6

И Н С Т И Т У Т
ЯДЕРНОЙ ФИЗИКИ СОАН СССР

ПРЕПРИНТ И Я Ф 78 - 15

O.P.Sushkov, V.V.Flambaum, and I.B.Khriplovich

STRONGLY FORBIDDEN M1 TRANSITIONS AND g-FACTOR ANOMALIES IN HEAVY ATOMS

Новосибирск
1978

STRONGLY FORBIDDEN M1 TRANSITIONS AND g-FACTOR ANOMALIES IN HEAVY ATOMS

O.P.Sushkov, V.V.Flambaum, and I.B.Khriplovich

Institute of Nuclear Physics
Novosibirsk 90, USSR

abstract

New mechanism for the origin of strongly forbidden M1 transitions and corrections to g-factors in heavy atoms with one external electron is pointed out. The expressions for these quantities in the case of external s or p electron are obtained. Numerical calculations are presented for cesium and thallium.

1. INTRODUCTION

The question why g-factor of an atom with one external electron deviates from that of free electron was under active discussion many years ago at the time of the first measurements of anomalous magnetic moment of electron[1-3]. Strongly forbidden M1 transitions in heavy atoms attracted attention recently due to the attempts to detect in them parity violation caused by weak interaction between electron and nucleus[4-10].

The experimental values of g-factor anomalies in alkalis[11-13] are presented in the Table 1. In light atoms the corrections to g-factors are almost constant, but in heavy ones they change sign and increase rapidly with Z. Therefore, one may conclude

	Li	Na	K	Rb	Cs
Z	3	11	19	37	55
$\delta g \cdot 10^4$	-0.173± ±0.024	-0.217± ±0.024	-0.241± ±0.022	0.127± ±0.020	2.218± ±0.024

Table 1

that the correction to g-factor in light and heavy atoms is due to different mechanisms. It is well known that to explain this anomaly in light atoms it is sufficient to take into account relativistic effects only[14,15]. As to the heavy atoms, it was conjectured long ago that here large contribution is given by interconfiguration interaction together with spin-orbit one[16]. It was natural to think that the last effect is essential also

for strongly forbidden M1 transitions in heavy atoms[5,6]. Namely, in the refs.[16,5,6] the corrections of the fourth order were considered: of the second order in Coulomb mixing of configurations and of the second order in spin-orbit interaction. But the corresponding quantitative calculations were absent. Therefore, the decisive argument in favour of this mechanism was the fact that all other attempts to explain the effects under discussion, say, in cesium, proved untenable.

However, when we carried out the corresponding calculations for cesium, we found to our surprise that their result was about 100 times smaller than the experimental value. This disagreement for cesium was noted also in the ref.[17] with which we became acquainted after this work had been over.

In the present work a new mechanism of the phenomena under discussion is pointed out. They can arise not in the fourth order of perturbation theory, but in the third one: in the first order in Coulomb mixing of configurations and in the second order in spin-orbit interaction. We have calculated g-factors of the $6s_{1/2}$ state of cesium, $6p_{1/2}$ and $6p_{3/2}$ states of thallium, as well as the amplitudes of M1 transitions $6s_{1/2} - 7s_{1/2}$ in cesium and $6p_{1/2} - 7p_{1/2}$, $8p_{1/2}$, $9p_{1/2}$ in thallium taking into account besides the interconfiguration interaction usual relativistic corrections. We do not consider the corrections caused by hyperfine interaction since their calculation is trivial and besides that they can be separated experimentally[5,17,19].

2. g-FACTOR OF CESIUM

To explain the origin of g-factor anomaly in cesium it is convenient to present the correction due to the interconfiguration interaction as

$$\frac{\delta g}{2} = \langle J, J_z=\tfrac{1}{2}|L_z+2S_z-2J_z|J,J_z=\tfrac{1}{2}\rangle = -\langle J,J_z=\tfrac{1}{2}|L_z|J,J_z=\tfrac{1}{2}\rangle \qquad (1)$$

In the LS coupling approximation the cesium atom has an external

6s electron above closed shells, i.e., the ground state is $^2S_{1/2}$. For the matrix element not to vanish, it is necessary to take into account the admixture to $^2S_{1/2}$ of the states with $L\neq 0$ both in the bra $\langle J, J_z=\frac{1}{2}|$ and the ket $|J, J_z=\frac{1}{2}\rangle$ vectors. To do it, one should evidently, firstly, break the closed shells, and secondly, switch on spin-orbit interaction which changes L. It was assumed in the refs.[16,5,6] that the shells can be broken only by Coulomb interconfiguration interaction. Thus the fourth order of perturbation theory arose.

