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Magnetic dipole and electric quadrupole amplitudes induced by the hyperfine interaction in the Cesium 6S-7S transition and the parity violation calibration

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 Résumé. — Une méthode possible pour calibrer l'amplitude électrique dipolaire violant la parité, E1(p.v), relative à la transition 6S → 7S du Césium est d'utiliser le rapport E1(p.v)/M1(h.f) où M1(h.f) est l'amplitude dipolaire magnétique induite par l'interaction hyperfine V(h.f). Nous montrons en évaluant les corrections relativistes et les effets à N-corps que M1(h.f) est donné, à mieux que 3.10^{-3}, par la moyenne géométrique des écarts hyperfins des états 6S et 7S ; M1(h.f) constitue donc une excellente calibration de E1(p.v). Lorsque l'on atteint le niveau du %, il n'est plus possible d'ignorer l'amplitude quadrupolaire électrique E2(h.f) qui, elle aussi, peut être induite par V(h.f). Nous avons montré que E2(h.f), calculée dans le cadre d'un modèle à une partie, est fortement inhibée par une règle de sélection approchée. Cette règle, cependant, ne s'applique pas en général aux effets à N-corps. En conséquence nous donnons une estimation du rapport E2(h.f)/M1(h.f) au premier ordre dans l'interaction électron-électron. Le résultat confirme la nécessité d'inclure E2(h.f) dans l'amplitude de transition radiative, ainsi que le suggère une analyse phénoménologique des données expérimentales. Par ailleurs, l'amplitude quadrupolaire E2(h.f) est une quantité intéressante par elle-même car elle est gouvernée presque exclusivement par les effets à N-corps.

Abstract. — A possible way to calibrate the Cesium 6S → 7S parity violating electric dipole amplitude E1(p.v) is to make use of the ratio E1(p.v)/M1(h.f) where M1(h.f) is the magnetic dipole amplitude induced by the hyperfine interaction V(h.f). We show by evaluating relativistic and many-body effects that M1(h.f) is given, to better than 3.10^{-3}, by the geometrical mean of the 6S and 7S hyperfine splittings and thus provides a very good calibration of E1(p.v). If one wishes to reach the 1% accuracy, it may be no longer legitimate to ignore the electric quadrupole amplitude E2(h.f) which can also be induced by V(h.f). We have shown that E2(h.f), computed within a one-particle model, is strongly suppressed by an approximate selection rule. This rule, however, does not work in general for many-body effects. Consequently we have made an estimate of the ratio E2(h.f)/M1(h.f) to first order in the electron-electron interaction ; we have found a value which confirms the necessity of including the quadrupole amplitude E2(h.f) in the 6S-7S radiative amplitude, as it is suggested by a recent phenomenological analysis of the experimental data. This quadrupole amplitude E2(h.f) is by itself an interesting quantity since it is governed almost exclusively by many-body effects.

Introduction.

The work reported here can be considered as part of a project aiming at a determination, to the 1% level, of the parity violating electric dipole amplitude E1(p.v), in the 6S → 7S transition of atomic Cesium. The motivations behind such a project have been given elsewhere [1]. In all experiments the numbers which are actually measured are amplitude ratios ; it means that one needs a known amplitude to calibrate the amplitude E1(p.v). Up to now the experimentalists have been using a Stark induced E1 amplitude determined by a semi-empirical method [2]. In this paper we suggest another procedure which involves the 6S-7S magnetic transition amplitude induced by the hyperfine interaction V(h.f), called thereafter

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We show that the amplitude $M_1(h.f)$ is given, to better than $2 \times 10^{-3}$, by the nondiagonal matrix element $\langle 7S | V(h.f) | 6S \rangle$ times a known energy denominator. We also prove, following the same kind of idea as in our recent work [3] on the amplitude $E_1(p.v)$, that the nondiagonal matrix element $\langle 7S | V(h.f) | 6S \rangle$ obeys, to an accuracy of $10^{-3}$, the simple factorization rule:

$$\langle 7S | V(h.f) | 6S \rangle = \left( \langle 7S | V(h.f) | 7S \rangle \right)^{1/2} \langle 6S | V(h.f) | 6S \rangle.$$  \hspace{1cm} (1)

The rule is automatically obeyed in a one-particle nonrelativistic model. The small deviation is coming from relativistic and many-body effects. Since the ratio $E_1(p.v)/M_1(h.f)$ is directly accessible to experiment, it is clear that $M_1(h.f)$ provides a very good calibration of the $p.v$ amplitude, free of theoretical uncertainties to better than $3 \times 10^{-3}$.

