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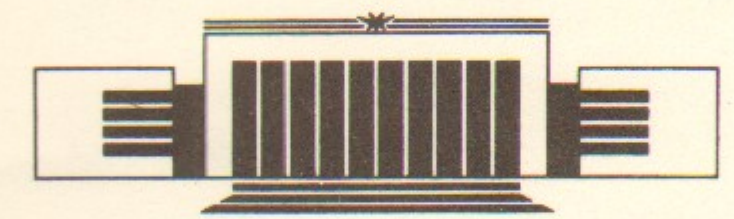
ИЯФ

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SUMMATION OF THE HIGH ORDERS OF PERTURBATION THEORY FOR THE PARITY NONCONCERVING E1-AMPLITUDE OF 6s — 7s-TRANSITION IN CAESIUM ATOM

Summation of the High Orders
of Perturbation Theory
for the Parity Nonconcerving E1-amplitude of
$6s — 7s$-transition in Caesium Atom

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ABSTRACT

Three dominating subsequences of diagrams in the correlation correction to amplitude are summed: screening of the electron-electron interaction, particle-hole interaction and the iterations of the self-energy. The result of calculations is: $E1(6s — 7s) = (0.91 \pm 0.01) \cdot 10^{-11} iea_B (-Q_W/N)$, Q_W is the weak charge of the nucleus, N is the number of neutrons. The experiment [1] and our calculation give the following value of the Weinberg angle: $\sin^2\theta_W = 0.226 \pm 0.007$ (exp.) ± 0.004 (theor.)

Recent measurements of the parity nonconservation (PNC) in the caesium atom [1] (see also the earlier works [2, 3]) have the accuracy about 2%. There are numerous calculations of the effect [4 — 18]. However only in the work [17] the accuracy of calculation 2% was declared. The improvement of both the experimental and theoretical accuracy allow us to make more precise the knowledge of electroweak theory parameter, Weinberg angle, and to improve the limits on the t-quark and extra Z-bozon masses (see e. g. Ref. [19]).

In the present work we have done the new calculation of PNC E1-amplitude for $6s — 7s$-transition in caesium (E_{PNC}). The calculation is based on the approach developed by us in the papers [20]. This approach provides the accuracy about 0.1% for the caesium energy levels and about 0.5% for the hyperfine structure constants and amplitudes of E1-transitions.

The way of calculation is as follows:

1. As zero approximation we use the wave functions and energies obtained by the relativistic Hartree — Fock method (RHF) in the frozen field of atomic core (V^{N-1}-potential [21]).
2. At the second step we calculate E_{PNC} taking into account the polarization of the closed shells by the electron-nucleon weak interaction and by the electromagnetic field of the photon. We use the time-dependent Hartree — Fock (TDHF) method to do this step. The result of corresponding calculation is presented in the first line of the Table 1.
3. The third and the most complicated step is the calculation of the correlation correction.

All the three points of this program have been realized by us in the work [17]. In the similar way the calculations have been carried out by the Indiana group [18]. The new result of the present paper is the more precise calculation of the correlation correction (point 3), and we will discuss only this point.

At the Fig. 1 we present the diagrams for the self-energy operator of an external electron $\Sigma(r_1, r_2, E)$ which is due to the many-body effects in second order in residual Coulomb interaction. The correlation correction to the energy level of an external electron in the linear approximation in Σ equals

$$\delta E_n = \langle n | \Sigma(r_1, r_2, E_n) | n \rangle. \qquad (1)$$

To produce the diagrams for the transition amplitude under discussion one should add the operators of weak interaction and of interaction with the photon into the electron lines. The most important are the diagrams where the interaction with external field (weak or electromagnetic) is introduced into external electron line (Fig. 2). These diagrams are enhanced by the small denominator ΔE_{ext}, which corresponds to the excitation of an external electron [10, 22]. 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 ΔE_{int} (see Fig. 3), and these diagrams are suppressed. For the contributions of the higher orders 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. The diagrams with the photon 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 calculate more accurately these contributions.

