52

ИНСТИТУТ ЯДЕРНОЙ ФИЗИКИ СО АН СССР

V.A.Dzuba, V.V.Flambaum and O.P.Sushkov

RELATIVISTIC MANY-BODY CALCULATION OF THE HYPERFINE-STRUCTURE INTERVALS IN THE CAESIUM AND FRANCIUM ATOMS

Preprint 83—82

НОВОСИБИРСК

RELATIVISTIC MANY-BODY CALCULATIONS OF THE HYPERFINE-STRUCTURE INTERVALS IN THE CAESIUM AND FRANCIUM ATOMS

V.A.Dzuba, V.V.Flambaum and O.P.Sushkov

Institute of Nuclear Physics,
630090, Novosibirsk 90, USSR

Abstract

The hyperfine structure of caesium and francium levels has been calculated using the relativistic Hartree-Fock (RHF) method and with the correlations being taken into account by means of the many-body perturbation theory. The hyperfine interaction has been included in the Hartree-Fock equations. The effect of the finite size of the nucleus has been considered. For the s and $p_{1/2}$ states, the agreement of our calculations with experiment is not worse than 3%. Using the experimental data on hyperfine structure the magnetic moments of isotopes $^{208\div 213}$Fr are obtained.

1. Introduction

The RHF method and many-body perturbation theory enables one to calculate the characteristics of heavy atoms with the good accuracy. In Refs. /1-5/ in such a way the hyperfine structure (HFS) constants of the s-levels of alkaline atoms from Li to Fr have been calculated. The energy levels and fine-structure intervals in Cs and Fr as well as the HFS constants of nine lower s and p-states of Cs have been calculated in Refs. /6-9/. At present, the calculation of the hyperfine structure of Fr seems to be urgent. The point is that the experimental data available on the g-factor of the nucleus of ^{211}Fr (Ref. /10/) and on the hyperfine splitting of the 7s-level of the francium atom (Ref. /11/) are not consistent with each other by 20%, according to the calculation which has been carried out in Ref. 5. There is the other calculation of Fr HFS /12/, but it does not take into account the correlation corrections

In the present paper the method of including of hyperfine interaction in the relativistic Hartree-Fock equations is developed. The hyperfine structure of a number of levels in Cs and Fr is calculated with correlation corrections taken into account. The result obtained for the 7s level in Fr is in disagreement with the calculation made in Ref. /5/ but is in agreement with the experimental data (see Refs /10,11/).

In calculating of the HFS constants in the frameworks of the relativistic Hartree-Fock method, at least, two approaches may be applied. In the first one, both the hyperfine interaction (HFI) together with the residual Coulomb one are taken into account using the many-body perturbation theory. Such an approach was used in all the papers of the New York group cited above (see Refs /1-5/) and in our previous work dealing with the HFS of Cs (see Refs /8,9/). In the second approach, the HFI operator enters in the Hartree-Fock equations, and only the correlation corrections are calculated in terms of the many-body perturbation theory. It is the approach that we use in the present paper. This approach takes into account the core polarization more accurately than first one, since it is equivalent to the summation of a certain infinite subsequence of diagrams. However, this difference from first method is not very significant. The main advantage of this second approach is purely technical: the calculations of correlations are simpler, although the very Hartree-Fock equations are somewhat complicated. This question will be discussed below in some detail.

2. Relativistic Hartree-Fock equations in an external field

The vector-potential $\vec{A}$, created by a magnetic moment, is of the form

$$\vec{A} = \frac{\vec{\mu}\times\vec{r}}{r^3} \qquad (1)$$

Correspondingly, the Hamiltonian of the hyperfine interaction between a relativistic electron and a point nucleus equals

$$\hat{H} = -\frac{e}{c}\vec{\alpha}\,\frac{\vec{\mu}\times\vec{r}}{r^3} = \frac{|e|}{c}\vec{\mu}\,\frac{\vec{r}\times\vec{\alpha}}{r^3} \qquad (2)$$

where $\vec{\alpha}$ is the Dirac matrix, $\vec{\mu}$ is the magnetic moment of the nucleus. In the calculation of the HFS of heavy atoms, the finite size of the nucleus needs to be taken into account. Let us use a simple model: we will assume that the nucleus represents an uniformly magnetized ball. Then,

$$\hat{H} = \frac{|e|}{c}\vec{\mu}\,\vec{F}(\vec{r})$$

$$\vec{F}(\vec{r}) = \begin{cases} \dfrac{\vec{r}\times\vec{\alpha}}{r_m^3} & r < r_m \\[2ex] \dfrac{\vec{r}\times\vec{\alpha}}{r^3} & r \geqslant r_m \end{cases} \qquad (3)$$

where $r_m = 1.1A^{1/3}$fm (A is the mass number of the nucleus). Of course, it is a rather rough approximation. The distribution of the currents in the nucleus is determined by external nucleons and is of the very complicated form. But it has turned out that the HFS is weakly dependent on a particular distribution. We shall discuss this problem below.

For the charge density of the nucleus, we use the standard formula

$$\rho(r) = \frac{N}{e^{\frac{r-r_N}{D}} + 1} \tag{4}$$

where N is the constant of normalization ($\int \rho(r)\,dv = Z$), according to Ref. /13/ $r_N \approx 1.10\,A^{1/3}\,fm$, $D \approx 0.57\,fm$. In the range of small r, the potential of the nucleus is determined by the numerical integration of the charge density.

Let us now consider how the HFI operator can be included in the Hartree-Fock procedure.

It is known that the approximation of the frozen core (or the $V^{(N-1)}$ approximation, see Refs /14, 1-9/) is convenient to use as the zero approximation for alkali atoms. In this approximation only the electrons of the core are included in self-consistence procedure. The states of an external electron are calculated in the field of the frozen core. Without the hyperfine interaction the Hartree-Fock equations for the orthogonal orbitals of the core are of the form

$$\hat{H}_0 \psi_a^{(0)} = \mathcal{E}_a^{(0)} \psi_a^{(0)} \tag{5}$$

where $\hat{H}_c$ is the Hartree-Fock Hamiltonian

$$\hat{H}_c = \vec{\alpha}\vec{p} + \beta(m_e - 1) - \frac{Ze^2}{r} + V_c^{(N-1)} \tag{6}$$

Here $\vec{p}$ is the electron momentum, $\vec{\alpha}$ and β are Dirac matrices, N is the number of electrons in the atom, and $V_0^{(N-1)}$ is the sum of the direct and exchange self-consistent electric potentials

$$V_0^{(N-1)} \psi_a^{(0)} = \sum_{b=1}^{N-1} \int d^3 r_2 \left| \psi_b^{(0)}(r_2) \right|^2 \frac{e^2}{r_{12}} \psi_a^{(0)}(r_1) - \sum_{b=1}^{N-1} \int d^3 r_2\, \psi_b^{(0)*}(r_2)\, \psi_a^{(0)}(r_2) \frac{e^2}{r_{12}} \psi_b^{(0)}(r_1) \tag{7}$$

Index " 0 " in formulae (5), (6) and (7) implies that the corresponding quantities are referred to the case without the HFI

being taken into account. It is well known that the states of an external electron in the frozen core approximation satisfy the same single-particle equation (5) (see, e.g., Ref. /6/). Thus, equation (5) generates the complete orthonormalized set of single-particles orbitals. Equations (5), (6) and (7) take into account exactly all the relativistic effects proportional to the powers of the parameter $Z\alpha$ which is rather large in heavy atoms. In this case, the magnetic interaction between electrons, retardation and radiative corrections are omitted. Their smallness is caused by the fact they are proportional to the lower powers of Z.