Up to now the only effect of the hyperfine interaction upon the $6S \rightarrow 7S$ radiative amplitude which has been considered is the modification $M_1(h.f)$ of the $M_1$ amplitude; it leads to appreciable deviations from the standard intensity rules obeyed by the various hyperfine components of the transition. When one reaches the 1% accuracy, another hyperfine mixing has to be considered: the tensor part of $V(h.f)$ gives rise to mixings between the $n'S_{1/2}$ and the $n'D_{3/2}$ states which lead to an electric quadrupole amplitude $E_2(h.f)$ in the $6S \rightarrow 7S$ transition. A rough order of magnitude estimate indicates that this effect has to be studied carefully. As a first step, we have evaluated the amplitude $E_2(h.f)$ within one-particle nonrelativistic and relativistic models. We have found results two orders of magnitude smaller than what was expected from a naïve estimate. This fact can be explained by the existence of an approximate selection rule which suppresses, for small binding energies, the one-particle matrix elements $\langle n'D_{3/2} | V(h.f) | n'S_{1/2} \rangle$. The selection rule works only within a single particle model and it is easy to find many-body processes which do not obey the selection rule. We have made an estimate of $E_2(h.f)$ to first order in the electron-electron interaction. The result is larger than the zero order one by more than two orders of magnitude. Within a suitable normalization, to be given later on, our estimated value for the ratio $E_2(h.f)/M_1(h.f)$ is $0.09 \pm 0.03$. This number is to be compared with the result of the detailed analysis of the empirical data concerning the $6S \rightarrow 7S$ transition performed in reference [4]: $E_2(h.f)/M_1(h.f) = 0.042 \pm 0.013$. Our work does confirm the necessity of including an electric quadrupole amplitude in the description of the $6S \rightarrow 7S$ radiative transition induced by $V(h.f)$, if one wishes to extract from experiment accurate values for the ratio $E_1(p.v)/M_1(h.f)$. Furthermore $E_2(h.f)$ is an interesting example of an atomic quantity dominated by many-body effects.

1. The factorization rule for the $M_1$ amplitude induced by the hyperfine interaction.

Let us begin by some conventions and definitions which we shall be using in the rest of the paper. The electron coordinate $r$, the binding energies $E(nlj)$ and the various interaction energies will be given in atomic units, respectively $a_0$ and $e^2/(2a_0)$, where $a_0$ is the Bohr radius. For a transition involving given radial quantum numbers $n$ and $n'$, it is convenient to introduce the most general parity conserving operator $T(n', n)$, linear in the electronic spin, acting in the tensor product of electronic and nuclear spin spaces, associated with a mixed $M_1 - E_2$ radiative transition:

$$T(n', n) = a_1 S \cdot \epsilon \wedge k + ia_2 (S \wedge I) \cdot (\epsilon \wedge k) + \epsilon \wedge k (S \cdot \epsilon) \cdot (I \cdot k) + (S \cdot k) \cdot (I \cdot \epsilon).$$ \hspace{1cm} (2)

$S$ and $I$ stand for the electronic and nuclear spin operators respectively; $k$ and $\epsilon$ are the momentum and the polarization of the photon. It follows from $T$ invariance that the $a_i$ are real quantities. The first term gives the normal $M_1$ amplitude, the second is associated with the $M_1(h.f)$ amplitude induced by the hyperfine interaction $V(h.f)$, the last term is the $E_2$ amplitude coming from the $S_{1/2} - D_{3/2}$ mixing produced by $V(h.f)$. Terms which do not contain the electron spin, like $(I \cdot k) \cdot (I \cdot \epsilon)$, can be neglected since they involve the coupling of the electron with the nuclear quadrupole moment of the Cesium nucleus which is rather small.