It is easy to check that the Brueckner type contributions to the transition amplitude are completely determined by the self-energy operator. The technique of calculation of Σ is described in detail in the Ref. [20]. Here we remind it very briefly. In the second order of perturbation theory one can obtain Σ by the direct summation over the intermediate states of the discrete and continuous spectrum. We have used this way in our earlier works, and the same way have been used by the Johnson group [18]. In the recent works [20] as well as in the present one we use the Green functions and the

Fig. 1. Second order correction to the self-energy operator (energy level). Wavy line denotes a residual Coulomb interaction.
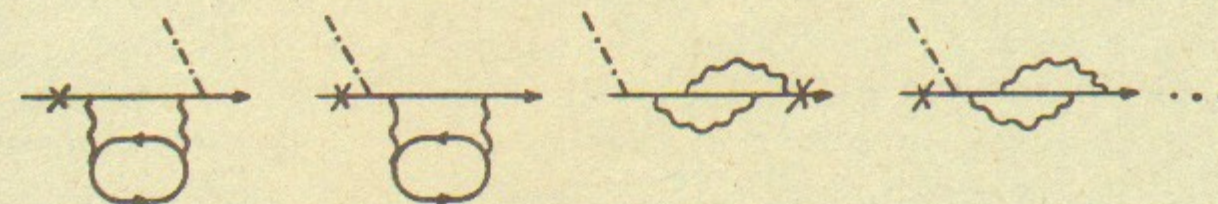

Fig. 2. Examples of Brueckner type correlation corrections to PNC E1-amplitude. Cross denotes weak interaction, dash-dotted line denotes photon field.
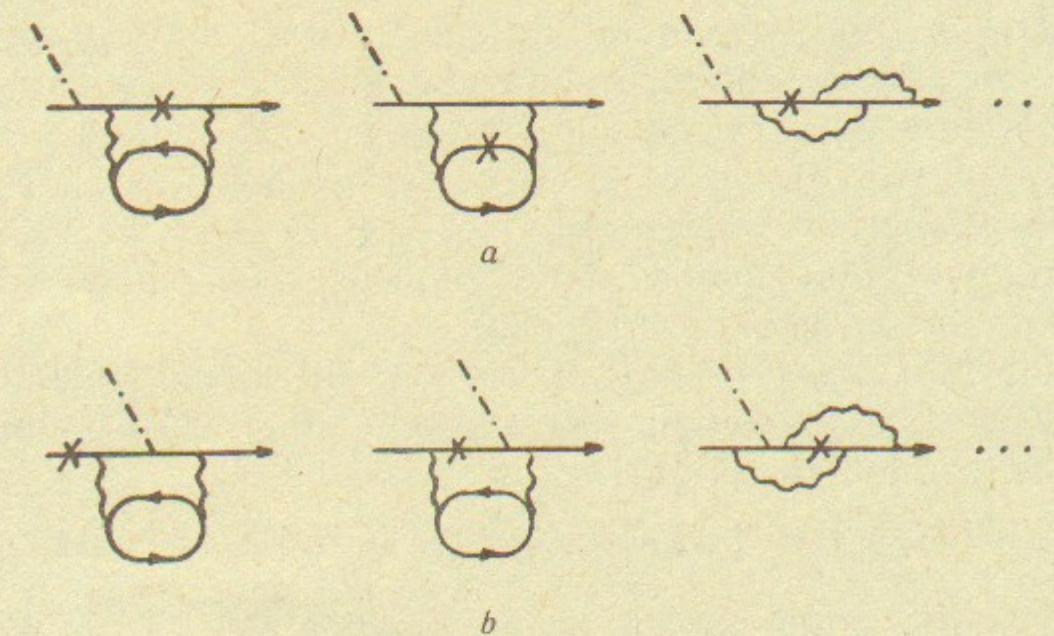

a

b

Fig. 3. Non-Brueckner correlation corrections to PNC amplitude: *a* — weak interaction inside the correlation correction (weak correlation potential); *b* — structural radiation.

Feynman technique. This way allows us to sum the dominaiting diagrams of higher orders and even in the second order it provides the better numerical accuracy.

We sum the three types of enhanced higher order diagrams. The most important contribution is the screening of residual Coulomb interaction. Corresponding sequence of diagrams is presented at Fig. 4. 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 [20]. The second contribution is the chain of diagrams in particle-hole interaction inside the electron loop (Fig. 5) which enters into the diagrams presented at Figs 1—4. 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. Finally the iterations of the self-energy operator Σ (Figs 6, 7) gives the sizable contribution. 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 diagrams of perturbation theory are proportional to the powers of the small parameter $Q_{nd}/\Delta E_{int}$ where Q_{nd} is a nondiagonal Coulomb integral and ΔE_{int} is a large energy denominator corresponding to excitation of the core electron.

