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ON HARTREE—FOCK CALCULATION OF ELECTRON ELECTRIC DIPOLE MOMENT ENHANCEMENT FACTOR FOR THE THALLIUM ATOM

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On Hartree—Fock Calculation of Electron Electric Dipole Moment Enhancement Factor for the Thallium Atom

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ABSTRACT

A perturbation theory expansion of the relativistic Hartree—Fock calculation of electron electric dipole moment enhancement in thallium is considered. The RPAE result appears to be highly overestimated because of an overestimation of the T-odd exchange polarization. The correlations, calculated in present work, reduce this result by 70%.

1. INTRODUCTION

It is known, that existence of electric dipole moment (EDM) of elementary particles would mean the violation of time invariancy. One of observable T-violating effects is the atomic EDM, induced by the EDM of electrons, which for heavy atoms may be essentially larger, than the electron EDM [1, 2].

In Refs [3, 4] the enhancement of electron EDM was calculated for some heavy atoms with one unpaired electron over the closed shells. For Tl atom a very strong difference was found between the relativistic Hartree—Fock result from one side, and the calculations in the model potentials and semi-empirical results [2, 5] from another side (Table 1).

In present work the relativistic Hartree—Fock calculation of EDM enhancement in thallium atom is done, some of the second-order correlations also are calculated. We analyze the reasons, which lead in the case of thallium atom to the large difference between the results of different methods and to the large value of correlations.

2. CALCULATION PROCEDURE

Calculation for the Tl atom, which has one unpaired electron $6p_{1/2}$ over the closed shells, is made in $V^{(N-1)}$ approximation. In this approximation the Hartree—Fock potential V is limited by a sum

over the closed shell electrons. This make it possible to apply the same potential both to the inner-shell and external electrons, the wave equations for inner electrons are solved self-consistently, for external — in frozen core approximation. A self-action, which formally appears in equations for inner electrons, is exactly cancelled in sum of direct and exchange potentials. Then the corrections, due to the difference between the Hartree — Fock potential and exact many-particle Hamiltonian, are calculated by the perturbation theory methods. The procedure of EDM calculation is very close to that of P-violating E1 transition amplitudes, caused by the weak electron-nucleon interaction [6]. This make it possible to use with a slight changes a complex of programs, developed in work [6].

To find the atomic EDM the shift of atomic energy in a static external electric field $\vec{E}_0$ was calculated: $\delta\varepsilon_{at} = -\vec{d}_{at}\cdot\vec{E}_0$. Energy shift for every electron is proportional to its angular momentum projection, so the energy shifts of inner-shell electrons cancel each other and only the external electron contribution remains. The dimensionless EDM enhancement coefficient is determined as $R = d_{at}/d_e = -\delta\varepsilon_{at}/(E_0 d_e)$.

The total one-particle perturbation operator looks as

$$\begin{aligned} W &= W_d + W_E + W_{Ed}, \\ W_d &= -d_e(\beta - 1)\,\vec{\Sigma}\vec{E}_{at}, \\ W_E &= -er\vec{E}_0, \\ W_{Ed} &= -d_e(\beta - 1)\,\vec{\Sigma}\vec{E}_0, \end{aligned} \qquad (1)$$

where W_d — T-violating interaction of electron EDM $\vec{d}_e$ with atomic own electric field $\vec{E}_{at}$, W_E and W_{Ed} — interactions of electron charge and EDM with external electric field, $\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ and $\vec{\Sigma} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix}$ — the Dirack matrices. Expressions for W_d and W_{Ed} are written with accounting of Schiff's theorem [7]. The matrix element of T-odd interaction with atomic field riches an order of $Z^3\alpha^2$, and with external field — α^2. So, in the heavy atoms, the interaction of external electric field with a direct electron EDM is much smaller, than that with the atomic EDM, induced by the T-odd interaction W_d, and the direct interaction W_{Ed} is neglected in present calculation.

