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

Institute of Nuclear Physics,
630090, Novosibirsk, U.S.S.R.

ABSTRACT

It is shown that the use of relativistic Hartree-Fock equations in an external field, Brueckner orbitals and a many-body perturbation theory provides, as a rule, a 1÷3% accuracy of atomic calculations. To control the accuracy, the energy levels and the fine and hyperfine structure intervals as well as the E1-amplitudes for s-p transitions in Cs have been calculated. The parity-violating E1-amplitude for the 6s-7s transition has been found: $\langle 7s|D_z|6s\rangle = (0.88\pm0.03)\cdot10^{-11}\times(-Q_W/N)(-ie a_B)$ where Q_W is the weak charge of the nucleus and N is the number of neutrons. The experimental data in Ref. /1/ make it possible to find a weak nuclear charge of ^{133}Cs, $Q_W = -73.4\pm8.1\pm6$, and the Weinberg angle $\sin^2\theta_W = 0.237\pm0.036\pm0.03$.

Recently, first results of the measurements of parity violating effects in the 6s → 7s transition in Cs have been published [1]. The more accurate measurements coupled with an increase in the accuracy of calculation have the potential of checking the unified theories of weak and electromagnetic interactions. The parity-violating E1-amplitude for the 6s-7s transition in Cs has previously been calculated by the effective potential method and by the other semi-empirical methods[2-6]. The accuracy of these calculations is not, however, sufficiently high. In the most recent and, apparently, most accurate calculation[6], the accuracy constitutes about 10%, according to the authors' estimation.

The other possible way is a calculation by the relativistic Hartree-Fock (RHF) method. However, without taking into account the correlation correction, up to the second order of perturbation theory in the residual Coulomb interaction, such calculations are not accurate enough (their accuracy ranges between 15 and 30%). At the same time, taking into account these corrections enables the calculational accuracy to be drastically improved (see, e.g., the energy, fine and hyperfine structure calculations in Refs. /7/ and /8/). In the present paper we have employed somewhat different method which reduces, in fact, to the summation of the series of dominating diagrams in all the orders of perturbation theory.

It was noted in Refs. /9/, /8/ and /7/ that the diagrams, which are equivalent to the introduction of an additional non-local potential acting on an external electron, give the main contribution to a correlation correction. These diagrams can be taken into account already in the single-particle orbitals. This approach is close to the method of Brueckner orbitals, or natural orbitals (see, e.g., Ref. /9/). The other many-body effects are taken into consideration by means of the Hartree-Fock method for the external field (the random phase approximation - RPA) and a many-body perturbation theory. For the parity-violating E1-amplitude of the 6s-7s transition in Cs, this calculation provides an accuracy of 1÷3%. We have also calculated, by the same method, a number of energy levels, fine and hyperfine structure intervals, and oscillator strengths.

Hartree-Fock calculation of E1($6s \to 7s$) - amplitude have been carried out in Ref. [29]. The result is in accordance with corresponding contribution calculated in present work (Table 4, HF, 1-form, columnа).

As it has become known to us from Ref. /6/, the many-body calculation of the E1-amplitude for the 6s-7s transition has been made in Ref. /10/. However, the result of this calculation, cited in Ref. /6/, is 20% larger than our result.

2. Choice of a single-particle Hamiltonian

In solving the problems of atomic physics, we usually divide the exact Hamiltonian of an atom by two parts: the first part is sum of the single-particle Hamiltonians allowing an exact numerical solution, and the second one represents the remaining ('residual') interaction which can be taken into account in terms of perturbation theory.

$$H = \sum_{i=1}^{N} H_0(\vec{r}_i) + U \qquad (1)$$

where

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

Here $\vec{\alpha}$ and β are Dirac matrices, Z is the nuclear charge and N is the number of electrons ($\hbar = c = 1$)

$$U = \sum_{i<j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} - \sum_{i=1}^{N} V(\vec{r}_i) \qquad (3)$$

The standard method of calculations (the RHF method) consists in that the potential V is chosen in such a way that there are no first-order corrections to the wave function with excitation of one electron. In other words the equation represented graphically in Figure 1 must be solved in a self-consistent way. If we consider the atom with one electron outside the closed shells (the core), it is natural to use the frozen-core approximation (the V^{N-1} approximation, see Refs. /11/ and /12/). In this case, only the core orbitals are determined according to the self-consistent equation represented in Figure 1. The potential has the form

$$V = V_d - V_{exch} \qquad (4)$$

Here V_d and V_{exch} are usual direct and exchange interactions occuring in Hartree-Fock equations:

$$V_d = e^2 \sum_{i=1}^{N-1} \int \frac{\psi_i^+(\vec{r}\,')\,\psi_i(\vec{r}\,')}{|\vec{r} - \vec{r}\,'|}\, d^3r'$$
$$V_{exch}\,\psi = e^2 \sum_{i=1}^{N-1} \int \frac{\psi_i^+(\vec{r}\,')\,\psi(\vec{r}\,')}{|\vec{r} - \vec{r}\,'|}\, d^3r'\, \psi_i(\vec{r}) \qquad (5)$$

The sum is taken over the electrons from the closed shells. The states of the external electron are calculated in the field of the frozen core. They turn out to be orthogonal to the closed orbitals, since all the states correspond to the same single-particle Hamiltonian (see, e.g., Refs. /7,11,12/). Thus, a complete set of single-particle states naturally arises. In this basis, there is no difficulty in calculating, for instance, the correlation correction to the ionization energy of an external electron, which is determined by the diagrams in Figure 2 (Ref. /7/).

The correlation correction to energy can be taken into consideration in the other way. Let us add to V in formula (4) the nonlocal correlation potential V_{corr} chosen so that its average value for the state of the external electron, coincides with the correlation correction to energy:

$$\delta E_\alpha = \langle \alpha | V_{corr} | \alpha \rangle$$
$$V = V_d - V_{exch} + V_{corr} \qquad (6)$$
$$V_{corr}\,\psi = \int \sum(\vec{r}_1, \vec{r}_2)\,\psi(\vec{r}_2)\, d^3r_2$$

It is easy to write the correlation potential explicitly. For example, a part of the mass operator Σ_{corr}, corresponding to Figure 2a, is of the form

$$\sum\nolimits_{corr}^{(a)}(\vec{r}_1, \vec{r}_2) = e^2 \sum_{n\beta\gamma} \iint d^3r_3\, d^3r_4 \frac{\psi_n^+(\vec{r}_3)\frac{1}{r_{13}}\psi_\gamma(\vec{r}_1)\psi_\gamma^+(\vec{r}_4)\psi_\beta(\vec{r}_3)\psi_\beta^+(\vec{r}_4)\frac{1}{r_{24}}\psi_n(\vec{r}_2)}{E + E_n - E_\gamma - E_\beta} \qquad (7)$$

