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NUCLEAR-SPIN-DEPENDENT PARITY-NONCONSERVING EFFECTS IN THALLIUM, LEAD AND BISMUTH ATOMS

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НОВОСИБИРСК

Nuclear-Spin-Dependent Parity-Nonconserving Effects in Thallium, Lead and Bismuth Atoms

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Abstract

Nuclear-spin-dependent P-odd optical activity in atomic Tl, Pb and Bi is calculated. Its magnitude is expressed analytically through the main contribution to the optical rotation, which is independent of nuclear spin. The accuracy of results is discussed.

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1 Introduction

Up to now only parity-nonconserving (PNC) effects independent of nuclear spin have been reliably observed in atomic experiments. The reason is that in heavy atoms, investigated experimentally, P-odd nuclear-spin-dependent (NSD) correlations are smaller than those observed, roughly by two orders of magnitude.

In heavy atoms the NSD P-odd effects were shown [1, 2] to be induced mainly by the anapole moment of a nucleus, its P-odd electromagnetic characteristic. The measurements of these effects would give valuable information on PNC nuclear forces.

P-odd interaction with nuclear spin leads to some difference in the magnitude of PNC effects at different hyperfine components of optical transitions [3]. Experiments aimed at the detection of NSD P-odd effects in cesium, thallium, lead, bismuth are underway in many groups. The first evidence of those correlations has been seen (at the level of two standard deviations) in cesium [4]. Meaningful upper limits on the NSD optical activity in bismuth and lead were obtained in Refs.[5, 6]. Recently the accuracy close to that necessary for the detection of NSD effects has been achieved in the thallium optical rotation experiment [7].

The first atomic calculations of the NSD P-odd effects were presented in Ref.[3]. More careful and accurate calculations of those correlations in cesium were carried out in Refs.[8, 9, 10, 11], the results of those last works being in good mutual agreement.

In view of the mentioned optical rotation experiments [5, 6, 7], a theoretical investigation of NSD PNC effects in thallium, lead and bismuth, alternative to that of Ref.[3], is relevant and timely. This is the subject of the present paper.

2 Thallium

The simplest case is that of the $6p_{1/2} \longrightarrow 6p_{3/2}$ transition in thallium. PNC weak interaction $\hat{W}$ admixes the states $ns_{1/2}$ to the initial one, and the mixing matrix element is proportional to (see, e.g., Ref.[12])

$$< s_{1/2}|\hat{W}|p_{1/2} >\sim i\left\{\frac{Q}{2} + \kappa_a \frac{2\gamma+1}{3} 2\mathbf{ji}\frac{K}{i(i+1)}\right\}. \qquad (1)$$

The weak nuclear charge Q in this expression is close numerically to $-N$, N being the neutron number; $N = 122$ and 124 for ^{203}Tl and ^{205}Tl respectively. The dimensionless anapole constant κ_a is close in Tl to 0.40 [2, 13]. As to other notations in expression (1), $j = 1/2$ is the electron angular momentum, i is the nuclear spin, $K = (l-i)(2i+1)$, l is the orbital angular momentum of the valence nucleon (for both thallium isotopes $i = 1/2$, $K = -1$, $l = 0$); $\gamma = \sqrt{1 - Z^2\alpha^2}$. An overall numerical factor omitted in the rhs of formula (1) is irrelevant for our treatment; the imaginary value of matrix element (1) is essential for the transition to the second-quantization representation (see below). Due to the short-range nature of the PNC electron-nucleus interaction $\hat{W}$, mixing of any other pair of opposite-parity one-electron states can be neglected.

There are other contributions to the NSD term in expression (1), due to the weak neutral currents, and to the combined effect of the weak neutral charge Q and usual hyperfine interaction [14, 15, 16]. Those contributions can be easily included into the consideration, but most probably they are numerically small as compared to κ_a.