In order to get $T(n'n')$ one starts from the purely electronic transition operator $t(e) = t(M_1) + t(E_2)$ given by:

$$t(M_1) = \mu_B (e \wedge k) \cdot \sum_i (g_e S_i + g_I L_i)$$ \hspace{1cm} (3)

$$t(E_2) = -i/2 \cdot \mu_B (E(n'S_{1/2}) - E(n'S_{1/2})) \times \sum_i (r_i \cdot k) \cdot (r_i \cdot \epsilon).$$ \hspace{1cm} (4)

The $M_1(h.f)$ contribution $T_2(n'n') = ia_2 (S \wedge I) \cdot (e \wedge k)$ is given, to first order in the hyperfine interaction $V(h.f)$ by:

$$\langle F' M' | T_2(n', n') | FM \rangle = \sum_{n'S_{1/2}} F' M' \langle \tilde{T}(M_1) | nS_{1/2} FM \rangle$$

where the perturbed $M_1$ transition operator reads as follows:

$$\tilde{T}(M_1) = V(h.f) \cdot (1 - P(n')) \cdot G(E(n'S_{1/2})) \times t(M_1) + (n' \langle - \rangle n)^I$$ \hspace{1cm} (5)

$G(E)$ stands for the atomic Green function and $P(n)$ for the projector $|nS_{1/2}\rangle \langle nS_{1/2}|$. The diagonal matrix elements of $t(M_1)$ dominate in the atomic
It is convenient to rewrite the matrix element of \( V(h.f) \) as:

\[
\langle n' S_{1/2} F M' \mid V(h.f) \mid n S_{1/2} F M \rangle = \langle n' S_{1/2} F M' \mid V(h.f) \mid n S_{1/2} F M \rangle \times \langle n S_{1/2} F M \mid t(M_1) \mid n S_{1/2} F M \rangle /
\]

\[
(E(n' S_{1/2}) - E(n S_{1/2})) + (n\langle - \rangle n')
\]

We shall not try to compute explicitly \( \langle n' S_{1/2} \mid V(h.f) \mid n S_{1/2} \rangle \), but as we have done in our recent work on parity violation, we shall introduce a matrix element rescaled by the geometrical mean of the h.f splittings of the \( n S_{1/2} \) and \( n' S_{1/2} \) states:

\[
Y(n' n) = \langle n' S_{1/2} \mid V(h.f) \mid n S_{1/2} \rangle / D(n' n) \tag{9}
\]

where:

\[
D(n' n) = (\langle n' S_{1/2} \mid V(h.f) \mid n' S_{1/2} \rangle \times \langle n S_{1/2} \mid V(h.f) \mid n S_{1/2} \rangle)^{1/2}. \tag{10}
\]

We note first that \( Y(n' n) \) is invariant upon a change of normalization of the states:

\[
|n S_{1/2}\rangle \rightarrow C(n) \mid n S_{1/2}\rangle, |n' S_{1/2}\rangle \rightarrow C(n') \mid n' S_{1/2}\rangle.
\]

In nonrelativistic single-particle model, the matrix element \( \langle n' S_{1/2} \mid V(h.f) \mid n S_{1/2} \rangle \) is proportional to the product of the wave functions evaluated at the origin \( R_{m}(0) \cdot R_{n'}(0) \), so that \( Y(n' n) \) is in this case equal to one. It is clear that such a result does not hold exactly when relativistic and many-body effects are taken into account.

Let us first study the relativistic corrections. We shall assume for simplicity that the nuclear magnetism is distributed over a thin spherical shell, of radius \( R \). Our argument applies equally to other distribution shapes. We write the Dirac amplitudes in a central potential \( V(r) \) as:

\[
\psi_{\alpha j m}(r) = \begin{pmatrix} g_{\alpha n}(r) \Omega_{\kappa m} \\ f_{\alpha n}(r) \Omega_{\kappa m}' \end{pmatrix}
\]

where \( \kappa = (\ell - j) \cdot (2 j + 1) \) and \( \ell' = 2 j - \ell \). \( \Omega_{\kappa m} \) are the conventional spherical spinors. Up to a constant factor the matrix element of \( V(h.f) \) is given by:

\[
\langle n' S_{1/2} \mid V(h.f) \mid n S_{1/2} \rangle = \int_{R} d r (f_{-1 n}(r) \cdot g_{-1 n}(r) + f_{-1 n}(r) \cdot g_{-1 n}(r)). \tag{12}
\]

