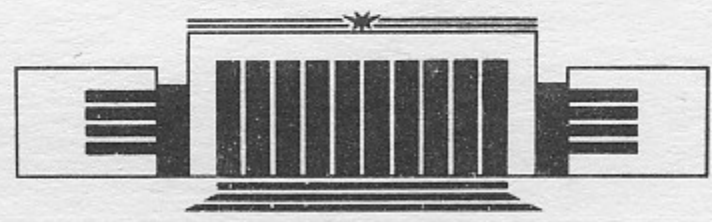V.A. Dzuba, V.V. Flambaum and O.P. Sushkov

SUMMATION OF THE PERTURBATION THEORY HIGH ORDERS CONTRIBUTIONS TO THE CORRELATION CORRECTION FOR THE ENERGY LEVELS OF CAESIUM ATOM

Summation of the Perturbation Theory High Orders Contributions to the Correlation Correction for the Energy Levels of Caesium Atom

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

Institute of Nuclear Physics
630090, Novosibirsk, USSR

ABSTRACT

Three dominating subsequencies of diagrams are sum-
marized: 1) screening of the residual Coulomb inte-
raction; 2) particle-hole interaction in the polarization
operator; 3) chaining of the self-energy correction. The
accuracy $\sim 0.1\%$ is obtained for the caesium energy
levels.

INTRODUCTION

Recent high precision experiments on the parity nonconservation
in the caesium atom [1] have shown that atomic experiments are
competitive in investigation of weak interaction between elementary
particles. Atomic calculations of high accuracy are necessary to
obtain information about the weak interaction constants. Atomic
energy levels are suitable as an object to develop the methods of
calculation.

Many-body perturbation theory gives a good accuracy. In the
papers [2, 3] the energy levels have been calculated in the second
order in residual Coulomb interaction (diagrams at Fig. 1). There
is a small disagreement between results of Refs [2] and [3] for the
second order correlation correction. The difference is about 10% of
the value of correlation correction or 1% of the value of the energy.
The reason of the difference is noncomplete summation over the vir-
tual high excited states ($E \geqslant 25$ Ry) in the Ref. [2]. It should be
noted that this inaccuracy does not exceed the higher orders contri-
butions which were not taken into account in the Refs [2, 3].

It was pointed in the Ref. [4] that taking into account the col-
lective screening of Coulomb interaction between electrons (summa-
tion of the diagrams, presented at Fig. 2) considerably improves the
convergence of perturbation theory. In the recent paper [5] the
third order diagrams were calculated for caesium. In agreement
with Ref. [4] the diagrams that correspond to the screening of the
second order (Fig. 3) give the largest contribution. However, accor-
ding to [5] diagram presented at Fig. 4 gives a large contribution

Fig. 1. Second order correction to the energy level. Dotted line denotes a residual Coulomb interaction.
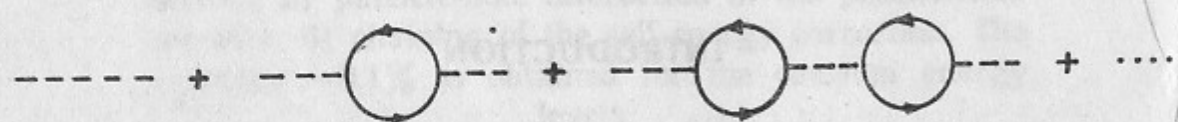

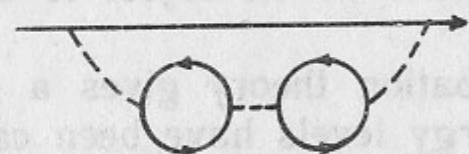Fig. 2. Renormalization of the Coulomb line: collective screening.

Fig. 3. The screening of the 1,a diagram.