Here we denote the core orbitals by the Latin letters n and m and the states outside the core by the Greek letters α, β and γ. The expressions for the contributions to V_{corr}, which correspond to the graphs b, c and d (Fig. 2) can be

written in a similar manner. In view of the fact that we take into account the interaction of the external electron with the closed shells, it is clear that V_{corr} conserves the orbital ℓ and total j angular momenta of the electron. Mathematically, this is a consequence of the fact that in formula (7) the sums are taken over all the projections of the angular momentum of the states n , β and γ . Thus, we have, really, a number of operators, each acting on the wave functions of electrons with definite ℓ and j . The angular coefficients in $V_{corr}^{(a)(b)(c)(d)}$ are calculated analytically and coincide with the coefficients for the corresponding graphs in Ref. /7/. Note that the parameter E in formula (7) is not yet fixed. It is obvious that one should put $E = E_\alpha$ in order that the average value $\langle\alpha|V_{corr}|\alpha\rangle$ coincide with the correction to the energy of the state α calculated according to the graphs in Figure 2. To get an orthonormalized set of orbitals, we are need in a common potential for all the states with fixed ℓ and j . In view of this, the parameter E for the given ℓ and j should be fixed. For instance, in Cs we usually put $E = E_{6s}$ for $\ell = 0$ and $j = \frac{1}{2}$, $E = E_{6p_{1/2}}$ for $\ell = 1$ and $j = \frac{1}{2}$, etc. Thus, E is chosen equal to the energy of the lowest external electron state with given ℓ and j . In this case, $\langle\alpha|V_{corr}|\alpha\rangle$ is exactly the same as the correlation correction only for these lowest states. For the other excited states of the atom, no exact coincidence occurs. However, the energy denominator in formula (7) always include the energy, at least, of one electron from the closed shells, which is considerably higher than the energy of the external electron. For this reason, the difference of $\langle\alpha|V_{corr}|\alpha\rangle$ from the correlation correction, calculated in terms of perturbation theory, does not exceed 5% for the states of the discrete spectrum and for the states of the continuous spectrum with not very high energy. The correlation corrections to the energies and wave functions of the internal electrons are taken into account by $V_{corr}(E_\alpha)$ substantially worse as compared with the external electrons. But these corrections have influence on the characteristics of the external electrons, we are finally interested in, only in the highest orders in the residual Coulomb interaction.

The method of calculating V_{corr} is similar to that used

for the calculation of correlation corrections in Refs. /7/ and /8/. The sums in formulae of the type (7) have been calculated explicitly, with the excited states with $\ell \leq 4$ taken into account. To calculate the sum over the discrete spectrum, for each ℓ and j three lower excited states have been taken into consideration. The contribution from the higher states has been taken into account by means of the quasiclassical asymptotic formula. Integration over the states of the continuous spectrum has been performed by the Sympson method within the region 0.1 Ry $\leq$ E $\leq$ 25 Ry. The contribution of the states with E < 0.1 Ry has been also taken into account by means of the asymptotic formula. The contribution of the energies E > 25 Ry is negligibly small. The 4d, 5p and 5s shells have been taken into account in the sum over the occupied states. The contribution from the deeper shells is negligibly small. According to control calculations made in Ref. /7/, the purely computational error of such a correlation-correction calculation constitutes 1÷2%. Since the correlation correction itself is not large, this accuracy well suits us. Note that at large distances, the potential V_{corr} is transformed into a local Van der Waals (polarization) potential:

$$V_{corr} \approx -\frac{\alpha e^2}{2r^4}$$

where α is the polarizability of the core. Having been obtained while calculating V_{corr} , the quantity $\alpha \approx 18\, a_B^3$ coincides with the polarizability of the Cs^+ ion calculated in Ref. /6/.

To eliminate the first- and second-order corrections in the residual interaction U to the energy of the external electron, (see equation (3)), it is necessary that all the wave functions, which enter into equations (5) and (7), be themselves the eigenfunctions of the Hamiltonian H_0 (see equation (2)). Therefore, equations (2), (5), (6) and (7), should be solved in a self-consistent way. This can be performed by means of iterations, starting with Hartree-Fock orbitals. However, the V_{corr} calculation takes a long computer time. Therefore practically we have calculated V_{corr} only once using the Hartree-Fock orbitals, and assuming it unchangeable in iterations.

For control, we have made one iteration, taking into account the variation of V_{corr}. The change of all the quantities, we are interested in, has turned out to be negligibly small.

The energies for the states of the external electron, which have been calculated by the way described above, are given in the last but one column of Table 1. The comparison with experiment /13/ demonstrates that the accuracy of calculation of the energies and fine-structure intervals for the s and p levels is about 1%. For comparison, we also present in the Table the energies obtained previously in Ref. /7/ within the framework of the RHF method without the correlation correction and with the correlation correction calculated using the perturbation theory. In the present paper we make allowance for V_{corr} not in the first order of perturbation theory but include it in the single-particle Hamiltonian, i.e. we sum a definite series of correlation diagrams, corresponding to iteration of the diagrams in Figure 2. For this reason, the values given in the third and fourth columns of Table 1 are somewhat different from each other, even for the lower 6s, 6p and 5d states.

It is worth emphasizing that the single-particle states, found in such a way, practically coincide with the Brueckner orbitals (see, e.g., Ref. /9/) and despite some distinction in their definitions, we will refer to the orbitals in the potential (6) as the Brueckner ones. It is known from the calculations of the hyperfine structure of alkaline atoms (see Refs. /9,12,14 and 8/) that the diagrams which reduce to the renormalization of the wave function of the external electron, give the main contribution to the correlation correction for the s and $p_{1/2}$ levels. In view of this, the Brueckner orbitals are adequate for calculation of the hyperfine-structure (see Section 5). In addition, the next Section will show that the amplitudes of the s-p E1-transitions are very well reproduced on the Brueckner orbitals. With this in mind, we think that this technique is also suited for calculation of the effects caused by weak interactions. We note that the employment of the Brueckner orbitals instead of the Hartree-Fock ones is useless if the correlation graphs, which do not reduce to the renormalization of the wave function of the external electron,

give a large contribution to the physical quantities we are going to calculate.

III. Calculation of the amplitudes of allowed E1-transitions

The interaction between an atom and an electromagnetic wave is usually described by means of the dipole-moment operator (length form):

$$\vec{D}^{(l)} = e\sum_{i=1}^{N} \vec{r}_i \qquad (8)$$

This corresponds to the choice of the gauge for the vector-potential of a wave, $\vec{A}(0)=0$. The other, often used form is the velocity form (gauge $\varphi = 0$):

$$\vec{D}^{(v)} = -\frac{ie}{\omega}\sum_{i=1}^{N} \vec{\alpha}_i \qquad (9)$$

where ω is the photon frequency and $\vec{\alpha}$ is the Dirac matrix. The amplitude of transition between the exact physical states is a gauge-invariant quantity. Hence, the comparison of the amplitudes, calculated according to equations (8) and (9), is a good test of the accuracy of calculations. The matter is that the nonlocal exchange and correlation potentials, occuring in the Hamiltonian (2) give rise to the violation of the gauge invariance, which should restore only after taking into account the remaining many-body effects.