The principal point of the present work is the observation that the shells can be broken also by non-diagonal spin-orbit interaction by itself. It can be easily shown by means of second quantisation formalism. Consider, e.g., the closed subshell $5p^6$. Let b_m^+ and c_m^+ be the creation operators of $5p_{1/2}$ and $5p_{3/2}$ electron with $j_z=m$. The wave function of the state $5p^6$ and the operator $\hat{L}_z$ in jj coupling scheme are

$$|5p^6\rangle_0 = b_{\frac{1}{2}}^+ b_{-\frac{1}{2}}^+ c_{\frac{1}{2}}^+ c_{\frac{1}{2}}^+ c_{-\frac{1}{2}}^+ c_{-\frac{3}{2}}^+ |0\rangle \qquad (2)$$

$$\hat{L}_z = \sum_m \left\{ \tfrac{4}{3} m b_m^+ b_m + \tfrac{\sqrt{2}}{3}(c_m^+ b_m + b_m^+ c_m) + \tfrac{2}{3} m c_m^+ c_m \right\} \qquad (3)$$

It can be easily shown that $\hat{L}_z|5p^6\rangle_0 \equiv 0$ as it should be for closed snell. Spin-orbit interaction mixes different p-states

$$|5p_{3/2}\rangle' = |5p_{3/2}\rangle + \frac{1}{2}\frac{\zeta_{56}}{E_{5p}-E_{6p}}|6p_{3/2}\rangle + \dots$$
$$|5p_{1/2}\rangle' = |5p_{1/2}\rangle - \frac{\zeta_{56}}{E_{5p}-E_{6p}}|6p_{1/2}\rangle + \dots \qquad (4)$$

Here $\zeta_{nn'}$ is radial matrix element of spin-orbit interaction. According to (4) the correct wave function will be obtained from (2) by the substitution

$$b_m^+ \to b_m^+ - \frac{\zeta_{56}}{E_{5p}-E_{6p}}\tilde{b}_m^+ + \dots, \quad c_m^+ \to c_m^+ + \frac{1}{2}\frac{\zeta_{56}}{E_{5p}-E_{6p}}\tilde{c}_m^+ + \dots ,$$

where $\tilde{b}_m^+$ and $\tilde{c}_m^+$ are creation operators of $6p_{1/2}$ and $6p_{3/2}$ electrons. Taking into account that besides the terms written down in the formula (3), there is an analogous contribution of 6p electrons into L_z, we get

$$\hat{L}_z|5p^6\rangle = \frac{\zeta_{56}}{\sqrt{2}(E_{6p}-E_{5p})}\left\{(\tilde{c}_{\frac{1}{2}}^+ b_{\frac{1}{2}}^+ + b_{\frac{1}{2}}^+ \tilde{c}_{-\frac{1}{2}}^+)c_{\frac{1}{2}}^+ c_{-\frac{1}{2}}^+ + b_{\frac{1}{2}}^+ b_{\frac{1}{2}}^+ (\tilde{b}_{\frac{1}{2}}^+ c_{-\frac{1}{2}}^+ + c_{\frac{1}{2}}^+ \tilde{b}_{\frac{1}{2}}^+)\right\} c_{\frac{3}{2}}^+ c_{-\frac{3}{2}}^+ |0\rangle \quad (5)$$

Therefore, after spin-orbit interaction is switched on, the wave function of a closed shell indeed is no more an eigenfunction of the operator $\hat{L}$ with L=0.[1] But of course the expectation value of L vanishes: $\langle 5p^6|\hat{L}|5p^6\rangle = 0$. For the matrix element of L_z in the formula (1) to be distinct from zero, the angular momentum of the excitation of a closed shell should be correlated with the spin of an external electron. It is sufficient for it to take into account exchange Coulomb interaction of internal electrons with an external one in the first order. Hence the effect arises in the third order of perturbation theory already: in the second order in spin-orbit interaction and in the first one in Coulomb.

Up to now we have spoken in the language of LS scheme considering spin-orbit interaction as perturbation. However, the calculation is much more compact in jj scheme with relativistic radial wave function where the effect arises formally in the first order of perturbation theory. In this approach it is sufficient to take into account the admixture by exchange Coulomb interaction of states with an excited internal electron to bra or ket vector in the matrix element (1). The corresponding correction to g-factor is

$$\delta g = -4\sum_{nn'lj'j_z} \frac{\langle 6s, nlj j_z|\frac{e^2}{r_2}|n'lj'j_z, 6s\rangle\langle n'lj'j_z|L_z+2S_z|nlj j_z\rangle}{E_{nlj}-E_{n'lj'}} \quad (6)$$

[1] V.G.Zelevinsky turned our attention to the fact that the same effect leads to presence of paramagnetic contribution to the magnetic susceptibility of inert gas. This question is considered in the Appendix 1.

where n,l,j,j_z refer correspondingly to principal quantum number, orbital angular momentum, total one and its projection for an electron. The states $|nljj_z\rangle$ lie below 6s, and $|n'lj'j_z\rangle$ above it. The matrix element $\langle n'lj'j_z|L_z+2S_z|nljj_z\rangle$ at $n \neq n'$ vanishes if $j = j'$, and does not vanish already in the first order in spin-orbit interaction at $j' = \tilde{j} = 2l - j$[18] (the fact that in heavy atoms it is not suppressed too much was discovered previously in the ref.[19] by means of numerical calculations). It can be shown that

$$\langle n'l\tilde{j}j_z|L_z+2S_z|nljj_z\rangle = -\frac{\sqrt{(l+\frac{1}{2})^2-j_z^2}}{2l+1}\,\alpha_{n'l\tilde{j};nlj} \quad (7)$$