Fig. 4. Insertion of the hole-particle interaction in the polarization operator.

as well. Its value is only the two times smaller than the value of screening diagram. This diagram appears due to the particle-hole interaction. This interaction contains diagonal zero multipolarity Coulomb integral which is very large and therefore enhances the corresponding contribution. In other words we can say that diagram 4 describes the alteration of the core potential due to the excitation of the particle from the core to the virtual intermediate state. The other third order diagrams according to Ref. [5] are very small.

The full third order contribution partially compensate the second order one and it makes worse the agreement with experiment [5]. Thus, the convergence of perturbation theory is very slow or absent at all. It was pointed out in the Ref. [4] that the convergence problem can be solved by summation of the screening diagrams (Fig. 2) and using the perturbation theory in screened interaction. Now we understand that to obtain high accuracy one needs in addition to take into account particle-hole interaction in the polarization operator in all orders (Fig. 5). It is well known that particle-hole interaction plays an important role in the photoexcitation of the noble gas atoms (see, e. g. Ref. [6]). In our case we have the similar situation: the virtual excitation of the closed core by the external electron field.

Thus, in the present paper to calculate the self-energy operator we work according to the following program. At first, the polarization operator with taking into account the particle-hole interaction is calculated (Fig. 5). Secondly, according to Fig. 6 we calculate the screened Coulomb interaction. Finally, the self-energy operator Σ is calculated according to diagrams presented at Fig. 7. In the first order in Σ correction to the energy is equal to average value of self-energy operator: $\delta\varepsilon = \langle\Sigma\rangle$. However we need to take into account self-energy operator iterations as well (Fig. 8). Such iterations are enhanced by small energy denominator ΔE_{ext} corresponding to excitation of the external electron only (in other diagrams denominator is about $\Delta E_{int} \gg \Delta E_{ext}$, where ΔE_{int} is the typical excitation energy of the core). The chaining of the second order self-energy operator have been done earlier in the papers [7, 3, 5].

Correlation correction taking into account three mentioned above dominating subsequencies of diagrams is calculated in the present paper. The accuracy of calculation by relativistic Hartree—Fock method in caesium is about 10%. Taking into account the second order correlation correction improves the accuracy to 1%. In the present work the accuracy ~0.1% is obtained.

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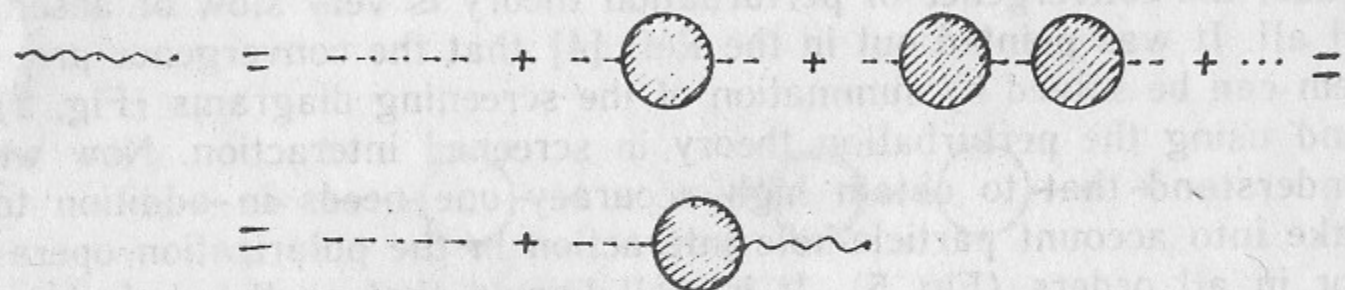Fig. 5. The hole-particle interaction in the polarization operator.