The reduced matrix elements of the operators (8) and (9) between the single particle orbitals $|1\rangle$ and $|2\rangle$ are of the form

$$\langle 2\|\vec{D}^{(l)}\|1\rangle = e\,(-1)^{j_1+\ell_{max}+\frac{1}{2}}\sqrt{(2j_1+1)(2j_2+1)\ell_{max}}\begin{Bmatrix} j_2 & 1 & j_1 \\ \ell_1 & \frac{1}{2} & \ell_2 \end{Bmatrix} \times$$

$$\times \int (f_2 f_1 + g_2 g_1)\, r\, dr \qquad (10)$$

$$\ell_{max} = \max(\ell_1, \ell_2)\,, \quad |\ell_2 - \ell_1| = 1$$

$$\langle 2\|\vec{D}^{(\omega)}\|1\rangle = \frac{e}{\omega}\sqrt{6(2j_1+1)(2j_2+1)}\,\chi$$

$$\chi\left[(-1)^{j_1+\ell_1-\frac{1}{2}}\begin{Bmatrix}\frac{1}{2} & j_2 & \ell_2\\ j_1 & \frac{1}{2} & 1\end{Bmatrix}\delta_{\ell_1\tilde{\ell}_2}\int f_2 g_1\,dr - (-1)^{j_2+\ell_1-\frac{1}{2}}\begin{Bmatrix}\frac{1}{2} & j_2 & \ell_1\\ j_1 & \frac{1}{2} & 1\end{Bmatrix}\delta_{\tilde{\ell}_2\ell_1}\int g_2 f_1\,dr\right] \qquad (11)$$

Here f and g are the upper and lower components of the wave function

$$\psi = \frac{1}{r}\begin{pmatrix} f\,\Omega_{jem} \\ ig\,\Omega_{j\tilde{e}m}\end{pmatrix} \qquad (12)$$

Ω_{jem} is the spherical spinor, and $\tilde{\ell}=2j-\ell$. At $r\to 0$ the sign of f is chosen positive.

The first column of Table 2 gives, as an illustration, the radial integrals in the $6s$-$6p_{1/2}$ transition in Cs, which have been calculated using the Hartree-Fock and Brueckner orbitals in the l and v forms. Here and below, in the v-form calculations we use the exact experimental difference in energies between the physical states as the frequency. However, it is worth mentioning that for the Brueckner orbitals, the difference between the experimental and calculated frequency is equal to about 1%. For convenience in the comparison with the previous works, we give, instead of the oscillator strengths, the effective radial integrals proportional to the amplitudes (10) and (11). Here, the common factor is such that in the l-form

$$R = \int_0^\infty (f_2 f_1 + g_2 g_1)\,r\,dr \qquad (13)$$

The radial integrals, presented in the Tables in the columns 'experiment', have been found from the corresponding experimental oscillator strengths (Refs. /15,16/) according to formula (10). We would like to note that we have always used the experimental frequencies. The signs of radial integrals have been determined only from calculation.

The corrections to the single-particle amplitude of the transition (10),(11) occur already in the first order in the residual interaction with taking into account the polarization of the closed shells by an external electric field. Figure 3

illustrates all four first-order diagrams contributing to the E1-amplitude. The corresponding expressions have the form

$$\langle 2\|\vec{D}\|1\rangle_a = \sum_{n\alpha}\frac{(-1)^{j_n-j_2+1}}{3}\,\frac{Q_1(21\alpha n)\langle n\|\vec{D}\|\alpha\rangle}{E_1+E_n-E_2-E_\alpha}$$

$$\langle 2\|\vec{D}\|1\rangle_b = \sum_{n\alpha}\frac{(-1)^{j_\alpha-j_2+1}}{3}\,\frac{Q_1(21n\alpha)\langle\alpha\|\vec{D}\|n\rangle}{E_2+E_n-E_1-E_\alpha}$$

$$\langle 2\|\vec{D}\|1\rangle_c = \sum_{n\alpha k}(-1)^{j_2+j_n+k}\begin{Bmatrix}1 & j_1 & j_2\\ k & j_n & j_\alpha\end{Bmatrix}\frac{Q_k(2n\alpha 1)\langle n\|\vec{D}\|\alpha\rangle}{E_1+E_n-E_2-E_\alpha} \qquad (14)$$

$$\langle 2\|\vec{D}\|1\rangle_d = \sum_{n\alpha k}(-1)^{j_2+j_\alpha+k}\begin{Bmatrix}1 & j_2 & j_1\\ k & j_n & j_\alpha\end{Bmatrix}\frac{Q_k(2\alpha n1)\langle\alpha\|\vec{D}\|n\rangle}{E_2+E_n-E_1-E_\alpha}$$

Here Q_k (1,2,3,4) is the matrix element of the Coulomb interaction:

$$Q_k(1234) = (-1)^{j_1+j_2+j_3+j_4+1}\sqrt{(2j_1+1)(2j_2+1)(2j_3+1)(2j_4+1)}\,\xi(k+\ell_1+\ell_2)\,\chi$$

$$\chi\,\xi(k+\ell_3+\ell_4)\begin{pmatrix} j_1 & j_2 & k\\ \frac{1}{2} & -\frac{1}{2} & 0\end{pmatrix}\begin{pmatrix} j_3 & j_4 & k\\ \frac{1}{2} & -\frac{1}{2} & 0\end{pmatrix}\int f_1(r_1)f_3(r_2)\frac{r_<^k}{r_>^{k+1}}f_2(r_1)f_4(r_2)\,dr_1\,dr_2 \qquad (15)$$

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

The zero-order amplitudes $\langle n\|\vec{D}\|\alpha\rangle$ in the right-hand sides of equations (14) are given by formulae (10), or (11). It is worth emphasizing that here the v-form (matrix element $\langle n\|\vec{D}\|\alpha\rangle$, formula (11)) includes the photon frequency in the $1\to 2$ transition rather than the energy difference E_n-E_α. The contribution of the core polarization (14) to the amplitude of the $6s\to 6p_{1/2}$ transition is given in Table 2. The third column presents the total contribution of the zeroth and first orders. The influence of the core polarization on the E1-amplitude is

ossible to take into account more exactly, by solving the Hart-ee-Fock equations in an external electric field. This is equi-alent to iteration of the graphs in Figure 3 (RPA approxima-tion). We have made such a calculation. The contribution of the igh orders to the core polarization has turned out to be very mall for the amplitudes corresponding to the transitions of ie external electron. Table 2 demonstrates that the using of ie Brueckner orbitals in calculations provides an accuracy of %. This considerably better than the accuracy of the calcula-on made with the help of Hartree-Fock orbitals. Thus, it is ssible to draw conclusion that the transition to Brueckner bitals has one to take into account the correlation correcti-s practically exactly. In addition, it is seen that the dif-rence between the amplitudes calculated in l and v forms is mparable with the deviation from experiment and can serve as e accuracy test in the cases when the experimental data are sent.