In taking into account the HFI, the using of the $V^{(N-1)}$ approximation seems to be natural. The equations for the orthonormalized orbitals of the core and external electron are of the form

$$\hat{H}\psi_a = \mathcal{E}_a \psi_a$$
$$\hat{H} = \vec{\alpha}\vec{p} + \beta(m_e - 1) - \frac{Ze^2}{r} + F_z + V^{(N-1)} \tag{8}$$

Since we consider the HFI in the linear approximation, the Hamiltonian (8) contains only the electron part of the operator, namely, the vector $\vec{F}(\vec{r})$ (see equation (3)). Note that $V^{(N-1)} \neq V_0^{(N-1)}$. The HFI has little influence on the wavefunctions (WF) and on the energies of electrons. Hence, we can write down

$$\psi_a = \psi_a^{(0)} + \delta\psi_a, \quad \mathcal{E}_a = \mathcal{E}_a^{(0)} + \delta\mathcal{E}_a \tag{9}$$

where $\delta\psi_a$ and $\delta\mathcal{E}_a$ are the small corrections to the WF and to the energy of the state with number a. Let us substitute the expansion (9) in the RHF equation (8) and omit $(\delta\psi)^2$, $\delta\mathcal{E}\cdot\delta\psi$, $(\delta\psi)^3$. Taking into account equation (5), we obtain the equation for $\delta\psi_a$

$$\left(\hat{H}_0 - \mathcal{E}_a^{(0)}\right)\delta\psi_a(r_1) = -F_z\psi_a^{(0)}(r_1) - \sum_{b=1}^{N-1} \int \delta\left|\psi_b(r_2)\right|^2 \frac{e^2}{r_{12}} \psi_a^{(0)}(r_1)\, d^3 r_2 + \tag{10}$$

$$+\sum_{b=1}^{N-1}\int \delta\left[\psi_b^{*}(r_2)\psi_b(r_1)\right]\frac{e^2}{r_{12}}\psi_a^{(0)}(r_2)\,d^3r_2 + \delta\varepsilon_a\psi_a^{(0)}(r_1) \qquad (10)$$

The second term in the right-hand side of equation (10) corresponds to correction to the direct Coulomb potential and the third one corresponds to the correction to the exchange potential. The above equation is written for an arbitrary small perturbation F_z (not necessarily for the HFI). As for the HFI, it is clear that the correction to the direct Coulomb potential equals zero, since the electron part of the HFI is a axial vector and, hence, it cannot change the Coulomb field of the closed shells in the linear approximation. An expression for $\delta\varepsilon_a$ is derived by multiplying equation (10) by $\psi_a^{(0)*}(r_1)$ and by integrating over r_1. (One should bear in mind that due to normalization of ψ_a the correction $\delta\psi_a$ is orthogonal to $\psi_a^{(0)}$).

$$\delta\varepsilon_a = \int\psi_a^{(0)*}(r)F_z\psi_a^{(0)}(r)\,d^3r - \sum_{b=1}^{N-1}\int\delta\left[\psi_b^{*}(r_2)\psi_b(r_1)\right]\frac{e^2}{r_{12}}\psi_a^{(0)*}(r_1)\psi_a^{(0)}(r_2)\,d^3r_1\,d^3r_2 \qquad (11)$$

The Hamiltonian $\hat{H}_0$ conserve the angular momentum. Therefore, $\delta\psi$ is convenient to expand in the states with definite orbital and total angular momenta of an electron l, j :

$$\delta\psi = \sum_{\varkappa}\delta\psi_{\varkappa} \qquad (12)$$

where $\varkappa = (-1)^{l+j+1/2}(j+1/2)$. The matrix elements of the HFI operator are different from zero for the transitions with Δl = 0,2 and Δj = 0,1. Correspondingly, the expansion (12) takes the form

If $\psi^{(0)} = |s_{1/2}\rangle$, then $\delta\psi = |s_{1/2}\rangle + |d_{3/2}\rangle$
If $\psi^{(0)} = |p_{1/2}\rangle$, then $\delta\psi = |p_{1/2}\rangle + |p_{3/2}\rangle$
If $\psi^{(0)} = |p_{3/2}\rangle$, then $\delta\psi = |p_{3/2}\rangle + |p_{1/2}\rangle + |f_{5/2}\rangle$
If $\psi^{(0)} = |d_{3/2}\rangle$, then $\delta\psi = |d_{3/2}\rangle + |s_{1/2}\rangle + |d_{5/2}\rangle$
If $\psi^{(0)} = |d_{5/2}\rangle$, then $\delta\psi = |d_{5/2}\rangle + |d_{3/2}\rangle + |g_{7/2}\rangle$ etc.

We will take into consideration only the corrections corresponding to Δl = 0. The contribution from the l-nondiagonal corrections is very small due to the smallness of the corresponding matrix elements. For example, $\langle 4s_{1/2}|F|4d_{3/2}\rangle/\langle 4s|F|4s\rangle = -0.52\cdot 10^{-3}$ and $\langle 4s_{1/2}|F|4d_{3/2}\rangle/\langle 4d_{3/2}|F|4d_{3/2}\rangle = -1.02\cdot 10^{-2}$ for Cs. The control calculations for Cs show that taking into account the l-nondiagonal corrections changes the HFS constant of the external electron not larger than by 0.2%. Thus, we have two corrections for the states of an electron with $l \neq 0$: diagonal and nondiagonal with respect to j. For the s-states there exists only the diagonal correction.

The dependence of the corrections to the wavefunction and to the energy on the projection of the electron angular momentum m is given by formulae

$$\delta\psi_{\varkappa m} = (-1)^{j-m}\begin{pmatrix} j & 1 & j_a \\ -m & 0 & m \end{pmatrix}\delta\psi_{\varkappa m}$$

$$\delta\varepsilon_m = (-1)^{j_a-m}\begin{pmatrix} j_a & 1 & j_a \\ -m & 0 & m \end{pmatrix}\delta\varepsilon \qquad (13)$$

Here j is the angular momentum corresponding to the correction, j_a is the angular momentum of the state to which the correction is calculated. The function $\delta\psi_{\varkappa m}$ is of the form

$$\delta\psi_{\varkappa m} = \frac{1}{r}\begin{pmatrix} f(r)\,\Omega_{jlm}\left(\frac{\vec{r}}{r}\right) \\ ig(r)\,\tilde{\Omega}_{jlm}\left(\frac{\vec{r}}{r}\right) \end{pmatrix} \qquad (14)$$

Here $\tilde{\Omega} = -(\vec{\sigma}\vec{n})\Omega$, Ω - spherical spinor.

The form of equation (13) is due to the fact that the HFI operator included in the Hartree-Fock equations, is an axial vector.

