname{Tr}(\mathbf{F} \mathcal{T} \mathcal{T}^\dagger)}{\operatorname{Tr}(\mathcal{T} \mathcal{T}^\dagger)} \\ &= \frac{4F(F+1)M_{1z}}{3g_F(2I+1)^2 \alpha E_0^2} \times \\ &\quad \times \left(1 + \frac{4F(F+1)M_{1z}^2}{3(2I+1)^2 \alpha^2 E_0^2} \right)^{-1} \hat{k} \wedge \mathbf{E}_0. \end{aligned}$$

This result can be expressed in terms of the electronic polarization :

$$\begin{aligned} \mathbf{P}_e &= \langle \boldsymbol{\sigma} \rangle = 2g_F \langle \mathbf{F} \rangle \\ &= \frac{8F(F+1)M_{1z}}{3(2I+1)^2 \alpha E_0^2} \times \\ &\quad \times \left[1 + \frac{4F(F+1)M_{1z}^2}{3(2I+1)^2 \alpha^2 E_0^2} \right]^{-1} \hat{k} \wedge \mathbf{E}_0. \quad (45) \end{aligned}$$

The measurement of \mathbf{P}_e as a function of E_0 yields M_{1z} with both sign and absolute value.

\mathbf{P}_e is maximum when :

$$E_0^2 = \frac{4}{3} \frac{F(F+1) |M_{1z}|^2}{(2I+1)^2 \alpha^2}; \quad (46)$$

$$\mathbf{P}_e^{\max} = \text{sign of } \left(\frac{\alpha E_0}{M_{1z}} \right) \times \frac{2}{2I+1} \left(\frac{F(F+1)}{3} \right)^{1/2} \frac{\hat{k} \wedge \mathbf{E}_0}{E_0}. \quad (47)$$

For example, if one takes $I = \frac{7}{2}$, $F = I + \frac{1}{2} = 4$, one finds :

$$|\mathbf{P}_e^{\max}| = \sqrt{\frac{5}{12}} \approx 0.64.$$

If one now chooses \mathbf{E}_0 parallel to $\boldsymbol{\varepsilon} \wedge \hat{k}$, the scalar term $\alpha \mathbf{E}_0 \cdot \boldsymbol{\varepsilon}$ does not contribute to the transition amplitude. One still finds an electronic polarization along $\mathbf{k} \wedge \mathbf{E}_0$, but now involving an interference between βE_0 and M_{1z} .

Let us remark that this electronic polarization cannot be confused with the one associated with a genuine parity violation discussed in the previous section which is directed along the momentum \mathbf{k} of the incident photon, paragraph 2.3.

3.3 INTERFERENCE BETWEEN THE ELECTRIC DIPOLE AMPLITUDES INDUCED BY PARITY VIOLATION AND BY AN EXTERNAL STATIC FIELD. — We would now like to discuss a new possible way to detect parity violation in $nS-n'S$ transitions which could be a valuable alternative to the methods described previously. If parity is violated in a S-S transition of an alkali atom, a new term of the form

$$E_{1z} \boldsymbol{\sigma} = \langle \widetilde{n'S}, \sigma' = 1 | d_z | \widetilde{nS}, \sigma = 1 \rangle \boldsymbol{\sigma}$$

has to be added to the effective transition matrix \mathcal{C} . If one considers an incident linearly polarized photon with the static field \mathbf{E}_0 parallel to $\boldsymbol{\varepsilon}$, no interference term of the type αE_1 appears and no new effects are predicted. However if the incident photon is circularly polarized, interference effects between the electric dipole amplitudes induced by the external static field and by parity violation do exist. In particular, they give rise to a component of the electronic polarization \mathbf{P}_e of the final atomic state along the vector $\hat{k} \wedge \mathbf{E}_0$ depending linearly upon the circular polarization ξ of the incident photon. The quantity $\xi(\hat{k} \wedge \mathbf{E}_0) \cdot \mathbf{P}_e$ being a pseudo-scalar, the observation of such an effect would clearly indicate that the atomic hamiltonian contains a term odd under space reflexion. The complete expression giving \mathbf{P}_e is rather involved in the general case. We shall only quote the result relative to a $F \rightarrow F$ transition with

