ИНСТИТУТ ЯДЕРНОЙ ФИЗИКИ СО АН СССР

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A b s t r a c t

Corrections to the g-factors of the Cs, Fr, Au and Hg^+ atoms as well as the amplitude of the 6S - 7S strongly forbidden M1 transition in Cs have been calculated. For this purpose, the relativistic Hartree-Fock equations involving the interaction between electrons and an external magnetic field are used. With such a method, the effect of polarization of the closed shells is taken into account exactly. The following values of the correction to the g-factor for Cs, Fr and Au have been obtained: $\delta g_{Cs} = 2.54 \cdot 10^{-4}$; $\delta g_{Fr} = 33.3 \cdot 10^{-4}$ and $\delta g_{Au} = 11.9 \cdot 10^{-4}$ (the experiment gives, correspondingly: $2.23(1)\,10^{-4}$; $26.5(8)\,10^{-4}$; $9.87(2) \cdot 10^{-4}$), and $\delta g_{Hg^+} = 10.2 \cdot 10^{-4}$ for the Hg^+ (refined value $8.5 \cdot 10^{-4}$). The amplitude of the 6S - 7S transition of Cs is equal to $-0.56 \cdot 10^{-4}\,|\mu_B|$ (and $-0.413(18) \cdot 10^{-4}$ in the experiment).

1. Introduction

The question on the difference of the g-factor of a atom with one external electron from that of a free electron was extensively discussed already in the course of the first measurements of the magnetic moment of the electron [1-3]. Strongly forbidden M1-transitions in heavy atoms have attracted attention in connection with the search for the parity violating effects in them.

The mechanism of appearing the correction to the g-factor is different for light and heavy atoms. For light atoms, only the relativistic effects should be taken into account [4,5,6]. For heavy atoms, the many-body effects mainly contribute to the g-factor [7,8]. In Ref. [7] the matter was concerned with the corrections appeared in the second order in the Coulomb interaction and in the second order in a spin-orbit one. However, in Ref. 8 the main contribution to the correction to the g-factor is shown to be appeared already in the first order in the residual Coulomb interaction (the second order in the spin-orbit interaction is, nevertheless, necessary). The amplitude of strongly forbidden M1-transitions in heavy atoms is due to the same effects. The reference 8 also presents the calculations of the correction to the g-factor and of the amplitude of the 6S - 7S transition in Cs, using the electron wave functions computed in the effective potential. The numerical values obtained are about 1.5 times larger as compared with the experimental ones. In Ref. 6 calculations were similarly made for the corrections to the g-factor in Li, Na, K and Rb.

The present paper deals with the calculation of the corrections to the g-factor of the heavy atoms of Cs, Fr, Au and Hg^+ as well as of the amplitude of the strongly forbidden M1-transition 6S-7S in Cs. For these quantities to be calculated, the relativistic Hartree-Fock equations including the interaction of electrons with an external magnetic field have been used. Such a method allows one to take into account correctly the effect of polarization of the closed shells of an atom and simplifies further application of a many-body perturbation the-

ory in the residual Coulomb interaction between the electrons. A similar method has previously been employed for calculation of the hyperfine structure (see, e.g., Ref. 9). The calculation of the corrections to the g-factors by the relativistic Hartree-Fock method proves to be more precise than the calculation in the effective potential [8].

II. Calculation of the correction to the g-factor

For an atom with one external s-electron, the correction to the g-factor, which is due to the mixing of configurations, is convenient to represent as follows:

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

It is clear that in order to find δg , it is necessary to take into consideration a spin-orbit interaction mixing the state with $L = 1$ to the state with $L = 0$, both in the bra $\langle J, J_z=\frac{1}{2}|$ and the Ket $|J, J_z=\frac{1}{2}\rangle$ vectors.

All the calculations become considerably simpler if the spin-orbital interaction is taken into account by an exact solution of the Dirac equation rather than with respect to a perturbation theory. True, here the correction to the g-factor will arise as a result of the cancellation of the terms up to the magnitudes of the order of $(Z\alpha)^4$ (we remind that the spin-orbital interaction is proportional to $(Z\alpha)^2$, Z is the charge of the nucleus, and $\alpha = 1/137$).