Using the Dirac equation, we write the radial wave function as:

\[
f_{-1 n}(r) = \alpha/2 (d/dr g_{-1 n}(r))/(1 + \alpha^2(E(n) - V(r))/4)
\]

where the central potential \( V(r) \), given in atomic unit, is such that \( \lim (r \rightarrow 0 r V(r)) = -2. Z \). For the states of interest, \( \alpha^2 E(n)/4 \) is smaller than \( 10^{-4} \) and can be ignored. With the help of an integration by part we rewrite the matrix element of \( V(h.f) \) as:

\[
\langle n' S_{1/2} \mid V(h.f) \mid n S_{1/2} \rangle = -\alpha/2 \cdot (g_{-1 n}(R) \cdot g_{-1 n}(R))/(1 - \alpha^2 V(R)/4) + I(n' n)
\]

where \( I(n' n) \) is given by:

\[
I(n' n) = \int_{R} d r g_{-1 n}(r) g_{-1 n'} \times
\]

\[
x d/dr(1/(1 - \alpha^2 V(r)/4)).
\]

Since \( Y(n' n) \) is independent of the wave function normalization, we can normalize \( g_{-1 n} \) \( g_{-1 n'} \) in such a way that: \( g_{-1 n}(R) = g_{-1 n}(R) = 1 \).

The integrant of \( I(n' n) \) is non zero for values of \( r \) such that \( -V(r) > 4/\alpha^2 \Rightarrow -E(n), -E(n') \). It fol-
lows then that $I(n', n)$ receives its main contribution from values of $r \leq Z \alpha^2$ for which the binding energies are negligible compared to the potential energy $V(r)$. This fact together with our normalization imply that the functions $g_{-1,n}$ and $g_{-1,n'}$ are independent of $E(n)$ and $E(n')$ in the domain of integration. Indeed, we have verified by an explicit calculation that $I(n', n)$ is independent of $n$ and $n'$ to better than $2 \times 10^{-4}$. We have found finally that the factorization relation (1) is satisfied to an accuracy of $10^{-4}$ in a single-particle relativistic model.

Let us turn now to the many-body corrections to $Y(n' n)$. From the above considerations, it follows that the many-body effects which can be described by a perturbation of the valence orbitals have practically no effects upon $Y(n' n)$. The mechanism which may lead to deviations from the factorization rule is the modification of the hyperfine interaction induced by the excitation of electron-hole pairs by the valence electron. This can be described by adding to the local interaction $V(h.f, r)$ a nonlocal part $V^{(1)}(h.f, r, r')$, the explicit form of which is given in reference [3]. We have computed the ratio $\delta (n', n) / \delta (n, n)$ of the matrix element of $V^{(1)}(h.f, r, r')$ to that of $V(h.f, r)$ for the states of interest; the results are given below:

$$\begin{array}{cccc}
(n', n) & (6.6) & (7.7) & (7.6) \\
\delta (n', n) / \delta (n, n) & 0.18354 & 0.17635 & 0.18060 \\
\end{array}$$

The resulting modifications of $Y(n' n)$ is:

$$\delta (7.6) - 1/2 \cdot (\delta (6.6) + \delta (7.7)) = 0.0007$$

We have not yet explored all the first order many-body effects which may correct the amplitude $M_1(h.f)$ as given by formula (6). In the summation over the intermediate states performed in the derivation of (6), we have left out the autoionizing states involving a valence electron plus an electron-hole pair. These states do contribute to first order in the electron-electron interaction. If the many-body effects are described by Q.E.D like diagrams these terms are associated with box diagrams, while the contributions discussed so far correspond to self-energy and vertex graphs. In figure 1 we have drawn two time ordered diagrams which describe the contribution of autoionizing states. There are two other diagrams which are obtained by changing the time ordering of $V(h.f)$ with respect to the electron-electron interaction. We have written down the amplitude $M(A) = M(A_1) + M(A_2)$ associated with $(A_1)$ and $(A_2)$:

$$M_1(h.f) = \sum \int V(|r_1 - r_2|) \cdot \psi_n(r_1) \cdot \left( \hat{G}(r_2, r, E(n) + \omega_0) - \hat{G}(r_2, r, E(n)) \right) / \omega_0 [M_1, V(h.f)] \times$$

$$\times \psi_n'(r_1) \cdot \psi_{6s}(r_1) \cdot \psi_{6s}(r_1) \cdot d^3 r_1 d^3 r_2 d^3 r$$