Here $\alpha_{n'l\tilde{j};nlj}$ is the integral of overlapping of the corresponding radial wave functions. In the first order in spin-orbit coupling (see (4))

$$\alpha_{n'l\tilde{j};nlj} \approx -\alpha_{n'lj;nl\tilde{j}} \approx (-1)^{l+\frac{1}{2}-j}(l+\tfrac{1}{2})\frac{\zeta_{nl,n'l}}{E_{nl}-E_{n'l}} \quad (8)$$

Now it can be easily seen that the expression (6) is indeed of the second order in spin-orbit coupling. The correction to g-factor of the ground state of cesium found in this way is

$$\delta g_3 = -\frac{8}{3}\sum_{nn'lj}\frac{l(l+1)}{(2l+1)^2}\,\frac{\zeta^l(6s,nlj;6s,n'l\tilde{j})}{E_{nlj}-E_{n'l\tilde{j}}}\,\alpha_{nlj;n'l\tilde{j}} \quad (9)$$

Here ζ^l is an exchange Coulomb integral

$$\zeta^l(a,b;c,d) = \int f_a(r_1)f_b(r_2)f_c(r_2)f_d(r_1)\frac{r_<^l}{r_>^{l+1}}\,dr_1\,dr_2 \quad (10)$$

f(r) is radial wave function. It should be noted that in the formula (9) the dependence of ζ^l on j and $\tilde{j}$ (i.e., on spin-orbit interaction) is essential no less than that of denominator $E_{nlj} - E_{n'lj}$.

Numerical calculation in an effective potential (see the Appendix 2) with the formula (9) gives

$$\delta g_3 = 3.66\cdot 10^{-4} \quad (11)$$

Consider now other mechanisms contributing to the correction to g-factor. Firstly, there are relativistic corrections to the magnetic moment operator of an external electron. Secondly, magnetic interaction of an external electron with internal ones. And finally, the mentioned above contribution of the fourth order of perturbation theory connected with the interconfiguration interaction.

Relativistic wave function of an external electron is

$$u = \frac{1}{r}\begin{pmatrix} f_{nlj}(r)\,\Omega_{ljj_z} \\ i g_{nlj}(r)\,\Omega_{l'jj_z} \end{pmatrix} \qquad (12)$$

where Ω_{ljj_z} is a spherical wave function with spin, $l' = 2j - l$, f(r) and g(r) are radial wave functions. Exact relativistic expression for the magnetic moment of an external electron can be reduced to

$$\vec{M} = \frac{e}{2}(\vec{l}+2\vec{s})\frac{4}{2\varkappa-1}\int r f(r) g(r)\, dr \qquad (13)$$

where $\varkappa = (-1)^{j+\frac{1}{2}-l}(j+\frac{1}{2})$, $e = -|e|$ is the charge of electron. By means of Dirac equation $\vec{M}$ can be easily transformed to the form where small corrections ($\sim\alpha^2$) are separated explicitly (we put $\hbar = c = 1$)

$$\vec{M} = -|\mu_B|(\vec{l}+2\vec{s})\left\{1 - \int\left[g^2(r) + \frac{\varepsilon - V(r)}{\varkappa - \frac{1}{2}} 2 f(r) g(r)\right] dr\right\} \qquad (14)$$

Here ε is the energy and V(r) is an effective potential. Numerical calculation for cesium (with $\varkappa = -1$ for the ground state) gives according to this formula

$$\delta g_{rel} = -0.38\cdot 10^{-4} \qquad (15)$$

The correction to g-factor caused by magnetic interaction of internal electrons with an external one arises from the diamagnetic term $\frac{e^2 A^2}{2mc^2}$ in the Hamiltonian (A1.1). In the present

case $\vec{A}(r_1) = \vec{A}_e(r_1) + \vec{A}_H(r_1)$, where $\vec{A}_H(r_1) = \frac{1}{2}[\vec{H}\times\vec{r}_1]$ is vector-potential of external field, and

$$\vec{A}_e(r_1) = \frac{e}{2mc}\left\{\frac{\vec{p}_2}{r_{12}} + \frac{\vec{r}_{12}(\vec{r}_{12}\vec{p}_2)}{r_{12}^3} + i\frac{\vec{\sigma}_2\times\vec{r}_{12}}{r_{12}^3}\right\} \qquad (16)$$

is vector-potential created by an external electron being at the point r_2. The corresponding correction to magnetic moment

$$\vec{M}_{dia} = \frac{e^2}{m}\left\langle[\vec{A}_e(r_1)\times\vec{r}_1]\right\rangle \qquad (17)$$

is reduced to

$$\vec{M}_{dia} = \frac{1}{3}|\mu_B|\alpha^2\left\langle(\vec{l}+2\vec{s})\left[\frac{2(\varkappa+1)}{2\varkappa-1}W_1 + W_2\right]\right\rangle \qquad (18)$$

$$W_1 = \frac{a_B}{r^3}\int_0^r n(r_1) r_1^2\, 4\pi r_1^2 dr_1\,, \quad W_2 = a_B\int_r^\infty \frac{n(r_1)}{r_1}\, 4\pi r_1^2 dr_1$$