Fig. 6. Renormalization of the Coulomb line.
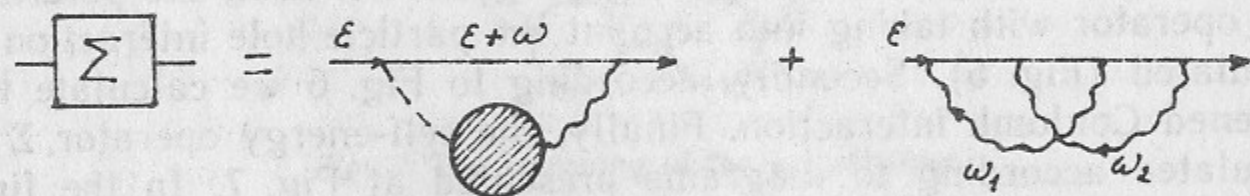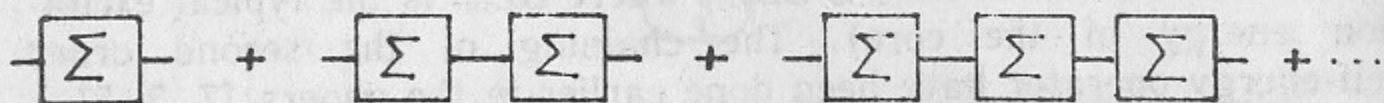

Fig. 7. The self-energy operator.

Fig. 8. Chaining of the self-energy.

As a starting approximation we use wave functions and energies obtained by the relativistic Hartree—Fock method (RHF) in the frozen field of atomic core.

$$V^{n-1} = V_d^{N-1} + V_{ex}^{N-1}.$$

Here N is the number of electrons, $N-1$ is the number of electrons of closed core, V_d and V_{ex} is the direct and exchange potential. Feynman technique is convenient for summation of high orders in correlation correction. The method of calculation is described in details in our previous papers [4, 7]. Here we would like only to remind of it briefly. It is well known that the radial electron Green function G_0 in the local potential can be expressed in terms of the solutions of Dirac equation χ_0 and χ_∞ which are regular at $r \to 0$ and $r \to \infty$ respectively: $G_0(r_1, r_2, \varepsilon) \infty \chi_0(r_<)\chi_\infty(r_>)$, $r_< = \min(r_1, r_2)$, $r_> = \max(r_1, r_2)$. We take into account nonlocal exchange interaction V_{ex} solving the Dyson equation for the exact Green function G

$$\hat{G} = (1 - \hat{G}_0 \hat{V}_{ex})^{-1} \hat{G}_0. \tag{1}$$

Here G, G_0 and V_{ex} are the matrices in the coordinate space.

The polarization operator $\hat{\Pi}$ (electron loop) can be calculated if we know G and the wave functions of the core occupied states Ψ_n

$$\Pi(r_1, r_2, \omega) = i \prod_{n=1}^{N-1} \Psi_n^*(r_1) | G(r_1, r_2, \varepsilon_n + \omega) + G(r_1, r_2 \varepsilon_n - \omega) | \Psi_n(r_2). \tag{2}$$

We have mentioned above that the chain of diagrams with particle-hole interaction in the loop describes the deviation of the direct potential for excited core particle from that for nonexcited particle. Actually, in Hartree—Fock calculation for nonexcited core one takes into account the direct self-interaction because it exactly cancels out by exchange self-interaction. There is no such cancelation for the electron excited from the core and therefore one should substract from the potential the part which is due to the self-interaction. The diagrams presented at Fig. 5 just correspond to this procedure. Physically it means that the excited core electron moves in the field of $N-2$ electrons. (The external electron moves at large distances and does not influence on the core). Let us denote by V_a the zero multipolarity potential of outgoing electron (e. g. $5p$-elect-

ron). Then the potential which discribes the excited and core states simultaneously looks as follow

$$V = V^{N-1} - (1 - \hat{P}) V_0 (1 - \hat{P}), \qquad (3)$$

Here $\hat{P}$ is the projection operator on the core orbitals

$$\hat{P} = \sum_{n=1}^{N-1} |n\rangle \langle n|. \qquad (4)$$

We introduce the projection operator $\hat{P}$ in potential because the excited states must be orthogonal to the core orbitals. For the occupied orbitals $\langle V \rangle = \langle V^{N-1} \rangle$, for excited orbitals $\langle V \rangle = \langle V^{N-1} \rangle - \langle V_0 \rangle$. Strictly speaking, one should do similar substractions for higher multipolarities and for exchange interaction as well. However, all these contributions are relatively small.