For the Dirac equation, it is easy to write the exact operator of magnetic moment, but it is more proper to divide it into two parts: nonrelativistic magnetic moment $M_z = -|\mu_b|(L_z + 2S_z)$ and proportional to α^2 relativistic corrections to it, for the convenience in control of the accuracy of calculations.

We have made use of the Hartree-Fock method in the frosen-core approximation (in other words, in the V^{N-1} approximati-

on [10-12]). The sense of this approximation consists in that only the electrons from the closed shells are involved in the self-consistency procedure. The states of the external electron are calculated in the 'frozen' field of the internal electrons. This method allow one to construct a complete set of orthonormalized atomic orbitals which includes both the closed and excitated states.

In this case the Hartree-Fock equations are of the form

$$H_0\psi = E\psi$$

$$H_0 = c\vec{\alpha}\cdot\vec{p} + (\beta-1)mc^2 - \frac{Ze^2}{r} + V^{N-1} \qquad (2)$$

Here $\vec{\alpha}$ and β are Dirac matrices, N is the number of electrons in an atom, and $V^{N-1} = V_d - V_{exch}$ is the sum of the direct and exchange potentials.

$$(V_d - V_{exch})\psi = e^2\sum_{i=1}^{N-1}\int \frac{\psi_i^+(\vec{r}')\psi_i(\vec{r}')}{|\vec{r}-\vec{r}'|}d\vec{r}'\,\psi(\vec{r}) - \\ -e^2\sum_{i=1}^{N-1}\int \frac{\psi_i^+(\vec{r}')\psi(\vec{r}')}{|\vec{r}-\vec{r}'|}d\vec{r}'\,\psi_i(\vec{r}) \qquad (3)$$

The sum is only taken over the electrons from the closed shells. Equation (2) is of the same form in cases when the function belongs to one of the 'core' electrons, or to the external electron. When calculating the wave function of the electron from the closed shell, we takes into account formally its interaction with itself. However, the Hartree-Fock equations are such that, for internal electrons, the direct and exchange self-interactions cancel each other.

With the complete set of eigenfunctions of the Hamiltonian (2), the correction to the g-factor could be calculated, using many-body perturbation theory in the residual Coulomb interaction. However, it is more convenient to find it, including the magnetic-interaction operator $H_z M_z$ in the self-consistent equations for single-particle orbitals:

$$(H_z M_z + H_0')(\psi+\delta\psi) = (E+\delta E)(\psi+\delta\psi) \qquad (4)$$

Here E and ψ are the energy and wave function satisfying equation (2), and δE and $\delta\psi$ are the corrections to them which are proportional to the magnetic field. We have written H_0' instead of H_0 in order to indicate that ψ_i should be replaced by $\psi_i + \delta\psi_i$ in the potential (3). In equation (4), only the terms linear in $\delta E, \delta\psi$ and $H_z M_z$ should be retained. If the factor $-|M_B| H_z/2$ is discarded in the operator $H_z M_z$, the energy correction δE will be equal to the g-factor. Taking into account equation (1) as well, we obtain

$$(E-H_0)\delta\psi = -2\tilde{\ell}_z\psi - \sum_{i=1}^{N-1} e^2 \left\{ \delta\psi_i(\vec{r}) \int \frac{\psi_i^+(\vec{r}')\psi(\vec{r}')}{|\vec{r}-\vec{r}'|} d\vec{r}' + \right.$$

$$\left. + \psi_i(\vec{r}) \int \frac{\delta\psi_i^+(\vec{r}')\psi(\vec{r}')}{|\vec{r}-\vec{r}'|} d\vec{r}' \right\} - \delta g \psi \qquad (5)$$

Here

$$\tilde{\ell}_z = \begin{pmatrix} \left(1+\frac{p^2}{4m^2c^2}\right)\ell_z & 0 \\ 0 & 0 \end{pmatrix} \qquad (6)$$