Table 3 lists the values of the E1-amplitudes, calculated th the use of Brueckner orbitals in l and v forms with the ce polarization taken into account. It is seen that for the ncipal 6s → 6p, 7s → 7p, and 6p → 7s transitions determi-ig the value of the p-odd E1-amplitude of the 6s → 7s tran-ion (see Ref. /3/), the accuracy is about 1%.

IV. The self-consistent equations with the weak interaction taken into account

In the Weinberg-Salam model, the Hamiltonian of a parity lating weak interaction between the electron and the nucleus, ch is due to the product of the electron axial current by a leon vector one, is of the form

$$h_{pv} = -\frac{G}{2\sqrt{2}}\rho(r)Q_W\gamma_5 \qquad (16)$$

re G is the Fermi constant, $Q_W \approx -[N+Z(4\sin^2\theta_W-1)]$ the weak charge of the nucleus, N and Z are the number of trons and protons in the nucleus, θ_W is the Weinberg angle, .- is the Dirac matrix,

$$\gamma_5 = \begin{pmatrix} 0 & -I \\ -I & 0 \end{pmatrix} \qquad (17)$$

and $\rho(r)$ is the nucleon density normalized per unity. We assume that the distributions of the neutron and proton densities coincide and make use of the standard formula

$$\rho(r) = \frac{C}{e^{\frac{r-r_N}{D}}+1} \qquad (18)$$

where C is the normalization constant, $r_N = 1.10A^{\frac{1}{3}}$ fm = = 5.61 fm and $D = 0.57$ fm (Ref. /17/). The matrix element of the operator (16) depend rather weakly on a particular form of density. For instance, in varying the radius of the nucleus by 10% (this is considerably larger as compared with the experimental error in the determination of r_N) the matrix element change less than by 1%.

The weak interaction is taken into account in a linear approximation. This is convenient to do, including the weak interaction in the self-consistent equations for single-particle orbitals (as this was done, e.g., in Ref. /18/) rather than in terms of many-body perturbation theory:

$$(h_{pv}+\tilde{H}_0)\tilde{\psi} = \varepsilon\tilde{\psi} \qquad (19)$$

where $\tilde{H}_0$ differs from H_0 by the substitution of the functions $\tilde{\psi}$ instead of ψ in formulae (5) and (7). In the linear approximation, $\tilde{\psi} = \psi + \delta\psi$ and $\tilde{H}_0 = H_0 + \delta H$. Since h_{pv} is a pseudoscalar, $\delta\psi$ corresponds to the same angular momentum j as ψ, but has the opposite parity and orbital angular momentum $\tilde{\ell} = 2j - \ell$. The energy correction in the first order in h_{pv} does not arise because the diagonal matrix elements of the parity-changing operator are equal to zero. In order to derive an equation for $\delta\psi$, the terms linear in h_{pv} and $\delta\psi$, should be separated from the expression (19):

$$(H_0-\varepsilon_\alpha)\delta\psi_\alpha = -h_{pv}\psi_\alpha + \sum_{n=1}^{N-1} e^2\left\{\delta\psi_n(\vec{r})\int\frac{\psi_n^+(\vec{r}')\psi_\alpha(\vec{r}')}{|\vec{r}-\vec{r}'|}d^3r' + \right. \qquad (20)$$

$$+\psi_n(\vec{r})\int\frac{\delta\psi_n^+(\vec{r}')\psi_\alpha(\vec{r}')}{|\vec{r}-\vec{r}'|}d^3r'\Big\}-\delta V_{corr}\psi_\alpha$$

Summation is carried out over the orbitals of the core. The expression in right-hand side of equation (20) is a correction to the exchange potential V_{exch} (see equation (5)). No similar correction to the direct potential occurs. It turns out also that the correction δV_{corr} to the correlation potential (7) is small (see below) and we neglect it in what follows.

The system of equations (20) for the corrections $\delta\psi$ is solved by iterations. To begin with, the corrections to the core orbitals are calculated for the case when only the term $h_{pv}\psi$ is taken into account in the right-hand side of equation (20). Making allowance for the correction to V_{exch} in the right-hand side of equation (20) is equivalent to the substitution of the renormalized operator $\tilde{h}_{pv}$ instead of h_{pv}. The operator $\tilde{h}_{pv}$ includes, in addition to h_{pv}, a chain of RPA diagrams (see, e.g., Ref. /19/) in the residual Coulomb interaction (core polarization by a weak interaction). The matrix elements of the operator $\tilde{h}_{pv}$ satisfy the graphic equation depicted in Figure 4, which is equivalent to equation (20). If one makes only one or two iterations when solving equation (20), this will mean that only the terms of the first or second order in the Coulomb interaction are taken into consideration in the chain of diagrams in Figure 4.

It is worth noting that we solve equation (20) for Brueckner orbitals since H_0 contains the correlation potential. In terms of Hartree-Fock orbitals, this corresponds to making allowance for the diagrams presented in Figure 5 and their iterations. At the same time, we do not take into account δV_{corr} in equation (20), i.e. we neglect the diagrams demonstrated in Figure 6. In Ref. /8/ when calculating the hyperfine structure of Cs and Fr all the diagrams of the second order in the residual interaction were taken into account. It has been shown that the diagrams of the type presented in Figure 5, give the main contribution to the correlation correction, whereas the contribution from the diagrams of the type presented in Figure 6, constitute about 1% of the magnitude of the hyperfine constant,

for the s and $p_{1/2}$ levels. Domination of the diagrams of the type shown in Figure 5 in hyperfine structure calculations has previously been mentioned in Ref. /9/. Moreover, as the preceding Section shows, to calculate the amplitudes of allowed E1-transitions with an accuracy of about 1%, it suffices to use the Brueckner orbitals, i.e. to take into account only the diagrams of the types demonstrated in Figure 5.

V. Calculation of the parity-violating E1-amplitude

In the preceding Section we have found the one-electron Brueckner orbitals $\tilde{\psi}=\psi+\delta\psi$ with the weak interaction taken into account. Since these functions are the eigenfunctions for a single-particle Hamiltonian (see equation (19)), they constitute the complete orthonormalized basis. For this reason, the parity-violating E1-amplitude problem is not different, in principle, from the allowed E1-amplitude problem treated in the foregoing Section. It is only necessary to replace ψ by $\tilde{\psi}=\psi+\delta\psi$ in all the diagrams. For instance, for the $6s\to 7s$ transition the contribution to the E1-amplitude without the core polarization by a photon field being taken into account, is equal to

$$\vec{d}^{(0)}=\int(\delta\psi_{7s}^+\vec{D}\psi_{6s}+\psi_{7s}^+\vec{D}\delta\psi_{6s})d^3r \qquad (21)$$

where $\vec{D}$ is the dipole-transition operator determined by formula (8), or (9). Formula (21) is equivalent to making allowance for four diagrams shown in Figure 7. Note that this formula takes into consideration the correlation effects, involved in the Brueckner orbitals (Figure 5), and the core polarization by a weak interaction (Figure 4). In addition to the contribution (21), we take into account, just as in the allowed E1-amplitudes, the first-order correction in the Coulomb interaction, which arises due to the core polarization by an electric field of the photon (Figure 3). There is no difficulty in doing it using formulae (14) with the substitution $\psi\to\tilde{\psi}=\psi+\delta\psi$ in them.

