ИНСТИТУТ ЯДЕРНОЙ ФИЗИКИ СО АН СССР

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# SUMMATION OF THE HIGH ORDERS OF PERTURBATION THEORY IN THE CORRELATION CORRECTION TO THE HYPERFINE STRUCTURE AND TO THE AMPLITUDES OF E1-TRANSITIONS IN CAESIUM ATOM

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НОВОСИБИРСК

# Summation of the High Orders of Perturbation Theory in the Correlation Correction to the Hyperfine Structure and to the Amplitudes of E1-Transitions in Caesium Atom

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ABSTRACT

Three dominating subsequences of diagrams in the correlation correction are summarized: screening of the residual electron-electron interaction, particle-hole interaction, and the iterations of the self-energy.



Up to the present time the most detailed calculations of the parity violating E1-amplitude of $6s-7s$-transition in Cs have been carried out in the works [1—3]. However the progress in experiment requires the progress in calculations. In the paper [4] we have developed the new technique which allows one to improve the accuracy of atomic calculations. The value of parity nonconserving amplitude depends on the wave function at the nucleus and at the large distances ($r \geqslant a_B$). It is well known that the hyperfine structure is a good probe of the wave function at small distances and amplitude of the allowed E1-transition is a probe at the large distances. For the control of accuracy of parity nonconservation calculation in the present work we calculate the hyperfine structure of $6s$-, $7s$-, $6p_{1/2}$-, $7p_{1/2}$-levels of Cs, as well as amplitudes of the E1-transitions $6s-6p,7p$; $7s-6p,7p$.

In our recent work [4] the energy levels of Caesium atom were calculated with higher order correlation corrections taken into account. As zero approximation we used the wave functions and energies obtained by the relativistic Hartree—Fock method (RHF) in the frozen field of atomic core ($V^{N-1}$-approximation [5]). Summation of the correlation diagrams were carried out using the Green functions and Feynman technique. The details of calculations of the Green function, polarization operator, and of the summation of diagrams are described in Refs [4, 6]. In the present work we use the same technique and therefore we remind it briefly. The diagrams of the second order in residual interaction for the correlation correc-

tion to energy are presented at Fig. 1. Three types of diagrams are enhanced in higher orders. The most important type is the screening of the residual Coulomb interaction. Corresponding sequence of diagrams is presented at Fig. 2. This is a collective effect similar to that in plasma. The enhancement parameter of these diagrams is the number of electrons in the external closed subshell. Use of the screened interaction essentially improves the convergence of the perturbation theory [6]. The second contribution is the chain of diagrams with particle-hole interaction inside the electron loop (Fig. 3) which should be included into the diagrams presented at Figs 1, 2. This interaction is enhanced due to the large diagonal Coulomb integral of zero multipolarity. Its importance is obvious from the following example: the existence of the discrete spectrum excitations in the noble gas atom is due just to the particle-hole interaction. The third contribution is due to the iterations of the self-energy operator $\Sigma(r_1, r_2, E)$ (Figs 4, 5). Correlation correction to energy in the first order in $\Sigma$ is equal to $\delta\varepsilon = \langle\Sigma\rangle$. The iterations are enhanced since in the intermediate states the small energy denominator corresponding to the excitation of the external electron arises. The all other perturbation theory diagrams are proportional to the powers of the small parameter $Q_{nd}/\Delta E_{int}$ where $Q_{nd}$ is a nondiagonal Coulomb integral and $\Delta E_{int}$ is a large energy denominator corresponding to excitation of the core electron.

In Caesium atom relativistic Hartree—Fock method provides the accuracy of calculation of energy levels about 10%. The second order correlation correction improves the accuracy to 1% [7, 8]. (The third order correction is calculated in the Ref. [9].) Summation of the pointed above sequences of higher order diagrams reduces the error to 0.1% [4].

In the present work we carry out the calculation of the hyperfine structure and of the E1-amplitudes basing on the approach developed in the papers [4, 6]. The three pointed above chains of correlation diagrams are taken into account. The accuracy is essentially better than in calculation in the second order in residual Coulomb interaction [10, 11, 8].

Let us remind the reader the structure of correlation correction to the transition amplitude and to the hyperfine structure [10, 11, 12]. The most important contributions are given by the diagrams where the interaction with external field (electric field of the photon for E1-amplitude, and magnetic field of the nucleus for hyperfine structure) is introduced into external electron line



*Fig. 1.* Second order correction to the self-energy. Wavy line denotes a residual Coulomb interaction.