Equations for radial components f, g are readily derived from equation (10) and are of the form

$$\frac{df_\alpha}{dr} + \frac{\varkappa_\alpha}{r} f_\alpha - (2m_e + \varepsilon_a^{(0)} - V_0) g_\alpha = -W_{\alpha a} G(r) f_a^{(0)} + \delta_{\alpha a} \cdot \delta\varepsilon_a \cdot g_a^{(0)}$$

$$\frac{dg_\alpha}{dr} - \frac{\varkappa_\alpha}{r} g_\alpha + (\varepsilon_a^{(0)} - V_0 - \hat{K}_0) f_\alpha = W_{\alpha a} G(r) g_a^{(0)} - \delta_{\alpha a} \cdot \delta\varepsilon_a f_a^{(0)} - \qquad (15)$$

$$-e^2 \sum_{b=1}^{N-1} \sum_{\kappa,\beta} C^{\kappa}_{a\alpha b\beta} \int f_\beta(r') f_b^{(0)}(r) f_a^{(0)}(r) \frac{r_<^\kappa}{r_>^{\kappa+1}} dr' - e^2 \sum_{b=1}^{N-1} \sum_{\kappa,\beta} \mathcal{D}^{\kappa}_{a\alpha b\beta} \int f_b^{(0)}(r') f_\beta(r) f_a^{(0)}(r) \frac{r_<^\kappa}{r_>^{\kappa+1}} dr'$$

$$G(r) = \frac{\mu e^2}{2m_p I} \times \begin{cases} \dfrac{r}{r_m^3}, & r < r_m \\ \dfrac{1}{r^2}, & r \geq r_m \end{cases}$$

; $\delta_{\alpha a}$ is the Kronecker symbol. μ is the nuclear magnetic moment in nuclear magnetons, I is the nuclear angular moment, m_p is the mass of the proton. Index α numerates the corrections to the WF $\psi_a^{(0)}$; index β numerates the corrections to the WF $\psi_b^{(0)}$; $f^{(0)}$ and $g^{(0)}$ are the radial components of the non-perturbed wavefunction. The self-consistent direct and exchange potentials V_0 and $\hat{K}_0$ are determined by the equalities

$$V_0(r) = -\frac{Ze^2}{r} + \frac{1}{r} \int_0^r n(r) dr + \int_r^\infty \frac{n(r)}{r} dr$$

where $n(r) = e^2 \sum_{b=1}^{N-1} (2j_b+1) \left[(f_b^{(0)}(r))^2 + (g_b^{(0)}(r))^2 \right]$

$$\hat{K}_0 f_\alpha(r) = -e^2 \sum_{b=1}^{N-1} \sum_{\kappa} (2j_b+1) \cdot \xi(\kappa + l_\alpha + l_b) \begin{pmatrix} \kappa & j_b & j_\alpha \\ 0 & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}^2 \int f_b^{(0)}(r') f_\alpha(r') f_b^{(0)}(r) \frac{r_<^\kappa}{r_>^{\kappa+1}} dr'$$

$$\xi(x) = \begin{cases} 1 & \text{for even } x \\ 0 & \text{for odd } x \end{cases}$$

The angular matrix elements $W_{\alpha a}$, $C^{\kappa}_{a\alpha b\beta}$ and $\mathcal{D}^{\kappa}_{a\alpha b\beta}$ are of the form

$$W_{\alpha a} = (-1)^{j_\alpha + l_\alpha + \frac{1}{2}} \sqrt{\tfrac{3}{2}(2j_a+1)(2j_\alpha+1)} \left[\begin{Bmatrix} \frac{1}{2} & j_\alpha & l_\alpha \\ j_a & \frac{1}{2} & 1 \end{Bmatrix} \delta_{l_\alpha l_a} + \begin{Bmatrix} \frac{1}{2} & j_\alpha & \tilde{l}_\alpha \\ j_a & \frac{1}{2} & 1 \end{Bmatrix} \delta_{\tilde{l}_a \tilde{l}_\alpha} \right]$$

$$\tilde{l} = 2j - l$$

$$C^{\kappa}_{a\alpha b\beta} = (-1)^{j_a + j_b + \kappa + 1} \begin{Bmatrix} 1 & j_\alpha & j_a \\ \kappa & j_\beta & j_b \end{Bmatrix} \cdot O_{a\beta} \cdot O_{\alpha b} \qquad (16)$$

$$\mathcal{D}^{\kappa}_{a\alpha b\beta} = (-1)^{j_a - j_\alpha} C^{\kappa}_{\alpha a b\beta} = (-1)^{j_a + j_b + \kappa + 1} \begin{Bmatrix} 1 & j_a & j_\alpha \\ \kappa & j_\beta & j_b \end{Bmatrix} \cdot O_{ab} \cdot O_{\alpha\beta}$$

where

$$O_{\alpha\beta} = \sqrt{(2l_\alpha+1)(2l_\beta+1)(2j_\alpha+1)(2j_\beta+1)} \begin{Bmatrix} l_\alpha & j_\alpha & \frac{1}{2} \\ j_\beta & l_\beta & \kappa \end{Bmatrix} \begin{pmatrix} l_\alpha & \kappa & l_\beta \\ 0 & 0 & 0 \end{pmatrix} =$$

$$= -\sqrt{(2j_\alpha+1)(2j_\beta+1)} \begin{pmatrix} j_\alpha & j_\beta & \kappa \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} \cdot \xi(\kappa + l_\alpha + l_\beta)$$

For the correction to energy $\delta\varepsilon_a$ we have

$$\delta\varepsilon_a = W_{aa} \int 2 f_a^{(0)} g_a^{(0)} G(r) dr - 2e^2 \sum_{b=1}^{N-1} \sum_{\kappa,\beta} C^{\kappa}_{aab\beta} \int f_b^{(0)}(r) f_\beta(r') f_a^{(0)}(r) f_a^{(0)}(r') \frac{r_<^\kappa}{r_>^{\kappa+1}} dr dr' \qquad (17)$$

Thus, if the eigenfunctions $f_a^{(0)}, g_a^{(0)}$ and the eigenvalues $\varepsilon_a^{(0)}$ of the Hartree-Fock Hamiltonian H_0 are known, the solution of equations (15-17) makes it possible to determine the corrections to them induced by the HFI. As seen from equation (15), the equation for each correction to the WF is dependent on the corrections to all the functions of the core. Therefore, equations (15) should be solved selfconsistently by iterations, for all the corrections to the functions of the core. As we have already mentioned, the correction to the WF of an external electron is calculated in the frozen-core approximation.

Let us introduce an abbreviation RHFH which denotes the relativistic Hartree-Fock equations with the hyperfine interaction. The used algorithms for solution of the RHF and RHFH equations for a discrete and continuous spectra are given in Ref. /15/. The HFS constant A_a is then obtained readily in the RHFH approximation:

$$A_a = \frac{\delta\varepsilon_a}{\sqrt{(2j_a+1)(j_a+1)j_a}} \qquad (18)$$

3. Calculation of correlations

In order to calculate the correlation corrections, we will use the perturbation theory. A perturbation operator is difference between the exact Hamiltonian and the RHFH one:

$$\hat{H}_1 = \hat{H} - \sum_{a=1}^{N} H_0(r_a) = \sum_{a<b}^{N} \frac{e^2}{r_{ab}} - \sum_{a=1}^{N} V^{(N-1)}(r_a) \qquad (19)$$

Due to the fact that the HFI operator has been included in the RHFH Hamiltonian, the calculation of the correlation correction to the HFS constants reduces to the calculation of the correlation corrections to energy. The first-order corrections with respect to the residual Coulomb interaction equal zero exactly, while the second-order corrections are described by four graphs in figure 1 (see Ref. /6/).

$$\delta\varepsilon^{(2)} = \delta\varepsilon_a^{(2)} - \delta\varepsilon_b^{(2)} + \delta\varepsilon_c^{(2)} - \delta\varepsilon_d^{(2)}$$

We use the conventional Rayleigh-Schrödinger perturbation theory and the second quantization technique . The letters m and n denote the states of the occupied shells and the letters u , v and w denote the excited states. Let the HFS constant of the state with number u is calculated. Let us consider as an example the contribution from the graph in Figure 1a to the HFS constant of the state u . The corresponding correction to the energy is given by the expression

$$\delta\varepsilon_a^{(2)} = \sum_{nvw} \frac{Q^2(\psi_u \psi_v \psi_n \psi_w)}{\varepsilon_u + \varepsilon_n - \varepsilon_v - \varepsilon_w} \qquad (20)$$

where $Q(\psi_u \psi_v \psi_n \psi_w) = \int \psi_u^*(r_1) \psi_n^*(r_2) \frac{e^2}{r_{12}} \psi_v(r_1) \psi_w(r_2)\, d^3r_1\, d^3r_2$.