Here n(r) is the density of internal electrons, a_B is Bohr radius. The expectation value in (18) is taken with respect to wave functions of external electron. In cesium for 6s electron ($\varkappa = -1$) numerical calculation by this formula gives

$$\langle W_2\rangle = 0.35\,; \qquad \delta g_{dia} = -0.12\cdot 10^{-4} \qquad (19)$$

The same result may be obtained from the Breit Hamiltonian of two electron interaction[20] by the substitution $\vec{p}\to\vec{p}-\frac{e}{c}\vec{A}_H$

$$\delta H_B = -\frac{e^3}{4m^2c^2}\left\{\frac{1}{r_{12}}\left[[\vec{r}_1\times\vec{H}]\vec{p}_2 + [\vec{r}_2\times\vec{H}]\vec{p}_1 + (\vec{n}[\vec{r}_1\times\vec{H}])(\vec{n}\vec{p}_2) + (\vec{n}[\vec{r}_2\times\vec{H}])\cdot\right.\right. \qquad (20)$$

$$\left.\left.\cdot(\vec{n}\vec{p}_1)\right] + \frac{1}{r_{12}^2}\left[(\vec{s}_1+2\vec{s}_2)[\vec{n}\times[\vec{r}_1\times\vec{H}]] - \underline{(s_2+2s_1)}\left[\vec{n}\times[\vec{r}_2\times\vec{H}]\right]\right]\right\}\,; \quad \vec{n} \equiv \vec{r}_{12}/r_{12}$$

It should be noted however that when calculating δg by means of Hamiltonian (20), one should drop in it the underlined term corresponding to spin-orbit interaction of external electron since it is taken into account already in the formulae (14), (15).

The exchange magnetic interaction also contributes to g-factor correction as well as direct one. To calculate it one should take into account all the terms in the Hamiltonian (20) of course. For cesium with external s-electron the calculation is rather simple and gives

$$\delta g_{exch} = \frac{\alpha^2}{2R_y} \sum_{nl} G^1(6s,nl;6s,nl) \qquad (21)$$

Here G^1 are usual exchange Slater integrals defined above, the summation is carried out over closed subshells. The numerical value of this correction is

$$\delta g_{exch} \lesssim 1\cdot 10^{-6} \qquad (22)$$

Thus, as it should be expected, the exchange magnetic interaction is essentially smaller than the direct one (19).

The contribution to g-factor of relativistic corrections and direct magnetic interaction was calculated previously in the refs.[5,6,17]. Our results agree with those obtained in the mentioned articles.

Give now an estimate of the mentioned above contribution of the fourth order of perturbation theory when closed subshells are broken by Coulomb interaction with an external electron only. There are many different types of excitations in this order - those of one or two electrons from closed s-, p-, d-subshells. We have carried out numerical calculations for the excitation of one electron from p- and d-subshells, this contribution being perhaps the dominating one. Let us consider as an example the excitation 5p→6p discussed previously in the refs. [16,5,6,17]. Here again the calculation is more conveniently carried out in jj scheme where the effect arises formally in the second order of perturbation theory already. The corresponding correction is

$$\delta g_4 = \frac{8}{243}\{-G_{11}^2 - 3G_{13}^2 + 4G_{11}G_{13} - 2G_{11}G_{31} + 2G_{13}G_{33} - 3G_{31}^2 - 5G_{33}^2 + 8G_{31}G_{33}\} \qquad (23)$$

Here

$$G_{ik} \equiv \frac{G^1(6s,5p_{i_{1/2}};6s,6p_{k_{1/2}})}{E_{5p_{i_{1/2}}} - E_{6p_{k_{1/2}}}} \qquad (24)$$

We stress that the Coulomb integrals G^1 are different for $p_{1/2}$ and $p_{3/2}$ electrons. If one neglects this difference, the magnitude of the correction (23) is smaller by two orders of magnitude. It can be shown expanding in fine splitting parameter the denominators and Coulomb integrals in (24) (the integrals are expanded by means of the formulae of the type (4)) that the expression (20) is in fact of the second order in spin-orbit interaction. The numerical value of the correction (23) is

$$\delta g_4 = -4\cdot 10^{-7} \qquad (25)$$

Thus, our calculations show that the fourth order contribution does not exceed perhaps some percent of the third order one (see (11)).

At the formal calculation of the fourth order contribution besides (23) the term arises which is dependent on direct zero multipole Coulomb integrals

$$\frac{8}{27}(F_{33} - F_{11})(G_{13} - G_{31}) \qquad (26)$$

where

$$F_{ik} = \frac{F^0(6s,5p_{i_{1/2}};6s,6p_{k_{1/2}})}{E_{5p_{i_{1/2}}} - E_{6p_{k_{1/2}}}}$$

It is evident, however, that this term should not be taken into account since the integrals F^0 are the matrix elements of spherically symmetric self-consistent field, and this field is taken into account already when the Dirac equation is solved. It can be easily shown, e.g., that the correction (26) is taken into account already in the formula (9). Assume that the Coulomb field of 6s electron is not included into the effective potential, but is taken into account as a perturbation. Then the mixing by this

field of the states 5p and 6p will lead to the term

$$(F_{11}-F_{33})\langle p_{1/2}|L_z+2S_z|p_{3/2}\rangle \qquad (27)$$

in the operator M_z (see (7)), and this term when inserted into the formula (6) gives the expression (26).