In 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% [23, 24]. Summation of the pointed above sequences of higher order diagrams reduces the error to 0.1% [20].

In the first order in Σ (i. e. without the chaining of the Σ) the Brueckner type correlation correction to the PNC E1-amplitude of $6s-7s$-transition equals [17]

$$\langle \Psi_{7s}|\Sigma|\delta X_{6s}\rangle + \langle \delta\Psi_{7s}|\Sigma|X_{6s}\rangle + \langle \delta Y_{7s}|\Sigma|\Psi_{6s}\rangle + \langle Y_{7s}|\Sigma|\delta\Psi_{6s}\rangle. \qquad (2)$$

Here Ψ is the single-particle wave function, $\delta\Psi$, X, Y, δX, δY are the corrections to this wave function. $\delta\Psi$ is induced by the weak interaction, X and Y are the positive frequency and negative frequency corrections induced by the electric field of the photon, and finally δX, ΔY are the positive and negative frequency corrections induced by the combined action of weak interaction and of the electric field of the photon (see Ref. [17]). The results of calculations of
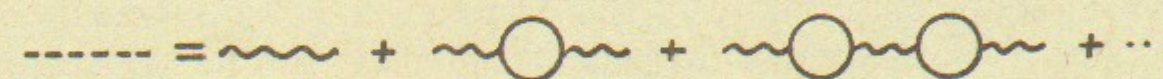
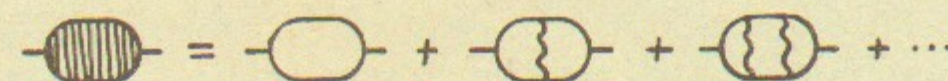Fig. 4. Screening of electron-electron interaction.

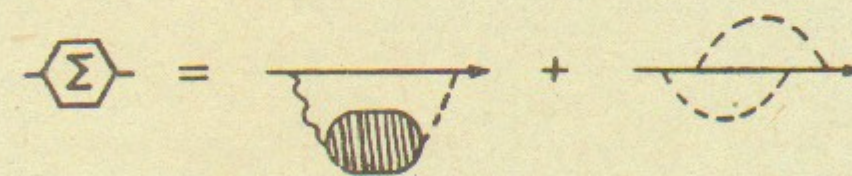Fig. 5. The hole-particle interaction in the polarization operator.
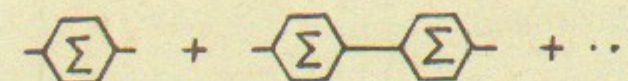

Fig. 6. The self-energy operator.

Fig. 7. Chaining of the self-energy.

the terms in the expression (2) with the operator Σ obtained in the way described above are presented in the Table 1.

The Brueckner type correlation corrections to the transition amplitude can be calculated by the correlation potential method [25, 10, 22]. 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 equations for the single-particle orbitals and corrections to these orbitals induced by the weak interaction and by the photon field are solved with the new potential. The transition amplitude can be found using these wave functions in the same way as in the usual time-dependent Hartree—Fock method [17]. The difference between the amplitude obtained in such a way and amplitude obtained using formula (2) is due to the nonlinear in Σ terms (the self energy chaining, Figs 6, 7). The corresponding value is presented in the line 6 of Table 1.

Table 1

Contributions into the E_{PNC}—Amplitude of 6s—7s-Transition in Caesium in Units $10^{-11} iea_B (-Q_W/N)$

TDHF value. The polarization of the closed shells by the weak interaction and by the photon field is taken into account	0.886
$s_1 = \langle \Psi_{7s} \mid \Sigma \mid \delta X_{6s} \rangle$	0.073
$s_2 = \langle \delta \Psi_{7s} \mid \Sigma \mid X_{6s} \rangle$	0.185
$s_3 = \langle \delta Y_{7s} \mid \Sigma \mid \Psi_{6s} \rangle$	−0.074
$s_4 = \langle Y_{7s} \mid \Sigma \mid \delta \Psi_{6s} \rangle$	−0.141
Nonlinear in Σ correction	−0.021
The contribution of diagrams with the weak interaction inside the correlation, but the photon at the external electron line (Fig. 3,a): $\langle Y_{7s} \mid \delta \Sigma \mid \Psi_{6s} \rangle + \langle \Psi_{7s} \mid \delta \Sigma \mid X_{6s} \rangle$	0.003
Structural radiation (Fig. 3,b)	0.003
The normalization contribution	−0.006
Final result: The sum of all contributions	0.908