According to equation (9), $\psi = \psi^{(0)} + \delta\psi$ and $\varepsilon = \varepsilon^{(0)} + \delta\varepsilon$, where $\delta\psi, \delta\varepsilon$ are the corrections connected with the HFI. Let us now expand equation (20) up to the first order:

$$\delta\varepsilon_a^{(2)} = \sum_{nvw} \frac{Q^2_{uvnw}}{\Delta E} + 2\sum_{nvw} \frac{Q_{uvnw}}{\Delta E} \left(Q_{\tilde{u}vnw} + Q_{u\tilde{v}nw} + Q_{uv\tilde{n}w} + Q_{uvn\tilde{w}} \right) - \sum_{nvw} \frac{Q^2_{uvnw}}{\Delta E^2} \left(\delta\varepsilon_u + \delta\varepsilon_n - \delta\varepsilon_v - \delta\varepsilon_w \right) \qquad (21)$$

Here $\Delta E = \varepsilon_u^{(0)} + \varepsilon_n^{(0)} - \varepsilon_v^{(0)} - \varepsilon_w^{(0)}$, $Q_{uvnw} = Q(\psi_u^{(0)} \psi_v^{(0)} \psi_n^{(0)} \psi_w^{(0)})$ is the Coulomb integral. The sign 'tilde' in the Coulomb integral

indicates that the RHFH correction is substituted instead of the corresponding function. For example,

$$Q_{u\tilde{v}nw} = Q(\psi_u^{(0)} \delta\psi_v \psi_n^{(0)} \psi_w^{(0)})$$

The first term in formula (21) is the same for all the components of the HF multiplet and, hence, can be omitted. This is a part of the correlation correction to the energy level calculated in Refs /6,7/. The remaining terms contribute to the HF constant. The correlation corrections corresponding to graphs 1b, 1c and 1d are expanded in a similar way. Figures 2a, 2b, 2c and 2d demonstrate graphically the different terms which contribute to the correlation correction. The cross on the line means that the corresponding $\delta\psi$ induced by the HFI should be taken instead of the wave function and the energy shift of the this orbital should be taken into account (see equation (21)). Figure 2a corresponds to the expansion of graph 1a, 2b corresponds to 1b, 2c corresponds to 1c, and 2d corresponds to 1d. As we have already pointed out in the Introduction, the relative simplicity of the calculation of correlations is the main reason for which the HFI is included in the Hartree-Fock equations rather than is taken into account using the many-body perturbation theory together with the residual Coulomb interaction. Although a variety of graphs appears in the expansion of the correlation correction to energy, their number is still less than in the standard many-body perturbation theory and all they are calculated in a completely uniform way. With formulae (13) taken into account, the summation over the projections of the moment of the states n, m, v and w in the corrections in figures 2a, 2b, 2c and 2d is made analytically. The corresponding formulae are given in the Appendix. All the intermediate orbitals with $l \leq 4$ have been taken into account in the numerical calculation of the correlation correction. As far as the RHFH corrections to the functions $\delta\psi$ are concerned, we have already mentioned that it is enough to take into account the l-diagonal corrections. Moreover, in calculating the correlations one can confine oneself to those which are diagonal with respect to j . Even for the $6p_{3/2}$ state of Cs the contribution of j-nondiagonal $\delta\psi$ to the correlation correction, constitute only 0.5% of the experimental value of the HFS. For the $s_{1/2}$ and $p_{1/2}$ states this contribution is much less.

Summation over the intermediate states of the discrete spectrum has been carried out up to $n = 8$ for the s and p states, up to $n = 7$ for the d states and up to $n = 5$ for the f states (n is the principal quantum number). The contributions from the higher states of the discrete spectrum have been evaluated according to the quasiclassical asymptotic formula, i.e. under the assumption that their energy dependence is $|E_n|^{3/2}$. The contribution from g- functions of the discrete spectrum has been omitted. Integration over the states of continuous spectrum has been performed by the Simpson method within the region $0.1 Ry \leq E \leq 25$ Ry. The contribution of the lower energies has been taken into account by means of the quasiclassical asymptotic formula. The contribution of the higher energies is negligibly small.

4. Results and discussion

Tables 1 and 2 list the results of the calculation of the HFI constants for the ^{133}Cs and ^{211}Fr isotopes by means of the RHFH method with the correlations taken into account. The spin of the nucleus ^{133}Cs is $I = 7/2$, the magnetic moment is $\mu = 2.578\,\mu_N$ (Ref. /16/); the spin of the nucleus ^{211}Fr is $I = 9/2$ and $\mu = 3.996\ (77)\,\mu_N$ (Ref. /10/) (the calculated HFS for ^{211}Fr corresponds to the average value: $\mu = 3.996\,\mu_N$). For comparison, the experimental values of the HF constants are presented in the Tables. It is seen that the HF structure of the s and $p_{1/2}$ states of Cs is reproduced with an accuracy not worse than 3%. The same error should be expected for the s and $p_{1/2}$ states of Fr. This error is likely to be connected with the higher orders of perturbation theory in the residual Coulomb interaction. Since the ratios of the calculated correlation corrections to the RHFH values for Cs and Fr are close (0.38 in Cs and 0.32 in Fr), it is naturally to accept that the relative contributions of the higher orders are the same as well. With this supposition, there is no difficulty to see that the value of the nuclear magnetic moment of ^{211}Fr, $\mu = 3.996\ (77)\,\mu_N$ ($g_I = 0.888\ (17)$), measured in

Ref. /10/ is in agreement with the HFS constants (Ref. /11/) with an accuracy not worse than the experimental errors (~ 2%).

For the 5d level in Cs, where the relative magnitude of the correlation correction is high, the accuracy is worse compared with that for the s and p states. The situation is the same for the fine structure of the 5d state of Cs (Ref./6/). Note that the inversion of the HF structure of the $5d_{5/2}$ state of Cs is reproduced already in the RHFH approximation. According to the calculation, the $6d_{5/2}$ state of Fr has the inverse HF structure, as well:

$$A_{RHFH}(6d_{5/2}) = -2.03 \cdot 10^{-3}\,cm^{-1}$$

The largest contribution to the correlation correction to the HF constant comes from the terms wich correspond to graph 2a (I). Taking into account only this graph and graph 2b (I) enables to achieve good coincidence of the calculated data with the experimental ones (about 3÷4% for s and $p_{1/2}$ states). At the same time, it is clear that these graphs describes, indeed, the renormalization of the Coulomb interaction of the external electron with the core. Therefore, this correction can be taken into account within the frames of the single-particle approach, by a choice of a certain additional potential acting on the external electron. (Really, it is the Brueсner or natural orbitals approach. See, for example, /17/). This fact explains the success of the semiempirical calculations of the HFS constants.

Tables 1 and 2 clearly indicate that the correlations increase the probability density of the external electron on the nucleus by 30-40%. In view of this, taking into account correlations is extremely important for the interactions which are singular on the nucleus, for example, for a parity-violating weak interaction. The same conclusion follows from the fine structure calculations of Cs (Ref. /6/). It is worth noting that the relative contribution of the correlation correction to the HF structure is much higher than to the energy. The mechanism of this enhancement is similar to that occuring for the fine structure (Ref. /6/), namely: the correlations "break" the occupied shells and lead to the effective inclusion of a large hyperfine interaction of the internal electrons.