Mixing (1) conserves obviously the total atomic angular momentum F which in this case refers to the initial state $6p_{1/2}$, and the matrix element reduces to

$$\frac{Q}{2} + \kappa_a \frac{2\gamma+1}{3}\begin{cases} 2, & F=0 \\ -2/3, & F=1 \end{cases}. \qquad (2)$$

The second type of excitation essential here is that of electrons belonging to the $6s^2$ subshell: the states of the configuration $6s_{1/2}6p_{1/2}6p_{3/2}$ are

admixed by the weak interaction to $6s^26p_{3/2}$. This contribution can be formally described as a transition of the $6p_{1/2}$ into the occupied $6s_{1/2}$ state, induced by the weak interaction, with the subsequent E1 transition from $6s_{1/2}$ to $6p_{3/2}$. No wonder therefore that the ratio between the nuclear-spin-independent (NSI) effect due to Q and that driven by the anapole moment (AM) interaction, proportional to κ_a, is controlled by the same relation (2) where F refers again to the initial state. This result can be as well obtained directly using the second-quantization representation and the completeness relation for the states belonging to the configuration $6s_{1/2}6p_{1/2}6p_{3/2}$ (see below).

In this way we obtain the following relation between the circular polarization P_a induced by the nuclear AM and that induced by the weak nuclear charge Q:

$$\frac{P_a}{\kappa_a} = \frac{P_Q}{Q}\frac{2\gamma+1}{3}\begin{cases} 4, & F=0 \\ -4/3, & F=1 \end{cases}. \qquad (3)$$

Taking for P_Q the result obtained in the phenomenological approach [17, 12]

$$P_Q = 3.4 \cdot 10^{-7}(-Q/N), \qquad (4)$$

we get finally

$$\frac{P_a}{\kappa_a} = \begin{cases} -0.96 \cdot 10^{-8}, & F=0 \longrightarrow F'=1 \\ 0.32 \cdot 10^{-8}, & F=1 \longrightarrow F'=1,\ 2 \end{cases}. \qquad (5)$$

Not only the result of Ref.[3] is reproduced[2], but it is clear now why for both transitions from the state of $F = 1$ the degree of circular polarization is the same.

In conclusion of this section it should be mentioned that relation (1) allows one to get immediately the magnitude of the NSD PNC effect in the strongly forbidden transition $6p_{1/2} \longrightarrow 7p_{1/2}$ in thallium at $F' = F = 1$, again in complete agreement with the result of Ref.[3]. This trick was applied previously in Ref.[8] (see also [11]) to the components with $F' = F$ of the transition $6s_{1/2} \longrightarrow 7s_{1/2}$ in cesium.

[2] In paper [3] we used different normalization for the NSD effect, natural for the neutral current interaction. For comparison with the present results (and with the numbers quoted in book [12]) the original ones should be multiplied by $(1-2K)/2K$. In thallium this factor equals $-3/2$.

3 Lead

The next case of experimental interest is the $^3P_0' \longrightarrow {}^3P_1$ transition in the odd isotope of lead, ^{207} Pb ($i = 1/2$, $K = 1$).

It is convenient here to use formula (1) in the second-quantization representation:

$$\hat{W} \sim i\Big\{\frac{Q}{2}(a_+^\dagger b_+ + a_-^\dagger b_- - b_+^\dagger a_+ - b_-^\dagger a_-)$$
$$+q[i_+(a_-^\dagger b_+ - b_-^\dagger a_+) + i_-(a_+^\dagger b_- - b_+^\dagger a_-)$$
$$+i_z(a_+^\dagger b_+ - a_-^\dagger b_- - b_+^\dagger a_+ + b_-^\dagger a_-)]\Big\}. \qquad (6)$$

Here $a^\dagger$ (a) and $b^\dagger$ (b) are the creation (annihilation) operators of the $s_{1/2}$ and $p_{1/2}$ electrons respectively, the subscripts refer to the signs of electron angular momentum projections $j_z = \pm 1/2$;

$$q = \kappa_a \frac{2\gamma+1}{3}\frac{K}{i(i+1)}.$$

We will need also the second-quantization representation for the operator of E1 $s-p$ transition. Up to an overall factor, which is again irrelevant for our purpose, this operator is (see, e.g., Ref.[12]):

$$\hat{D}^+ \sim -i\Big\{\rho_{1/2}\sqrt{2}(a_+^\dagger b_- + b_+^\dagger a_-)$$
$$+\rho_{3/2}(\sqrt{3}c_{3/2}^\dagger a_+ + c_{1/2}^\dagger a_- - \sqrt{3}a_-^\dagger c_{-3/2} - a_+^\dagger c_{-1/2})\Big\}. \qquad (7)$$