Note that just the correction (26) without the account for difference of Coulomb integrals for $p_{1/2}$ and $p_{3/2}$ electrons was considered previously in the refs.[6,5,6,17,1)].

Adding up all the calculated contributions (11), (14), (19), we get

$$\delta g = \delta g_3 + \delta g_{rel} + \delta g_{dia} = 3.2\cdot 10^{-4} \qquad (28)$$

Since our calculation of Coulomb integrals in the same for all electrons effective potential is very approximate one, the agreement with the experimental value[11-13] $\delta g = 2.18\ 10^{-4}$ appears to be quite satisfactory.

Note that by means of formulae (9),(14),(18) one can calculate the correction δg not only in cesium, but in other alcalis as well. The qualitative dependence of this correction on the atomic number Z (see Table 1) canbe easily understood. In light atoms relativistic and diamagnetic corrections (14), (18) dominate, and their contribution is negative. In heavy atoms from rubidium on the contribution of interconfiguration interaction (9) becomes important, it is positive and increases rapidly with Z ($\delta g \sim \zeta^2 \sim Z^4$).

---

1) One of the authors(I.B.Khriplovich) takes the opportunity to note that an error in the preprint of his work[6] was corrected by him after the acquaintance with the paper[5].

3. AMPLITUDE OF STRONGLY FORBIDDEN TRANSITION $6s_{1/2} - 7s_{1/2}$ IN CESIUM

The amplitude of M1 transition $6s_{1/2} \to 7s_{1/2}$ $M_z = \langle J, J_z=1/2|\hat{M}_z|J, J_z=1/2\rangle$ is calculated just in the same way as the correction to g-factor. (We define $\hat{M}_z$ in such a way that in nonrelativistic limit $\hat{M}_z \to -|\mu_B|(L_z+2S_z)$. All radial wave functions are assumed to be positive at $r\to 0$.) The contribution of interconfiguration interconfiguration interaction is (cf. (9)):

$$M_3 = \frac{2}{3}|\mu_B| \sum_{nn'lj} \frac{l(l+1)}{(2l+1)^2} \frac{G^1(6s,nlj;7s,n'lj)+G^1(7s,nlj;6s,n'lj)}{E_{nlj}-E_{n'lj}} \times \qquad (29)$$

$$\times a_{nlj;n'lj} = -0.76\cdot 10^{-4}|\mu_B|$$

Relativistic correction to an amplitude of M1 transition of an external electron $1(nlj) \to 2(n'lj)$ is (cf. (14))

$$\vec{M}_{rel} = |\mu_B|(\vec{l}+2\vec{s})\left\{\int_0^\infty \left[g_1 g_2 + \frac{1}{2\varkappa-1}\left((\varepsilon_2-V(2))f_1 g_2 2 + (\varepsilon_1-V(2))f_2 g_1 2\right)\right]dz + \right. \qquad (30)$$

$$\left. + \frac{m}{5(2\varkappa-1)}\int_0^\infty (f_1 g_2 + f_2 g_1)\kappa^2 z^3 dz\right\}$$

where $\kappa = \varepsilon_2 - \varepsilon_1$ ($\hbar = c = 1$). The second term in the curly brackets appeared from the expansion of the exponent in photon wave function. For $6s_{1/2} \to 7s_{1/2}$ transition in cesium ($\varkappa = -1$)

$$M_{rel} = 0.10\cdot 10^{-4}|\mu_B| \qquad (31)$$

The contribution of magnetic corrections is calculated by means of formula (18)

$$M_{dia} = 0.03\cdot 10^{-4}|\mu_B| \qquad (32)$$

Both M_{rel} and M_{dia} are in agreement withthe results of refs.[5,6,17,21,22]. All the other contributions to the M1 amplitude are very small, as well as those to g-factor anomaly. The total amplitude is

$$\langle 6S,\ j_z=\tfrac{1}{2}|M_z|7S,\ j_z=\tfrac{1}{2}\rangle = M_3+M_{2el}+M_{dia} = -0.63\cdot10^{-4}|\mu_B| \qquad (33)$$

The experimental value[17] is $M_z = -(0.424 \pm 0.034)\cdot10^{-4}|\mu_B|$. Note that the ratio $M_z/\delta g$ is reproduced by our calculation with high accuracy.

4. g-FACTORS OF $6P_{1/2}$ AND $6P_{3/2}$ STATES AND AMPLITUDES OF STRONGLY FORBIDDEN M1 TRANSITIONS $6P_{1/2} - nP_{1/2}$ (n = 7,8,9) IN THALLIUM

In thallium for the correction to g-factor of the ground state $6p_{1/2}$ and for the amplitudes of M1 transition $6p_{1/2}$-$np_{1/2}$ the mechanism of third order, principal for cesium, does not work since , as it can be easily seen, Coulomb interaction cannot cause a transition $p_{1/2},1j - p_{1/2},1j$.