$\beta \ll \alpha$, $\mathbf{E}_0 \cdot \hat{k} = 0$, keeping only the first order term in

$$\frac{|M_{1z}|}{\alpha E_0} \quad \text{and} \quad \frac{|E_{1z}|}{\alpha E_0};$$

$$\mathbf{P}_e \approx \frac{8}{3} \frac{(M_{1z} + i\xi E_{1z}) F(F+1)}{(2I+1)^2 \alpha E_0^2} \hat{k} \wedge \mathbf{E}_0 \quad (5). \quad (48)$$

The detection of a variation of \mathbf{P}_e with the sign of the circular polarization of incident photons could be the only possible procedure to see a parity violation if, for some reasons, the magnetic dipole amplitude is strongly suppressed, say much below the level of $10^{-5} \mu_B/c$, leading to a very small excitation cross-section $\sigma_e \lesssim 10^{-27} \text{ cm}^2$ in absence of a static electric field.

APPENDIX I

We would like to present an evaluation of the electric dipole amplitude $E_{1z} = \langle \widetilde{n'S}_{1/2} | d_z | \widetilde{nS}_{1/2} \rangle$ induced by the weak parity violating electron-nucleus potential where the summation over intermediate P states appearing in eq. (1) is no longer performed explicitly.

Let us first rewrite the first order perturbation expression for E_{1z} in terms of one particle radial wave functions :

$$E_{1z} = i \frac{ea_0}{8\pi} \frac{G_F m_e^2 c}{\sqrt{2} \hbar^3} \alpha^2 Q_W \times$$

$$\times \left[\sum_{n''} \left\{ \frac{u_{n_0}(\rho)}{\rho} \Big|_{\rho=0} \frac{u_{n_1}(\rho)}{\rho^2} \Big|_{\rho=0} \right. \right.$$

$$\times \frac{1}{\varepsilon_n - \varepsilon_{n''}} \int_0^\infty u_{n_1}(\rho) u_{n_0}(\rho) \rho \, d\rho$$

$$\left. - \sum_{n''} \frac{u_{n_0}(\rho)}{\rho} \Big|_{\rho=0} \frac{u_{n_1}(\rho)}{\rho^2} \Big|_{\rho=0} \frac{1}{\varepsilon_{n''} - \varepsilon_n} \right.$$

$$\left. \times \int_0^\infty u_{n_1}(\rho) u_{n_0}(\rho) \rho \, d\rho \right\} \Big]. \quad (\text{A.I.1})$$

In this formula, ρ is the radial distance in atomic units and the u_n radial functions obey the normalization condition :

$$\int_0^\infty u_n(\rho) u_{n'}(\rho) \rho \, d\rho = \delta_{n,n'}.$$

Let us introduce the Green's function $g_1(\varepsilon, \rho, \rho')$ given by :

$$g_1(\varepsilon, \rho, \rho') = \sum_{n''} \frac{u_{n_1}(\rho) u_{n_1}(\rho')}{\varepsilon - \varepsilon_{n''}}, \quad (\text{A.I.2})$$

(5) In the expression of \mathbf{P}_e given here, we have omitted a component along \hat{k} involving terms proportional to ξM_{1z}^2 and $\xi \alpha \beta E_0^2$ which could be easily distinguished.

(the sum $\sum_{n''}$ in (A.I.1) and (A.I.2) includes also the continuum part of the spectrum), and define the function :

$$\bar{u}_1(\varepsilon, \varepsilon_n, \rho) = \int_0^\infty g_1(\varepsilon, \rho, \rho') u_{n_0}(\rho') \rho' d\rho'$$

which is the regular square integrable solution of the differential equation :

$$\left(\frac{d^2}{d\rho^2} - \frac{2}{\rho^2} + v(\rho) + \varepsilon \right) \bar{u}_1(\varepsilon, \varepsilon_n, \rho) = \rho u_{n_0}(\rho). \quad (\text{A.I.3})$$

where $v(\rho)$ is the ion core potential in atomic units. The dipole amplitude E_{1z} takes then the simple form :