Here $c_m^\dagger$ (c_m) is the creation (annihilation) operator of the $p_{3/2}$ electron with $j_z = m$; ρ_j is the scalar radial integral of E1 $s-p_j$ transition.

The ground state wave function of the lead $6p^2$ configuration is expanded as follows in the jj basis (see, e.g., Ref.[12]):

$$|^3P_0' >= a_1|1/2\ 1/2>_0 + a_2|3/2\ 3/2>_0;\ \ a_1 = 0.974,\ a_2 = -0.227. \qquad (8)$$

The symbol $|j_1\ j_2>_J$ denotes the normalized wave function of two p-electrons with angular momenta j_1 and j_2, and total angular momentum J. The first excited state of that configuration is pure both in the LS and jj-scheme:

$$|^3P_1 >= |1/2\ 3/2>_1 . \qquad (9)$$

In the second-quantization representation the basic wave functions are

$$|1/2\ 1/2>_0 = b_+^\dagger b_-^\dagger|0>, \qquad (10)$$

$$|3/2\ 3/2>_0 = \frac{1}{\sqrt{2}}(c_{3/2}^\dagger c_{-3/2}^\dagger - c_{1/2}^\dagger c_{-1/2}^\dagger)|0>, \qquad (11)$$

$$|1/2\ 3/2>_1 = \frac{1}{2}(\sqrt{3}c_{3/2}^\dagger b_-^\dagger - c_{1/2}^\dagger b_+^\dagger)|0> . \qquad (12)$$

Here $|0>$ is the wave function of the closed shells.

The admixed E1 transition from one of the ground state jj components, $|1/2\ 1/2>_0$, to $|1/2\ 3/2>_1$ proceeds via states of the type $ns_{1/2}6p_{1/2}$ (including the subshell $6s^2$ excitation, as it was the case in thallium) and is described by the effective operator $\hat{D}^+\hat{W}$. Small spin $i = 1/2$ of the isotope ^{207}Pb simplifies the calculations essentially. The total atomic angular momentum of the ground state is fixed, $F = 1/2$, and coincides with the nuclear spin. Elementary calculations demonstrate that

$$\hat{D}^+\hat{W}|1/2\ 1/2>_0\ |->\sim (Q-q)\sqrt{2/3}\,|1/2,1/2) + (Q+q/2)\sqrt{1/3}\,|3/2,1/2). \qquad (13)$$

Here $|->$ denotes the nuclear spin state with $i_z = -1/2$ (at $J = 0$ it corresponds to $F_z = -1/2$), $|F, F_z)$ refers to atomic eigenstate of given F and F_z.

The transition from the second ground state component, $|3/2\ 3/2>_0 \longrightarrow |1/2\ 3/2>_1$, corresponds to the effective operator $\hat{W}\hat{D}^+$. As easily one gets

$$\hat{W}\hat{D}^+|3/2\ 3/2>_0\ |->\sim (Q+q)\sqrt{1/3}\,|1/2,1/2) + (Q-q/2)\sqrt{2/3}\,|3/2,1/2). \qquad (14)$$

Therefore, the admixed E1 amplitude of the $F = 1/2 \longrightarrow F' = 1/2$ transition is proportional to

$$Q(a_1\sqrt{2/3} + a_2\sqrt{1/3}) - q(a_1\sqrt{2/3} - a_2\sqrt{1/3});$$

that of $F = 1/2 \longrightarrow F' = 3/2$ to

$$Q(a_1\sqrt{1/3} + a_2\sqrt{1/6}) + q/2(a_1\sqrt{1/3} - a_2\sqrt{1/6}).$$

Finally, we get

$$\frac{P_a}{\kappa_a} = \frac{P_Q}{Q}\,\frac{2\gamma+1}{3}\,\frac{2}{3}\,\frac{1-a_2/(a_1\sqrt{2})}{1+a_2/(a_1\sqrt{2})}\begin{cases} -2, & F' = 1/2 \\ 1, & F' = 3/2 \end{cases}. \qquad (15)$$