It is easy to see that in going from the Dirac equation to a Schredinger one the operator $\tilde{\ell}_z$ transforms into a usual ℓ_z within an accuracy up to the terms $(v/c)^4$ (cf. Ref. 13). In equation (5), $\psi, E, \delta\psi$, and δg can also belong either to one of the internal electrons or to the external electron. The second term in the right-hand side part of equation (5) is a correction to the exchange potential V_{exch} (see equation (3)). A similar correction to the direct potential does not arise because the pseudovector ℓ_z is not capable of changing, in the

first order of magnitude, the Coulomb field of the closed shells. The point is that in the linear approximation a state with the unperturbed value of the total momentum, $J = 0$, can has only the dipole moment under the action of an external vector field, but the dipole moment is a true vector. In order that the atomic orbitals remain orthonormalized while including the external field, the corrections $\delta\psi$ should be orthogonal to the functions ψ themselves.

From equation (5), it is easy to derive

$$\delta g = -2\int \psi^+(\vec{r})\tilde{\ell}_z\psi(\vec{r})d\vec{r} - 2e^2\sum_{i=1}^{N-1}\iint \frac{\psi^+(\vec{r})\psi_i^+(\vec{r}')\delta\psi_i(\vec{r})\psi(\vec{r}')}{|\vec{r}-\vec{r}'|} d\vec{r}\,d\vec{r}' \qquad (7)$$

Equations (5) and (7) are solved by iterations. The results obtained is possible to explain in the following way. Taking into account the correction to Vexch in the r.h.s. part of equations (5) and (7) is equivalent to the substitution of $\tilde{\ell}_z$ by the renormalized operator w for which these equations take the form

$$(H_0 - E_i)\delta\psi = -w|i\rangle \qquad (8)$$

and

$$\delta g_i = \langle i|w|i\rangle \qquad (9)$$

Here $\langle k|w|i\rangle = \int \psi_k^+(\vec{r}) w \psi_i(\vec{r}) d\vec{r}$. Substituting equation (8) into the right-hand side part of equation (5), we have the following relation for the matrix elements of the operator w :

$$\langle k|w|i\rangle = -2\langle k|\tilde{\ell}_z|i\rangle -$$

$$-\sum_{n=1}^{N-1}\sum_{\mu=N}^{\infty}\left\{ \frac{\langle n|w|\mu\rangle\langle k\mu|\frac{e^2}{|\vec{r}-\vec{r}'|}|ni\rangle}{E_n - E_\mu} + \frac{\langle kn|\frac{e^2}{|\vec{r}-\vec{r}'|}|\mu i\rangle\langle\mu|w|n\rangle}{E_n - E_\mu} \right\} \qquad (10)$$

where

$$\langle kn|\frac{e^2}{|\vec{r}-\vec{r}'|}|\mu i\rangle = e^2\iint \frac{\psi_k^+(\vec{r})\psi_n^+(\vec{r}')\psi_\mu(\vec{r})\psi_i(\vec{r}')}{|\vec{r}-\vec{r}'|}d\vec{r}\,d\vec{r}'$$

Thus, the self-consistency of Hartree-Fock equations in an external field is equivalent to the solution of a graphic equation (Figure 1) for the vertex operator W (corresponding to the approach of the RPA to an exact equation for the vertex operator [14,15,16]).

When solving the system of equations for the quantities $\langle k|w|i\rangle$ (see equation (10)) by iterations, it is easy to show what diagrams of many-body perturbation theory are included in equation (7) (see Figure 1). These diagrams take into account an interaction between the valent electron and the core polarized by an external field.

The Hamiltonian H_0 corresponds to a centrally-symmetric field. In view of this, it is convenient to expand $\delta\psi$ in the states with definite orbital and total electron moments ℓ and j.