Atomic electrical field in $V^{(N-1)}$ approximation is determined by

the summary charge density of nucleus and closed-shell electrons. So it is spherically symmetrical and T-odd interaction looks as

$$W_d = 2d_e \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} E_{at}(r)\,(\vec{\sigma}\cdot\vec{n}), \qquad (2)$$

where $\vec{n} = \vec{r}/r$. Strictly speaking, here it is necessary to exclude the self-action (interaction between the electron EDM and its own field) and consider the influence of external electron field on the inner-shell electron EDMs. But both this effects gives the contributions of the same order as W_{Ed}, so they also are neglected.

The wave function corrections, due to the T-violating interaction (W_d) and electric (W_E) are calculated independently with accounting of direct and exchange polarizations. Then the mixed corrections, proportional to $E_0 d_e$, are calculated. The energy shift $\delta\varepsilon$ can be determined from the equations for these $E_0 d_e$ corrections.

The total Hartree — Fock result, obtained with accounting of all the polarizations, corresponds to the random phase approximation with exchange (RPAE). At Fig. 1 the diagrams of zero and first order in the Coulomb interaction, giving a nonzero contribution to the total result, are shown. In the RPAE-approximation the first-order corrections in the residual Coulomb interaction, which corresponds to the shielding of external electric field inside the atom, are already taken into account. The calculation with only T-odd polarization taken into account is equal to the sum of 1,*a* and 1,*b* diagrams which corresponds to the «zero order» approximation in Refs [3, 4]. The second-order corrections in residual Coulomb interaction are calculated by the correlation potential method [8]. The diagrams, composing this correlation potential Σ are shown at Fig. 2, the second-order correction diagrams in terms of this potential — at Fig. 3.

3. THE RESULTS OF CALCULATION

The results of calculation in RPAE approximation are listed in Table 2. These results for the calculations with T-odd and all the polarizations taken into account coinside up to the possible numerical uncertainties with the corresponding results of Refs [3, 4]. The calculated second-order corrections are listed in Table 3. Except the total contributions of different diagrams, the simple estimations of

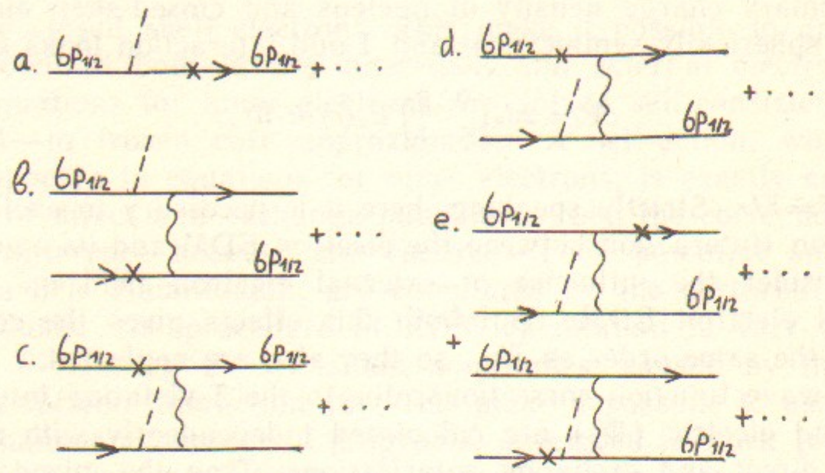


Fig. 1. Zero- and first-order diagrams, giving a nonzero contribution to the RPAE result:

~~ — Coulomb electron-electron interaction. × — T-odd interaction of electron EDM with atomic field. — — — — Interaction with external field.

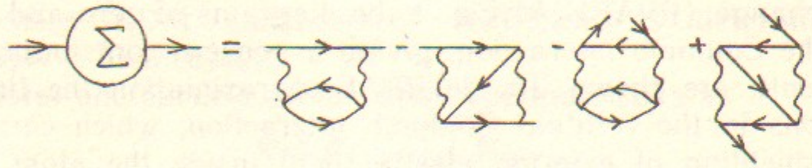


Fig. 2. Second-order diagrams, composing the correlation potential.