$$E_{1z} = i \frac{ea_0}{8\pi} \frac{G_F m_e^2 c}{\sqrt{2} \hbar^3} \alpha^2 Q_W \times \left[\frac{u_{n_0}(\rho)}{\rho} \Big|_{\rho=0} \frac{\bar{u}_1(\varepsilon_n, \varepsilon_n, \rho)}{\rho^2} \Big|_{\rho=0} - \frac{u_{n_0}(\rho)}{\rho} \Big|_{\rho=0} \frac{\bar{u}_1(\varepsilon_n, \varepsilon_n, \rho)}{\rho^2} \Big|_{\rho=0} \right]. \quad (\text{A.I.4})$$

The above expression is certainly the best starting point for refined numerical computation of E_{1z} . If one knows accurate 6S and 7S wave functions, the differential eq. (A.I.3) can be solved numerically. Here we shall use it to obtain a simple approximate expression involving the Coulomb radial integrals tabulated by Bates and Damgaard.

Let us introduce the two functions $\mathcal{U}_l(\varepsilon, \rho)$ and $\mathcal{V}_l(\varepsilon, \rho)$ solutions of the differential equation :

$$\left(\frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} + v(\rho) + \varepsilon \right) f = 0 \quad (\text{A.I.5})$$

such that :

$$\left. \begin{aligned} \lim_{\rho \rightarrow 0} \frac{\mathcal{U}_l}{\rho^{l+1}} &= 1 \\ \lim_{\rho \rightarrow \infty} \mathcal{V}_l(\varepsilon, \rho) &= 0 \end{aligned} \right\} \quad (\text{A.I.6})$$

$$W(\mathcal{U}_l, \mathcal{V}_l) = \mathcal{U}_l \frac{\partial}{\partial \rho} \mathcal{V}_l - \frac{\partial \mathcal{U}_l}{\partial \rho} \mathcal{V}_l = 1$$

The functions \mathcal{U}_l and \mathcal{V}_l exist provided ε is not an eigenvalue of the operator

$$- \left[\frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} + v(\rho) \right].$$

One can then verify immediately that the Green's

function $g_1(\varepsilon, \rho, \rho')$ can be written in terms of the functions $\mathcal{U}_1(\varepsilon, \rho)$ and $\mathcal{V}_1(\varepsilon, \rho)$ as :

$$g_1(\varepsilon, \rho, \rho') = \theta(\rho' - \rho) \mathcal{U}_1(\varepsilon, \rho) \mathcal{V}_1(\varepsilon, \rho') + \theta(\rho - \rho') \mathcal{U}_1(\varepsilon, \rho') \mathcal{V}_1(\varepsilon, \rho) \quad (\text{A.I.7})$$

where $\theta(x)$ is the usual step function.

Inserting this for $g_1(\varepsilon, \rho, \rho')$ in (A.I.2), the following expression for $\bar{u}_1(\varepsilon, \varepsilon_n, \rho)$ is obtained :

$$\bar{u}_1(\varepsilon, \varepsilon_n, \rho) = \mathcal{U}_1(\varepsilon, \rho) \int_\rho^\infty \mathcal{V}_1(\varepsilon, \rho') u_{n_0}(\rho') \rho' d\rho' + \mathcal{V}_1(\varepsilon, \rho) \int_0^\rho \mathcal{U}_1(\varepsilon, \rho') u_{n_0}(\rho') \rho' d\rho'.$$

Remembering that near the origin \mathcal{U}_1 behaves like ρ^2 and \mathcal{V}_1 like $1/\rho$, one can see that the first term in the above expression behaves like ρ^2 while the second like ρ^4 . Writing $u_{n_0}(\rho)$ as :

$$u_{n_0}(\rho) = \frac{u_{n_0}(\rho)}{\rho} \Big|_{\rho=0} \mathcal{U}_0(\varepsilon_n, \rho),$$

one finally arrives at the following expression for the electric dipole amplitude :

$$E_{1z} = iea_0 \frac{G_F m_e^2 c}{8\pi \sqrt{2} \hbar^3} \alpha^2 Q_W \frac{u_{n_0}(\rho)}{\rho} \Big|_{\rho=0} \frac{u_{n_0}(\rho)}{\rho} \Big|_{\rho=0} \times [I(\varepsilon_n, \varepsilon_n) - I(\varepsilon_n, \varepsilon_n)] \quad (\text{A.I.8})$$

with

$$I(\varepsilon, \varepsilon') = \int_0^\infty \mathcal{V}_1(\varepsilon, \rho) \mathcal{U}_0(\varepsilon', \rho) \rho d\rho.$$