There is the contribution to the E_{PNC} which is due to the diagrams with the weak interaction inside the correlation, but photon field attached to the external electron line (weak correlation potential, Fig. 3,a). In the notations of the Ref. [17] this is

$$\langle Y_{7s} \mid \delta \Sigma \mid \Psi_{6s} \rangle + \langle \Psi_{7s} \mid \delta \Sigma \mid X_{6s} \rangle. \qquad (3)$$

Its value calculated in Refs [17, 18] is very small (Table 1).

The structural radiation (Fig. 3,b) and the normalization contributions [17] are presented in the Table 1 as well.

In the last line of the Table 1 the sum of all contributions is presented. This is the result of the present work.

Before to proceed to discussion of the accuracy we would like to consider the disagreement between the results of the papers [17, 18]. This discussion will be useful in the analysis of present calculation accuracy. The values of E_{PNC} in the units of $iea_B \cdot 10^{-11} (-Q_W/N)$ are:

our earlier value [17]	0.90(2),
W. Johnson et al. [18]	0.95(5).

Within the pointed errors the results agree. However in the formal calculation there is disagreement. Our result [17]: 0.904. The Indiana group result [18]: 0.951. It should be noted that the results should not coincide exactly. Actually, in the Ref. [17] the electromagnetic polarization is taken into account in the correlation correction, while in the Ref. [18] this effect is neglected. Besides that there are the cortributions of the structural radiation and normalisation in the Ref. [17]. These effects reduce the disagreement from 0.047 to 0.03.

Table 2

Brueckner Type Second Order Correlation Corrections in Terms of the Contributions to the Expression (2) in Units $10^{-11} iea_B (-Q_W/N)$

	s_1	s_2	s_3	s_4	$s_1 + s_2$	$s_3 + s_4$	$s_1 + s_2 + s_3 + s_4$
Present work	0.123	0.197	−0.115	−0.144	0.320	−0.259	0.061
Ref. [18]					0.321	−0.263	0.058

We should say that in the work [17] we had not high numerical accuracy in the calculation of the correlation correction (accuracy was about 10% in each term). In the present work we use Green functions and Feynman technique which give better numerical accuracy. We have recalculated the second order correlation correction without the electromagnetic polarization and structural radiation. The result of this calculation in terms of contributions to the formula (2) is presented in the Table 2. In the same Table the results of

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Ref. [18] are presented. Thus we see that formal second order practically coincides with the result of the Johnson and collaborators [18], but not with our old one [17]. The couse of small dicrepancy with Ref. [17] was the limited basis set used in work [17] in the integration over continuous spectrum.

However we insist that the result of Ref. [17] has better physical accuracy than the result of Ref. [18]. Calculation which we carried out in the Ref. [17] was not pure ab initio calculation. The statement about the accuracy was based on the analysis of experimental data on energy levels, hyperfine structure, and E1-amplitudes. Let us elucidate this statement. The structure of PNC-amplitude in terms of expansion in physical states is as follows:

$$\frac{\langle 7s|r|7p\rangle\langle 7p|H_W|6s\rangle}{E_{6s}-E_{7p}} + \frac{\langle 7s|r|6p\rangle\langle 6p|H_W|6s\rangle}{E_{6s}-E_{6p}} + \frac{\langle 7s|H_W|6p\rangle\langle 6p|r|6s\rangle}{E_{7s}-E_{6p}}. \quad (4)$$

The other states np give rather small contribution. These three terms have the same magnitude but the different signs. Let us consider the correlation corrections. There are the corrections to the matrix elements and to the energy denominators. The denominators are relatively small and we would like to discuss the corrections to them.

