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**TO THE QUESTION OF PARITY NONCONSERVATION
IN FORBIDDEN ATOMIC TRANSITIONS**

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TO THE QUESTION OF PARITY NONCONSERVATION
IN FORBIDDEN ATOMIC TRANSITIONS

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The mechanism of forbidden M1 transition 6s - 7s in cesium is discussed. The contribution of relativistic effects to this transition and to g-factor of valent electron is computed. 6s - 7s transition is shown to proceed mainly because of configurations mixing. Due to weak parity violating eN interaction, a circular polarization of photons at the level 10^{-5} may arise in this transition. Atomic transitions are pointed where one may expect somewhat larger effects of parity violation.

1. INTRODUCTION

For many years the theorists discuss the question of the possibility to observe in atomic transitions the effects caused by the existence of weak interaction between electrons and nucleons (eN interaction) /1,2/. The new out-break of interest to this problem (see recent works/3,4/ and/5-7/) is caused by creation of renormalized unified models of electromagnetic and weak interactions. The important role was played also by recent experiments at CERN/8/ and Batavia/9/ that pointed at the existence of neutral currents involving neutrinos.

Since the hypothetical eN interaction at the energies of atomic order of magnitude is evidently extremely small, it can be detected in this region by qualitative effects only. Parity violation is meant. The presence of P-odd interaction would lead to the mixing of levels with the same total angular momentum and opposite parity. Then the radiation amplitudes for right- and left-polarized photons would be different, in other words, the radiation would be circularly polarized.

The mixing of levels with opposite parity is evidently the larger, the smaller is the interval ΔE between them. At the first sight, atomic hydrogen is out of competition in this respect since its levels $2s_{1/2}$ and $2p_{1/2}$ are separated due to Lamb shift only. Moreover, in the $1s-2s$ transition an additional enhancement in the effect arises. It is connected with the fact that the one-quantum transition (M1 if parity is conserved) is strongly suppressed here, it proceeds only due to relativistic effects. However, even in this extremely favourable situation the degree of circular polarization is $4 \cdot 10^{-4}$ only. In my opinion, the experiments of this kind with atomic hydrogen are hardly practicable at present.

An important step that allowed to pass to the discussion of realistic experiments, was made by Bouchiat/3/. They have shown that in heavy atoms where all energy intervals between levels are of normal magnitude, a new enhancement of the effect $\sim Z^3$ arises due to a large value of the wave function near the nucleus (and of course, to a large number of nucleons in the nucleus). Moreover, since the motion of the electrons near

the nucleus is relativistic, an additional enhancement of the effect takes place/3/. The corresponding factor is

$$R = 4 \left(2r_0 Z / a_0 \right)^{2x-2} / \Gamma^2(2x+1) \quad (1)$$

Here a_0 is the Bohr radius, r_0 is the radius of the nucleus, $\delta = \sqrt{1 - Z^2 \alpha^2}$. Bouchiat/3/ estimated the degree of circular polarization of photons in the 6s-7s transition in atomic cesium to constitute 10^{-4} . At such a magnitude of the effect the experiment on the detection of parity non-conservation in cesium vapour, discussed in the work/3/, would be quite practicable already at present.

However, the estimate of the matrix element of M1 transition 6s-7s, presented in the paper/3/, is in my opinion essentially understated, and the estimate of the degree of circular polarization is correspondingly overstated. Discuss now this question in detail.

2. COMPUTATION OF RELATIVISTIC EFFECTS. ESTIMATE OF RADIATIVE CORRECTIONS

One-quantum $6s_{1/2} - 7s_{1/2}$ transition proceeds via electron spin-flip and is strongly forbidden because of orthogonality of coordinate wave functions. As well as in hydrogen the strict ban is lifted if one takes into account the relativistic effects. The simplest way, as it seems to me, to obtain relativistic corrections to the Hamiltonian of interaction of many-electron atom with external field is as follows. Consider at first one electron. Its Hamiltonian of interaction with external field \bar{A} , accounting for the terms $\sim (v/c)^3$, is found by means of usual transformations (see/10/):

$$\begin{aligned} H_{int} = & -\frac{e}{2mc} [\bar{p}_i \bar{A}(r_i) + \bar{A} \bar{p}_i] - \mu \left(1 - \frac{\hbar |\bar{k}|}{4mc} \right) \bar{\sigma}_i \bar{\mathcal{H}}(r_i) + \frac{e^2}{mc^2} \bar{A} \bar{A}_i + \\ & + \frac{e}{8m^2 c^3} [p_i^2 (\bar{p}_i \bar{A} + \bar{A} \bar{p}_i) + (\bar{p}_i \bar{A} + \bar{A} \bar{p}_i) p_i^2] + \\ & + \frac{e \hbar}{8m^2 c^3} [p_i^2 (\bar{\sigma}_i \bar{\mathcal{H}}) + (\bar{\sigma}_i \bar{\mathcal{H}}) p_i^2] - \frac{e \hbar}{4m^2 c^2} \bar{\sigma}_i [\bar{\mathcal{E}} \times \bar{p}_i] - \\ & - \frac{e \hbar}{4m^2 c^3} \bar{\sigma}_i [\bar{v} U \times \bar{A}] \end{aligned} \quad (2)$$