$$\delta\psi = \sum_{\varkappa} \delta\psi_{\varkappa} \qquad (11)$$

where $\varkappa = (-1)^{\ell+j+\frac{1}{2}}(j+\frac{1}{2})$. The pseudovector operator can have the non-zero matrix elements for the transitions with $\Delta j = 0,1$ and $\Delta\ell = 0,2$. The corrections to the functions with $\Delta\ell = 2$ are omitted. One can show that for an atom with the external s-electron these corrections contribute to the g-factor in the third order in the Coulomb residual interaction and in the fourth ($\sim(\alpha Z)^8$) in a spin-orbital one. Indeed, the spin-orbit interaction operator is the only operator, which can give rise to the mixing of the states with different values of the total atomic orbital moment L. However, taking into account the admixture of the function with the angular momentum $\ell \pm 2$ to the wave function of one electron with the angular momentum ℓ, we thereby take into account the admixture of the state with $L = 2$ to the full wave function of an atom with $L = 0$. The first-order spin-orbit interaction can change L only by

unity. For this reason, the admixture itself of the state with $L = 2$ to the state with $L = 0$ appears only in the second order in the spin-orbit interaction, whereas the presence of this admixture has influence on the energy (since δg is, as a matter of fact, the atomic energy in a magnetic field) in the fourth order only.

For the wave functions of electrons with $\ell \neq 0$, we thus have two corrections for each: diagonal over j and non-diagonal over j (with $j' = 2\ell - j$). For s electrons, there is only one j-diagonal correction. The corrections to the wave function and to the g-factor as a function of the projection of the total electronic ungular momentum m are given by formulae

$$\delta\psi_{m\varkappa} = (-1)^{j'-m}\begin{pmatrix} j' & 1 & j \\ -m & 0 & m\end{pmatrix}\frac{1}{r}\begin{pmatrix}\delta f(r)\,\Omega_{j'\ell m}(\vec{n}) \\ i\,\delta g(r)\,\widetilde{\Omega}_{j'\ell m}(\vec{n})\end{pmatrix}$$

$$\delta g_m = (-1)^{j-m}\begin{pmatrix} j & 1 & j \\ -m & 0 & m\end{pmatrix}\delta g \qquad (12)$$

Here $\widetilde{\Omega} = -(\vec{\sigma}\cdot\vec{n})\Omega$ and Ω is a spherical spinor, $\vec{n} = \vec{r}/r$.

Reference /9/ where the hyperfine structure (HFS) of the levels in Cs and Fr is calculated presents a more complete description of the solution of type-(5) equations. To find both the HFS constants and corrections to the g-factor, one needs to consider an interaction between the electrons and a magnetic field. In the first case, this will be an inhomogeneous magnetic field of the atomic nucleus, while in the second case this is a homogeneous external field. Therefore the angular dependence of appropriate corrections to the wave functions and the form of an equation which is satisfied by their radial components practically coincide in both cases.

As has already been mentioned, the correction to the g-factor, calculated according to formula (7), also includes, in addition to the zero order ($-2\int\psi^+\tilde{\ell}_z\psi\,d^3r$), the chain of many-body perturbation theory diagrams. When calculating the

HFS constant, making allowance for a similar chain of diagrams leads to an insignificant refinement of the value of the HFS appeared already in the zero order. Unlike the HFS, there is no contribution to the anomaly of the g-factor in the zero order (i.e. without the residual Coulomb interaction being taken account). In our case of the atom with one external s electron, $\int \psi^+ \tilde{\ell}_z \psi \, d^3r = 0$, and, hence, the effect under discussion occurs while taking into account the second term in the r.h.s. of equations (7) and (5).

The first-order correction to the g-factor in the Coulomb interaction (which have been calculated in Ref. /8/) is possible to find according to formula (7) if when calculating the corrections to the wave functions of electrons from the closed shells we do not perform the self-consistency procedure (i.e. take into account only the first term in equation (5)). The matrix elements of the operator $\tilde{\ell}_z$ between the wave functions of the states with equal ℓ and j , and with different principal quantum numbers n and n' are equal to zero because of the orthogonality of the radial wave functions. In view of this without the self-consistency being taken into account, only the j-nondiagonal correction to the wave functions arises. The first-order correction to the g-factor in the Coulomb interaction is as follows (Ref. /8/):

$$\delta g_{1i} = 4 \sum_{k=1}^{N-1} \sum_{\mu=N}^{\infty} \frac{\langle k|\tilde{\ell}_z|\mu\rangle\langle i\mu|\frac{e^2}{|\vec{r}-\vec{r}'|}|ki\rangle}{E_k - E_\mu} \qquad (13)$$

where k correspond to the sets of quantum numbers $njlm$ and $\mu - n'j'lm$, respectively, and $j' = 2l - j$. In the first order in the spin-orbit interaction $\langle njlm|\tilde{\ell}_z|n'j'lm\rangle = -\langle nj'lm|\tilde{\ell}_z|n'jlm\rangle$ (Ref. /8/). Making use of this, it is easy to show that δg_1 in equation (13) is, indeed, the quantity of the second order in the spin-orbit interaction.