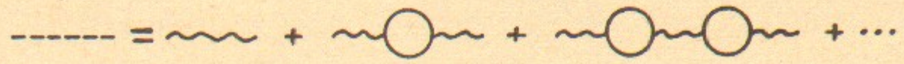

*Fig. 2.* Screening of electron-electron interaction.

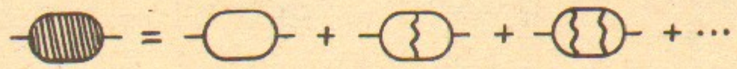

*Fig. 3.* The hole-particle interaction in the polarization operator.

*Fig. 4.* The self-energy operator with the renormalizations described by the Figs 2, 3 taken into account.

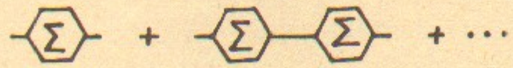

*Fig. 5.* Chaining of the self-energy operator.

(Fig. 6). These diagrams are enhanced by the small denominator $\Delta E_{ext}$, which corresponds to the excitation of an external electron. If an external field is attached to the internal electron line then the perturbation theory denominator is of the order of large energy of electron excitation from the closed shells $\Delta E_{int}$ (see Fig. 7), and

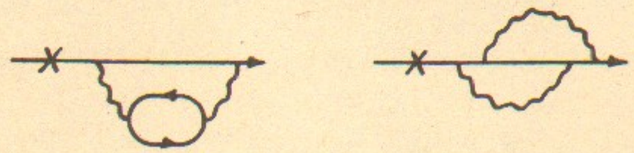

*Fig. 6.* Brueckner type correlation correction to hyperfine constant or E1-amplitude in the second order in residual Coulomb interaction. The cross denotes the external field.

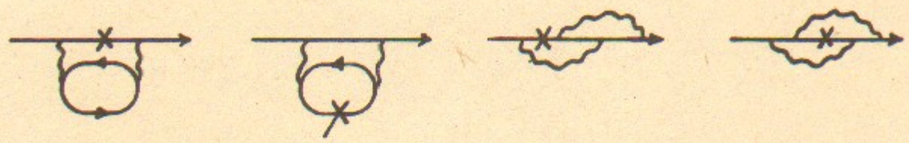

*Fig. 7.* Correlation diagrams of the type of structural radiation.

these diagrams are suppressed. For the contributions of the higher order in residual Coulomb interaction there is similar enhancement of the diagrams with the single-particle operator on the external electron line. We call such diagrams the Brueckner type diagrams, and the diagrams with the external field attached to the internal electron line are called structural radiation. In the alkaline atoms the enhancement factor for Brueckner type diagrams is of the order of $\Delta E_{int}/\Delta E_{ext} \sim 10$. Therefore to improve the accuracy of calculation we should first of all to calculate more accurately these contributions.

The Brueckner type correlation corrections can be calculated by the correlation potential method [13, 12]. In this method one should add the self-energy operator $\Sigma(r_1, r_2, E)$ to the Hartree—Fock potential: $V^{N-1} \to V^{N-1} + \Sigma$. The single-particle orbitals obtained in this potential can be used for the calculation of matrix elements of electric dipole moment or hyperfine interaction. In this way we take into account the diagrams presented at Fig. 6 and all the diagrams with the iterations of $\Sigma$ (Fig. 5). The self-energy operator $\Sigma$ is calculated with the screening correction (Fig. 2) and particle-hole interaction (Fig. 3) taken into account. Thus we see that evolution of Brueckner type correlation correction to the matrix element of



single-particle operator is not more complicated than that for the energy level.

Besides the correlations we must take into account polarization correction which is due to the polarization of the atomic core by the external electric field or by magnetic field of the nucleus. We do it in standard way using the time-dependent Hartree—Fock method in the external field. The details of this calculation are described in the Refs [10, 11]. Let us stress that even in evolution of correlation correction we use the single-particle operator with the core polarization taken into account.