Here

$$U = -\frac{Ze^2}{r_i} + e^2 \sum_{j \neq i} \frac{1}{r_{ij}}, \quad \bar{r}_{ij} = \bar{r}_i - \bar{r}_j \quad (3)$$

$$\bar{\mathcal{H}}(\bar{r}_i) = \text{rot } \bar{A} = \bar{\mathcal{H}} e^{-i\bar{k}\bar{r}_i}, \quad \bar{\mathcal{E}} = -\frac{\bar{k}}{|\bar{k}|} \times \bar{\mathcal{H}} \quad (4)$$

The vector-potential \bar{A}_i is created by other electrons. It is equal to

$$\bar{A}_i = \frac{e}{mc} \sum_{j \neq i} \left(\bar{p}_j / r_{ij} + \frac{\hbar}{2} \bar{\sigma}_j \times \bar{r}_{ij} / r_{ij}^3 \right) \quad (5)$$

The coordinate, momentum and spin of the electron under consideration are marked by index i , and the corresponding operators for other electrons of the atom are marked by index j . The total interaction Hamiltonian for many-electron system is found by summation of H_{int} over all electrons. Here as usually one should be cautious not to take into account twice the interaction between the same pair of electrons.

After simple transformations, accounting for spherical symmetry of initial and final states, the matrix element of interaction Hamiltonian is reduced to

$$\langle H_{int} \rangle = -\frac{1}{3} \mu \bar{\mathcal{H}} \sum_i \left\langle \frac{\bar{\sigma}_i p_i^2}{m^2 c^2} + \frac{e^2 \bar{\sigma}_i}{mc^2} \sum_{j \neq i} \frac{(\bar{r}_i \bar{r}_{ij})}{r_{ij}^3} \right\rangle \quad (6)$$

Note that to transform the terms $k^2 r_i^2$ (they arise in particular after expansion into series of the exponent in $\bar{\mathcal{H}}(r_i)$) the following identity

$$k^2 \langle r_i^2 \rangle = \frac{1}{\hbar^2 c^2} \langle [H_0, [H_0, r_i^2]] \rangle = \frac{2}{mc^2} \langle \bar{r}_i \cdot \bar{v}_i U - \frac{p_i^2}{m} \rangle \quad (7)$$

is convenient.

In the case of two electrons the expression (6) coincides with the result obtained previously for helium-like systems by other methods in the works/11,12/.

For cesium, taking into account that all the electrons, except the valent one, may be combined into pairs with zero total spin, transform the expression (6) to the following form

$$\langle H_{int} \rangle = -\frac{1}{3} \mu \bar{\sigma} \bar{p} \left\langle \frac{p^2}{m^2 c^2} + \frac{1}{m c^2} \frac{d}{dr} (r \bar{U}) \right\rangle \quad (8)$$

Here $\bar{\sigma}$, \bar{p} and \bar{U} are the spin, momentum and effective potential of the valent electron.

The matrix element (8) was computed in two ways.

1) The Thomas-Fermi approximation for the potential, created by other electrons, and quasiclassical expressions for wave functions were used. In the integration region that gives the principal contribution to the matrix element, the energies of 6s and 7s states may be neglected in comparison with the effective potential \bar{U} . Then the wave functions differ only in normalization factor which is equal to/13/

$$\frac{\sqrt{2} m e^2}{\sqrt{\pi} \hbar^2} \nu^{-3/2} \quad (9)$$

where ν is the effective principal quantum number. Finally, the problem is reduced to computation of integrals

$$\int_0^\infty \frac{dx \varphi'(x)}{\sqrt{x} \varphi(x)}, \quad \int_0^\infty \frac{dx \varphi'^2(x)}{\varphi^2(x)} \quad (10)$$

where $\varphi(x)$ is the universal Thomas-Fermi function. (The tables of $\varphi(x)$ and $\varphi'(x)$ are contained in the book/14/)

2) The effective potential, found in the work/15/, was used as well as wave functions obtained by numerical integration of the Schroedinger equation with this potential.