Taking again for P_Q the result of the phenomenological calculations [17, 12]

$$P_Q = 2.4\cdot 10^{-7}(-Q/N), \qquad (16)$$

we come to the following numerical predictions:

$$\frac{P_a}{\kappa_a} = \begin{cases} 0.31 \cdot 10^{-8}, & F' = 1/2 \\ -0.15 \cdot 10^{-8}, & F' = 3/2 \end{cases} \tag{17}$$

in complete agreement with Ref.[3].

4 Bismuth

Of experimental interest in bismuth are the transitions from the ground state into the first and second excited ones. All those levels belong to the configuration $6p^3$. The ground state and the first excited one have $J = 3/2$. The coefficients of their expansion in jj basis

$$a_1|1/2\ 1/2\ 3/2>_{3/2} + a_2|1/2\ 3/2\ 3/2>_{3/2} + a_3|3/2\ 3/2\ 3/2>_{3/2},$$

as derived in Ref.[18] (and quoted in Ref.[12]), are presented in Table 1. Their standard values [19] are given in brackets in the same Table. The second excited state is pure $|1/2/;3/2/;3/2>_{5/2}$.

Table 1: Expansion of bismuth $6p^3$ states in jj basis

	a_1	a_2	a_3
Ground state	-0.929 (-0.935)	0.323 (0.308)	-0.179 (-0.172)
First excited state	-0.336 (-0.324)	-0.940 (-0.944)	0.053 (0.066)

In the second-quantization representation the basic jj functions with maximum projections are:

$$|1/2\ 1/2\ 3/2>_{3/2} = c^\dagger_{3/2} b^\dagger_+ b^\dagger_- |0>, \tag{18}$$

$$|1/2\ 3/2\ 3/2>_{3/2} = \frac{1}{\sqrt{5}} c^\dagger_{3/2}(2c^\dagger_{1/2} b^\dagger_- - c^\dagger_{-1/2} b^\dagger_+)|0>, \tag{19}$$

$$|3/2\ 3/2\ 3/2>_{3/2} = c^\dagger_{3/2} c^\dagger_{1/2} c^\dagger_{-1/2}|0>, \tag{20}$$

$$|1/2\ 3/2\ 3/2>_{5/2} = c^\dagger_{3/2} c^\dagger_{1/2} b^\dagger_+)|0> . \tag{21}$$

The only stable bismuth isotope ^{209}Bi has spin $i = 9/2$ ($K = 5$). Due to large J's and i both transitions from the ground state, into the first excited one (876 nm) and into the second (648 nm), have a lot of hyperfine components, 10 and 12 respectively. This makes us to resort, instead of the elementary treatment of lead and especially of thallium, to heavy artillery of $3nj$ symbols.

In the single-electron language the following chains contribute to both transitions:

$$p_{1/2} \longrightarrow s_{1/2} \longrightarrow p_{1/2},$$
$$p_{1/2} \longrightarrow s_{1/2} \longrightarrow p_{3/2},$$
$$p_{3/2} \longrightarrow s_{1/2} \longrightarrow p_{1/2}.$$

The first of chain is described by the effective operator $\hat{D}^+\hat{W} + \hat{W}\hat{D}^+$ which reduces in this case to

$$\hat{D}^+\hat{W} + \hat{W}\hat{D}^+ \sim q\sqrt{2}\{i_+(b^\dagger_+ b_+ - b^\dagger_- b_-) - 2i_z\, b^\dagger_+ b_-\} = q\, 2\sqrt{2}[\hat{V}_1 \times i]^1_+. \tag{22}$$

In this expression vector

$$\hat{V}^1 = \{-\sqrt{2}b^\dagger_+ b_-, b^\dagger_+ b_+ - b^\dagger_- b_-, \sqrt{2}b^\dagger_- b_+\} \tag{23}$$

is nothing else but the operator $2\mathbf{j}$ for $p_{1/2}$ electron in the second-quantization representation; the symbol $[\hat{V}^1 \times i]^1_+$ denotes as usual the tensor product of two operators coupled into a vector with projection $+1$.