Table 4 lists the results of the calculation of the parity-violating E1-amplitude in the 6s → 7s transition in Cs. To control the accuracy, the calculation has been made in the l and v forms. For comparison, we also give the results of the calculation for Hartree-Fock orbitals. The column 'a' corresponds to zero - order contribution in the residual Coulomb interaction (the correlation corrections which are included in the line renormalization, of course, are taken into account in Brueckner orbitals, see Figure 2). The column 'b' shows the contribution caused by the core polarization by a weak interaction, in the first order in the residual Coulomb interaction (the first-order graphs in the chain of diagrams in Figure 4). The column 'c' corresponds to the contribution, caused by the core polarization, in the second and higher orders in the residual Coulomb interaction (the second- and higher- order graphs in Figure 4). With our method of calculation using formula (21) we immediately find the sum of the contributions: a+b+c. To get the contribution 'a' when solving equation (20), we should confine ourselves to the zeroth iteration and then substitute the found corrections $\delta\psi$ into equation (21). The sum 'a + b' corresponds to one iteration in equation (20) and, finally, 'a + b + c' is referred to the self-consistent solution. The column 'd' in Table 4 gives the contribution to the parity-violating E1-amplitude, which is due to the core polarization by an electric field of the photon in the first order in the residual Coulomb interaction. This contribution corresponds to the substitution $\psi \to \tilde{\psi} = \psi + \delta\psi$ in the graphs depicted in Fig. 3.

As seen from Table 4, the contribution, which is associated with the core polarization by a weak interaction ('b + c'), is 3÷5 times larger as compared with that (d) associated with the core polarization by a photon field. Just for this reason, we have restricted ourselves to the leading order in the residual Coulomb interaction in the latter case, while the closed-shell polarization by a weak interaction is taken into account in all the orders.

Thus, we see (Table 4) that taking account of the correlation corrections using the transition to Brueckner orbitals of the core polarization effects enables the gauge invariance of

the amplitude to be restored. The parity-violating E1-amplitude of the 6s → 7s transition is equal to

$$\langle \tilde{7s} \,|\, D_z \,|\, \tilde{6s} \rangle = 0.856 \cdot 10^{-11} \left(-\frac{Q_w}{N}\right)(-ie a_B) \qquad (22)$$

where e is the electron charge and a_B is the Bohr radius. The results of the calculations in the l and v forms are different by 0.2% (by 20% in the RHF method). Of course, such a good coincidence in this case is occasional. So, for the 6s → 8s transition the amplitudes are as follows:

$$\langle \tilde{8s} \,|\, D_z^{(el)} \,|\, \tilde{6s} \rangle = 0.370 \cdot 10^{-11} \left(-\frac{Q_w}{N}\right)(-ie a_B)$$

$$\langle \tilde{8s} \,|\, D_z^{(vl)} \,|\, \tilde{6s} \rangle = 0.367 \cdot 10^{-11} \left(-\frac{Q_w}{N}\right)(-ie a_B) \qquad (23)$$

i.e. the difference constitutes o.8%.

In solving the inhomogeneius equation (20) for the correction to the wave function, we take into account the admixture not only of the positive-frequency intermediate states but also negative-frequency states ($E < -2m$). In the v-form calculation, the contribution of the negative-frequency states is not, generally speaking, negligibly small. To estimate this contribution, it is convenient to come to the nonrelativistic limit. Then the Hamiltonian (16) takes the form

$$h_{pv}^{nr} = \frac{G Q_w}{4\sqrt{2}\, m} \left(\vec{\sigma}\cdot\vec{p}\,\delta(\vec{r}) + \delta(\vec{r})\vec{\sigma}\cdot\vec{p}\right) \qquad (24)$$

where $\vec{\sigma}$ is the Pauli matrix and $\vec{p}$ is the electron momentum. The contribution of the positive-frequency intermediate states to the E1-amplitude in the v-form is equal to

$$E1_+ = \sum_i \left\{ \frac{\langle 7s | h_{pv}^{nr} | i \rangle \langle i | -\frac{e}{m}\vec{p}\vec{A} | 6s \rangle}{E_{7s} - E_i} + \frac{\langle 7s | -\frac{e}{m}\vec{p}\vec{A} | i \rangle \langle i | h_{pv}^{nr} | 6s \rangle}{E_{6s} - E_i} \right\} \qquad (25)$$

where $\vec{A}$ is the vector-potential of the electromagnetic wave. In addition to the contribution (25), the contact term appears in the E1-amplitude while substituting $\vec{p} \to \vec{p} - e\vec{A}$ in equation (24):

$$E1_- = -\frac{G Q_w e}{2\sqrt{2}\, m} \langle 7s | \vec{\sigma}\cdot\vec{A}\,\delta(r) | 6s \rangle \qquad (26)$$

It is well known that E1- corresponds to the contribution of the negative-frequencies intermediate states in terms of relativistic language (in the relativistic case, this equation arises when replacing the denominator $E_s - E_i \to 2m$). Let us take into account the fact that in equation (25) $E \sim m\alpha^2$, the velocity of the external electron at large distances ($r \sim a_B$) is equal to α , and $v \sim Z\alpha$ near the nucleus. Thus, we obtain that the E1_is suppressed by Z times as compared with the E1$_\nu$. It is worth emphasizing once more that our method of calculation authomatically takes into account the negative-frequencies contribution.

VI. Hyperfine structure of the levels

The hyperfine interaction is localized in the vicinity of the nucleus, just as a weak one. Therefore, as is known, the hyperfine-structure calculation is suited for testing the accuracy of the parity-violating effects calculation. Previously, we have calculated the hyperfine structure of Cs making allowance for the core polarization and all the second-order correlation corrections (see Ref. /8/). This calculation provides an accuracy of about 1÷2% for the hyperfine constants of the s and $p_{1/2}$ levels and of about 3÷4% for the $p_{3/2}$ levels. In the present paper we take into consideration only the correlation corrections, which are included in the renormalization of single-particle orbitals. It is noted in Ref. /8/ that for the s and $p_{1/2}$ levels (which are significant for a weak interaction) these graphs dominate and, hence, one should expect that the calculation, which is performed using Brueckner orbitals with the core polarization taken into account, provides an accuracy of the order of several percent. Calculations are made in the same way as for the weak interaction. The procedure of including the hyperfine interaction into the self-consistent equations (core polarization) is described in Ref. /8/. It is only necessary to go from Hartree-Fock to Brueckner orbitals in all the formulae. The results of the calculation are listed in Table 5. For comparison, the results of the calculation on the Hartree-Fock orbitals are also presented. It is seen that the calculation with the Brueckner orbitals provides an accuracy