Table 1 lists the values of δg_1 and δg_{HF} , the corrections to the g-factor in the first order in Coulomb interaction and after the consistency procedure for Cs, Fr, Au, and for the Hg^+ ion. It is seen that the contribution from the diagrams of the second and higher orders of many-body perturbation theory (taken into account in equation (7)) is not small as well.

Let us consider the other mechanisms contributing to the correction to the g-factor.

First, this is the above mentioned relativistic corrections to the operator $-|\mu_B|(\ell_z + 2s_z)$. The relativistic wave function is of the form

$$\psi = \frac{1}{r}\begin{pmatrix} f(r)\,\Omega_{jlm} \\ ig(r)\,\tilde{\Omega}_{jlm} \end{pmatrix} \qquad (14)$$

The electron magnetic moment is then equal, with an accuracy up to $(v/c)^4$, to ($\hbar = c = 1$, see Ref. /8/)

$$H_{rel} = -|\mu_B|(\vec{\ell} + 2\vec{s})\left\{1 - \int\left[g^2(r) + \frac{E - V(r)}{r} - \frac{1}{2} f(r)g(r)\right]dr\right\} \qquad (15)$$

Here $V(r) = -\frac{Ze^2}{r} + V_d(r)$

We have evaluated also how the correlation effects influence the magnitude of the relativistic correction to the magnetic moment. In Cs, the contribution to the correction to the g-factor, which occurs when taking into account the relativistic corrections to the magnetic moment operator and the first-order corrections in the residual Coulomb interaction, constitutes about 1% of the experimental value of δg .

The correction to the g-factor, which is due to the magnetic interaction between the external electron and the internal electrons, arises from the diamagnetic term $\frac{e^2\vec{A}^2}{2m_e c^2}$ in the Hamiltonian. $\vec{A} = \vec{A}_e + \vec{A}_H$, where $\vec{A}_H$ and $\vec{A}_e$ are the vector-potentials of the external field and external electron, respectively. The corresponding correction to the magnetic moment of the external electron with $\ell = 0$ reduces to the form/8/

$$H_{dia} = \frac{1}{3}|\mu_B|\alpha^2 \left\langle 2\vec{s}\left[a_B \int_r^\infty \frac{n(r')}{r'} 4\pi r'^2 dr'\right]\right\rangle \qquad (16)$$

where $n(r')$ is the density of internal electrons and a_B is the Bohr radius. The matrix element in equation (16) is taken over the wave function of the external electron.

The correction to the g-factor, which is due to the exchange magnetic interaction, has been calculated in Ref. /8/ and has proven to be negligibly small.

The values of the relativistic corrections δg_{rel} and δg_{dia} to the g-factor are given in Table 1.

Table 2 presents the sums of these three contributions taken into account, $\delta g_{HF} + \delta g_{rel} + \delta g_{dia}$, and the experimental values of the correction to the g-factor for Cs, Fr, Au, and Hg^+. It is seen that the computational results are 15-20% larger in comparison with the experimental values.

As has already been noted above, the correction to the g-factor arises as a result of the cancellation of the terms which could be a possible reason for the increase of the errors. In the corrections δg_{rel} and δg_{dia}, caused by the relativistic effects, the small factor α^2 is separated explicitly. Substantial cancellation occurs only when calculating the corrections δg_1 and δg_{HF} caused by the many-body effects. If this cancellation is made sufficiently exactly, the result should depend, in a definite manner, on the fine structure constant: $\delta g_1, \delta g_{HF} \sim (Z\alpha)^4$. Changing the magnitude of the parameter α, we have the possibility of checking the accuracy of the calculations being made. This check has been made and one can affirm that the difference between the calculational and experimental results (Table 2) is determined not by the errors in calculations but by the not-being-taken into-account contributions to δg in the second and higher orders in the residual Coulomb interaction (see, e.g., Figure 2). It is seen from Table 1 that the corrections to the g-factor, which are due to the correlation effects, are rather close, for Au and Hg^+. The contributions, which are not being taken into account, may be expected to be also close, for these two cases. With this argument taken into consideration, we obtain the refined value for the Hg^+ ion:

$$\delta g_{Hg^+} = 8.5 \cdot 10^{-4} \qquad (17)$$

III. Amplitude of the 6s-7s transition in caesium

To calculate the amplitude of the M1-transition, let us analyse the interaction of an atom with an external periodic field:

$$H_z \left(e^{-\frac{i\omega}{\hbar}t} + e^{\frac{i\omega}{\hbar}t} \right) \qquad (18)$$

The influence of this field gives rise, in particular, to the polarization of the closed shells. In the V^{N-1} approximation, the electrons from the closed shells are unaware of the existence of the external electron at all. For this reason one can assume that the 6s-7s transition proceeds in a purely single-particle way, and the influence of the internal shells reduces to the fact that the field (18) is complemented by the induced field of the core.

To determine the closed-shell polarization effect, we will use the 'time-dependent Hartree-Fock equation' method /14,15,16/.

The wave functions of electrons will be searched for as follows:

$$\psi'(t) = \psi(r) + \chi(r) e^{-\frac{i\omega}{\hbar}t} + \gamma(r) e^{\frac{i\omega}{\hbar}t} \qquad (19)$$

where $\chi(r)$ and $\gamma(r)$ are the corrections to the unperturbed wave function, which are proportional to the weak external field. The Hartree-Fock equations then take form

$$\left[H_z M_z\left(e^{-\frac{i\omega}{\hbar}t}+e^{\frac{i\omega}{\hbar}t}\right)+H_o'\right]\left(\psi+\chi e^{-\frac{i\omega}{\hbar}t}+\gamma e^{\frac{i\omega}{\hbar}t}\right)=$$

$$=E\psi+(E+\omega)\chi e^{-\frac{i\omega}{\hbar}t}+(E-\omega)\gamma e^{\frac{i\omega}{\hbar}t} \qquad (20)$$

Here H_o' is obtained from the Hamiltonian H_o with the substitution of ψ_i' for ψ_i in the potential (3). From equation (20), remaining only the first-order terms in the external field, we obtain

$$(E+\omega-H_o)\chi=-\tilde{\ell}_z\psi-\sum_{i=1}^{N-1}e^2\left\{\chi_i(\vec{r})\int\frac{\psi_i^+(\vec{r}')\psi(\vec{r}')}{|\vec{r}-\vec{r}'|}d\vec{r}'+\right.$$

$$\left.+\psi_i(\vec{r})\int\frac{\gamma_i^+(\vec{r}')\psi(\vec{r}')}{|\vec{r}-\vec{r}'|}d\vec{r}'\right\}$$

$$(E-\omega-H_o)\gamma=-\tilde{\ell}_z\psi-\sum_{i=1}^{N-1}e^2\left\{\gamma_i(\vec{r})\int\frac{\psi_i^+(\vec{r}')\psi(\vec{r}')}{|\vec{r}-\vec{r}'|}d\vec{r}'+\right. \qquad (21)$$

$$\left.+\psi_i(\vec{r})\int\frac{\chi_i^+(\vec{r}')\psi(\vec{r}')}{|\vec{r}-\vec{r}'|}d\vec{r}'\right\}$$

When deriving the above equation, we have discarded the common factor $-|\mu_e|H_z$ and have taken into account the fact that the total angular momentum operator J_z cannot have the nondiagonal matrix elements.