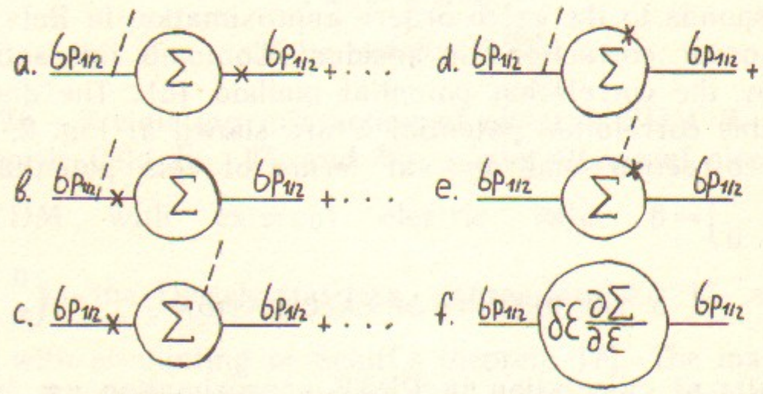
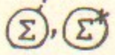


Fig. 3. Diagrams of correlation corrections to the atomic energy shift:



— Diagrams with corresponding interactions on internal lines.

— Contribution of renormalization of correlation potential, due to the shifts of atomic energy levels in external field.

these contributions are listed. This estimations are obtained by summing over the limited number of intermediate states: 6*s*, 7*s*, 8*s*, 9*s* for zero-order diagrams 1,*a* and 6*s*, $6p_{1/2}$ for all other diagrams (Fig. 4). This part of contributions can be expressed through the Coulomb integrals and the matrix elements of T-violating interaction and of electron interaction with external field.

The most unexpected result of correlations calculation (Table 3) is an extremely large contribution of 3,*d* diagrams, including the

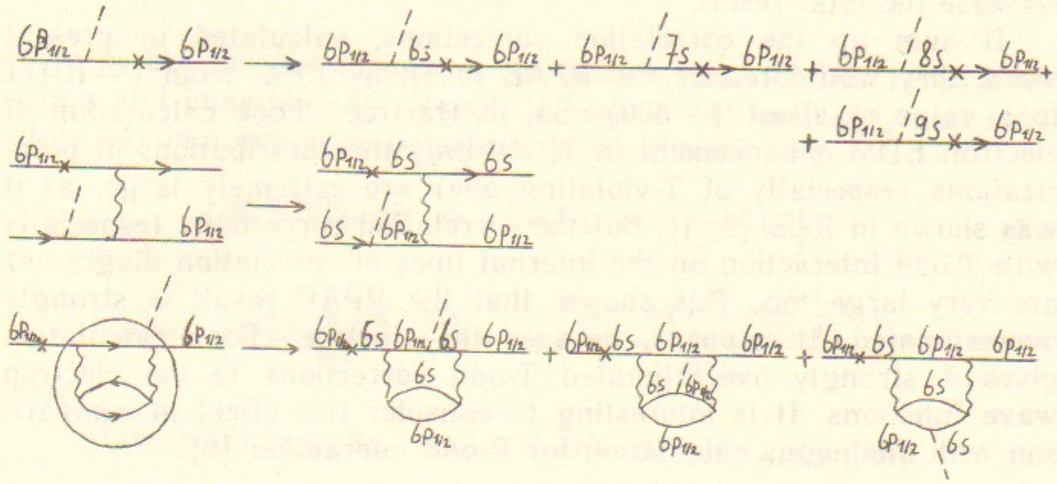


Fig. 4. Estimations of different order diagrams by sum over the limited number of intermediate states.

T-violating interaction on the internal lines of the correlation potential diagrams. In Ref. [6], when such correlations were calculated for the P-odd effects, it was supposed, that the diagrams like 3,*c*, 3,*d*, including one of the interactions (weak or electric one) on the internal lines, were less, than the 3,*a*, 3,*b* ones, containing both interactions on the external lines. Correspondingly, the 3,*e* diagram, including both interactions on the internal lines, should be less, than 3,*c* and 3,*d* ones. The ratio of typical energies of external and inner-shell electrons was considered as a parameter of this suppression. For Tl atom in $V^{(N-1)}$ approximation $\varepsilon_{6p_{1/2}}/\varepsilon_{6s}=0.29$. So in Ref. [6] the calculation of total contribution of diagrams like 3,*c* was changed by an approximate expression [8]:

$$\delta\varepsilon \simeq \langle \tilde{\varphi}_{6p_{1/2}} \left| W_E \frac{\partial\Sigma}{\partial\varepsilon} + \frac{\partial\Sigma}{\partial\varepsilon} W_E \right| \tilde{\varphi}_{6p_{1/2}} \rangle /2 , \qquad (3)$$

where $\tilde{\varphi}_{6p_{1/2}}$ was the $6p_{1/2}$ wave function with T-odd correction. The 3,*e* diagram contribution was approximately estimated by the contribution of 6*s* and $6p_{1/2}$ intermediate states. In our case such estimations are not sufficient because of the large magnitude of 3,*d* diagrams, and the total contributions of 3,*c* and, especially, 3,*e* diagrams are not determined. We can only suppose, that this contributions have the same signes, as estimations, obtained for them, and, so, they reduce to some extent the total correlation correction and increase the total result.

If sum up the correlation corrections, calculated in present work, they would reduce the RPAE result by 70%: from (−1041) to a value of about (−300). So, in Hartree—Fock calculation of electron EDM enhancement in Tl not only the contributions of polarizations (especially of T-violating one) are extremely large, as it was shown in Refs [3, 4], but the correlation corrections (especially with T-odd interaction on the internal lines of correlation diagrams) are very large too. This shows, that the RPAE result is strongly overestimated. It happens, besause the Hartree—Fock calculation gives a strongly overestimated T-odd corrections to the electron wave functions. It is interesting to consider this effect in comparison with analogous calculation for P-odd interaction [6].

4. THE REASONS OF THE P- AND T-ODD CORRECTIONS OVERESTIMATION IN HARTREE—FOCK CALCULATION

The P-odd weak electron-nucleon interaction, considered in Ref. [6], and T-odd interaction of electron EDM with spherically symmetrical atomic field have the identical transformation qualities: they both are the pseudoscalar interactions. Significant difference between these two interactions is, that the matrix elements of the T-odd interaction are real and the P-odd — imaginary.

In Hartree-Fock calculation of P- and T-odd wave function corrections the self-consistent procedure converge slowly, and the resulting matrix elements $\langle \varphi_j | \delta\varphi_i \rangle = -\langle j | W + \delta V | i \rangle / \Delta\varepsilon_{ji}$ are much larger, than the initial matrix elements $-\langle j | W | i \rangle / \Delta\varepsilon_{ji}$, especially for $i, j = 6s, 6p_{1/2}$ (Table 4). Here W is P- or T-odd interaction, δV — corresponding exchange polarization (the direct polarization in first order in $\delta\varphi$ is equal to zero).

The reasons of such behaviour can be understood in the model,

taking into account the polarization of only one closed shell and neglecting the polarizations of other shells. The $6s^2$ shell is the most interesting for us because, firstly, for this shell the considered effect is large enough, and, secondly, the polarization of this shell makes the major contribution to the RPAE result (Table 2). Then in exchange polarization δV_{6s^2} only the sum over two 6*s* electrons remains. We can write the correction to the 6*s* wave function like

$$\delta\varphi_{6s} = \sum_n a_n \varphi_{np_{1/2}}, \tag{4}$$

where a_n are the decomposition coefficients, real for the T-odd interaction and imaginary for P-odd. If keep in (4) only $\varphi_{6p_{1/2}}$ and substitute (4) into exchange polarization, we obtain

$$\langle 6p_{1/2} | \delta V_{6s^2} | 6s \rangle = -\left\{ a_6 F_0(s,p) + \frac{1}{3} a_6^* G_1 \right\}, \tag{5}$$

$$a_6 = -\frac{\langle 6p_{1/2} | W + \delta V | 6s \rangle}{\Delta\varepsilon_{6p6s}} = -\frac{W_{6p6s} - a_6\left(F_0(s,p) \pm \frac{1}{3} G_1\right)}{\Delta\varepsilon_{6p6s}},$$

where

$$F_0(s,p) = F_0(6s, 6s, 6p_{1/2}, 6p_{1/2}), \quad G_1 = G_1(6s, 6p_{1/2}, 6p_{1/2}, 6s),$$