We shall split the integral $I(\varepsilon, \varepsilon')$ into two parts

$$I(\varepsilon_n, \varepsilon_n) = I_c(\varepsilon_n, \varepsilon_n) + \Delta I(\varepsilon_n, \varepsilon_n),$$

where $I_c(\varepsilon_n, \varepsilon_n)$ is obtained by replacing everywhere $\mathcal{V}_1(\varepsilon_n, \rho)$ and $\mathcal{U}_0(\varepsilon_n, \rho)$ by their Coulomb form $\mathcal{V}_1^c(\varepsilon_n, \rho)$ and $\mathcal{U}_0^c(\varepsilon_n, \rho)$ which are supposed to be valid only for $\rho > \rho_c$. The remaining part $\Delta I(\varepsilon_n, \varepsilon_n)$ is given in terms of integrals involving the interval region $0 < \rho < \rho_c$

$$\Delta I(\varepsilon, \varepsilon') = \int_0^{\rho_c} \mathcal{V}_1(\varepsilon, \rho) \mathcal{U}_0(\varepsilon', \rho) \rho d\rho - \int_0^{\rho_c} \mathcal{V}_1^c(\varepsilon, \rho) \mathcal{U}_0^c(\varepsilon', \rho) \rho d\rho. \quad (\text{A.I.9})$$

We shall show that if ε and ε' are assumed to have the form :

$$\begin{aligned} \varepsilon = \varepsilon_n &= (n - \mu_0(\varepsilon_n))^{-2} \\ \varepsilon' = \varepsilon_{n'} &= (n' - \mu_0(\varepsilon_{n'}))^{-2}, \end{aligned} \quad (\text{A.I.10})$$

n, n' being two integers and $\mu_0(\varepsilon)$ the quantum defect associated with the spectrum of S states, $\Delta I(\varepsilon_n, \varepsilon_{n'})$ can be expanded in power-series in ε_n and $\varepsilon_{n'}$. When n and n' go to infinity with $n - n'$ remaining fixed, the difference $\Delta I(\varepsilon_n - \varepsilon_{n'})$ is of the order of $\varepsilon_n - \varepsilon_{n'} \sim 1/n^3$:

$$\Delta I(\varepsilon_n, \varepsilon_{n'}) - \Delta I(\varepsilon_{n'}, \varepsilon_n) \approx \left(\frac{\partial \Delta I}{\partial \varepsilon} \Big|_{\varepsilon=\varepsilon'=0} - \frac{\partial \Delta I}{\partial \varepsilon'} \Big|_{\varepsilon=\varepsilon'=0} \right) (\varepsilon_n - \varepsilon_{n'}) \sim \frac{1}{n^3} .$$

On the other hand, it will appear that in the same limit, the difference between the Coulomb integrals $I_c(\varepsilon_n, \varepsilon_{n'}) - I_c(\varepsilon_{n'}, \varepsilon_n)$ behaves as n^4 so in this way we shall be led to the approximation :

$$I(\varepsilon_n, \varepsilon_{n'}) - I(\varepsilon_{n'}, \varepsilon_n) \approx I_c(\varepsilon_n, \varepsilon_{n'}) - I_c(\varepsilon_{n'}, \varepsilon_n) . \tag{A.I.11}$$

Let us first construct the function $\mathcal{U}_1(\varepsilon, \rho)$ for $\rho > \rho_c$. Using the results and notations of Appendix I of reference [2], we write \mathcal{U}_1 as :

$$\begin{aligned} \mathcal{U}_1(\varepsilon, \rho) &= \mathcal{U}_1^c(\varepsilon, \rho) = K_1(\varepsilon) U_1(\varepsilon, \rho) \\ &= K_1(\varepsilon) [y_{11}(\varepsilon, \rho) - \beta(\varepsilon) y_{41}(\varepsilon, \rho)] . \end{aligned}$$