Table 1

**The Hyperfine Constants For $^{133}$Cs. Units $10^{-3}$ cm$^{-1}$**

| | *a* | *b* | *c* | *d* | *c*+*d* | *e* | *f* |
|---|---|---|---|---|---|---|---|
| 6*s* | 47.54 | 57.19 | 77.40 | −0.80 | 76.60 | 76.66 | −0.1% |
| 7*s* | 13.06 | 15.66 | 18.14 | −0.09 | 18.05 | 18.21 | −0.9% |
| $6p_{1/2}$ | 5.368 | 6.671 | 9.691 | 0.06 | 9.751 | 9.737 | 0.1% |
| $7p_{1/2}$ | 1.922 | 2.370 | 3.116 | 0.03 | 3.146 | 3.147 | 0.0% |

*a*—Calculation by the Relativistic Hartree—Fock method (RHF);
*b*—RHF+polarization;
*c*—RHF+polarization+Brueckner type correlation;
*d*—contribution of non-Brueckner type correlation (Fig. 7 and normalization correction) multiplied by a screening factor $K=0.8$.
*c*+*d*—Result of calculation;
*e*—experimental values [14, 15];
*f*—accuracy of calculation with respect to experiment (per cent).

The results of hyperfine structure calculations are presented at the Table 1. The diagrams of the type of structural radiation (Fig. 7, the hyperfine interaction inside the correlation correction) as well as the normalization contribution we calculate by the direct summation over the intermediate states in the same way as in Ref. [10]. To take into account the screening of the residual Coulomb interaction in the structural radiation and normalization correction we introduce the effective screening factor $K_{scr}=0.8$. The value of the factor is determined from the some explicitly calculated diagrams. This factor is not very important since the structural radiation is small by itself.

For the sake of analysis of the accuracy of calculation we can try to refine the theoretical values by fitting the energy levels. The

energies can be reproduced exactly if we introduce by hands the coefficients into self-energy operators calculated by us:

$$\Sigma_{6s} \to 1.010\,\Sigma_{6s}\,,$$
$$\Sigma_{7s} \to 1.023\,\Sigma_{7s}\,,$$
$$\Sigma_{6p} \to 0.978\,\Sigma_{6p}\,,$$
$$\Sigma_{7p} \to 0.970\,\Sigma_{7p}\,. \qquad (1)$$

After this procedure we recalculate the Brueckner contribution to the hyperfine constant. The results are presented at the column «*c*» of the Table 2.

Table 2

**The Hyperfine Constants for $^{133}$Cs Calculated with the Fit of the Energy Levels. Units $10^{-3}$ cm$^{-1}$**

| | *c* | *c*+*d* | *f* |
|---|---|---|---|
| 6*s* | 77.60 | 76.80 | 0.2% |
| 7*s* | 18.19 | 18.10 | −0.6% |
| $6p_{1/2}$ | 9.613 | 9.677 | −0.6% |
| $7p_{1/2}$ | 3.093 | 3.125 | −0.7% |

*c* — RHF + polarization + Brueckner type correlation refined according to eq. (1);
*c*+*d* — result of calculation;
*f* — accuracy of calculation with respect to experiment (per cent).

There is the radiation correction to the hyperfine constant of the *s*-levels. At $Z\alpha \ll 1$ its relative value is (see Ref. [15])

$$\frac{\alpha}{2\pi} - Z\alpha^2\left(\frac{5}{2} - \ln 2\right) \approx -0.4\%\,. \qquad (2)$$

However it should be noted that in the energy fit (1) we do not take into account the Lamb shift which has the same origin as the correction (2). Therefore one can say that fit (1) effectively takes into account the correction (2). Thus the Tables 1, 2 represent the final versions of the calculations. Accuracy is not worse than 1%.

We carry out the calculation of the radial integrals (amplitudes of the E1-transitions) in the same way as that for hyperfine structure. The only difference is that instead of direct calculation of the structural radiation we use the approximate formula derived in the



paper [12]:

$$\Gamma_{str} = -\frac{1}{2}\langle f|\; D\frac{\partial\Sigma}{\partial E} + \frac{\partial\Sigma}{\partial E}D\;|i\rangle\,, \qquad (3)$$

*D* **is** the dipole moment operator. The normalization contribution which is due to the admixing of many-body excitations is

$$\Gamma_{norm} = \frac{1}{2}\langle f|\,D\,|i\rangle\left(\langle f|\;\frac{\partial\Sigma}{\partial E}\;|f\rangle + \langle i|\;\frac{\partial\Sigma}{\partial E}\;|i\rangle\right). \qquad (4)$$

The results of radial integrals calculations are presented in the Table 3.