$$F_0(\varphi_1, \varphi_2, \varphi_3, \varphi_4) = \iint f_1^+(r_1)\, f_2(r_1)\, \frac{e^2}{r_>} f_3^+(r_2)\, f_4(r_2)\, r_1^2\, dr_1\, r_2^2\, dr_2,$$

$$G_1(\varphi_1, \varphi_2, \varphi_3, \varphi_4) = \iint f_1^+(r_1)\, f_2(r_1)\, \frac{e^2 r_<}{r_>^2} f_3^+(r_2)\, f_4(r_2)\, r_1^2\, dr_1\, r_2^2\, dr_2,$$

are radial Coulomb integrals of zero and first multipolarity. Here in the sign (±) (+) corresponds to the case of T-odd interaction, (−) — to the P-odd one ($a_6^* = \pm a_6$). Then we obtain

$$a_6 = -\frac{W_{6p6s}}{\left\{ \varepsilon_{6p} - \varepsilon_{6s} - \left(F_0(s,p) \pm \frac{1}{3} G_1 \right) \right\}}. \tag{6}$$

In self-consistent procedure expression (6) appears as a result of iterations, equal to summing up the diagrams, shown at Fig. 5. This gives us a sum of geometrical progression:

$$a_6^0 = -\frac{W_{6p6s}}{\Delta\varepsilon_{6p6s}}, \quad a_6^1 = -\frac{W}{\Delta\varepsilon} + a_6^0\left(\frac{F_0 \pm \frac{1}{3} G_1}{\Delta\varepsilon}\right) = -\frac{W}{\Delta\varepsilon}\left(1 + \frac{F_0 \pm \frac{1}{3} G_1}{\Delta\varepsilon}\right) \ldots$$

$$a_6^N = -\frac{W}{\Delta\varepsilon} + a_6^{N-1}\left(\frac{F_0 \pm \frac{1}{3}G_1}{\Delta\varepsilon}\right) = -$$

$$= -\frac{W}{\Delta\varepsilon}\left(1 + \frac{F_0 \pm \frac{1}{3}G_1}{\Delta\varepsilon} + \ldots + \left(\frac{F_0 \pm \frac{1}{3}G_1}{\Delta\varepsilon}\right)^N\right),$$

$$a_6^N \xrightarrow[N\to\infty]{} -\frac{W}{\Delta\varepsilon}\,\frac{1}{1 - \frac{F_0 \pm \frac{1}{3}G_1}{\Delta\varepsilon}}.$$

The slow convergence of this progression is connected with a large values of Coulomb integrals of $6s$, $6p_{1/2}$ wave functions in Tl.

The difference between P- and T-odd interactions is connected in this model with a Coulomb integral of first multipolarity $\pm\frac{1}{3}G_1$. If we keep in δV_{6s^2} only the Coulomb integrals of zero multipolarity,

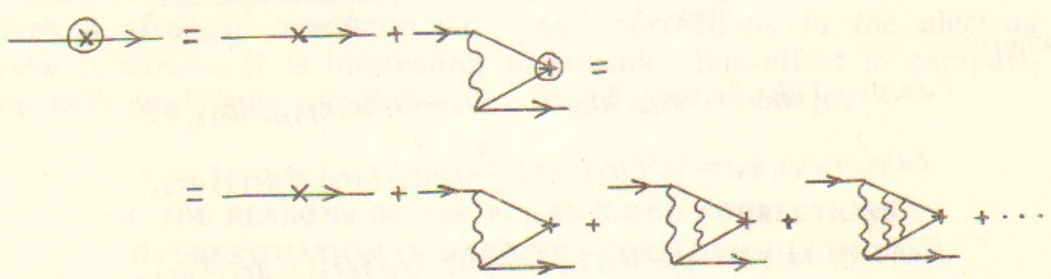


Fig. 5. Diagrams of Hartree—Fock self-consistent calculation of P- and T-odd wave function corrections.