The constant $K_1(\varepsilon)$ is obtained from the condition :

$$\lim_{\rho \rightarrow 0} \frac{\mathcal{U}_1(\varepsilon, \rho)}{\rho^2} = K_1(\varepsilon) \lim_{\rho \rightarrow 0} \frac{U_1(\varepsilon, \rho)}{\rho^2} = 1 .$$

With the help of formulas ((A.I.19), (A.I.27) and (A.I.48)) of reference [2], one obtains :

$$K_1(\varepsilon) = \frac{\sin(\pi\mu_1(\varepsilon))}{\frac{2}{3}(Z^*)^{3/2} \beta(\varepsilon) \left[1 + \frac{\varepsilon}{2} + O(\varepsilon^2) \right]} , \tag{A.I.12}$$

with $Z^* = Z(1 - \frac{2}{3}\zeta)$.

To construct $\mathcal{U}_1 = \mathcal{U}_1^c$ for $\rho > \rho_c$, we write :

$$\mathcal{U}_1(\varepsilon, \rho) = L_1(\varepsilon) \bar{y}_{51}(\varepsilon, \rho) \tag{A.I.13}$$

where we have defined :

$$\bar{y}_{51}(\varepsilon, \rho) = \frac{\Gamma(l+1-v)}{\pi v^l} y_{51}(\varepsilon, \rho)$$

$y_{51}(\varepsilon, \rho) = W_{v, l+1/2} \left(\frac{2\rho}{v} \right)$ is the Whittaker function.

The coefficient $L_1(\varepsilon)$ is obtained by writing that the Wronskian $W(\mathcal{U}_1, \mathcal{U}_1) = 1$. In order to do that, we write \mathcal{U}_1 in terms of y_1 and \bar{y}_5 using identities given by Seaton [21] :

$$\begin{aligned} \mathcal{U}_1(\varepsilon, \rho) &= K_1(\varepsilon) \{ y_{11}(\varepsilon, \rho) (1 + \beta(\varepsilon) \times \\ &\times [(1 + \varepsilon) \cotg \pi v + G(\varepsilon, 1)]) + \beta(\varepsilon) \bar{y}_{51}(\rho, \varepsilon) \} . \end{aligned}$$

The Wronskian of the functions $y_1(\varepsilon, \rho)$ and $\bar{y}_5(\varepsilon, \rho)$ can be found in Magnus, Oberhettinger and Soni [20]

$$W(y_1, \bar{y}_5) = -\frac{2}{\pi} .$$

This leads

$$\begin{aligned} L_1(\varepsilon) &= -\frac{\pi}{2} K_1^{-1}(\varepsilon) \times \\ &\times [1 + \beta(\varepsilon) ((1 + \varepsilon) \cotg \pi v + G(\varepsilon, 1))]^{-1} . \end{aligned}$$

By noting that $\mathcal{U}_1(\varepsilon, \rho)$ should be proportional to \bar{y}_5 when ε is equal to the bound state energy of a p state, one obtains the well known relation between $\beta(\varepsilon)$ and the interpolated quantum defect $\mu_1(\varepsilon)$ of p states :

$$\beta(\varepsilon) = [A(v, 1) \cotg \pi\mu_1(\varepsilon) - G(\varepsilon, 1)]^{-1} . \tag{A.I.14}$$

If we restrict ourselves to values of ε such that :

$$\varepsilon = \varepsilon_n = -(n - \mu_0(\varepsilon))^{-2}$$

the above relation leads to the following expression of $L_1(\varepsilon)$:

$$L_1(\varepsilon_n) = \frac{+\frac{\pi}{3} Z^{*3/2} \left(1 - \frac{\varepsilon_n}{2} + O(\varepsilon_n^2) \right) \sin \pi\mu_0(\varepsilon_n)}{\sin \pi(\mu_1(\varepsilon_n) - \mu_0(\varepsilon_n))} . \tag{A.I.15}$$

We note that the two coefficients $K_1(\varepsilon)$ and $L_1(\varepsilon)$ can be expanded in powers series in ε , provided ε is of the form (A.I.10).