of about 1% for the lower $6s_{1/2}$ and $6p_{1/2}$ states. The worse accuracy for the 7s, 8s and $7p_{1/2}$ states is connected with that we have underestimated the magnitude of the correlation correction, taking $\Sigma_s(\varepsilon = \varepsilon_{6s})$ and $\Sigma_{p_{1/2}}(\varepsilon = \varepsilon_{6p_{1/2}})$ instead of $\Sigma_s(\varepsilon = \varepsilon_{7s})$ and $\Sigma_{p_{1/2}}(\varepsilon = \varepsilon_{7p_{1/2}})$. For instance, the calculation of the hyperfine structure of the $7p_{1/2}$ level with $\Sigma_{p_{1/2}}(\varepsilon_{7p_{1/2}})$ refines the accuracy up to -3% (from -5%). The values of the p-odd and usual E1 amplitudes remain, practically, the same, since the relative contribution of correlations to them is a factor of 3, less than that to the hyperfine structure.

VII. Discussion of the accuracy of calculation of the parity-violating E1-amplitude and comparison with experiment

In the present paper the following tests have been performed in order to estimate the accuracy of calculation:

1. Estimation of the sensitivity to the parameters of the nucleon distribution in the nucleus. The accuracy is better than 0.2%.

2. Coincidence of the amplitudes calculated in the l and v forms. The difference constitutes about 0.2%. Remind that for the E1-amplitudes of the usual allowed transitions, the discrepancy in the l and v forms is of the same order as the disagreement with the experimental data.

3. Calculation of the atomic parameters known from the experiment. This test is of extreme importance since our calculations are based on the first-principles analysis and contain no fitting parameters. The calculated values of the energies are different from the experimental ones less than by 1%. An accuracy of about 1% is also obtained when calculating the allowed E1-amplitudes between the lower states. The error in calculation of the fine and hyperfine structure proves to be a little larger. It is probably for the reason that here the correlation corrections, which we calculate with some inaccuracy turn out to be large (about 30%). For the energies and E1-amplitudes, these corrections constitute about 10%. These are not large for the parity-violating E1-amplitude, too: -3% in the l

form and 13% in the v form. In view of this, one can expect that the accuracy for this amplitude is about 1%, just as in the calculation of the energies and usual E1-amplitudes.

Table 5 demonstrates that all the calculated hyperfine constants have turned out to be less than the experimental ones: for the 6s by 0.4%, 7s by 2.7%, $6p_{1/2}$ by 1.8%, and for the $7p_{1/2}$ is less by 5% at $\Sigma_{p_{1/2}}(E_{6p_{1/2}})$ and by 3% at $\Sigma_{p_{1/2}}(E_{7p_{1/2}})$. From these data, one can form the impression that we underestimate the wave function of electrons in the vicinity of the nucleus and, hence, underestimate the magnitude of the weak electron-nucleus interaction. For control, we have made a calculation which gives the hyperfine constants larger than the experimental ones: by 4% for the 6s, by 0.2% for the 7s, and by 0.6% for the $6p_{1/2}$. Only for the $7p_{1/2}$, the calculated value is smaller than the experimental one: by 3% at $\Sigma_{p_{1/2}}(E_{6p_{1/2}})$ and by 1% at $\Sigma_{p_{1/2}}(E_{7p_{1/2}})$. This version is obtained if in going from the Hartree-Fock single-particle potential $V = V_d - V_{exch}$ to the Brueckner potential, $V = V_d - V_{exch} + V_{corr}$ (see formulae (4), (5) and (6)), the core orbitals are frozen, i.e. V is calculated using the Hartree-Fock orbitals. The difference of the first version from the second one consists in that the former takes into account some additional graphs of the third order in the residual Coulomb interaction. In the second version, the usual E1-amplitudes for the allowed transitions between the lower states are different from those obtained in the first version by less than 1%. The P-odd amplitude also remains nearly the same:

$$\langle \tilde{7s} | D_z^{(1)} | \tilde{6s} \rangle = 0.868 \cdot 10^{-11} \left(-\frac{Q_W}{N}\right)(-ie a_B) \qquad (27)$$

$$\langle \tilde{7s} | D_z^{(v)} | \tilde{6s} \rangle = 0.873 \cdot 10^{-11} \left(-\frac{Q_W}{N}\right)(-ie a_B) \qquad (28)$$

One can substitute $\delta\tilde{\psi}$, obtained by means of the usual perturbation theory in h_{pv}, into the formula for the p-odd amplitude (21). Then the largest contribution to the P-odd amplitude comes from the mixing of the 7s and $6p_{1/2}$ -states:

$$\langle \tilde{7s} | E1 | \tilde{6s} \rangle \sim \frac{\langle 7s | \tilde{h}_{pv} | 6p_{1/2} \rangle \langle 6p_{1/2} | D_z | 6s \rangle}{E_{7s} - E_{6p_{1/2}}} \qquad (29)$$

The matrix element $\langle \psi_{7s} | h_{pv} | \psi_{6p_{1/2}} \rangle$ is determined by the behaviour of the wave functions in the vicinity of the nucleus. The hyperfine-structure constants are sensitive to the same region. For instance, $A_s \sim |\psi_s(0)|^2$ in the nonrelativistic limit. Therefore, it is reasonable to compare, with experiment, the quantity which is similar, in structure, to the p-odd E1-amplitude:

$$\frac{\sqrt{A_{7s} A_{6p_{1/2}}} \langle 6p_{1/2} | D_z | 7s \rangle}{E_{7s} - E_{6p_{1/2}}} \qquad (30)$$

It turns out that the calculation with the first-version Brueckner potential underestimates this quantity by 5.4% in the l form and by 3.1% in the v-form, while for the case of the second-version Brueckner potential this quantity is underestimated by 3.5% in the l form and by 0% in the v form. If we add the contribution of the other large terms from the expansion of $\delta\psi_{6s}$ to the r.h.s. of equations (29) and (30), the situation remains the same. This fact it is possible to consider as the indication to that we have underestimated the value of the P-odd E1-amplitude. To guarantee the correctness of the result, we have slightly increased the average point in the theoretical value of the E1-amplitude (see equations (22), (27) and (28)), increasing simultaneously the interval of its possible variation:

$$E1 \equiv \langle \tilde{7s} | D_z | \tilde{6s} \rangle = (0.88 \pm 0.03) \cdot 10^{-11} \left(-\frac{Q_W}{N}\right)(-ie a_B) \qquad (31)$$

The results of the calculations made by the other groups are presented in Table 6. In the experimental works (see Ref. /1/), the following quantity has been measured:

$$\frac{\mathrm{Im}\, E1}{\beta} = 1.56 \pm 0.17 \pm 0.12 \ \mathrm{mV/cm} \qquad (32)$$