The effective operator for the second chain is

$$\hat{D}^+\hat{W} \sim Q\frac{1}{2}(\sqrt{3}c^\dagger_{3/2} b_+ + c^\dagger_{1/2} b_-)$$

$$+q[i_+ c^\dagger_{1/2} b_+ + i_- c^\dagger_{3/2} b_- \sqrt{3} + i_z(\sqrt{3}c^\dagger_{3/2} b_+ - c^\dagger_{1/2} b_-)]$$
$$= Q\,\hat{V}_+ + q\,\{2\sqrt{2}[\hat{V} \times i]^1_+ + \sqrt{10}[\hat{T} \times i]^1_+\}. \tag{24}$$

The tensor operator $\hat{T}$ is defined in such a way that

$$\hat{T}_{+2} = c^\dagger_{3/2} b_- .$$

The definition of the vector operator $\hat{V}$ is clear from the equation itself.

Quite analogously the third chain is described by the effective operator

$$\hat{W}\hat{D}^+ \longrightarrow Q\frac{1}{2}(\sqrt{3}\, b\dagger_- c_{-3/2} + b\dagger_+ c_{-1/2})$$

$$+q[i_+b\dagger_+c_{1/2}+i_-b\dagger_-c_{3/2}\sqrt{3}+i_z(-\sqrt{3}b\dagger_-c_{-3/2}+b\dagger_+c_{-1/2})]$$
$$=Q\,\hat{\tilde{V}}_+ + q\,\{-2\sqrt{2}[\hat{\tilde{V}}\times i]^1_+ + \sqrt{10}[\hat{\tilde{T}}\times i]^1_+\} \qquad (25)$$

where

$$\hat{\tilde{T}}_{+2}=b^\dagger_+c_{-3/2}.$$

Now the standard technique of the angular momentum theory allows one to obtain closed expressions for the reduced matrix elements of those operators between the hyperfine states. For the infrared transition it is

$$\sqrt{(2F'+1)(2F+1)}\Bigg[(-)^{F+1}\left\{\begin{array}{ccc}3/2 & F' & i\\ F & 3/2 & 1\end{array}\right\}$$
$$\times Q\sqrt{6}(a_1a'_2+a_2a'_3-a_2a'_1-a_3a'_2)+q\sqrt{i(i+1)(2i+1)}$$
$$\times\Bigg(\left\{\begin{array}{ccc}3/2 & 3/2 & 1\\ i & i & 1\\ F' & F & 1\end{array}\right\}6(a_1a'_2+a_2a'_3+a_2a'_1+a_3a'_2-2\sqrt{2/5}\,a_2a'_2)$$
$$+\left\{\begin{array}{ccc}3/2 & 3/2 & 2\\ i & i & 1\\ F' & F & 1\end{array}\right\}(-2\sqrt{15})(a_1a'_2-a_2a'_3-a_2a'_1+a_3a'_2)\Bigg)\Bigg] \qquad (26)$$

Here unprimed and primed factors a_i refer to the ground and first excited states respectively. For the red transition the analogous formula is

$$-\sqrt{(2F'+1)(2F+1)}\Bigg[(-)^F\left\{\begin{array}{ccc}5/2 & F' & i\\ F & 3/2 & 1\end{array}\right\}Q\sqrt{3/2}\,(a_1+a_3)$$
$$+3q\sqrt{i(i+1)(2i+1)}\Bigg(\left\{\begin{array}{ccc}5/2 & 3/2 & 1\\ i & i & 1\\ F' & F & 1\end{array}\right\}(a_1+a_3+8\sqrt{2/5}\,a_2)$$
$$+\left\{\begin{array}{ccc}5/2 & 3/2 & 2\\ i & i & 1\\ F' & F & 1\end{array}\right\}\sqrt{35}\,(a_1+a_3)\Bigg)\Bigg]. \qquad (27)$$

We have used in both formulae (26) and (27) the explicit values of the reduced matrix elements of the operators V^1, V, $\tilde{V}$, T and $\tilde{T}$ between the jj states (18) - (21) which can be found easily.