For any fixed value of ρ , Ham has shown that $\mathcal{U}_l(\varepsilon, \rho)$ is an analytic function of ε . For $\rho > \rho_c$, $\mathcal{U}_1(\varepsilon, \rho)$ is not analytic in ε , but for values of ε such that $\varepsilon = -[n - \mu_0(\varepsilon)]^{-2}$ it has an asymptotic expansion in ε . This can be seen by writing \bar{y}_{51} in terms of $y_{11}(\varepsilon, \rho)$ and $y_{31}(\varepsilon, \rho)$:

$$\begin{aligned} \bar{y}_{51}(\varepsilon, \rho) &= -y_{31}(\varepsilon, \rho) - (1 + \varepsilon) \cotg \pi v y_{11}(\varepsilon, \rho) \\ &= -y_{31}(\varepsilon, \rho) + (1 + \varepsilon) \cotg(\pi\mu_0(\varepsilon)) y_{11}(\varepsilon, \rho) . \end{aligned} \tag{A.I.16}$$

$y_{11}(\varepsilon, \rho)$ is analytic in ε and $y_{31}(\varepsilon, \rho)$ although non analytic in ε can be expanded in asymptotic series near $\varepsilon = 0$.

This result can be extended to the internal region $\rho < \rho_c$ and the first two terms of the ε expansion of $\mathcal{U}_1(\varepsilon, \rho)$ can be obtained following the techniques developed in Appendix I of reference [2].

From the above considerations, it follows immediately that $\Delta I(\varepsilon, \varepsilon')$ can be expanded in asymptotic power-series in ε and ε' provided ε and ε' are of the form (A.I.10).

The final step of the derivation consists in expressing the Coulomb integral :

$$I_c(\varepsilon, \varepsilon') = \int_0^\infty \mathcal{U}_1^c(\varepsilon, \rho) \mathcal{U}_0^c(\varepsilon', \rho) \rho \, d\rho,$$

in terms of the integrals $I^{\text{B.D.}}(\varepsilon, \varepsilon')$ tabulated by Bates and Damgaard :

$$I^{\text{B.D.}}(\varepsilon_n, \varepsilon_{n'}) = \int_0^\infty u_1^{\text{B.D.}}(\varepsilon_n, \rho) u_0^{\text{B.D.}}(\varepsilon_{n'}, \rho) \rho \, d\rho, \quad (\text{A.I.17})$$

where the functions $u_l^{\text{B.D.}}(\varepsilon, \rho)$ are given by :

$$u_l^{\text{B.D.}}(\varepsilon, \rho) = [\nu^2 \Gamma(\nu - l) \Gamma(\nu + l + 1)]^{-1/2} y_{sl}(\varepsilon, \rho), \quad (\text{A.I.18})$$

with $\varepsilon = -1/\nu^2$.

The S bound state wave function $\mathcal{U}_0(\varepsilon_n, \rho)$ for $\rho > \rho_c$ is equal to its Coulomb form $\mathcal{U}_0^c(\varepsilon_n, \rho)$ which is given using eq. (A. I. 10) and (A. I. 51) of reference [1] by the following expression :

$$\mathcal{U}_0^c(\varepsilon_n, \rho) = -\frac{1}{2\sqrt{Z}} (-1)^n \nu_n^{3/2} u_0^{\text{B.D.}}(\varepsilon_n, \rho). \quad (\text{A.I.19})$$

$$\lim_{n \rightarrow \infty} \frac{I^{\text{B.D.}}\left(-\frac{1}{n^2}, -\frac{1}{(n+1)^2}\right)}{n^2} = J_0(1) - J_1(1),$$

$$\lim_{n \rightarrow \infty} \frac{I^{\text{B.D.}}\left(-\frac{1}{n^2}, -\frac{1}{(n+1)^2}\right) - I^{\text{B.D.}}\left(-\frac{1}{(n+1)^2}, -\frac{1}{n^2}\right)}{n} = -2J_1(1),$$

where $J_n(x)$ is the Bessel function of order n . A similar result is expected to hold true in the more general case of non integer values of ν_n and $\nu_{n'}$ when $\nu_n \rightarrow \infty$, $\nu_{n'} \rightarrow \infty$ with $\nu_n - \nu_{n'}$ fixed. A close inspection of the tables found in reference [5] supports this conclusion.