In conclusion, to an accuracy of $2 \times 10^{-3}$, $M_1(h.f)$ is proportional to the nondiagonal matrix element $\langle 7S_{1/2} | V(h.f) | 6S_{1/2} \rangle$ which is given, up to corrections smaller than $10^{-3}$, by the geometrical mean of the $6S_{1/2}$ and $7S_{1/2}$ hyperfine splittings.

2. The electric quadrupole amplitude induced in the $6S \rightarrow 7S$ transition by the hyperfine interaction.

The hyperfine interaction is able to produce mixings of $nS_{1/2}$ to $n'D_{3/2}$ states and, as a consequence, the $6S_{1/2} \rightarrow 7S_{1/2}$ radiative transition amplitude will contain a small electric quadrupole part $E_2(h.f)$ given by the quantity $a_3$ in equation (2). In reference [4], the existing experimental data [5] concerning the $6S_{1/2} \rightarrow 7S_{1/2}$ transition have been carefully analysed.
using the effective transition operator \( T(n', n) \) given by formula (2). The following value for the ratio \( a_3/a_2 \) comes out from a best fit with \( a_1, a_2, a_3 \) as free parameters:

\[
a_3/a_2 = 0.042 \pm 0.013.
\]

The experimental ratio is three standard deviations away from zero and the quality of the fit is much improved (smaller \( \chi^2 \) if \( a_3 \) is assumed to be non-zero.

In view of the above result, a theoretical analysis was undertaken within the framework of nonrelativistic and relativistic one-particle models. The \( E_2(h.f) \) amplitude \( a_3 \) is given by:

\[
a_3 = -1/5 \cdot \mu_B C \sum_{\pi'} (W(n'S_{1/2}, n''D_{3/2}) \cdot Q(n''D_{3/2}, nS_{1/2}) \times \)
\[\times (E(n'S_{1/2}) - E(n''D_{3/2})^{-1}) + (n \leftrightarrow n')) \quad (14)
\]

with:

\[
W(nS_{1/2}, n'D_{3/2}) = 2/(3 \alpha) \int_0^\infty (f_{-1+n}(r) \cdot g_{2n}(r) + f_{2n}(r) \cdot g_{-1+n}(r)) dr \quad (15)
\]

\[
Q(n'D_{3/2}, nS_{1/2}) = \int_0^\infty (g_{-1+n}(r) \cdot g_{2n}(r) + f_{-1+n}(r) \cdot f_{2n}(r)) r^4 dr. \quad (16)
\]

A little to our surprise, we have found that the one-particle result obtained with the Norcross potential is much smaller than one might have expected on the basis of simple minded estimates. The explanation is to be found in the existence of an approximate selection rule for the non-diagonal matrix element of \( V(h.f) \) between single particle states. Let us consider the following radial integral:

\[
X(\kappa, \kappa') = \int_0^\infty (g_\kappa(r) \cdot f_\kappa'(r) + f_\kappa(r) \cdot g_\kappa'(r)) dr. \quad (17)
\]

where

\[
X_0(\kappa, \kappa') = - (\kappa + \kappa' - 1) / 2/\alpha \int_0^\infty f_\kappa(r) \cdot f_\kappa'(r)/(rV(r)) dr
\]

\[
\Delta_1X(\kappa, \kappa') = \int_0^\infty (E(n') \cdot g_\kappa(r) \cdot f_\kappa'(r) + E(n') \cdot f_\kappa(r) \cdot g_\kappa'(r))/V(r) dr
\]

\[
\Delta_2X(\kappa, \kappa') = 2/\alpha \int_0^\infty r dr / dr \log (rV(r)) \cdot f_\kappa(r) \cdot f_\kappa'(r)/(rV(r)) dr
\]