Table 3

**The Radial Integrals (E1-Amplitudes) for Cs in the Units of Bohr Radius**

| | *a* | *b* | *c* | *d* | *c*+*d* | *e* | *f* |
|---|---|---|---|---|---|---|---|
| $6s-6p_{1/2}$ | −6.463 | −6.091 | −5.531 | 0.021 | −5.510 | −5.535(14) | −0.45±0.25 |
| $6s-6p_{3/2}$ | −6.430 | −6.073 | −5.505 | 0.021 | −5.484 | −5.509(8) | −0.45±0.15 |
| $6s-7p_{1/2}$ | −0.459 | −0.296 | −0.299 | −0.019 | −0.318 | −0.348(3) | −8±1 |
| $6s-7p_{3/2}$ | −0.606 | −0.445 | −0.460 | −0.027 | −0.487 | — | — |
| $7s-6p_{1/2}$ | 5.404 | 5.450 | 5.210 | −0.037 | 5.173 | 5.185(27) | −0.2±0.5 |
| $7s-6p_{3/2}$ | 5.779 | 5.816 | 5.636 | −0.037 | 5.599 | 5.611(27) | −0.2±0.5 |
| $7s-7p_{1/2}$ | −13.48 | −13.37 | −12.66 | 0.023 | −12.64 | −12.50(2 | 1.1±0.2 |
| $7s-7p_{3/2}$ | −13.29 | −13.18 | −12.44 | 0.023 | −12.42 | −12.28(2) | 1.1±0.2 |

*a* — RHF;
*b* — RHF + polarization;
*c* — RHF + polarization + Brueckner type correlation;
*d* — contribution of the structural radiation and of the normalization correction;
*c*+*d* — result of calculation;
*e* — experimental values [17, 18, 19];
*f* — accuracy of calculation with respect to experiment (per cent).

Similar to hyperfine structure for the sake of analysis of accuracy we recalculate the E1-radial integrals with the refined self-energy operator (1). The results of this calculation are tabulated in the Table 4. Thus the Tables 3, 4 represents the final results for the E1-amplitudes. Excluding the small $6s-7p$ radial integral the accuracy is not worse than 1%.

Table 4

**The Radial Integrals (E1-Amplitudes) for Cs Calculated with the Fit of the Energy Levels. Units of Bohr Radius**

| | $c$ | $c+d$ | $f$ |
|---|---|---|---|
| $6s-6p_{1/2}$ | −5.525 | −5.504 | $-0.55\pm0.25$ |
| $6s-6p_{3/2}$ | −5.499 | −5.478 | $-0.55\pm0.15$ |
| $6s-7p_{1/2}$ | −0.318 | −0.337 | $-3\pm1$ |
| $6s-7p_{3/2}$ | −0.478 | −0.505 | — |
| $7s-6p_{1/2}$ | 5.246 | 5.209 | $0.5\pm0.5$ |
| $7s-6p_{3/2}$ | 5.672 | 5.635 | $0.4\pm0.5$ |
| $7s-7p_{1/2}$ | −12.62 | −12.60 | $0.8\pm0.2$ |
| $7s-7p_{3/2}$ | −12.40 | −12.38 | $0.8\pm0.2$ |

$c$ — RHF + polarization + Brueckner type correlation refined according to eq. (1);
$c+d$ — result of calculation;
$f$ — accuracy of calculation with respect to experiment (per cent).

We would like to note that we do not understand the reason of the error about 1% in the calculation of $7s-7p$-amplitude. At the first sight the error about 1% is comparable with that about 0.5% obtained for example for the $6s-6p$-amplitude. However it is not so. For the $6s-6p$-transition the structural radiation and normalization contributions considerably compensate each other: $0.021=0.072-0.051$. (The sum is presented in the column «$d$» of the Table 3.) We calculate the structural radiation ($-0.051$) using the approximate formula (3). Therefore we may assume the error ~100% in the sum of structural radiation and normalization. This is enough to explain the inaccuracy 0.5% in the calculation of $6s-6p$ E1-amplitude.

For the $7s-7p$-transition the structural radiation is very small (0.032 is the normalization contribution, and $-0.009$ is the structural radiation contribution). Therefore its approximate evolution can not influence on the final accuracy.



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*В.В. Фламбаум, О.П. Сушков*

**Суммирование высших порядков теории возмущений в корреляционной поправке к сверхтонкой структуре и амплитудам E1-переходов в атоме цезия**

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