Let us now proceed to the discussion of the influence of the finite size of the nucleus on the HFS. The matrix elements of a hyperfine Hamiltonian between the Hartree-Fock wavefunctions for Cs and Fr are given in Tables 3 and 4. The first lines corresponds to the zeroth size of the nucleus, the next to the finite one. Note that for the second lines the charge density and the HFI operator are defined by formulae (3) and (4) (i.e. this is the case for that the calculations have been made in the present paper). It is seen that the correction to the finite size of the nucleus constitutes 3% for Cs and 19% for Fr. This is consistent with the standard estimates (Ref. /18/) and with Ref. /12/. Thus, the correction is substantially larger than that indicated in the Ref. /5/, where the HFS of the 7s level in Fr has been calculated at the zeroth nuclear size. It is worth mentioning that if one decreases the result of Ref. /5/ by 19% (that corresponds to taking into account the finite size of the nucleus), the number obtained will be in good agreement with that calculated in the present paper.

Thus, introduction of the effect of the finite nuclear size needs to be done. As far as the charge density is concerned, formula (4), apparently, corresponds quite correctly to the real distribution, whereas formula (3) only corresponds to a certain model: the uniformly magnetized ball.

In order to clarify the question on the sensitivity of the HFS to the magnetic moment distribution, the third and fourth lines of Tables 3 and 4 give the matrix elements calculated with Hamiltonian (3) at different values of the magnetic radius (the charge distribution is fixed, equation (4)). Finally, the fifth line presents the matrix elements at the completely other distribution of magnetic moment: the uniformly magnetized surface of the sphere, i.e.

$$\hat{H}_s = \frac{|e|}{c}\vec{\mu}\vec{F}(\vec{r})$$

$$\vec{F}(\vec{r}) = \begin{cases} 0 & r < r_m \\ \dfrac{\vec{r}\times\vec{\alpha}}{r^3} & r \geqslant r_m \end{cases} \qquad (22)$$

It is known from the nucleus-electron scattering experiments that the mean square radii for the charge and magnetic distributions usually coincide within good accuracy (Ref. /19/). In this connection, the model of an uniformly magnetized ball with $r_m = r_N$ seems to be most reasonable. The case of a magnetized sphere (22) is likely to be scarcely realistic and can serve only for the limiting estimation of a feasible error. Referring to Tables 3 and 4, one can conclude that the error in the HFS calculations, which is due to an unknown distribution of the magnetic moment of the nucleus, does not exceed, for the s -electrons, ±0.3% in Cs and ±1% in Fr. As for the p and d electrons, the error is yet less. This is confirmed by the experimental data. According to paper /11/ value of the ratio $A(^2S_{1/2})/A(^2P_{3/2})$ is constant to better than 0.5% for different Fr isotopes. It is natural to believe that the magnetic moment distributions for different isotopes differ from each other. Since this distribution influences on $A(7S_{1/2})$and $A(7P_{3/2})$ in different ways, this fact directly confirm the above statement.

Using the known HFS constants (Ref. /11/) and the results of the present paper, it is easy to calculate the magnetic moments of the Fr isotopes, which are not directly measured. The corresponding numbers are given in Table 5. The precision of the prediction is approximately 1%.

In conclusion, we would like to thank I.B.Khriplovich for discussions and his interest in the work and P.G.Silvestrov for the help in calculations.

Appendix

Here we consider the derivation of formula for correlation corrections. To do this, we first calculate the Coulomb integral for the functions with given l and j :

$$Q_{1234}=\int \psi_1^*(r_1)\psi_3^*(r_2)\frac{1}{r_{12}}\psi_2(r_1)\psi_4(r_2)\,d^3r_1 d^3r_2 \tag{A.1}$$

Let us use the expansion

$$\frac{1}{r_{12}}=4\pi\sum_{\kappa m}\frac{1}{2\kappa+1}\,Y^*_{\kappa m}(\vec{n}_1)\,Y_{\kappa m}(\vec{n}_2)\,\frac{r_<^{\kappa}}{r_>^{\kappa+1}} \tag{A.2}$$

The relative contribution of the lower components of the WF to the Coulomb integrals does not exceed 10^{-3} and can be omitted. Hence,

$$\psi(r)=f(r)\,|jlm\rangle \tag{A.3}$$

The expansion of the state $|jlm\rangle$ is of the form

$$|jlm\rangle=\sum_{\alpha\sigma}C^{jm}_{l\alpha\frac{1}{2}\sigma}|l\alpha\rangle|\tfrac{1}{2}\sigma\rangle=\sum_{\alpha\sigma}(-1)^{l-\frac{1}{2}+m}\sqrt{2j+1}\begin{pmatrix} l & \frac{1}{2} & j\\ \alpha & \sigma & -m\end{pmatrix}|l\alpha\rangle|\tfrac{1}{2}\sigma\rangle \tag{A.4}$$

Substituting (A4), (A3) and (A2) into (A1) and using the known expression for the integral of the product of three Y -functions, we obtain

$$Q_{1234}=\sum_{\kappa q}(-1)^{j_1+j_2+j_3+j_4+q+m_1+m_3+1}\times$$

$$\times\sqrt{(2j_1+1)(2j_2+1)(2j_3+1)(2j_4+1)(2l_1+1)(2l_2+1)(2l_3+1)(2l_4+1)}\times$$

$$\times\begin{pmatrix} l_1 & \kappa & l_2\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} j_1 & \kappa & j_2\\ -m_1 & q & m_2\end{pmatrix}\begin{Bmatrix} j_1 & \kappa & j_2\\ l_2 & \frac{1}{2} & l_1\end{Bmatrix}\begin{pmatrix} l_3 & \kappa & l_4\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} j_3 & \kappa & j_4\\ -m_3 & -q & m_4\end{pmatrix}\begin{Bmatrix} j_3 & \kappa & j_4\\ l_4 & \frac{1}{2} & l_3\end{Bmatrix}\times \tag{A.5}$$

$$\times\int f_1(r_1)f_3(r_2)\frac{r_<^{\kappa}}{r_>^{\kappa+1}}f_2(r_1)f_4(r_2)\,dr_1 dr_2 =$$

$$=\sum_{\kappa q}(-1)^{q+m_1+m_3}\begin{pmatrix} j_1 & \kappa & j_2\\ -m_1 & q & m_2\end{pmatrix}\begin{pmatrix} j_3 & \kappa & j_4\\ -m_3 & -q & m_4\end{pmatrix}Q_\kappa(1\,2\,3\,4)$$

The notation $Q_\kappa(1\,2\,3\,4)$ for the matrix element of the Coulomb interaction is here introduced:

$$Q_\kappa(1\,2\,3\,4)=(-1)^{j_1+j_2+j_3+j_4+1}\sqrt{(2j_1+1)(2j_2+1)(2j_3+1)(2j_4+1)}\cdot\xi(\kappa+l_1+l_2)\times$$

$$\times\xi(\kappa+l_3+l_4)\cdot\begin{pmatrix} j_1 & j_2 & \kappa\\ \frac{1}{2} & -\frac{1}{2} & 0\end{pmatrix}\begin{pmatrix} j_3 & j_4 & \kappa\\ \frac{1}{2} & -\frac{1}{2} & 0\end{pmatrix}\cdot\int f_1(r_1)f_3(r_2)\frac{r_<^{\kappa}}{r_>^{\kappa+1}}f_2(r_1)f_4(r_2)\,dr_1 dr_2 \tag{A.6}$$

and the relation

$$\begin{pmatrix} j_1 & j_2 & \kappa\\ \frac{1}{2} & -\frac{1}{2} & 0\end{pmatrix}\cdot\xi(\kappa+l_1+l_2)=-\sqrt{(2l_1+1)(2l_2+1)}\begin{pmatrix} l_1 & l_2 & \kappa\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} j_1 & j_2 & \kappa\\ l_2 & l_1 & \frac{1}{2}\end{Bmatrix}$$

$$\xi(x)=\begin{cases} 1 & \text{for even } x\\ 0 & \text{for odd } x\end{cases}$$

is taken into account (Ref. /21/).