When we use the perturbation theory we expand the denominators, e. g.

$$\frac{1}{E_{6s}+\Sigma_{6s}-E_{6p}-\Sigma_{6p}} = \frac{1}{E_{6s}-E_{6p}} - \frac{\Sigma_{6s}}{(E_{6s}-E_{6p})^2} + \frac{\Sigma_{6p}}{(E_{6s}-E_{6p})^2}. \quad (5)$$

We can do it because the total correction to the denominator is not very large. At the same time each term in expansion (5) is large: $\Sigma_{6p}/(E_{6s}-E_{6p})=0.4$. This is the reason why the relatively small second order correction to the PNC-amplitude arises as the compensation of the large contributions. We know that exact second order calculation overestimates the correlation correction by 5—20% [24, 20]. This is just about 1% of the energy, but due to the small denominator the inaccuracy is enhanced in expansion (5).

In the Ref. [17] our idea was that we did not need the numerical accuracy of the second order to be better than the contribution of higher orders. However keeping in mind the situation with the small denominators we tried to fit carefully the energy levels. If our ab initio calculation did not reproduce the energy level we multiplied the correlation correction by some numerical factor to fit

energy. One can say that this is effective accounting of both the higher orders and numerical inaccuracy in most sensitive part: energy denominators (note that hyperfine structure and E1-amplitude calculations also gave better results after energy fit procedure). The result of the present work with the summation of the higher orders confirms this idea.

Accuracy of Calculation

We can estimate the numerical error of the computer codes comparing our evolution of TDHF value and second order correlation correction with that obtained in Refs [12, 18]. The conclusion is that this error does not exceed 0.3%.

The more complicated question is the physical accuracy of calculation, i. e. estimation of unaccounted diagrams. Let us start with the contribution of an unaccounted diagrams in Σ. In the Ref. [25] all diagrams of the third order in residual interaction have been calculated for the energy level shift. The third order contributions which are not absorbed by the sequences which we have summed exactly proved to be about 1—3% of the correlation correction value [20]. The maximal Brueckner type correction to the E_{PNC}, $\langle\delta\Psi_{7s}|\Sigma|X_{6s}\rangle$, is about 20% of E_{PNC}-value. Basing on the experience on energy we can estimate the error which comes from the Brueckner type diagrams as 0.2—0.6%. We estimate the structural radiation using the approximate formula obtained in Ref. [22]. Therefore the error in its evolution could be about 100%, but the structural radiation is small by itself: 0.3%.

The reasonable estimation of inaccuracy one can obtain comparing the calculated values of the energy levels, hyperfine structure intervals, and E1-amplitudes with the experimental data. For the energy levels we have the accuracy about 0.1% [20]. For the hyperfine structure and E1-amplitudes accuracy is not worse than 1% (except small E1-amplitude of $7s—6p$-transition) [20].

We can try to refine the calculated values by fitting the available experimental data. It was mentioned above that the E_{PNC} is very sensitive to the energy splitting between the levels of opposite parity ns and np. Main contribution to the amplitude depends on the $6s$-, $6p$-, $7s$-, $7p$-states (expression (4)). The corresponding energy levels can be reproduced exactly if we introduce by hands the coefficients into self energy operators calculated by us:

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

After this procedure the theoretical values of E1-amplitudes and hyperfine intervals become somewhat more close to the experimental values [20]. The value of E_{PNC} after fit (6) practically does not change due to the compensation between different contributions.

<div align="right">T a b l e   3</div>

<div align="center">Results of Calculations and Measurements of 6s—7s PNC
Caesium Amplitude in Units $10^{-11} i e a_B(-Q_W/N)$</div>

	Bouchiat and Bouchiat	[4]	1.33
	Loving and Sandars	[5]	1.15
	Neuffer and Commins	[6]	1.00
	Kuchiev et al.	[7]	0.75
	Das et al.	[8]	1.06
	Bouchiat et al.	[9]	0.97 ± 0.10
	Dzuba et al.	[10]	0.88 ± 0.03
Calculations	Schaffer et al.	[11]	0.74
	Martensson-Pendrill	[12]	0.886
	Plummer and Grant	[13]	0.71
	Schaffer et al.	[14]	0.92
	Johnson et al.	[15]	0.890
	Bouchiat and Piketty	[16]	$0.935 \pm .02 \pm .03$
	Dzuba et al.	[17]	0.90 ± 0.02
	Johnson et al.	[18]	0.95 ± 0.05
	Present work		0.91 ± 0.01
Experiment: values divided by $(-Q_W/N) = 0.9207$ corresponding to $\sin^2(\theta_W) = 0.230$	Bouchiat et al.	[2]	$0.89 \pm .10 \pm .07$
	Noecker et al.	[1]	0.90 ± 0.02