The contribution to δg of relativistic corrections to the operator of magnetic moment of $6p_{1/2}$ (electron) is calculated by formula (14) at $\mathcal{L} = 1$ (the effective potential used by us is described in the Appendix 2)

$$\delta g_{rel} = -1.07\cdot10^{-4} \qquad (34)$$

This value coincides with that obtained previously in ref.[19]

The calculation by the formula (18) of magnetic interaction of an external electron with internal ones gives

$$\langle W_1\rangle = 2.280\ ;\ \langle W_2\rangle = 1.275\ ;\ \delta g_{dia} = -1.23\cdot10^{-4} \qquad (35)$$

Our formula (18) does not agree with analogous expression obtained previously in ref.[19] (remind that for comparison one should put $\mathcal{L} = 1$ in (18)). However, numerically this disagreement is not too essential.

The calculation of exchange matrix element of magnetic interaction Hamiltonian (20) is rather tedious. It can be somewhat simplified if the angular part of the wave function of $6p_{1/2}$ (electron) is

written as $|p_{1/2}\rangle = -(\vec{\sigma}\vec{n})|s_{1/2}\rangle$. The final result for the magnetic moment of the transition $6p_{1/2} - np_{1/2}$ is ($M(n=6) = -\frac{1}{2}|\mu_B|\delta g_{6p_{1/2}}$)

$$M_{exch} = -|\mu_B|\frac{\alpha^2}{6R_y}\sum_{nl}\Big\{\frac{2l(l-1)}{(2l-1)(2l-3)}G^{l-3} + \Big[\frac{2(2l^2+2l-1)}{(2l+3)(2l-1)} + \frac{l(l-1)}{(2l-3)} - \frac{3l^2}{2(2l-1)}\Big]G^{l-1} +$$
$$+\Big[\frac{2(2l^2+2l-1)}{(2l+3)(2l-1)} - \frac{(l+1)(l+2)}{(2l+5)} + \frac{3(l+1)^2}{2(2l+3)}\Big]G^{l+1} + \frac{2(l+1)(l+2)}{(2l+5)(2l+3)}G^{l+3} +$$
$$+\frac{2(l^2+l-1)}{(2l+3)(2l-1)}(I^l - R^l) - \frac{(l+1)(l+2)}{(2l+5)(2l+3)}(I^{l+1} - R^{l+1}) - \frac{l(l-1)}{(2l-1)(2l-3)}(I^{l-1} - R^{l-1})\Big\} \qquad (36)$$

$$I^n \equiv \int f_{nl}(r_1) f_{nl}(r_2)\Big[f_{\varepsilon p_{1/2}}(r_1) r_1 \frac{\partial f_{\kappa p_{1/2}}(r_2)}{\partial r_2} + f_{\kappa p_{1/2}}(r_2) r_2 \frac{\partial f_{\varepsilon p_{1/2}}(r_1)}{\partial r_1}\Big]\frac{r_<^n}{r_>^{n+1}}\,dr_1\,dr_2$$

$$R^n \equiv m\Big(\frac{\varepsilon_{\varepsilon p} + \varepsilon_{\kappa p}}{2} - \varepsilon_{nl}\Big)\int f_{nl}(r_1) f_{nl}(r_2) f_{\varepsilon p_{1/2}}(r_1) f_{\kappa p_{1/2}}(r_2)\frac{r_<^{n+1}}{r_>^n}\,dr_1\,dr_2$$

$$G^n \equiv \int f_{nl}(r_1) f_{nl}(r_2) f_{\varepsilon p_{1/2}}(r_1) f_{\kappa p_{1/2}}(r_2)\frac{r_<^n}{r_>^{n+1}}\,dr_1\,dr_2$$

G^n is an usual exchange Coulomb integral. Note that the index n can be here negative as well. Numerical calculation by the formula (36) gives

$$\delta g_{exch} = 0.19\cdot10^{-4} \qquad (37)$$

Therefore, the exchange magnetic contribution to δg is by an order of magnitude smaller than that of direct one. As to the fourth order correction, here it is smaller than $2\cdot10^{-6}$. The total correction to g-factor of the $6p_{1/2}$ state is

$$\delta g = \delta g_{rel} + \delta g_{dia} + \delta g_{exch} = -2.1\cdot10^{-4} \qquad (38)$$

This value of δg is in a good agreement with the experimental number[23] $\delta g = -2.012(18)\ 10^{-4}$ and is close numerically to the result of calculation[19].