This procedure is equivalent to the use of a new field, instead of (18), which takes account of the closed-shell polarization:

$$-|\mu_e|H_z\left(we^{-\frac{i\omega}{\hbar}t}+w^+e^{\frac{i\omega}{\hbar}t}\right) \qquad (22)$$

The matrix elements of the operator w satisfy the following relation:

$$\langle k|w|i\rangle=-\langle k|\tilde{e}_z|i\rangle-$$

$$-\sum_{n=1}^{N-1}\sum_{\mu=N}^{\infty}\left\{\frac{\langle kn|\frac{e^2}{|\vec{r}-\vec{r}'|}|\mu i\rangle\langle\mu|w|n\rangle}{E_n+\omega-E_\mu}+\frac{\langle n|w|\mu\rangle\langle k\mu|\frac{e^2}{|\vec{r}-\vec{r}'|}|ni\rangle}{E_n-\omega-E_\mu}\right\} \qquad (23)$$

The amplitude of the 6s-7s transition in the field (22) is equal to

$$M=-|\mu_e|\langle 7s|w|6s\rangle=-|\mu_e|\sum_{i=1}^{N-1}e^2\left\{-\iint\frac{\psi_{7s}^+(\vec{r})\psi_i^+(\vec{r}')\chi_i(\vec{r})\psi_{6s}(\vec{r}')}{|\vec{r}-\vec{r}'|}d\vec{r}d\vec{r}'-\right.$$

$$\left.-\iint\frac{\psi_{7s}^+(\vec{r})\gamma_i^+(\vec{r}')\psi_i(\vec{r})\psi_{6s}(\vec{r}')}{|\vec{r}-\vec{r}'|}d\vec{r}d\vec{r}'\right\} \qquad (24)$$

The frequency in equation (21) must be taken equal to the difference in the Hartree-Fock values of the energy: $\omega = E_{7s}-E_{6s}$. Just as when calculating the correction to the g-factor, equation (24) make allowance for the series of diagrams of many-body perturbation theory and among them there are all the first-order diagrams in the Coulomb interaction.

The transition amplitude in the first order in the Coulomb interaction equals $M_1 = -0.432\cdot10^{-4}\,|\mu_e|$, and $M_{HF} = -0.641\cdot10^{-4}\,|\mu_e|$ after the consistency procedure.

The M1-amplitude (24) is very weakly dependent on the frequency at what equations (21) have been solved. This occurs because the transition frequency ω is much less than the energy of internal electrons E, entering into equation (21). In addition, for the 6s-7s transition in Cs, the linear term in the expansion (24) in powers ω/E is strongly suppressed because of the cancellation of the corresponding linear terms in the expansion of the first and second terms.

The relativistic correction to the M1-transition amplitude is of the form /8/ ($\hbar=c=1$)

$$M_{rel}=|\mu_e|(\ell_z+2s_z)\left\{\int_0^\infty g_1g_2+\frac{1}{2\varkappa-1}\left((E_1-V(r))f_1g_2r+\right.\right.$$

$$\left.\left.+(E_1-V(r))f_2g_1r\right)\right]dr+\frac{m}{5(2\varkappa-1)}\int_0^\infty(f_1g_2+f_2g_1)\omega^2r^3dr\Big\} \qquad (25)$$

For the transition under consideration, $M_{rel} = 0.062\cdot10^{-4}|\mu_e|$ The contribution from the diamagnetic corrections is calculated according to formula (16): $M_{dia} = 0.019\cdot10^{-4}|\mu_e|$.

The total amplitude equals

$$M = M_{HF} + M_{rel} + M_{dia} = -0.560 \cdot 10^{-4} |\mu_B| \qquad (26)$$

The experimental value is the following:

$$M = -(0.424 \pm 0.034) \cdot 10^{-4} |\mu_B| \quad [20]$$
$$M = -(0.369 \pm 0.024) \cdot 10^{-4} |\mu_B| \quad [21]$$
$$M = -(0.413 \pm 0.018) \cdot 10^{-4} |\mu_B| \quad [22]$$

IV. Conclusion

Following from all the calculations presented in the paper, we can say that the value of the correction to the g-factor in heavy atoms and the amplitude of strongly forbidden M1-transitions are both determined by the effect of closed--shell polarization in an external field. The largest contribution to δg and $M1$ comes from the diagrams appearing in the first order in the residual Coulomb interaction and in the second order in the spin-orbital interaction (considered in Ref. /8/). However, taking into account the second- and higher-order diagrams in the Coulomb interaction, which enter 'core' polarization, proves to be significant, too. Unlike the light atoms, purely relativistic corrections have little influence on the δg and $M1$ -amplitudes. The contribution of the not-taken-into-account higher-order correlation effects to δg, which explain, in our opinion, the discrepancy between calculation and experiment, should be at a level of 15-25%.