We are interested in the ratios of the NSD terms in those matrix elements, which are proportional to q, to NSI ones, which are proportional to Q. The following identity is useful here[20]:

$$\sqrt{i(i+1)(2i+1)}\left\{\begin{array}{ccc}j' & j & 1\\ i & i & 1\\ F' & F & 1\end{array}\right\} \qquad (28)$$
$$=\frac{(F'-j')(F'+j'+1)-(F-j)(F+j+1)}{2\sqrt{6}}(-)^{j'+i+F+1}\left\{\begin{array}{ccc}j' & F' & i\\ F & j & 1\end{array}\right\}.$$

Somewhat less general and elegant identities [20] relate

$$\sqrt{i(i+1)(2i+1)}\left\{\begin{array}{ccc}j' & j & 2\\ i & i & 1\\ F' & F & 1\end{array}\right\}$$

to

$$\left\{\begin{array}{ccc}j' & F' & i\\ F & j & 1\end{array}\right\}.$$

Finally, we come to the following results for NSD optical activity in bismuth.

Infrared line (876 nm):

$$\frac{P_a}{\kappa_a}=\frac{P_Q}{Q}\,\frac{2\gamma+1}{3}\,\frac{K}{i(i+1)}\,(a_1a'_2+a_2a'_3-a_2a'_1-a_3a'_2)^{-1}$$
$$\times\Bigg\{(a_1a'_2+a_2a'_3+a_2a'_1+a_3a'_2-2\sqrt{2/5}\,a_2a'_2)\begin{pmatrix}F+1\\ 0\\ -F\end{pmatrix}$$
$$+(a_1a'_2-a_2a'_3-a_2a'_1+a_3a'_2)\frac{1}{2}\begin{pmatrix}(F+1)^2-26\\ \frac{F^2(F+1)^2-52F(F+1)+546}{F(F+1)-21}\\ F^2-26\end{pmatrix}\Bigg\}$$
$$=-10^{-9}\Bigg\{0.645\begin{pmatrix}F+1\\ 0\\ -F\end{pmatrix}+0.274\begin{pmatrix}(F+1)^2-26\\ \frac{F^2(F+1)^2-52F(F+1)+546}{F(F+1)-21}\\ F^2-26\end{pmatrix}\Bigg\}. \qquad (29)$$

Red line (648 nm):

$$\frac{P_a}{\kappa_a}=\frac{P_Q}{Q}\,\frac{2\gamma+1}{3}\,\frac{K}{i(i+1)}\,(-a_1+a_3)^{-1}\cdot\Bigg\{(-a_1-a_3-8\sqrt{2/5}\,a_2)\begin{pmatrix}F-3/2\\ -5/2\\ -F-5/2\end{pmatrix}$$

$$+(-a_1-a_3)\begin{pmatrix} -2F^2+F+105/2 \\ -2F^2-2F+99/2 \\ -2F^2-5F+99/2 \end{pmatrix}\Bigg\}$$

$$=10^{-9}\Bigg\{0.370\begin{pmatrix} F-3/2 \\ -5/2 \\ -F-5/2 \end{pmatrix}-0.780\begin{pmatrix} -2F^2+F+105/2 \\ -2F^2-2F+99/2 \\ -2F^2-5F+99/2 \end{pmatrix}\Bigg\}. \quad (30)$$

We use here for P_Q the results of the phenomenological calculations [17, 12]

$$P_Q(876)=2.9\cdot 10^{-7}(-Q/N), \quad (31)$$

$$P_Q(648)=3.8\cdot 10^{-7}(-Q/N) \quad (32)$$

for the infrared and red line. In formulae (29) and (30) the first, second and third lines in each column refer to the transitions $F\longrightarrow F+1, F\longrightarrow F$ and $F\longrightarrow F-1$ correspondingly.