Thus, we do not calculate the diagrams presented at Fig. 5 in direct way. Instead of this we calculate the Green function in the potential (3) and then use it in the expression (2) for polarization operator. This procedure is equivalent to the summation of the chain Fig. 5.

There are diagrams in correlation correction that describe the interaction of the particle and hole with external electron (Fig. 9). However the diagrams 9,a and 9,b are of the opposite sign and cancel each other almost exactly. Actually, the interaction with small
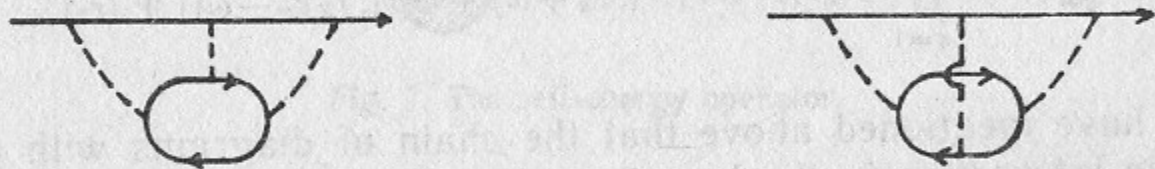

Fig. 9. Interaction of a hole and particle from the loop with an external electron.

and almost constant potential of distant external electron shifts the energies of the core and excited orbitals on the same value and practically does not influence on the wave functions. The fact of cancelation was proved by direct calculation of the third order in the Ref. [3].

The sum of the screening diagrams presented at Fig. 6 (effective screening operator) is of the form

$$\pi(\omega) = \Pi(\omega) [1 + i\hat{Q} \Pi(\omega)]^{-1}. \qquad (5)$$

The angular variables are separated and this equation is written down for fixed multipolarity. Q is the multipole component of Coulomb interaction: $Q_k = r_<^k / r_>^{k+1}$. Screened Coulomb interaction (Fig. 6) looks as follow:

$$\bar{Q} = Q - iQ\pi Q. \qquad (6)$$

The self-energy operator Σ is defined by diagrams presented at Fig. 7. In the leading order correction to the energy of the level equals to the average value of the Σ:

$$\delta E = \langle \Psi | \Sigma | \Psi \rangle. \qquad (7)$$

To take into account to chain of diagrams presented at Fig. 8 it is enough to add Σ to the potential V^{N-1} in the Dirac equation for the orbital of an external electron

$$V^{N-1} \to V^{N-1} + \Sigma. \qquad (8)$$

It is easy to take into account the insertion of the Σ in the internal electron orbitals (see Fig. 10). However, it was proved in Ref. [7] that this contribution to the external electron energy is very small.
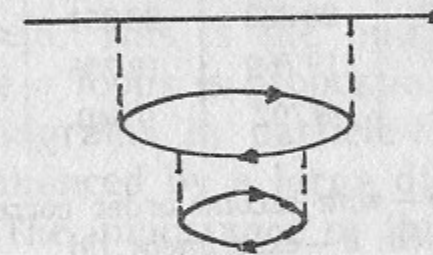

Fig. 10. Insertion of the self-energy correction in the orbitals of closed shells.

For the calculation of self-energy operator we integrate over frequency ω in Fig. 7,a and over frequencies ω_1, ω_2 in Fig. 7,b numerically in the complex plane. For example, the contribution 7,a looks as follow

$$\Sigma^a(r_1, r_2, E) = -i \sum_{k,j,l} C(k, j, l) \int \frac{d\omega}{2\pi} G_{jl}(r_1, r_2, E + \omega) Q_k. \qquad (9)$$

Here $C(k, j, l)$ is the angular coefficient. The technical details of calculations are described in the Ref. [4].