× — P- or T-odd interaction; ⊗ — corresponding interaction with exchange polarization.

the P- and T-odd corrections would behave itself equally. For the T-odd interaction expression (6) gives a value, significantly less, than a total result of corresponding calculation of isolated $6s^2$-shell polarization (Table 4). This difference decreases to some extent when the $n = 5p_{1/2}$, $7p_{1/2}$, $8p_{1/2}$ states are also taken into account in decomposition (4) and a system of linear equations on a_n is solved. The rest difference is probably connected with contributions of continious specter states in expression (4). The difference between the total calculation and the calculation in our model (with δV_{6s^2}) is due to the polarization of other inner shells.

As we have seen, the self-consistent Hartree—Fock calculation

shifts the energetical denominators in expression (6). For the T-odd interaction this shift is of most significance: $F_0 + \frac{1}{3}G_1 \simeq 0.72\Delta\varepsilon$ (for P-odd interaction this shift is $F_0 - \frac{1}{3}G_1 \simeq 0.48\Delta\varepsilon$, for interaction with external field W_E: $F_0 - \frac{5}{9}G_1 \simeq 0.40\Delta\varepsilon$). For the T-odd interaction the reduced one-particle $6s - 6p_{1/2}$ energetical denominator is even less, than the exact energetical denominators—the energy differences between the atomic states $6s^2 6p_{1/2}$ and $6s6p_{1/2}^2$, or ionic states $6s$ and $(6s6p_{1/2})_{00}$, mixing together by a parity violating interaction (Fig. 6). This reduced energetical denominators leads to a highly overestimated T-odd wave function corrections of $6s$ and $6p_{1/2}$ states and, in turn, to a highly overestimated electron EDM enhancement in Tl atom. In semiempirical calculations this does not happen, because the correct many-particle energies are used there.

$6s$ Hartree-Fock calculation	$6s^2$ Tl^+ ion	$6s^2 6p_{1/2}$ Tl atom
$\frac{6p_{1/2}}{(0.487)}$		
$\frac{\varepsilon_{6p_{1/2}} - \varepsilon_{6s} - \left(F_0(s,p) - \frac{1}{3}G_1\right)}{(0.252)}$		
$\frac{\varepsilon_{6p_{1/2}} - \varepsilon_{6s} - \left(F_0(s,p) + \frac{1}{3}G_1\right)}{(0.138)}$	$\frac{(6s6p_{1/2})_{00}}{(0.195)}$	$\frac{6s6p_{1/2}^2}{(0.212)}$

If we calculate the corrections to the Hartree—Fock result in all orders in the residual Coulomb interaction, which is equal to the exact solution, the terms with reduced energetical denominators

$\Delta\varepsilon - \left(F_0 \pm \frac{1}{3}G_1\right)$ would be cancelled and the exact energetical denominators would take their places. We can calculate only the first- and second-order corrections, which reduce the Hartree—Fock result and make it closer to the exact one. The result with this corrections must coincide with the exact result, expanded on powers of the Coulomb integrals up to the first or second power correspondingly.

We can observe the ratio between the RPAE result, second-order corrections and the exact result in a model, equal to that, which leads to the expression (6). Let us consider the three-electron wave functions, corresponding to three external electrons of Tl atom, composed by only two one-particle Hartree—Fock functions: $6s$ and $6p_{1/2}$. According to the Pauli principle, we have only two such functions Ψ_1: $|6s^2 6p_{1/2}\rangle$, Ψ_2: $|6s 6p_{1/2}^2\rangle$. These functions are the eigenfunctions for the three-particle Hartree—Fock Hamiltonian, equal to a sum of three one-particle ones.

In this approximation the exact unperturbed three-particle wave functions (the eigenfunctions for the exact three-particle Hamiltonian without parity violation) formally coincide with Hartree—Fock three-particle unperturbed functions. It happens because the unperturbed Coulomb interaction does not mix together the Ψ_1 and Ψ_2 functions, having an opposite parity. By the same reason, the exact energies of 1 and 2 states differ from Hartree—Fock energies only in the first order in Coulomb interaction:

$$\varepsilon_1 = \varepsilon_{6s} - F_0(s, s)\,,$$

$$\varepsilon_2 = \varepsilon_{6p_{1/2}} + F_0(p, p) - F_0(s, s) - 2F_0(s, p) + \frac{1}{3}G_1\,,$$