According to Refs. /21/ and /6/, the vector polarizability β is equal to $27.3 \pm 0.5\, a_B^3$. Then

$$E1_{exp} = 0.828\,(1 \pm 0.11 \pm 0.08) \cdot 10^{-11}(-ie a_B) \qquad (33)$$

Using equation (31), we obtain that for ^{133}Cs the weak nuclear charge is the following:

$$Q_W = -73.4 \pm 8 \pm 6 = q_n N + q_p Z \qquad (34)$$

where q_n and q_p are the weak charges of the neutron and proton. In the Weinberg-Salam model,

$$q_n = -1, \quad q_p = 1 - 4\sin^2\theta_W$$

Because of the electro-weak radiation corrections, these constants depend on the momentum transfer. If the W-boson's mass M_W is chosen as a normalization point, according to Ref. /22/, then at low transfers

$$q_n = -0.974, \quad q_p = 0.974 - 3.908\sin^2\theta_W(M_W) \qquad (35)$$

From the W-boson mass measurements it follows that $\sin^2\theta_W(M_W) = 0.226 \pm 0.008 \pm 0.014$ (see Ref. /23/) and hence the weak charge of the ^{133}Cs nucleus is

$$Q_W = -71.0 \pm 1.7 \pm 3.0 \qquad (36)$$

The value of Q_W from equation (34) is well consistent with this number. In addition, formulae (34) and (35) can be used for an independent determination of $\sin^2\theta_W$:

$$\sin^2\theta_W(M_W) = 0.237 \pm 0.036 \pm 0.03 \qquad (37)$$

The discovery of the parity-violation effect in atoms (Ref. /24/), which was confirmed in Refs. /25-28,1/, was a very important verification of the unified theory of electroweak interactions, suggested by Weinberg and Salam. An exact measurement of the weak charge of the nucleus can prove to be a new step in this field.

VIII. Conclusion

In conclusion we would like to note that the high accuracy of atomic calculations, achieved ir the present paper, is due apparently, to the following circumstances. For homogeneous matter, the RPA method (summation of the diagrams in Figure 4) is the approximation of a high density. The Brueckner method

(summation of the diagrams similar to those demonstrated in Figures 2 and 5) corresponds to the low-density approximation. We take into account both classes of diagrams and it is probably for this reason we obtain a good accuracy in the intermediate region as well. The other point is the fact that we take into account all the first-order diagrams and the main second- and higher order diagrams in the residual Coulomb interaction. The correlation graphs we take into account (Figure 5) dominates because only these graphs contain a small energy denominator corresponding to the excitation of the external electron. In all the remaining graphs of this order, in the intermediate states, there is at least one electron excited from the core, i.e. all the energy denominators are large.

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Table I. Energy levels of Cs (cm^{-1})

State	HF	HF+correlations in perturb.theory	Brueckner orbitals	Experiment /13/
6s	27926	31440	31703	31407
7s	12104	12924	12851	12871
8s	6790	7116	7080	7090
$6p_{1/2}$	18792	20223	20349	20228
$7p_{1/2}$	9230	9663	9635	9641
$6p_{3/2}$	I8388	I9667	19779	19674
$7p_{3/2}$	9079	9478	9455	9460
$5d_{3/2}$	I4146	16381	16634	16907
$5d_{5/2}$	14168	16318	16514	16810

Table 2. Radial integral $6s\text{-}6p_{1/2}$ in the units of Bohr radius

		Zero order	Core polarization	Sum	Experiment
HF	ℓ	-6.47	0.41	-6.07	-5.535(14)
	v	-5.05	0.06	-4.99	
Brueck-ner orb.	ℓ	-5.90	0.45	-5.45	
	v	-5.67	0.09	-5.58	

Table 3. Allowed E1-amplitudes (radial integrals) in Cs, in the units of Bohr radius

Transition	ℓ	v	Experiment /15,16/
$6s - 6p_{1/2}$	-5.45	-5.58	-5.535(14)
$6s - 7p_{1/2}$	-0.32	-0.36	-0.348(3)
$6s - 8p_{1/2}$	-0.076	-0.114	-0.099(2)
$6s - 6p_{3/2}$	-5.43	-5.54	-5.509(7)
$6s - 7p_{3/2}$	-0.48	-0.52	-0.505(9)
$6s - 8p_{3/2}$	-0.17	-0.20	-0.188(5)
$7s - 6p_{1/2}$	5.16	5.14	
$7s - 7p_{1/2}$	-12.63	-12.51	
$7s - 8p_{1/2}$	-1.14	-1.12	
$7s - \overline{7p}$	-12.48	-12.36	-12.30(3)

Table 4. E1-amplitude of the $6s \to 7s$ transition

$$\frac{i}{e a_B} \langle \widetilde{7s} | D_z | \widetilde{6s} \rangle \left(-\frac{N}{Q_w}\right) \cdot 10^{11}$$

		a	Core polarization			Σ
			b	c	d	
HF	ℓ	0.740	0.132	0.048	-0.039	0.880
	v	0.504	0.131	0.065	0.038	0.739
Bru.	ℓ	0.734	0.128	0.045	-0.051	0.856
	v	0.594	0.155	0.072	0.033	0.854

a - without taking into account the core polarization ;
b - core polarization by a weak interaction, the first order;
c - higher orders;
d - core polarization by an electric field of the photon.

Table 5. Hyperfine-structure constants in ^{133}Cs (x 10^3 cm^{-1})

State	HF	HF+correlations, /8/	Brueckner orbitals	Experiment /20/
6s	56.79	78.27	76.38	76.66
7s	15.59	18.73	17.72	18.22(10)
8s	6.51	7.46	7.09	7.30(5)
$6p_{1/2}$	6.67	9.54	9.56	9.737(4)
$7p_{1/2}$	2.37	3.15	2.99	3.147(I)

Table 6. The values of the 6s → 7s E1-amplitude obtained by various authors

$$\frac{i}{ea_6}\langle \tilde{7s}|D_z|\tilde{6s}\rangle\left(-\frac{N}{Q_w}\right)\cdot 10^{11}$$

E1	Reference
I.33	/3/
I.15	/4/
I.00	/5/
0.75	/29/
1.06	/10/
0.97 ± 0.1	/6/
0.88 ± 0.03	our number