The first term \( X_0(\kappa, \kappa') \) is the only one which remains for a Coulomb potential when the limit of small binding energies is taken. It obeys a strict selection rule with respect to the quantum number \( \kappa \): \( X_0(\kappa, \kappa') \) vanishes if \( \kappa + \kappa' = 1 \); this relation is clearly satisfied for \( S_{1/2} - D_{3/2} \). Under normal conditions, say \( \kappa = \kappa' = 1 \), \( X_0(\kappa, \kappa') \) is the dominant term and it receives its main contribution from low values of \( r \): \( 0 \leq r \leq 1/Z \). For such values of \( r \) the integrant of \( \Delta_1X(\kappa, \kappa') \) is suppressed, in the case of valence states, by the factor

\[
E(n)/V(r) < 10^{-4}. \quad (18)
\]

The suppression factor for \( \Delta_2X(\kappa, \kappa') \) is the dimensionless screening function \( rd/dr \log (rV(r)) \) which vanishes for \( r = 0 \) and stays below 0.1 when \( 0 \leq r \leq 1/Z \). From the above considerations, it follows that the selection rule should work pretty well for the valence states while its validity is dubious for deeply bound states and for the scattering states. It is then necessary to perform exactly the summation over the \( D_{3/2} \) states with the help of a Green function technique. We have completed the computations of \( a_3 \) using the finite
sum and the Green function methods, both with relativistic and nonrelativistic potential models. The four numbers obtained in this way differ in detail but they lead to values for the ratio $|a_3/a_2|$ which are all below 0.001 and consequently too small to affect the empirical determination of $M_1(h.f)$ at the 1% level. So one may think that, after all, the neglect of $E_2(h.f)$ was justified. However the selection rule which suppresses the one-particle matrix element $\langle n' D_{3/2} | V(h.f) | n S_{1/2} \rangle$ has no reason to do so when $V(h.f, r)$ is replaced by the nonlocal interaction $V^{(1)}(h.f, r, r')$ induced by the core polarization; indeed it will then appear unsuppressed matrix elements between one-particle P states, associated with the excitation of electron-hole pairs by the dipole-dipole electron-electron interaction. Consequently we have computed the core polarization amplitude contributions described by the time ordered diagrams given in figure 2. The summation over the $n' P$ states and $n'' D_{3/2}$ states has been performed exactly using Green functions techniques. We have obtained for the ratio $a_3/a_2$ the following result:

$$a_3/a_2 = 0.09.$$  \hfill (19)

We have neglected in $V^{(1)}(h.f, r, r')$ the quadrupole-quadrupole electron-electron interaction. This is quite legitimate since the h.f splittings for D states, which are then involved, are in general one order of magnitude smaller than the corresponding quantities for the P states. The many body effects which can be described as a modification of the valence orbitals are expected to be suppressed by the selection rule discussed previously. The most important first order effects which have been left out are the contributions of the box diagrams of the type given in figure 1, they involve two large energy denominators and are usually smaller than the ones we have considered.

Among the higher order effects the one which is potentially the most important is the screening of the quadrupole radiation field by the core polarization; it is expected to lead to a decrease of the $E_2$ amplitude involved in the computation of the first order diagrams of figure 2. Similarly we know that the P states h.f matrix elements used in our computation overestimate the h.f splittings by about 10% so a corresponding reduction factor should be applied to the result given in equation (19).

It is, of course, rather difficult to estimate, without an explicit calculation, the theoretical uncertainty affecting the number given in equation (19), due to the contributions we have neglected. In view of what happens in similar computations, 30-40% seems to us a reasonable guess for the theoretical error.

From we have said before, it is likely that our evaluation of $E_2(h.f)$ overestimates the actual value, so the fact our result is larger by about a factor two than the central experimental value should not be taken too seriously.

In conclusion, it appears to be reasonably well established that, in order to extract from experiments an accurate value of $M_1(h.f)$, it is necessary to incorporate in the phenomenological analysis the $E_2(h.f)$ amplitude which, by itself, is a rather interesting physical quantity since it is governed almost exclusively by many-body effects.

References