The results of both calculations agree within 10% and give

$$\langle H_{int} \rangle = -0,2 \alpha^2 \mu \bar{\sigma} \bar{p} = -0,1 \cdot 10^{-4} \mu \bar{\sigma} \bar{p} \quad (11)$$

The obtained coefficient at $\mu \bar{\sigma} \bar{p}$ is by an order of magnitude smaller than the estimate given in the work/3/. Its authors proceeded from the known value of g-factor of 6s electron and from the assumption that both effects are caused by relativistic corrections. Experiment gives for the difference of g-factor of 6s electron in cesium and free electron the following value/16,17/

$$\Delta g_{Cs} = 1,1 \cdot 10^{-4} \quad (12)$$

It is natural to see what is the magnitude of relativistic corrections to g-factor. Proceeding in the same way as at the deduction of the formula (8), it can be easily shown that this correction is equal to

$$\Delta g_r = -\frac{1}{3} \left\langle \frac{p^2}{m^2 c^2} + \frac{1}{m c^2} \frac{d}{dr} (r \bar{U}) \right\rangle \quad (13)$$

The computation made again in two ways gives

$$\Delta g_{r,Cs} = -0,4 \alpha^2 = -0,2 \cdot 10^{-4} \quad (14)$$

in sharp disagreement with the experimental value both in magnitude and in sign. And just the negative sign of the relativistic correction causes no doubts since not only p^2 , but $\frac{d}{dr}(r\bar{U})$ as well, are, as can be easily seen, positively defined quantities.

Therefore, the correction to g-factor is in no way defined by considered relativistic effect. Then where does it arise from?

Would not lead to needed result the difference in radiative corrections for bound and free electron? It is convenient to use for estimates the non-covariant perturbation theory and the non-covariant Coulomb gauge. The main contribution to Δg is given by the graph 1 where the wavy line corresponds to

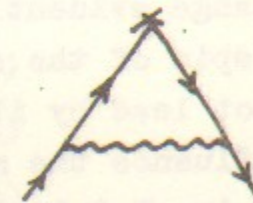


fig.1

three-dimensionally transverse quantum. Both virtual electrons should be considered as non-relativistic since the contribution of relativistic region is the same for free and bound electron. But then every interaction vertex for the intermediate

quantum contains an additional small factor $p/mc \sim \alpha$. The arising small energy denominators are compensated by the integral $\omega d\omega$ over the frequencies of intermediate quantum. Therefore, this correction is of the order of magnitude α^3 and is undoubtedly inessential for the explanation of the effect we are interested in.

It can be easily understood that the radiative correction due to instantaneous Coulomb interaction demands inevitably the presence of a positron in the intermediate state. However, all the graphs with positrons, both for Coulomb quantum and three-dimensionally transverse one in the intermediate state, due to large energy denominators give the contribution even smaller than α^3 to the effect under consideration. Just in the same way the contribution of radiative corrections to the matrix element of M1 transition is negligible. The last conclusion was obtained previously in the work/11/ by means of direct computations.

3. CONFIGURATIONS MIXING. ESTIMATE OF CIRCULAR POLARIZATION

The correct qualitative explanation of the quantity Δg_{cs} was given many years ago by Phillips/18/. As it is known, in complex atoms due to residual Coulomb interaction between electrons that is not accounted for by the effective potential \bar{U} , the so-called configurations mixing takes place. Say in cesium the true stationary state contains the admixture of a state with two electrons and a hole in a closed shell. Since the Coulomb interaction does not change evidently neither total orbital momentum, nor the total spin of the system, the Coulomb configurations mixing does not lead by itself to the change of g-factor. Neither does it influence the matrix element of the transition we are interested in. But in the admixture state for the hole in the shell strong spin-orbit interaction takes place. Just it does lead to the change in g-factor. Quite standard, although rather lengthy, calculations lead to the following result:

$$\Delta g = -\frac{4}{3} FG \zeta^2 / E^4 \quad (15)$$

Here $F = F_0(6s, 5p; 6s, 5p)$, $G = G_1(6s, 5p; 6s, 6p)$ are the direct and exchange Coulomb integrals correspondingly. The symbols in brackets denote one-electron states with respect to which the matrix elements are taken. $\zeta = \zeta(5p)$ is the parameter of spin-orbit interaction for the hole in the 5p shell; E is the energy interval between the mixing states, shift of the levels due to fine structure is neglected. Notations of the book/19/ are used. (The magnitude of the electrostatic mixing turned out $\sqrt{2}$ times larger and the final result (15) 2 times larger than by Phillips.)