As an illustration, let us now consider the derivation of formulae for the graph in Fig. 2a(I) (the second term in the right-hand side of the expression (21)).

$$\delta\varepsilon_u^{(2)}=2\sum_{nvw}\frac{Q_{uvnw}\,Q_{\tilde{u}vnw}}{\Delta E}$$

We bear in mind the HF correction to the WF is proportional to the 3j-symbol (see equation (13)) and use the expression (A.5). Then,

$$\delta\varepsilon^{(2)}_{u m_u}=2\sum_{nvw\tilde{u}}\ \sum_{\substack{\kappa m_n m_v\\ m_w m_{\tilde{u}} q}}(-1)^{j_{\tilde{u}}-m_{\tilde{u}}+m_u+m_n+m_w+m_v}\begin{pmatrix} j_{\tilde{u}} & 1 & j_u\\ -m_{\tilde{u}} & 0 & m_u\end{pmatrix}\times$$

$$\times\begin{pmatrix} j_{\tilde u} & \kappa & j_v \\ -m_{\tilde u} & q & m_v \end{pmatrix}\begin{pmatrix} j_n & \kappa & j_w \\ -m_n & -q & m_w \end{pmatrix}\begin{pmatrix} j_v & \kappa & j_u \\ -m_v & -q & m_u \end{pmatrix}\begin{pmatrix} j_w & \kappa & j_n \\ -m_w & q & m_n \end{pmatrix}\frac{Q_\kappa(uvnw)\,Q_\kappa(\tilde u vnw)}{\Delta E_{uvnw}}=$$

$$=2(-1)^{j_u-m_u}\begin{pmatrix} j_u & 1 & j_u \\ -m_u & 0 & m_u \end{pmatrix}\delta_{j_u j_{\tilde u}}\sum_{vwn\kappa}\frac{1}{(2j_u+1)(2\kappa+1)}\,\frac{Q_\kappa(uvnw)\,Q_\kappa(\tilde u vnw)}{\Delta E_{uvnw}} \qquad (A.7)$$

The sign 'tilde' denotes the correction to the corresponding function.

In order to make the summation over the projections m_v, m_w, m_n and q, we make use of the standard formula for the sum of the products of the 3j symbols (Ref. /21/). It is clear that the value of the projection m_u is fixed. The shift in energy, given by the expression (A.7), is recalculated in the HFS constant by means of formulae (13) and (18).

The general method of deriving the formulae is evident from the above example. It is necessary, first of all, to separate the dependence on the values of the angular moment projections. To do this, we note that each Coulomb vertex is proportional to the 3j-symbol $(-1)^{j_2+m_1}\begin{pmatrix} j_1 & \kappa & j_2 \\ -m_1 & q & m_2 \end{pmatrix}$ and each hyperfine HF vertex is proportional to the 3j-symbol as well $(-1)^{j_1-m_1}\begin{pmatrix} j_1 & 1 & j_2 \\ -m_1 & 0 & m_2 \end{pmatrix}$ Summation over the projections is made by means of standard formulae (Ref. /21/). The result is then multiplied by the corresponding matrix elements of the Coulomb interaction (A.6). It is worth mentioning that the result does not contain the matrix elements of the HF interaction because they are already taken into account in calculating the correction to the WF. At the same time, the dependence of the correction on the projection $j_z=m$ is only determined by the fact that the HFI operator is a vector.

For the third, fourth and fifth terms in the expression (21), we obtain, in a similar way (see Figures 2a (II), 2a (III) and 2a (IV) respectively),

$$\frac{Q_{u\tilde v nw}Q_{uvnw}}{\Delta E_{uvnw}}=\sum_{\kappa,j_{\tilde v}}\frac{(-1)^{j_{\tilde v}+j_u+\kappa+1}}{2\kappa+1}\begin{Bmatrix} j_u & 1 & j_u \\ j_v & \kappa & j_{\tilde v} \end{Bmatrix}\frac{Q_\kappa(u\tilde v nw)\,Q_\kappa(uvnw)}{\Delta E_{uvnw}} \qquad (A.8)$$

$$\frac{Q_{uv\tilde n w}\cdot Q_{uvnw}}{\Delta E_{uvnw}}=\sum_{\kappa,j_{\tilde n}}(-1)^{j_u+j_n+j_v+j_w+1}\begin{Bmatrix} 1 & \kappa & \kappa \\ j_w & j_n & j_{\tilde n} \end{Bmatrix}\begin{Bmatrix} 1 & j_u & j_u \\ j_v & \kappa & \kappa \end{Bmatrix}\cdot\frac{Q_\kappa(uv\tilde n w)\cdot Q_\kappa(uvnw)}{\Delta E_{uvnw}} \qquad (A.9)$$

$$\frac{Q_{uvn\tilde w}\cdot Q_{uvnw}}{\Delta E_{uvnw}}=\sum_{\kappa,j_{\tilde w}}(-1)^{j_u+j_v+j_n+j_w}\begin{Bmatrix} 1 & \kappa & \kappa \\ j_n & j_{\tilde w} & j_w \end{Bmatrix}\begin{Bmatrix} 1 & j_u & j_u \\ j_v & \kappa & \kappa \end{Bmatrix}\frac{Q_\kappa(uvn\tilde w)\cdot Q_\kappa(uvnw)}{\Delta E_{uvnw}} \qquad (A.10)$$

In these formulae the factor $(-1)^{j_u-m_u}\begin{pmatrix} j_u & 1 & j_u \\ -m_u & 0 & m_u \end{pmatrix}$ is omitted.

As for the terms obtained from the expansion of the energy denominator (see Eq. (21)), since $\delta\psi$ and $\delta\varepsilon$ are proportional to the same 3j-symbol (see Eq. (13)) the angular parts of the expressions, containing $\delta\psi$ and $\delta\varepsilon$, are the same. For the graph in Figure 1b we obtain in a similar way (see also Figure 2b)

$$\frac{Q_{\tilde u vnw}Q_{uwnv}}{\Delta E_{uvnw}}=\sum_{\kappa_1\kappa_2}\frac{(-1)^{\kappa_1+\kappa_2+1}}{(2j_u+1)}\cdot\delta_{j_u j_{\tilde u}}\begin{Bmatrix} j_v & \kappa_1 & j_u \\ j_w & \kappa_2 & j_n \end{Bmatrix}\frac{Q_{\kappa_1}(\tilde u vnw)\,Q_{\kappa_2}(uwnv)}{\Delta E_{uvnw}} \qquad (A.11)$$