The amplitude of M1 transition $6p_{1/2} \to 7p_{1/2}$ is also ca-

used mainly by the relativistic and diamagnetic corrections, their contribution, calculated by the formulae (14), (18) and (36), being

$$M_{rel} = 0.17\cdot10^{-4}\,|\mu_B|\,;\ \langle W_1\rangle = 0.62\,;\ \langle W_2\rangle = 0.42\,;$$
$$M_{dia} = 0.17\cdot10^{-4}\,|\mu_B|\,;\quad M_{exch} = -0.18\cdot10^{-5}\,|\mu_B| \qquad (39)$$

Here, however, of some importance are the effects of interconfiguration interaction arising in the fourth order of perturbation theory. Most important is perhaps the contribution of the excitations $6s6p_{1/2}$ - ns,mp. It is equal to

$$M_4 = -\frac{4}{243}\,|\mu_B|\Big\{\sum_{m\geq6;n>6}\big[G(6;m\tfrac{3}{2},n)-G(6;m\tfrac{1}{2},n)\big]\big[G(m\tfrac{3}{2},n;7)-G(m\tfrac{1}{2},n;7\big]- \qquad (40)$$
$$-\sum_{n>6;\,j;\,\substack{m,k\geq6\\ m\neq k}}\alpha_{mj;k\tilde{j}}\,G(6;mj,n)\,G(k\tilde{j},n;7)\Big\}$$

where

$$G(6;mj,n)\equiv\frac{G^1(6p_{1/2},6s;mp_j,ns)}{E_{6p_{1/2}}+E_{6s}-E_{mp_j}-E_{ns}}$$
$$G(mj,n;7)\equiv\frac{G^1(mp_j,ns;7p_{1/2},6s)}{E_{7p_{1/2}}+E_{6s}-E_{mp_j}-E_{ns}}$$
$$\alpha_{mj;k\tilde{j}}\equiv\int_0^\infty f^{(2)}_{mp_j}f^{(2)}_{kp_{\tilde{j}}}\,dz\ ;\ \tilde{j}=2l-j$$

Taking into account the inaccuracy in the value of Coulomb integrals mentioned above, we get from here an estimate $M_4 = -(0.1 \div 0.5)\cdot10^{-5}\,|\mu_B|$. Therefore, the calculated value of the transition amplitude is close to

$$M_z = 2.9\cdot10^{-5}\,|\mu_B| \qquad (41)$$

This value of M differs in sign both from the experimental one $M_z = (-2.11 \pm 0.30)\cdot10^{-5}\,|\mu_B|$ [8] and from that calculated previously $M_z = (-3.2 \pm 1)\cdot10^{-5}\,|\mu_B|$ [19]. However, it cannot be excluded that this discrepancy in sign is due to different definitions of the transition amplitude. Our definition of M_z is given *before* the formula (29). Unfortunately, we were not able to find unambiguously with which sign is M_z defined in the refs. [8,19].

The analogous calculation of other M1 amplitudes gives

$$M(6p_{1/2}\to8p_{1/2}) = 0.18\cdot10^{-4}\,|\mu_B|$$
$$M(6p_{1/2}\to9p_{1/2}) = 0.12\cdot10^{-4}\,|\mu_B| \qquad (42)$$

As to the correction to g-factor of the state $6p_{3/2}$, the contribution to it of the third order mechanism considered in the section 2, is

$$\delta g_3 = -\frac{4}{5}\sum_{nn'lj}\left\{\frac{(l-1)l(l+1)}{(2l-1)(2l+1)^2}G^{l-1}+\frac{l(l+1)(l+2)}{(2l+1)^2(2l+3)}G^{l+1}\right\}\frac{\alpha_{nlj;n'lj}}{E_{nlj}-E_{n'lj}} \qquad (43)$$

$$G^k\equiv G^k(6p_{3/2},nlj;6p_{3/2},n'lj)$$

According to numerical calculations

$$\delta g_3 = 2.6\cdot10^{-4} \qquad (44)$$

The relativistic and diamagnetic corrections are calculated by the formulae (14) and (18) at $\varkappa = -2$

$$\delta g_{rel}+\delta g_{dia} = -0.63\cdot10^{-4}-0.38\cdot10^{-4} = -1.01\cdot10^{-4} \qquad (45)$$

Usually our calculations overestimate Coulomb integrals for the excitation of an electron from closed subshell by a factor of 1.5 - 2.5 (see the above calculations for cesium and the calculations of hyperfine structure for thallium, lead and bismuth in the ref. [24]). In this situation, when considerable cancellation between the contributions (44) and (45) takes place, we can give only a tentative estimate of this g-factor ano-

maly:

$$\delta g \lesssim 1\cdot 10^{-4} \qquad (46)$$

The experimental value of this correction is unknown to us.

APPENDIX 1

Let us calculate the paramagnetic correction to the magnetic susceptibility of inert gas. It is well-known that the Hamiltonian of an electron in a magnetic field (in the Coulomb gauge $\mathrm{div}\vec{A} = 0$) is transformed to

$$\mathcal{H} = \frac{(\vec{p} - \frac{e}{c}\vec{A})^2}{2m} + |\mu_B|\vec{\sigma}\vec{H} \to \frac{p^2}{2m} + |\mu_B|(\vec{L}+2\vec{S})\vec{H} + \frac{e^2A^2}{2m^2c^2} \qquad (A1.1)$$

It is assumed usually that only the last term with A^2 contributes to the magnetic susceptibility of inert gas leading to diamagnetism. However, as it was shown in the section 2, if one takes into account spin-orbit interaction, the ground state of an inert gas atom is not pure $^1S_0$. Therefore, in the second order of perturbation theory the term $|\mu_B|(\vec{L}+2\vec{S})$ gives a paramagnetic contribution $\sim(Z\alpha)^4$ to the magnetic susceptibility. Really, using the formula (7), we get easily

$$\delta\chi_p = -2\mu_B^2 \sum_m \frac{|\langle m|L_z+2S_z|0\rangle|^2}{E_0 - E_m} = -\frac{4}{3}\mu_B^2 \sum_{nn'lj} \frac{l(l+1)}{2l+1} \frac{|\alpha_{nlj;n'lj}|^2}{E_{nlj} - E_{n'lj}} \qquad (A1.2)$$

The notations are the same as in (6) and (7).