The numerical predictions for all hyperfine components of the two transitions are collected in Table 2. They are obviously in a reasonable agreement with those of Ref.[3] which are included for comparison into the Table.

Table 2: $(P_a/\kappa_a)\cdot 10^8$ at hyperfine components of infrared and red transitions

		876 nm this work	876 nm [3]	648 nm this work	648 nm [3]
F	F'				
6	7	–	–	1.22	1.01
6	6	-0.17	-0.15	2.60	2.39
6	5	0.11	0.08	3.78	3.57
5	6	-0.66	-0.56	-0.46	-0.48
5	5	0.35	0.29	0.73	0.70
5	4	0.35	0.29	1.71	1.69
4	5	-0.30	-0.24	-1.82	-1.69
4	4	-2.58	-2.17	-0.83	-0.70
4	3	0.54	0.45	-0.05	0.09
3	4	0.02	0.03	-2.87	-2.61
3	3	0.20	0.18	-2.08	-1.82
3	2	–	–	-1.49	-1.23

5 Accuracy of results

It is proper now to compare the accuracy of the present results with that of the results of Ref.[3] and with that of theoretical predictions for the NSI optical rotation.

Let us start with thallium. Here in the phenomenological approach adopted in Refs.[17, 3] and here, both NSI and NSD weak interactions admix to the initial state $6p_{1/2}$ exactly same simple excitations $ns_{1/2}$. As to the excitations of the type $6s6p^2$, when treating both effects the energy splitting between them was neglected. There is no special reasons to expect that such an averaging can influence NSD and NSI effects in essentially different ways. Therefore, for the accuracy of our thallium result (5) one can accept the same estimate 15% as was given in Refs.[17, 12] for the NSI prediction (4). It should be mentioned that, taking account of the mentioned 15% error, the phenomenological NSI result (4) agrees well with the most accurate subsequent theoretical calculation [21] which gives for this transition $P_Q=3.20(10)\cdot 10^{-7}(-Q/N)$. The experimental result [22], $P_Q=2.50(38)\cdot 10^{-7}$, does not contradict the theoretical predictions (at $-Q/N=0.947$).

A close situation takes place in lead. Usual excitations of the $6p$ electron belong to the configurations $ns\ 6p$ which are well described by the jj coupling approximation. The NSI and NSD weak interactions admix to the dominating, $|1/2\ 1/2>_0$, component of the ground state wave function states of different total electronic angular momentum J, $|\cdot\ 1/2>_0$ and $|\cdot\ 1/2>_1$ respectively (here the dot denotes the ns-electron). However, the energy interval between the states $|\cdot\ 1/2>_0$ and $|\cdot\ 1/2>_1$ is tiny, about 300 cm^{-1} even at $n=7$. In the contribution to the effect of the second ground state component, $|3/2\ 3/2>_0$, the usual ns excitations are admixed to the final state $|^3P_1>=|1/2\ 3/2>_1$; the NSI weak interaction admixes the excitations $|\cdot\ 3/2>_1$, and the NSD one admixes both $|\cdot\ 3/2>_1$ and $|\cdot\ 3/2>_2$. The energy interval between the last two states is also small (1250 cm^{-1} for $n=7$). And finally as concerns the contributions of the $6s$-electron excitations, the same arguments apply as in the case of Tl. Therefore the averaged treatment of all the excited states when evaluating the NSD effects in lead in Ref.[3] is practically of the same accuracy as the phenomenological calculation of NSI effects in Ref.[17].

However, in the present approach an extra approximation is made as compared to Ref.[3]. From the above argument concerning the admixture of $ns\ 6p$ excitations it follows that to treat both ground state components on the same footing one has to neglect the energy interval between the ground state and $|^3P_1>=|1/2\ 3/2>_1$. But this interval, 7819 cm^{-1}, is not as negligible.

