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V.V. FLAMBAUM

TO THE QUESTION OF ELECTRIC-DIPOLE MOMENT ENHANCEMENT
IN HEAVY ATOMS

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TO THE QUESTION OF ELECTRIC-DIPOLE MOMENT ENHANCEMENT

(EM) ENHANCEMENT IN HEAVY ATOMS

pointed out by Salpeter [1], later Gendens, Struchiner

[2,3] and Ignatovich [4]. The first calculation found

V.V. FLAMBAUM

It was found that

Institute of Nuclear Physics

in heavy atoms the enhancement factors are more than 100

Novosibirsk 90, USSR

times. In the present paper the expressions for EM of

alkalis and thallium are obtained as a function of the

quantum numbers of the ground state and the excited state

showing that the enhancement factors are significantly larger

than in the case of the ground state. The simple way to calculate the factors of electron

electric-dipole moment enhancement in heavy atoms is pre-

sented. The dipole moments of alkalis and thallium are fo-

und. The results are discussed below.

The Hamiltonian of electron interaction with electric

field is of the form [1]

$$H = -eU - \frac{d \cdot \vec{E}}{c} \quad (1)$$

where \vec{E} is the electric field, U is the potential, d is the

dipole moment of electron, β, Z are the Dirac matrices. Thanks to the

electron EM interaction with the total electric field of

the atom wave function of the ground state mixes with the

states of the opposite parity and of the same total angular

momentum (because the perturbation operator $-\frac{d \cdot \vec{E}}{c}$

is paravector)

$$|0\rangle \rightarrow |0\rangle - \frac{d \cdot \vec{E}}{c} \frac{1}{E_0 - H_0} |0\rangle \quad (2)$$

where $\vec{E} = \sum_{i=1}^Z \vec{E}_i$ (the sum over i is performed

over all atom electrons), H_0, E_0 are the energies of the

The possibility of electron electric -dipole moment (EDM) enhancement in atoms for hydrogen example was first pointed out by Salpeter /1/. Later Sandars, Sternheimer /2,3/ and Ignatovich /4/ using numerical calculation found dipole moments of alkalis and thallium. It was found that in heavy atoms electron EDM can be enhanced more than 100 times. In the present paper the expressions for EDM of alkalis and thallium dependent only on the quantities known experimentally are obtained. Comparison of the result shows that for alkalis our formula agrees with numerical computations in /2/ and /4/. But our results for thallium disagrees with that obtained in /3/. The roots of the disagreement are discussed below.

Hamiltonian of electron interaction with electric field is of the form /1/

$$H_{int} = -eU - d_e \beta \vec{\Sigma} \vec{E} \quad (1)$$

where \vec{E} is the electric field, U is the potential, d_e is EDM of electron, $\beta, \vec{\Sigma}$ are the Dirac matrices. Thanks to the electron EDM interaction with the total electric field of an atom wave function of the ground state mixes with the states of the opposite parity and of the same total angular momentum (because the perturbation operator $d_e \beta \vec{\Sigma} \vec{E}$ is pseudoscalar)

$$|0'\rangle = |0\rangle - d_e \sum_K \frac{V_{K0}}{E_c - E_c} |K\rangle \quad (2)$$

where $V = \sum_{i=1}^N \beta_i \vec{\Sigma}_i \vec{E}_i$ (the sum over i is performed over all atom electrons), E_0, E_K are the energies of the

ground and excited states. The resulting total atomic dipole moment is equal to

$$d_A = \langle 0 | d_e \sum_{i=1}^N \beta' \vec{z}_i' - e \sum_{i=1}^N \vec{z}_i | 0' \rangle =$$

$$= 2 d_e e \sum_K \operatorname{Re} \frac{\langle 0 | \sum_{i=1}^N (\beta' - 1) \vec{z}_i' \vec{E}^i | K \rangle \langle K | \sum_{i=1}^N \vec{z}_i' | 0 \rangle}{E_0 - E_K} +$$

$$+ \langle 0 | \sum_{i=1}^N d_e (\beta' - 1) \vec{z}_i' | 0 \rangle$$

Here we use the identity $\vec{z} \vec{E} = \frac{1}{2} [\vec{z} \vec{\nabla}, H_0]$ /5,6/. Operator of interaction $V' = (\beta' - 1) \vec{z} \vec{E}$ falls off rapidly as the distance from nucleus increases ($V' \sim \frac{e Z_{eff}}{r^3}$), and the region $r \sim \frac{a}{Z}$ gives the main contribution to its matrix element (a is the Bohr radius, Z is the nucleus charge).