In heavy atoms the Lamb shift can be sizable. However for Cs it is not large: $\Delta E_{6s} = 28$ cm^{-1}, $\Delta E_{7s} = 7$ cm^{-1} [8].

Table 1

The Correlation Corrections to the Energy in Units (-1 cm^{-1})

	a	b	c	d
$6s$	3 886	2 419	3 087	3 425
$7s$	941	579	740	761
$6p_{1/2}$	1 533	966	1 297	1 461
$6p_{3/2}$	1 374	858	1 164	1 310

a — second order of perturbation theory (Fig. 1); b — second order with screened residual Coulomb interaction (Fig. 2); c — screening and particle-hole interaction taken into account (Figs 5—7); d — the final result: second order + screening + particle-hole interaction + chaining of self-energy (Fig. 8).

Table 2

Caesium Energy Levels in Units (-1 cm^{-1})

	a	b	c	d
$6s$	27 949	31 835	31 374	31 407
$7s$	12 110	13 051	12 871	12 872
$6p_{1/2}$	18 800	20 333	20 261	20 229
$6p_{3/2}$	18 395	19 769	19 705	19 675
$7p_{1/2}$	9 225	9 702	9 640	9 641

a — relativistic Hartree — Fork; b — with second order correlation correction; c — with final value of correlation correction; d — experiment [9].

RESULTS

The results of calculations are presented in the Tables 1 and 2. The difference between calculated and experimental values of energy is ~0.1%. However such a good agreement with experiment may prove to be accidental and it is useful to estimate accuracy in the independent way. Firstly, about the numerical accuracy of calculation. The Hartree — Fock values of energies are in agreement with that obtained in the Ref. [3] with accuracy better than 0.1%. The values of the second order correlation correction agree with Ref. [3] with accuracy ~1%, but the contribution of this correction to the energy is ≤10% and therefore once more we have the esti-

mation of the error ≤0.1%. Concerning the perturbation theory convergency we can refer to the paper [5] where all diagrams of the 3-d order are calculated. The contributions of the 3-d order diagrams which are not absorbed by the subsequencies calculated in the present work is 0.1—0.3% with respect to the energy. The Breit correction is small as well because its relative value is ~α^2 (it is calculated in [5]). Thus, we can claim that the theoretical accuracy of present calculation (the accuracy determined not from the comparison with experiment but from the estimation of higher orders of perturbation theory) is better then 0.3%.

CONCLUSION

Three dominating subsequencies of diagrams contributing to the correlation correction are calculated.

1. Screening of the residual Coulomb interaction (Fig. 2). These diagrams are enhanced due to the collective contribution of the electrons into the loop. For example, the external electric field is screened to zero at $r \rightarrow 0$ (Schiff theorem). The enhancement parameter is the number of electrons in the external closed subshells N_e [4]. For caesium $N_e \approx 6$. This is the number of $5p$-electrons. The diagram containing the n loops is proportional to N_e^n.

2. The chain of diagrams in particle-hole interaction (Fig. 5). These diagrams are enhanced by a large diagonal Coulomb integral of zero multipolarity. The importance of this contribution 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.

3. Self-energy chaining (Fig. 8). The enhancement arises due to the small energy denominator ΔE_{ext} corresponding to the excitation of the external electron. The enhancement factor is $\Delta E_{ext}/\Delta E_{int}$.

The all other diagrams of perturbation theory are proportional to the powers of the small parameters $Q_{nd}/\Delta E_{int}$, where Q_{nd} is a nondiagonal Coulomb integral and ΔE_{int} is a large energy denominator corresponding to excitation of the core electron. In the perturbation theory with screened residual interaction this parameter is suppressed in adition by the screening factor. Thus, one may hope that the way of calculation used in the present work provides high accuracy not only in the alkaline atoms but in the other atoms as well.

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

Summation of the Perturbation Theory High Orders Contributions to the Correlation Correction for the Energy Levels of Caesium Atom

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

Суммирование высших порядков теории возмущений в корреляционной поправке к уровням энергии атома цезия