The parameters ζ and E can be determined by the spectrum of Xe. As to the Coulomb integrals F and G, Phillips produces indirect arguments in favour of these integrals being of opposite sign and of such magnitude that guarantees the correct order for Δg . The decisive argument in favour of Phillips considerations is in my opinion the fact that all other efforts to explain the effect (see, e.g.,/20/) are undoubtedly untenable.

In the case of the 6s-7s transition the analogous calculation leads to the following expression for the coefficient α at $\mu B \hbar$ in the matrix element of radiation

$$\alpha = -\frac{2\zeta^2}{3E^4} \left[2(F_7 F'_6 + F F'_7 + G_7 G'_6 + G G'_7) - (G_7 F'_6 + F_7 G'_6 + G F'_7 + F G'_7) \right] \quad (16)$$

Here

$$\begin{aligned} F'_6 &= F_0(6s, 5p; 7s, 6p) & G'_6 &= G_1(6s, 5p; 7s, 6p) \\ F'_7 &= F_0(7s, 5p; 6s, 6p) & G'_7 &= G_1(7s, 5p; 6s, 6p) \\ F_7 &= F_0(7s, 5p; 7s, 6p) & G_7 &= G_1(7s, 5p; 7s, 6p) \end{aligned} \quad (17)$$

Pass to the quantitative estimate of the obtained result. It is convenient to rewrite the direct Coulomb integral in the form

$$2 \int_0^{\infty} dx_1 dx_2 u_{6l}(x_1) u_{5l}(x_1) \int_0^{x_1} dx u_{n_0'}(x) u_{n_0}(x) \left(\frac{1}{x_1} - \frac{1}{x} \right) \quad (18)$$

Here u_{nl} is the radial wave function of a state with a principal quantum number n and an orbital one l ; atomic units are used. The dependence of the wave functions of 6s and 7s electrons on the corresponding energies at the distances characteristic for 5p electron may be neglected. But then in this region the mentioned functions differ in normalizing factors only, their ratio being equal (see (9)) to $(\nu_6/\nu_7)^{3/2}$ where $\nu_6 = 1,9$ and $\nu_7 = 2,9$ are the effective principal quantum numbers of 6s and 7s states. Finally, the following relations take place:

$$F_6' \approx F_7' \approx 0,51F; \quad F_x \approx 0,26F \quad (19)$$

As to the exchange integral, presenting it in the form

$$\frac{1}{3} \int_0^{\infty} dx dx_1 \left[\theta(x_1 - x) \frac{x}{x_1^2} + \theta(x - x_1) \frac{x_1}{x^2} \right] u_{n_0'}(x) u_{5l}(x) u_{n_0}(x_1) u_{6l}(x_1) \quad (20)$$

we find just in the same way that

$$G_6' \approx 0,51G, \quad G_7' \approx 0,51G \quad (21)$$

For the following estimates take into account the factor $1/3$ in the formula (20) and the circumstance that the exchange integral is determined by the overlapping of wave functions over both integration variables, and the direct one contains the square of the wave function of 6s state. Then it is natural to expect that the quantity F is 6 - 7 times larger than G . As to the quantities G and G_7' , there are no special grounds to expect that they differ considerably. Finally, comparing the expressions (16) and (15) and taking into account that the last one should be equal to $\Delta g_{6s} - \Delta g_{7s} = 1,3 \cdot 10^{-4}$, we find that constitutes $(6 \div 7) \cdot 10^{-4}$.

Of course, the estimates presented in the preceding paragraph are not sufficiently reliable, and the experimental determination of the matrix element of 6s-7s transition is, as it was noted in the work/3/, a necessary stage for the detection

of parity violation. However, when planning the experiment, one should be oriented, evidently, rather at $\alpha \sim 10^{-3}$ and at the degree of circular polarization $P \sim 10^{-5}$, but not at $\alpha \sim 10^{-4}$ and $P \sim 10^{-4}$ as it was predicted in the work/3/. Although the diminishing of the effect is accompanied by the quadratic growth of the statistics, however, taking into account the smallness of the expected effect and the inevitability of systematic errors, the experimental detection of the parity violation in the 6s-7s transition in cesium seems to be more difficult problem than it would follow from the estimates by Bouchiat/3/.

In conclusion note that there are many strongly forbidden M1 transitions in mercury, thallium and lead that proceed also due to configurations mixing. Because of the growth of the effect with Z and the relativistic enhancement, one may expect in these transitions the circular polarization indeed close to 10^{-4} . Unfortunately, all these transitions lie in the region 2000 - 3000 Å that complicates the experiment strongly.

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