$$\frac{Q_{u\tilde v nw}Q_{uwnv}}{\Delta E_{uvnw}}=\sum_{\kappa_1\kappa_2 j_{\tilde v}}(-1)^{\kappa_2+j_u+j_{\tilde v}}\begin{Bmatrix} 1 & j_u & j_u \\ \kappa_1 & j_v & j_{\tilde v} \end{Bmatrix}\begin{Bmatrix} \kappa_1 & j_u & j_v \\ \kappa_2 & j_n & j_w \end{Bmatrix}\frac{Q_{\kappa_1}(u\tilde v nw)\,Q_{\kappa_2}(uwnv)}{\Delta E_{uvnw}} \qquad (A.12)$$

$$\frac{Q_{uv\tilde n w}Q_{uwnv}}{\Delta E_{uvnw}}=\sum_{\kappa_1\kappa_2 j_{\tilde n}}(-1)^{j_u+j_n+j_v+j_w+\kappa_1+\kappa_2}\begin{Bmatrix} 1 & j_u & j_u \\ j_n & \kappa_2 & j_v \\ j_{\tilde n} & j_w & \kappa_1 \end{Bmatrix}\frac{Q_{\kappa_1}(uv\tilde n w)\,Q_{\kappa_2}(uwnv)}{\Delta E_{uvnw}} \qquad (A.13)$$

$$\frac{Q_{uvn\tilde w}Q_{uwnv}}{\Delta E_{uvnw}}=\sum_{\kappa_1\kappa_2 j_{\tilde w}}(-1)^{\kappa_1+j_u+j_{\tilde w}}\begin{Bmatrix} 1 & j_u & j_u \\ \kappa_2 & j_w & j_{\tilde w} \end{Bmatrix}\begin{Bmatrix} \kappa_2 & j_u & j_{\tilde w} \\ \kappa_1 & j_n & j_v \end{Bmatrix}\frac{Q_{\kappa_1}(uvn\tilde w)\,Q_{\kappa_2}(uwnv)}{\Delta E_{uvnw}} \qquad (A.14)$$

Formulae for the graphs in Fig. 2C (I,II,III,IV) can be obtained by means of the substitution $\nu \to m$, $n \to \nu$, $w \to n$ from (A7), (A9), (A10), A(8) correspondingly. And for the graphs in Fig. 2d (I,II,III,IV) - from A(11), A(13), A(14), A(12) by means of the same substitution.

References

I. E.S.Chang, R.T.Pu and T.P.Das. Phys. Rev., 174, 1 (1968).

2. T.Lee, N.C.Dutta and T.P.Das. Phys. Rev., A1, 995 (1970).

3. M.Vajed-Samii, S.N.Ray, J.Andriessen and T.P.Das. Phys. Rev., A20, 1787 (1979).

4. B.P.Das, S.N.Ray, T.Lee, J.Andriessen and T.P.Das. Bull. Am. Phys. Soc., 24, 476 (1979).

5. M.Vajed-Samii, J.Andriessen, B.P.Das, S.N.Ray, T.Lee and T.P.Das. Phys. Rev. Lett., 48, 1330 (1982).

6. V.A.Dzuba, V.V.Flambaum and O.P.Sushkov. J. Phys., B16, 715 (1983).

7. V.A.Dzuba, V.V.Flambaum and O.P.Sushkov. Phys. Lett., 95A, 230 (1983).

8. V.A.Dzuba, V.V.Flambaum and O.P.Sushkov. Abstracts of the conference on physics of vacuum ultra-violet radiation (VUF-82), p. 41, 42. Moscow, 1982.

9. V.A.Dzuba, V.V.Flambaum and O.P.Sushkov. VIII ICAP, Abstracts, p. A29, B27, Göteborg, Sweden, 1982.

10. C.Ekström, L.Robertson. VIII ICAP, Abstracts, p. B44, Göteborg, Sweden, 1982.

11. S.Liberman et al. Phys. Rev., A22, 2732 (1980).

12. A.-M.Martensson and J.-L.Heully. VIII ICAP, Abstracts, p. B25, Göteborg, Sweden, 1982.

13. Y.N.Kim, Mesic Atoms and Nuclear Structure, North-Holland Publishing Company, Amsterdam, 1971 (Russ. transl. Moscow, 1975).

14. H.P.Kelly. Phys. Rev., 131, 684 (1963); 136B, 896 (1964); 144, 39 (1966).

15. V.A.Dzuba, V.V.Flambaum and O.P.Sushkov. Preprint INP 82-89, Novosibirsk, 1982.

16. Tables of physical values. Ed. I.K.Kikoin. Moscow, Atomisdat, 1976.

17. I.Lindgren, A.-M.Martensson. Z. Physik A279, 113-125 (1976).

18. I.I.Sobelman. Introduction to the theory of Atomic Spectra, Moscow, Nauka, 1977.

19. H.Collard et al. Phys. Rev. Lett., 11, 132 (1963).
H.Theissen, H.Fink and H.A.Bentz. Z. Phys. 231, 475 (1970).

20. A. de Shalit and I.Talmi. Nuclear Shell Theory, New York, Academic Press, 1963.

21. D.A.Varshalovich, A.N.Moskalev, V.K.Khersonsky. Quantum theory of angular momentum, Nauka, Leningrad, 1975.

22. E.Arimondo, M.Inguscio and P.Violino. Rev. Mod. Phys. 49(1), 31-75, 1977.

23. G.H.Fuller. J.Phys. Chem. Ref. Data 5, 947 (1976).

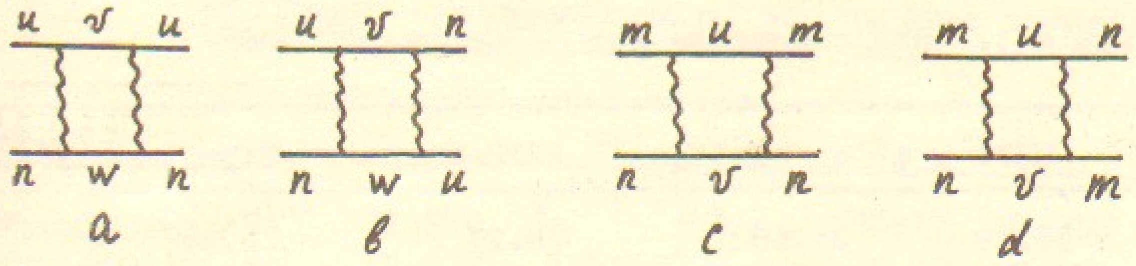

Fig. 1.

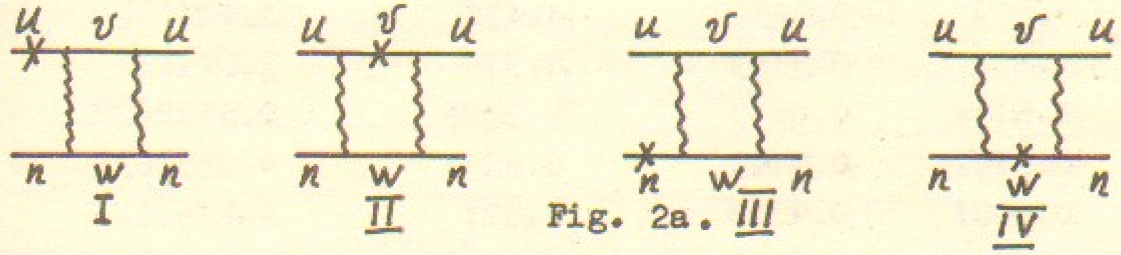

Fig. 2a.