As at this distances the field of the nucleus is not shielded ($U = \frac{Z e^2}{r}$), the solutions of the single-particle Dirac equation in this region are relativistic Coulomb functions corresponding to energy $E \approx 0$ (see, for example, /7/).

Normalization factor in these functions is determined by comparison with non-relativistic quasi-classical solution which is valid at the large distances from a nucleus /8/. The hyperfine structure ^{computed using these particles} agrees with the experimental value within some percent. Single-particle matrix element of operator V' obtained using these functions is equal to ($\hbar = c = 1$)

$$Z e \langle j, j_z, \ell = j + \frac{1}{2} | \frac{1}{r^3} (\beta' - 1) \vec{z} | j, j_z, \ell = j - \frac{1}{2} \rangle =$$

$$= - \frac{4i (Z a)^2 Z e}{\gamma (4\gamma^2 - 1) a^2 (n_o^* n_k^*)^{3/2}} \quad (4)$$

where $\gamma = \sqrt{(j + \frac{1}{2})^2 - (Z a)^2}$, a is the Bohr radius, n_o^* , n_k^* is the effective principal quantum number ($E = -\frac{m \alpha^2}{2 n^2}$)

of the ground state and excited state, J, l are the total and orbital angular momenta of an electron. Single-particle matrix element of radius-vector are expressed through radial integral $r = \int_0^\infty R_o r R_k r^2 dr$

$$\langle j, j_z, \ell = j - \frac{1}{2} | z | j, j_z, \ell = j + \frac{1}{2} \rangle = - \frac{i j_z}{2 j(j+1)} \chi_{ok} \quad (5)$$

The absolute value of r_{ok} one can obtain from the experimental oscillator strength data. Sign of r_{ok} is defined from the Bates-Damgaard tables /9/. It is necessary to take into account that in /9/ radial wave functions used for calculation r_{ok} have been taken positive at $r \rightarrow \infty$, but in our calculation their signs must be defined by the conjunctions with Coulomb solution /7/. Using (3), (4), (5) and expressing atom wave function as the products of single-particle functions we could calculate EDM of an atom. But really it is enough to take into account in the sum (3) only excitations of the electrons from the incomplete shell. (for example in Cs the contribution of the excitations of 5s and 5p electrons is not larger than some percents). Thus the final result for alkalis is of the form

$$R = \frac{d_A}{j_z d_e} = \frac{4 (Z a)^3 \hbar c}{(j+1) \gamma (4\gamma^2 - 1) a^2 (n_o^*)^{3/2}} \sum_K \frac{\chi_{ok}}{(n_k^*)^{3/2} (E_k - E_0)} \quad (6)$$

where the sum is performed over excitations of the external electron, and it is enough with some percents accuracy to take into account only one term, corresponding to mixing with nearest level. One can see from the expression (6) that the factor R is large when the charge of the nucle-

us is large and the total angular momentum is small ($d_A \sim \frac{1}{(j+\frac{1}{2})^4}$). For example, in the ground state of cesium ($Z=55, J=\frac{1}{2}$) $R_{Cs} = 138$. This value agrees with $R_{Cs} = 133$ and 131 obtained earlier in the works /2,4/. The value R comparable to R_{Cs} is obtained also for the lowest metastable state with s-electron (3P_2) in xenon ($R_{Xe} \sim 120$; see also /12a/).

Let us now calculate EDM of thallium. Its ground state $6s^2 6p_{1/2}$ can be mixed with both states with excited p-electron ($6s^2 ns_{1/2}$) and with excited s-electron ($6s6p^2$), and their contributions to EDM prove to be approximately equal. One can take into account mixing with $6s^2 ns_{1/2}$ using formula (6). But for calculation of s-electron excitations it is needed to know the "true" wave functions of the $6s6p^2$ states with total angular momentum $J=\frac{1}{2}$. According to work /10/ the expansion of this functions in terms of the functions with definite total spin and total orbital angular momentum is of the form¹⁾

$$\begin{aligned} (E=76880) &= 0,444 \ ^2S_{1/2} + 0,894 \ ^2P_{1/2} - 0,056 \ ^4P_{1/2} \\ (E=66960) &= 0,846 \ ^2S_{1/2} - 0,439 \ ^2P_{1/2} - 0,302 \ ^4P_{1/2} \\ (E=45220) &= 0,295 \ ^2S_{1/2} - 0,087 \ ^2P_{1/2} + 0,952 \ ^4P_{1/2} \end{aligned} \quad (7)$$