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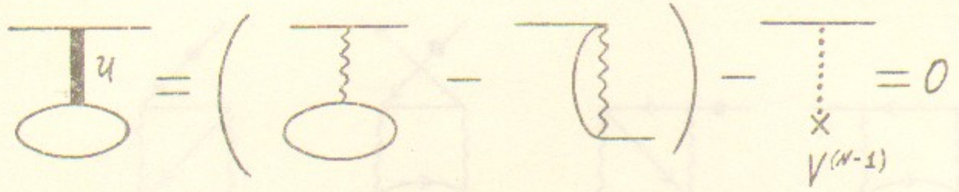
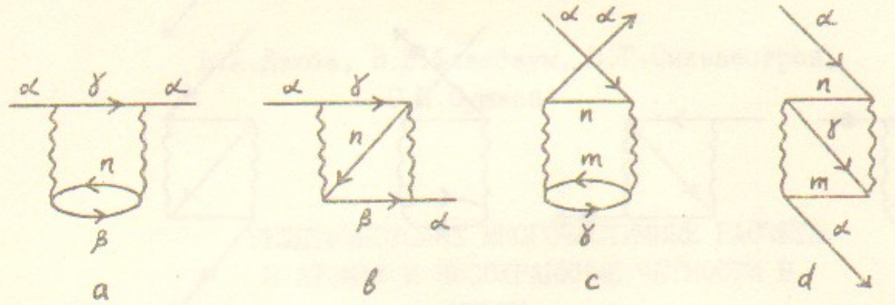


Fig. 1



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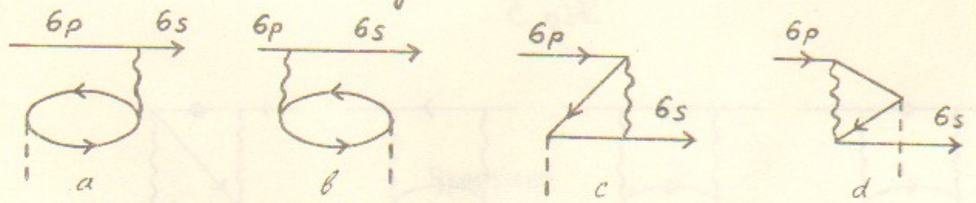

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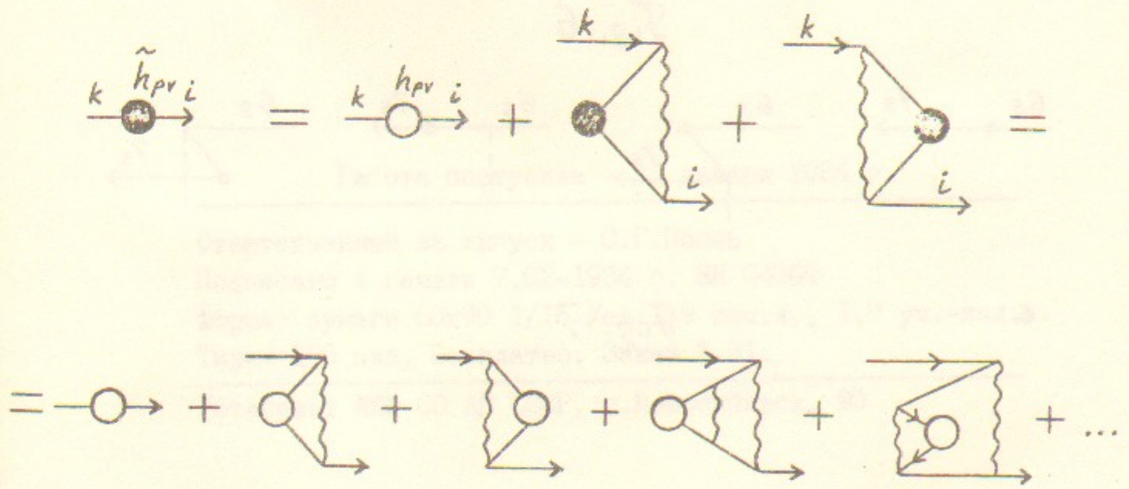

Fig. 4

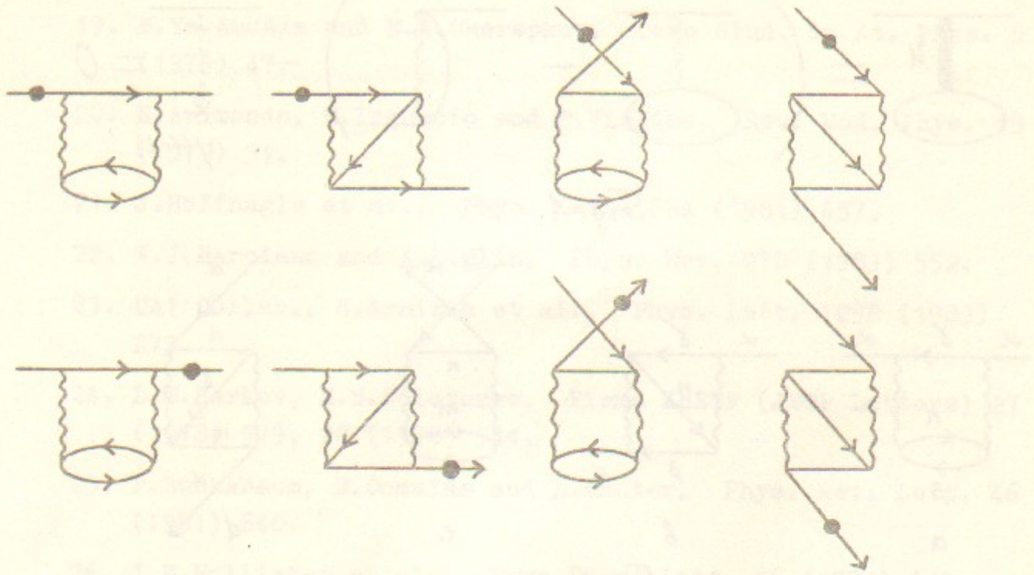

Fig. 5

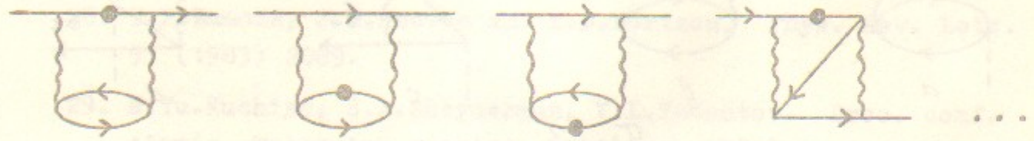

Fig. 6

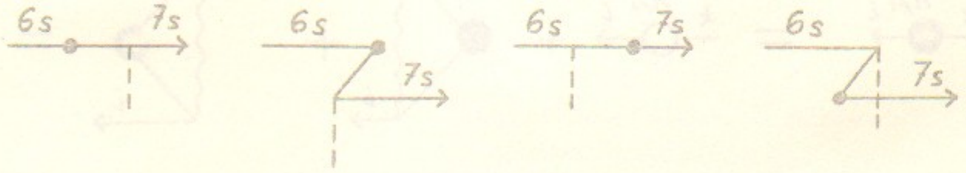

Fig. 7

В.А.Дзюба, В.В.Фламбаум, П.Г.Сильвестров,
О.П.Сушков

РЕЛЯТИВИСТСКИЕ МНОГОЧАСТИЧНЫЕ РАСЧЕТЫ В АТОМАХ И НЕСОХРАНЕНИЕ ЧЕТНОСТИ В ЦЕЗИИ

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