Fortunately, the ground state of lead is also close to pure jj coupling, the relative admixture of the $|3/2\ 3/2>_0$ component in it is small (see (8)). Thus the error introduced by that extra approximation gets negligible, and the present result coincides numerically with that of Ref.[3]. The accuracy of both can be estimated to be the same, 20%, as that of the phenomenological NSI one (16). It is worth noting here that the phenomenological NSI result (16) agrees within the indicated error with subsequent theoretical calculations [23, 24] and experiment [6].

In bismuth the situation is rather different. In spite of the reasonable agreement between the present results and previous ones [3] (see Table 2), the neglect of the energy intervals between the states belonging to the $6p^3$ configuration is more essential than in lead. Furthermore, in bismuth, as distinct from thallium and lead, the chain

$$p_{1/2} \longrightarrow s_{1/2} \longrightarrow p_{1/2},$$

becomes operative. Therefore, not only $ns \longrightarrow 6p_{3/2}$ E1 transitions, but $ns \longrightarrow 6p_{1/2}$ ones contribute to the effect. In our treatment we have tacitly assumed that the corresponding radial integrals are equal. However, they are not, at least for the E1 transition $7s \longrightarrow 6p$ [17].

The latter correction can be introduced easily into our consideration. Numerical calculations [25] give the following values for the radial integrals of $7s \longrightarrow 6p$ transitions (in the units of the Bohr radius)

$$\rho_{3/2} = 2.2; \quad \rho_{1/2} = 1.5$$

The relative contributions of the $7s\,6p^2$ excitations to the effect constitute, according to Ref.[17], 30% and 24% for the infrared and red transitions respectively. So, the effect discussed can be accounted for by the introduction of the correction factors 0.89 into the term $2\sqrt{2/5}\,a_2 a_2'$ in formula (29) and 0.92 into the term $8\sqrt{2/5}\,a_2$ in formula (30). Both those terms are due to the $ns \longrightarrow 6p_{1/2}$ E1 transitions.

The present results for Bi were recalculated at the standard set of the intermediate-coupling coefficients a_i (see Table 1) used in Ref.[3], and the above correction was made, accounting for the difference between $\rho_{3/2}$ and $\rho_{1/2}$. The numbers obtained in this way are indeed even more close to the results of Ref.[3].

A specific consequence of the neglect of the energy splitting inside the $6p^3$ configuration is the absence in expression (22) of the contribution

$$i_+ \frac{b_+^\dagger b_+ + b_-^\dagger b_-}{\sqrt{2}}$$

scalar in electron variables. Such terms arise at q both in $\hat{D}^+\hat{W}$ and $\hat{W}\hat{D}^+$, but cancel out in their sum. The cancellation is no more exact if the energy splitting does not vanish. The comparison with the results of Ref.[3] demonstrate that the scalar contribution to the infrared transition does not exceed few percent. Obviously, it cannot contribute to the red transition with $\Delta J = 1$.

Of course, the aim and outcome of the above procedures is to establish the correspondence between the two results for bismuth, to have one more check for both of them. Clearly, in bismuth the present calculation by itself is less accurate than that of Ref.[3].

But what is the accuracy of the latter? In spite of an extra approximation, that of averaging over the positions of all intermediate states belonging to the same configuration, its error should be about the same as that of the phenomenological calculation [17] of NSI optical activity in bismuth. The accuracy of the latter was stated to be 20%. Indeed the phenomenological result (31) for the infrared transition within this error contradicts neither most refined theoretical investigations [24, 26], nor experimental results [27, 28, 5].

As to the red transition, the situation is less clear. There is no agreement between the phenomenological result (32) for it and that of the Hartree-Fock calculation [26]: $P_Q = 1.5(1.0) \cdot 10^{-7}(-Q/N)$. Moreover, there is a discrepancy between experiments at this line. One of them [29] gives $P_Q = 4.04(0.54) \cdot 10^{-7}$, two other [30, 31] $1.56(0.36) \cdot 10^{-7}$ and $1.96(0.18) \cdot 10^{-7}$ respectively. Both discrepancies, theoretical and experimental, still are not resolved.

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