where

$$F_0(s, s) = F_0(6s, 6s, 6s, 6s)\,,$$

$$F_0(p, p) = F_0(6p_{1/2}, 6p_{1/2}, 6p_{1/2}, 6p_{1/2})\,.$$

The three-particle matrix elements of parity violating and electric interactions coincide with the one-particle matrix elements between $6s$ and $6p_{1/2}$ states. All this makes it possible to obtain analytically (to express trough the Coulomb integrals and one-particle matrix elements) not only the Hartree—Fock result with polarization and correlation corrections, but also the exact result. For example, the shift of atomic energy in RPAE approximation looks in $6s^2 6p_{1/2} - 6s 6p_{1/2}^2$ basis as

$$\delta\varepsilon^{RPAE} = -2a_6 b_6\left[\Delta\varepsilon_{6p6s} - F_0(p, p) - \frac{1}{9}G_1\right],$$

the correlation correction

$$\delta\varepsilon^{cor} = -\frac{2a_6 b_6}{\Delta\varepsilon_{6p6s}}\left[F_0(s, p) - F_0(p, p) - \frac{2}{3}G_1\right]\left[F_0(s, p) - F_0(p, p) + \frac{2}{9}G_1\right],$$

and the exact result

$$\delta\varepsilon' = -2\langle 6p_{1/2}\downarrow|W_d|6s\downarrow\rangle\langle 6s\downarrow|W_E|6p_{1/2}\downarrow\rangle/(\varepsilon_2 - \varepsilon_1)\,,$$

where $a_6 = -\langle 6p_{1/2}|W_d + \delta V_d|6s\rangle/\Delta\varepsilon_{6p6s}$ is determined by expression (6), analogously

$$b_6 = -\langle 6p_{1/2}\downarrow|W_E + \delta V_E|6s\downarrow\rangle/\Delta\varepsilon_{6p6s} = -\frac{W_{6p\downarrow 6s\downarrow}}{\Delta\varepsilon - \left(F_0 - \frac{5}{9}G_1\right)},$$

where sign $\downarrow$ means $-\frac{1}{2}$ spin projection (it corresponds to the $6s\uparrow 6s\downarrow 6p_{1/2}\uparrow$ — $6s\uparrow 6p_{1/2}\downarrow 6p_{1/2}\uparrow$ matrix element). The results of calculation in $6s^2 6p_{1/2} - 6s 6p_{1/2}^2$ basis for the T-odd mixing coefficient $A = \langle\Psi_2|\delta\Psi_1\rangle$ and the electron EDM enhancement coefficient R are listed in Table 5. We can see, that the corrections of third and higher orders in the residual Coulomb interaction are even higher, than the second order ones.

In the $6s^2 6p_{1/2} - 6s 6p_{1/2}^2$ basis all the correlations are connected with the energetical denominators correction. In the total calculation the corrections, due to the mixing of Hartree—Fock states into exact unperturbed states by residual Coulomb interaction, appears. Moreover, the total value of correlations is much higher, than in our $6s^2 6p_{1/2} - 6s 6p_{1/2}^2$ approximation. So we can not estimate the contribution of higher-order corrections in the total calculation. It is clear only, that they can also be very large.

5. CONCLUSION

So, in Hartree—Fock calculation of EDM enhancement in Tl atom, not only the first-order corrections in the residual Coulomb interaction, but the second-order ones too are extremely large. The sum of correlations, calculated in present work, +740, and total enhancement coefficient —300 can not be considered as the com-

plete results, because the total contribution of the correlation diagrams, containing the interaction with the external electric field on internal lines, is not calculated, and the higher-order corrections are not determined.