To control the accuracy it is useful to consider the «weaklike» expression which reproduces the dependence of E_{PNC} (4) on the energy intervals, wave functions at the nucleus, and E1-amplitudes (see, e. g. Ref. [10])

$$\sum_{n=6,7} \frac{\langle 7s|r|np \rangle \sqrt{A_{np} A_{6s}}}{E_{6s} - E_{np}} - \frac{\langle 6s|r|np \rangle \sqrt{A_{np} A_{7s}}}{E_{7s} - E_{np}}\,. \qquad (7)$$

Theoretical values of the E1-amplitudes $\langle f|r|i \rangle$ and hyperfine constants A are presented in the Ref. [20]. Expression (7) calculated with the values of $\langle f|r|i \rangle$ and A obtained in pure ab initio way is by 0.35% less than that with the experimental values. We would like to note that there is the partial compensation of errors between the terms in (7). Evolution of (7) with the parameters obtained after fit (6) gives value by 1% less than «experimental» value. The fit reduces the error in each term, but destroy the compensation. In any case it should be noted that the «experimental» error in (7) is 1.3%.

We think that all above arguments show that the accuracy of the present calculation is about 1%. Thus the final result of the present work looks as follows:

$$E_{PNC} = (0.91 \pm 0.01) \cdot 10^{-11} i e a_B(-Q_W/N)\,. \qquad (8)$$

Results of other calculations and measurements are presented in Table 3.

Comparison with Experiment

Measurement [1] and our calculation (8) lead to the following value of caesium weak charge:

$$(-Q_W/N) = 0.909 \pm 0.020 \text{ (exp.)} + 0.010 \text{ (theor.)} \qquad (9)$$

In the standard model of weak interaction with radiative corrections [27] weak charge is expressed trough the Weinberg angle:

$$\sin^2(\theta_W) = 1 - M_W^2/M_Z^2\,,$$
$$(-Q_W/N) = 0.9793 - Z/N \cdot (0.9793 - 3.8968 \sin^2(\theta_W))\,. \qquad (10)$$

Using (9), (10) we obtain Weinberg angle:

$$\sin^2(\theta_W) = 0.226 \pm 0.007 \text{ (exp.)} + 0.004 \text{ (theor.)} \qquad (11)$$

This value agrees with world average value $\sin^2(\theta_W) = 0.230 \pm 0.005$ [27] and has the accuracy comparable with the best measurements of Weinberg angle.

Using our new experience of high order correlation calculations we together with P.G. Silvestrov reanalysed our old calculation of parity nonconservation in Bismuth [28]. Now we think that it is better to present the results of calculations [28] as follow:

$$Bi(\lambda=876): \quad E_{PNC}=26.2, \quad R=-11.0\pm1.3,$$
$$Bi(\lambda=648): \quad E_{PNC}=4 \quad , \quad R=-7.5\pm5 . \tag{12}$$

$R=\mathrm{Im}(E_{PNC}/M1)$ is given in the units $(-Q_W/N)\cdot10^{-8}$, λ is a wavelength in nanometers. The values for $\lambda=876$ transition differ a little from the values presented in paper [28] ($E_{PNC}=25$, $R=10.4\pm1$) due to change of estimate of high order $6p-6p$-correlations (Bismuth ground state configuration is $...6s^26p^3$). The values for $\lambda=648$ transition calculated in the work [28] are presented for the first time. Large error in this transition is due to strong cancellation of different contributions to E_{PNC}: TDHF amplitude is 9.9, correlation with electron core gives -0.5, first order $6p-6p$-correlation is -8.5, high orders $6p-6p$-correlations give 3. Corresponding contributions to $\lambda=876$ transition amplitude are: 32.8, -1.7, -10.4, 5.5). The references on the measurements and other calculations can be found e. g. in Refs [28—30].

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**Summation of the High Orders of Perturbation Theory
for the Parity Nonconcerving E1-amplitude of
6s — 7s-transition in Caesium Atom**

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

**Суммирование высших порядков теории возмущений
в нарушающей четность E1-амплитуде
перехода 6s — 7s в цезии**