APPENDIX 2

For all our calculations in cesium we used the effective potential

$$V(r) = -\frac{(Z-1)}{r(1+\eta r)^2} \frac{e^{-r/d}+1}{e^{\frac{r-\mu}{d}}+1} - \frac{1}{r} \qquad (A2.1)$$

$Z = 55$, $\mu = 3.1 a_B$, $d = 0.4 a_B$, $\eta = 2.235 a_B^{-1}$

It is in fact the "Tietz" potential [25] in which we introduce shielding factor. At $r < \mu$ $V(r)$ yields a good approximation of Thomas-Fermi potential.

The potential (A2.1) yields agreement between calculated and observed values of energies and fine splittings of all one particle states (including the states of inner electrons) to withing several per cent. (We assume that $5p$ fine splitting equals to difference between ionization potentials of the $5p_{3/2}$ and $5p_{1/2}$ electrons: $E_{5p_{3/2}} - E_{5p_{1/2}} = 15\cdot 10^3\,cm^{-1}$ [26]).

In thallium we use the potential given in ref. [19].

$$V(r) = -\frac{(Z-1)}{r(1+\eta r)^2} e^{-r/d} - \frac{1}{r} \qquad (A2.2)$$

$Z = 81$, $d = 3.8775 a_B$, $\eta = 2.5937 a_B^{-1}$

This potential fits the energy levels and fine splittings with an accuracy to several per cent.

References

1. P.Kusch and H.M.Foley. Phys. Rev. 74, 250, 1948.
2. P.Kusch and H.Taub. Phys. Rev. 75, 1477, 1949.
3. A.K.Mann and P.Kusch. Phys. Rev. 77, 435, 1950.
4. M.A.Bouchiat and C.C.Bouchiat. Phys. Lett. 48B, 111, 1974.
5. M.A.Bouchiat and C.C.Bouchiat. J.de Phys. 35, 899, 1974; 36, 493, 1975.
6. I.B.Khriplovich. Yadernaya Fizika 21, 1046, 1975.
7. M.A.Bouchiat and L.Pottier. Phys. Lett. 62B, 327, 1976.
8. S.Chu, E.D.Commins and R.Conti. Phys. Lett. 60A, 96,1977.
9. O.P.Sushkov, V.V.Flambaum, I.B.Khriplovich. Pis'ma v ZhETF 24, 502, 1976.
10. V.N.Novikov, O.P.Sushkov, V.V.Flambaum, I.B.Khriplovich. ZhETF 73, 802, 1977.
11. K.D.Böklen et al., Zeitschr. für Phys. 200, 467, 1967.
12. P.A.Vandenbout et al. Phys. Rev. 165, 88, 1968.
13. C.W.White et al. Phys. Rev. A7, 1178, 1973.
14. A.Abragam, J.H.Van Vlec, Phys. Rev. 92, 1448, 1953.
15. W.E.Lamb, Jr. Phys. Rev. 60, 817, 19.
16. M.Phillips, Phys. Rev. 88, 202, 1952.
17. D.V.Neuffer and E.D.Commins. Phys. Rev. A16, 1760, 1977.
18. O.P.Sushkov, V.V.Flambaum, I.B.Khriplovich. ZhETF, 74, 868, 1978.
19. D.V.Neuffer and E.D.Commis. Phys. Rev. A16, 844, 1977.
20. A.I.Akhiezer and V.B.Berestetsky. Quantum Electrodynamics.
21. G.Feinberg and J.Sucher. Phys. Rev. Lett. 26, 681, 1971.
22. G.W.F.Drake. Phys. Rev. A3, 908, 1971.
23. T.R.Fowler. Ph.D.thesis (UCRL-18321), University of California, Berkeley, 1968. (cited on ref. /17/).
24. O.P.Sushkov, V.V.Flambaum, I.B.Khriplovich. Optica i Spectroskopiya 44, 3, 1978.
25. T.Tietz. J.Chem. Phys. 22, 2094, 1954.
26. Ch. E.Moore. Atomic Energy Levels, Vol. 3, NBS 467, Washington, 1958.

Работа поступила - 23 января 1978 г.

Ответственный за выпуск - С.Г.ПОПОВ
Подписано к печати 26.I-1978 г. МН 02631
Усл. 1,4 печ.л., 1,2 учетно-изд.л.
Тираж 200 экз. Бесплатно
Заказ № 15.

Отпечатано на ротапринте ИЯФ СО АН СССР