The reasons of highly overestimated Hartree—Fock result with T-odd polarization and of large magnitude of corrections to this result are connected with the calculation of T-odd corrections to the wave functions. Especial features of T-odd interaction (reality and transformation qualities of its matrix elements) makes the Coulomb integrals of zero and first multipolity to add one with another in T-odd polarization, and not to subtract, as in P-odd or electric polarizations. The certain ratio between the Coulomb integrals of $6s$, $6p_{1/2}$ wave functions and the energies of corresponding states in Tl atom makes the matrix elements of the T-odd polarization large. This in self-consistent calculation leads to an essentially overestimated T-odd wave function corrections, especially for $6s$, $6p_{1/2}$ wave functions, which, in turn, gives an overestimated result in initial approximation (with T-odd polarization) and a large corrections of first and second order in the residual Coulomb interaction. These corrections reduce the result and make it closer to the semi-empirical results. The noncalculated corrections of higher orders also may be large, because of a large value of Coulomb integrals.

The combination of features of T-odd interaction, Hartree—Fock calculation in $V^{(N-1)}$ approximation and certain atomic characteristics leads in the case of Tl atom to the loss of accuracy of the Hartree—Fock method, even if the second-order corrections are calculated. We can note, that in this calculation the features of Hartree—Fock method, presenting in every such calculation, become significant: the shift of energetical denominators, due to the self-consistent calculation with polarization, the correlations, correcting these denominators. So, in estimation of accuracy of RPAE result in Hartree—Fock method, the estimation of first-order corrections is not sufficient. The RPAE result, even with second-order corrections calculated, has a satisfactory accuracy only if these second-order corrections are small enough.

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Table 1

The Previous Results of Electron EDM Enhancement Calculation in Thallium Atom (d_{at}/d_e)

	Hartree—Fock result [3, 4]	Model potentials [3, 4]		Semiempirical results	
		Green	Norcross	[2]	[5]
The initial approximation	−1906	−689	−687	−716	−500
The result with first-order corrections	−1041	−607	−562		

Table 2

The Contributions of Different Zero- and First-Order Grafics to the Hartree—Fock Result With Polarizations (R_{at}/d_e Coefficient)

Grafics	Without polarizations	With T-odd polarization	With all polarizations
1,*a*	−422 /−362/*	−422 /−362/	−422 /−362/
1,*b*	—	−1493 /−858/	−1769 /−1148/
1,*c*	—	—	1118 /252/
1,*d*	—	—	−1228 /−1023/
1,*e*	—	—	1260 /1023/
Summary	−422 /−362/	−1915 /−1220/	−1041 /−1258/

* In / /—the sum over the limited number of intermediate states.

Table 3

The Correlation Grafics Contributions to the Result.

Grafics	3,*a*	3,*b*	3,*c*	3,*d*	3,*e*	3,*f*	sum
Total result	346	−26	−9*	420		21	740
$6s$, $6p_{1/2}$ contributions	22	11	−9	31	−16		39

* Approximate expression (3).

Table 4

The Hartree—Fock Matrix Elements of P- and T-odd Interactions

	Multipolarity of δV	P-odd*		T-odd**		
		Total	Expr.(6)	Total	Expr.(6)	$m=5p,\ldots,8p$
$-\frac{\langle 6p_{1/2}\|W\|6s\rangle}{\Delta\varepsilon_{6p6s}}$		9.4		−91		
$-\frac{\langle 6p_{1/2}\|W+\delta V\|6s\rangle}{\Delta\varepsilon_{6p6s}}$	0 ,..., 7	22.2		−701		
$-\frac{\langle 6p_{1/2}\|W+\delta V_{6s^2}\|6s\rangle}{\Delta\varepsilon_{6p6s}}$	0, 1	20.2	18.2	−540	−320	−360
$-\frac{\langle 6p_{1/2}\|W+\delta V_{6s^2}\|6s\rangle}{\Delta\varepsilon_{6p6s}}$	0	30.5	23.5	−290	−230	−240

* In units $i10^3\alpha GQ_W/2\sqrt{2}$ (atomic units).
** In units d_e.

Table 5

The Results of Calculation in $6s^26p_{1/2}$ — $6s6p_{1/2}^2$ Basis

	A*	R
Without polarizations	−91	−155
With T-odd polarization	−322	−549
With ail polarizations	−273	−408
Second-order correction	27.5	23
Higher-order corrections	36.5	29
The exact result	−209	−356

* In units d_e.

A.Ya. Kraftmakher

On Hartree-Fock Calculation of Electron Electric Dipole Moment Enhancement Factor for the Thallium Atom

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