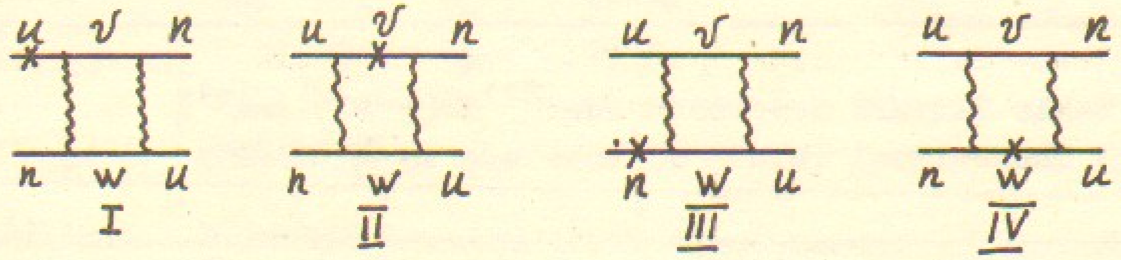

Fig. 2b.

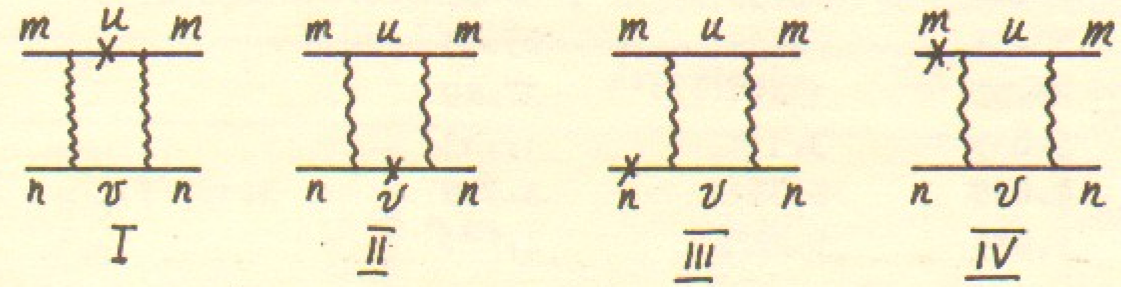

Fig. 2c.

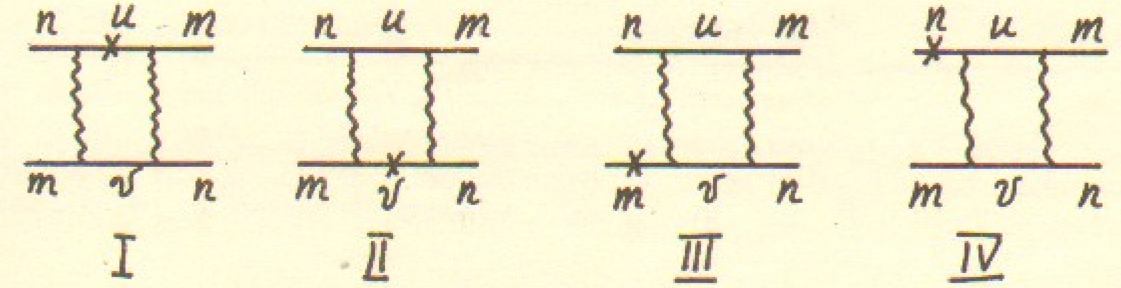

Fig. 2d.

Table 1. HFS constants for ^{133}Cs (x 10^{+3} cm^{-1})

Level	RHFS	Correlations	RHFH+Corr.	Experiment /22/
6s	56.79	21.48	78.27	76.66
7s	15.59	3.139	18.73	18.22(10)
8s	6.507	0.950	7.457	7.30(5)
$6p_{1/2}$	6.672	2.864	9.537	9.737(4)
$7p_{1/2}$	2.371	0.7834	3.154	3.147(1)
$8p_{1/2}$	1.109	0.3256	1.434	1.433(3)
$6p_{3/2}$	1.427	0.3113	1.738	1.679(2)
$7p_{3/2}$	0.5116	0.0613	0.5729	0.5539(2)
$8p_{3/2}$	0.2402	0.0129	0.2531	0.2528(3)
$5d_{3/2}$	0.5507	0.9703	1.521	1.621(7)
$5d_{5/2}$	-0.8119	-0.2293	-1.041	-0.74(2), -0.707(3)

Table 2. HFS constants for ^{211}Fr(x 10^{+3} cm^{-1})
Theoretical values corresponds to g_I = 0.888

Level	RHFH	Correlations	RHFS+Corr.	Experiment /11/
7s	228.4	72.39	300.8	289.94(35)
8s	58.54	7.19	65.73	
$7p_{1/2}$	25.59	11.91	37.49	
$8p_{1/2}$	9.013	3.114	12.13	
$7p_{3/2}$	2.818	0.5911	3.409	3.157(7)
$8p_{3/2}$	I.034	0.1412	I.175	

Table 3. Matrix elements of the HFIx10^3cm^{-1} for the 6s, $6p_{1/2}$, $6p_{3/2}$ functions of Cs in the RHF approximation at different distributions of the nuclear magnetic moment (for explanations see the text)

		6s	$6p_{1/2}$	$6p_{3/2}$
	Point nucleus ($r_m = r_N = 0$)	48.77	5.39I	0.7974
r_N = 5.61 fm	Ball with r_m = 5.61 fm	47.31	5.373	0.7974
	Ball with r_m = 6.73 fm	47.20	5.372	0.7974
	Ball with r_m = 4.68 fm	47.39	5.374	0.7974
	Sphere with r_m = 5.61 fm	47.11	5.371	0.7974

Table 4. Metrix elements of the HFIx10^3cm^{-1} for the 7s, $7p_{1/2}$, $7p_{3/2}$ functions of Fr in the RHF approximation (g_I = 0.888)

		7s	$7p_{1/2}$	$7p_{3/2}$
	Point nucleus ($r_m = r_N = 0$)	231.7	22.04	1.639
r_N = 6.57 fm	Ball with r_m = 6.57 fm	194.2	20.81	1.639
	Ball with r_m = 7.88 fm	192.6	20.75	1.639
	Ball with r_m = 5.47 fm	195.5	20.88	1.639
	Sphere with r_m = 6.57 fm	191.9	20.72	1.639

Table 5. Magnetic moments of Fr isotopes (in unites μ_N) The errors pointed in lest column are due to the uncertanty of the magnetic moment distribution in nuclear and to the error of extrapolation from Cs to Fr the contribution of higher order correlations

A	I	Experiment	Values obtained from HFS
208	7	-	4.67(7)
209	$\frac{9}{2}$	-	3.88(6)
210	6	-	4.33(7)
211	$\frac{9}{2}$	3.996(77)^a	3.93(6)
212	5	-	4.54(7)
213	$\frac{9}{2}$	3.996(14)^b	3.95(6)

a Ref. /10/

b Ref. /23/. Values obtained by extrapolation with use of results of g-factor measurements for $(h_{9/2})^k$ proton states of nuclei with neutron number 126.

В.А.Дзюба, В.В.Фламбаум, О.П.Сушков

РЕЛЯТИВИСТСКИЙ МНОГОЧАСТИЧНЫЙ РАСЧЕТ СВЕРХТОНКОЙ СТРУКТУРЫ ЦЕЗИЯ И ФРАНЦИЯ

Препринт
№ 83-82

Работа поступила - 4 марта I983 г.

Ответственный за выпуск - С.Г.Попов
Подписано к печати I2.05-I983 г. МН I7536
Формат бумаги 60х90 I/I6 Усл.I,3 печ.л., I,I учетно-изд.л.
Тираж 290 экз. Бесплатно. Заказ № 82.

Ротапринт ИЯФ СО АН СССР, г.Новосибирск, 90