From this, one concludes that the difference $I_c(\varepsilon_n, \varepsilon_{n'}) - I_c(\varepsilon_{n'}, \varepsilon_n)$ goes like ν_n^4 when $\nu_n \rightarrow \infty$. So that the use of the approximate equality

$$E_{1z} \approx iea_0 \frac{G_F m_e^2 c}{12\sqrt{2} \hbar^3} (Z\alpha)^2 (1 - \zeta) Q_w(Z, N) (1 + \delta_0(\varepsilon_n)) (1 + \delta_0(\varepsilon_{n'})) (-1)^{n+n'+1} \times \left\{ \frac{I^{\text{B.D.}}(\varepsilon_n, \varepsilon_{n'})}{\sin \pi[\mu_1(\varepsilon_n) - \mu_0(\varepsilon_n)]} - \frac{I^{\text{B.D.}}(\varepsilon_{n'}, \varepsilon_n)}{\sin \pi[\mu_1(\varepsilon_{n'}) - \mu_0(\varepsilon_{n'})]} \right\} \quad (\text{A.I.21})$$

with :

$$1 + \delta_0(\varepsilon_n) = \left(1 + \frac{\partial \mu_0}{\partial \nu}\right)^{-1/2} (1 + O(\varepsilon_n^2)).$$

Using eq. (A.I.13), (A.I.15), together with eq. (A.I.18), we obtain :

$$\mathcal{U}_1(\varepsilon_n, \rho) = (-1)^n \frac{\pi Z^{*3/2} \nu_n^{3/2} u_1^{\text{B.D.}}(\varepsilon_n, \rho)}{3 \sin \pi(\mu_1(\varepsilon_n) - \mu_0(\varepsilon_n))}. \quad (\text{A.I.20})$$

We have all we need to express the integral $I_c(\varepsilon_n, \varepsilon_{n'})$ in terms of Bates and Damgaard integrals :

$$I_c(\varepsilon_n, \varepsilon_{n'}) = (-1)^{n+n'+1} \frac{\pi Z(1 - \zeta) (\nu_n \nu_{n'})^{3/2} I^{\text{B.D.}}(\varepsilon_n, \varepsilon_{n'})}{6 \sin \pi(\mu_1(\varepsilon_n) - \mu_0(\varepsilon_n))}.$$

Let us now discuss briefly the difference

$$I_c(\varepsilon_n, \varepsilon_{n'}) - I_c(\varepsilon_{n'}, \varepsilon_n)$$

when n and n' go to infinity, $n - n'$ remaining fixed. Consider first the difference

$$I^{\text{B.D.}}(\varepsilon_n, \varepsilon_{n'}) - I^{\text{B.D.}}(\varepsilon_{n'}, \varepsilon_n).$$

We have not studied the problem in full generality but limited ourselves to the particular case of hydrogenic wave functions corresponding to $\varepsilon_n = -1/n^2$ and $\varepsilon_{n'} = -1/(n+1)^2$.

Using the Gordon formula and asymptotic properties of Jacobi polynomials, we have been able to prove the asymptotic formula :

$$I(\varepsilon_n, \varepsilon_{n'}) - I(\varepsilon_{n'}, \varepsilon_n) \approx I_c(\varepsilon_n, \varepsilon_{n'}) - I_c(\varepsilon_{n'}, \varepsilon_n)$$

introduces a relative error of the order $\nu_n^{-7} = (-\varepsilon_n)^{7/2}$, in the limit of large ν_n or small energy $\varepsilon_n = -1/\nu_n^2$.

Using the above equality, together with the value of $\left. \frac{u_0(\rho)}{\rho} \right|_{\rho=0}$ derived in reference [2], one gets from eq. (A.I.8) the final formula :

This formula has to be multiplied by the relativistic correction factor $K_r(Z, R)$ and ignores the core polarization and spin-orbit effects on the electric dipole matrix element.

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