1) I thank V.N.Novikov and I.B.Khrilovich who have placed at my disposal their calculation of $6s6p^2$ states in thallium.

where E is the energy in cm^{-1} counted off the ground state. Then expressing wave functions of the ground and excited states as the sum of products of the single-particle functions and using (3), (4) and (5), find

$$R_{Tl} = \frac{d_A}{\frac{y_2}{y} d_e} = R(6p \rightarrow ns) + R(6s \rightarrow 6p) \approx -188 - 183 \approx -370 \quad (8)$$

Note, that in the ground state of thallium the proper dipole moment of the electron is directed oppositely to \vec{J} too ($\langle d_e \hat{e}_z \rangle = -\frac{2}{3} y_2 d_e$). The experimental value of d_{Tl} is $(1,3 \pm 2,4) \cdot 10^{-21} \text{ e.cm} / \text{II}$, hence for d_e we obtain $d_e = (-3,5 \pm 6,5) \cdot 10^{-24} \text{ e.cm}$. It is comparable to $|d_e| < 3 \cdot 10^{-24} \text{ e.cm}$ and $d_e = (0,7 \pm 1,5) \cdot 10^{-24} \text{ e.cm}$ obtained in works /12,12a/ from measurements on cesium and xenon EDM.

The numerical calculation of thallium EDM has been performed earlier in work /3/. However in this work contribution of mixing with $6s6p^2$ states has not been taken into account. Besides that, the contribution of single-particle excitations presented in /3/ is four times larger than one obtained in our work. The reason of this difference could be on our mind the following. In papers /2,3,4/ authors have used Sternheimer equation²⁾ /13/

$$(H - E_0) |p\rangle = \sum_k |k\rangle \langle k|z|0\rangle = z|0\rangle \quad (9)$$

2) One can obtain this equation also "multiplying" the equation for electron Green function $G = \sum_k \frac{|k\rangle \langle k|}{E_k - E}$ by $z|0\rangle$.

where $|p\rangle = \sum_k \frac{|k\rangle\langle k|Z|0\rangle}{E_k - E_0}$, H is unperturbed Hamiltonian of the electron in atomic electric field. Then single-particle function $|p\rangle$ obtained from this equation (numerically) is used to calculate d_A . However, if $|0\rangle$ and $|k\rangle$ are single-particle electron functions in the self-consistent field, functions $|k\rangle$ form a complete set only if the sum $|p\rangle$ contains transitions to occupied levels really unexisting, in particular to $6s_{1/2}$ ³⁾. As $6s_{1/2}$ level is in the same shell that $6p_{1/2}$, their mixing would be the strongest one. It is the reason, on our mind, that R_{T1} is so large in the work /3/. The well known example when analogous situation appears, is the calculation of the oscillator strength sum /14,15/. Because of theoretic oscillator strength sum for transitions from the ground state with $l=1$ to $l=0$ includes really unexisting transitions to occupied levels, it has an opposite sign than experimental one /15/. Note that for alkalis transitions to the occupied states change the result quite a little because the transition inside shell $ns \rightarrow np$ really exists in this case and contribution of the mixing with other shells is small (for example, in Cs transition $6s \rightarrow 7p$ gives 2% $6s \rightarrow 6p$).

In conclusion dwell on the question about influence of the electron core on the EDM created by valence electrons.

3) This problem is absent if $|0\rangle$ and $|k\rangle$ are the total antisymmetric atomic wave functions, but the equation (9) will not be single-particle one in this case.

When interacting with external electric field, the core is polarized by it and changes the field acting on the valence electrons. However, we have taken into account the considerable part of this effect already using the radial matrix elements obtained from the experiment. The point is that when the photon frequency is small in comparison to frequency of the inner electrons, the polarizability of the core is the same as in the constant external field. In the alkalis radial matrix element can be obtained also from the experimental data of atomic polarizability and its value is found approximately the same /16/.

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