Thus, the relativistic Hartree-Fock equation method in an external field allows one to obtain relatively easily the values of δg and $M1$, which are in rather good agreement with the experiment.

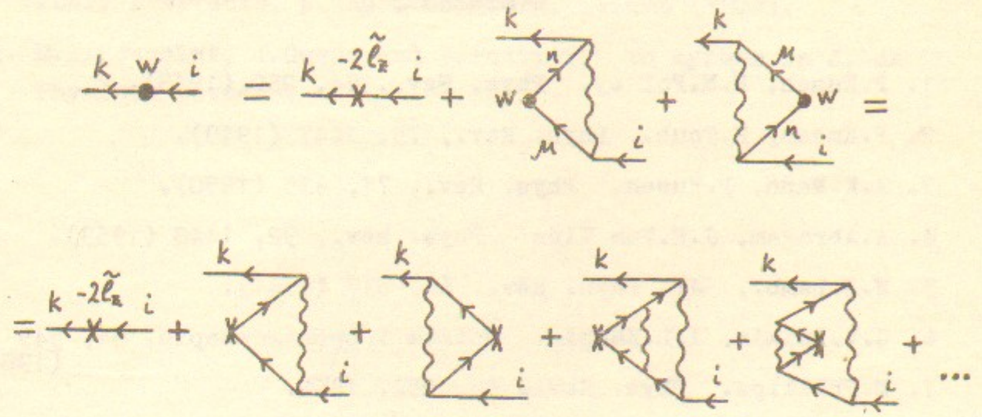

Fig. 1. The cross denotes the matrix element of the operator $-2\tilde{\ell}_z$ and the black point denotes w. The index n numerates the states from the closed shells and μ stands for the virtual excited states.

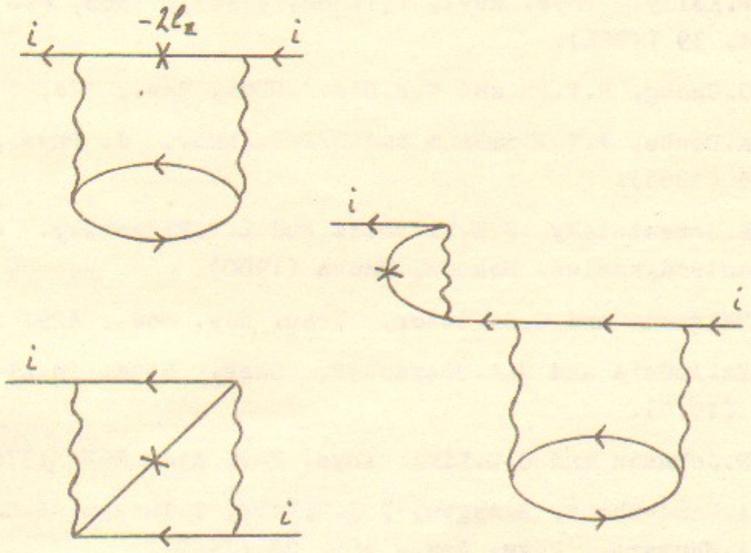

Fig. 2. Some of the diagrams we do not taken into account when calculating the correction to the g-factor.

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Table I

	$\delta g_1 \cdot 10^4$	$\delta g_{HF} \cdot 10^4$	$\delta g_{rel} \cdot 10^4$	$\delta g_{dia} \cdot 10^4$
Cs	I.87	2.84	-0.23	-0.07
Fr	2.5	33.7	-0.33	-0.10
Au	9.23	13.6	-1.20	-0.44
Hg^+	9.25	12.7	-1.82	-0.61

Table II

	$(\delta g_{HF} + \delta g_{rel} + \delta g_{dia}) \cdot 10^4$	$\delta g_{exp} \cdot 10^4$
Cs	2.54	2.23 (I) [17]
Fr	33.3	26.5 (8) [18]
Au	II.9	9.87 (2) [19]
Hg^+	10.2	-

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