

Calculation of energy levels, $E1$ transition amplitudes and parity violation in francium

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Many-body perturbation theory in the screened Coulomb interaction was used to calculate energy levels, $E1$ transition amplitudes, and the parity-nonconserving (PNC) $E1$ amplitude of the $7s-8s$ transition in francium. The method takes into account the core-polarization effect, the second-order correlations, and the three dominating sequences of higher-order correlation diagrams: screening of the electron-electron interaction, particle-hole interaction, and the iterations of the self-energy operator. The result for the PNC amplitude for ^{223}Fr is $E1(7s-8s) = (1.59 \pm \sim 1\%) \times 10^{-10} ie a_B (-Q_W/N)$, where Q_W is the weak charge of the nucleus, $N = 136$ is the number of neutrons $e = |e|$ is the elementary charge, and a_B is the Bohr radius. Our prediction for the position of the $8s$ energy level of Fr, which has not been measured yet, is $13\,110\text{ cm}^{-1}$ below the limit of the continuous spectrum. The accuracy of the calculation was controlled by comparison with available experimental data and analogous calculations for cesium. It is estimated to be $\sim 0.1\%$ for the energy levels and $\sim 1\%$ for the transition amplitudes.

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I. INTRODUCTION

Until now francium has remained one of the least studied atoms. There was a lot of progress from 1978 to 1990 when many energy levels, hyperfine structure intervals, and isotope shifts were measured [1–6]. During the same period of time we performed *ab initio* many-body calculations of the energy levels and hyperfine structure intervals of francium [7,8]. Energy levels were in fact predicted by us because nothing was measured at that time except the wavelength of the $7s-7p_{3/2}$ transition. Hyperfine structure intervals were in turn used to extract magnetic moment values of a number of francium nucleus isotopes. Recently an interest in francium has been revived due to a proposed experiment to measure parity nonconservation (PNC) in this atom [9]. So far, the most accurate measurements of PNC effects in atoms (on the level of 1–2%) were carried out for the four atoms: cesium [10], lead [11], thallium [12], and bismuth [13]. Nevertheless, until now cesium had remained the only atom for which the accuracy of both experiments and theory [14,15] is about 1%. (Comparisons of our calculations and experiments for other atoms are presented in Sec. III.) Francium is a heavier analog of cesium and, due to the similar electron structure, a similar accuracy of the PNC calculations may be expected for it. On the other hand, for the francium atom the PNC effect must be considerably larger than for cesium due to the larger value of nuclear

charge Z . These facts make the proposal of PNC measurements in francium very promising.

In our works [14,16–18] an accurate method of atomic calculations has been developed. As shown for cesium, the method gives an accuracy of about 0.1% for the calculations of the energy levels [17] and about 1% for the hyperfine structure intervals and $E1$ transition amplitudes, including the PNC effect [14,18]. In the present paper we apply the approach developed in [14,16–18] to the calculation of energy levels, $E1$ transition amplitudes, and the PNC amplitude in francium.

II. METHOD OF CALCULATION

The method of calculation was described in [14,16–18]. Here we repeat the most important aspects of it for future reference. We use the relativistic Hartree-Fock (RHF) method in the V^{N-1} approximation to obtain a complete set of one-electron orbitals. The core states are then frozen and the states outside the core are found by solving the single-particle equation (Brueckner approximation)

$$(\hat{H}_0 + \hat{\Sigma})\psi_a = E_a\psi_a, \quad (1)$$

where \hat{H}_0 is the relativistic Hartree-Fock-Dirac Hamiltonian

$$\hat{H}_0 = c\vec{\alpha} \cdot \mathbf{p} + (\beta - 1)mc^2 - \frac{Z(r)e^2}{r} + \hat{V}^{N-1}, \quad (2)$$

$\hat{V}^{N-1} = \hat{V}_{\text{dir}} + \hat{V}_{\text{exch}}$ is the sum of the direct and the nonlocal exchange Hartree-Fock potentials created by the $N - 1$ electrons of the atomic core, and $\hat{\Sigma}$ is the nonlocal correlation potential (self-energy operator) which describes the correlation interaction of the external electron with the core.

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For accurate calculations of the PNC effect in heavy atoms finite nuclear size must be taken into account. We use the standard formula for the charge distribution in the nucleus

$$\rho(r) = \frac{C}{\exp[(r - r_N)/D] + 1}, \quad (3)$$

where C is the normalization constant, $r_N = 1.10A^{1/3}$ fm, and $D = 0.57$ fm [19]. The nuclear part of the Coulomb potential at small distances is calculated by integrating (3). ($\int_0^\infty \rho(r)r^2 dr = 1$.)

There are no specific experimental data for the proton and neutron distributions in the Fr nucleus, but usually these distributions for the most stable isotopes are very close (see, e.g., Refs. [19–22]). Therefore we assume that the distributions of the neutron and proton densities coincide and the Hamiltonian of the parity-violating (PV) weak interaction between the electrons and the nucleus has the form

$$H_{PV} = -\frac{1}{2\sqrt{2}}G\rho(r)Q_W\gamma_5 \quad (4)$$

with nuclear density given by Eq. (3). In this Hamiltonian G is the Fermi constant, Q_W is the weak charge of the nucleus, and γ_5 is the Dirac matrix. The next question concerns the sensitivity of the PNC effect to the nuclear radius r_N . We have proved that it takes a 3% variation of r_N in (3) to change the PNC result for Fr by 1%. Since an average nuclear radius is known with an accuracy better than 3% (see, e.g., Refs. [19–22]), we believe that this uncertainty in the PNC is also negligible. Probably the main question concerns the shape of the Fr nucleus. It is a deformed or at least a soft nucleus. On the other hand, the distribution (3) corresponds to a spherical nucleus. To imitate the effect of a quadrupole deformation we change the parameter D in the distribution (3). Matching the values of $\langle r^2 \rangle$ one can prove that the 20% quadrupole deformation corresponds to the variation of D from 0.57 fm to 0.64 fm. At this variation of D the PNC effect is changed by 0.9%. However, for the Fr nucleus a 20% quadrupole deformation is certainly an overestimation. Therefore, we can conclude that the uncertainty in the calculated PNC effect due to the nuclear part of the problem is smaller than 1%. We have to note that due to the large nuclear charge this uncertainty for Fr is much greater than that for Cs and is actually rather close to 1%. Thus it would be very important to do a more detailed analysis of the nuclear part of the problem, similar to that carried out in Refs. [23–25] for Cs and Pb.

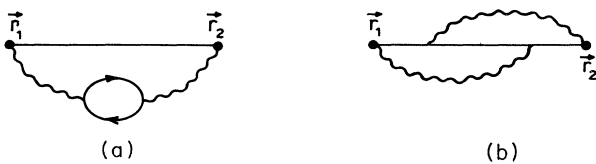


FIG. 1. Second-order diagrams for $\hat{\Sigma}$ in the Feynman diagram technique.

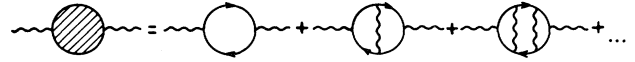


FIG. 2. Hole-particle interaction in the polarization operator.

The calculation of $\hat{\Sigma}$ is the most complicated part of the method. In the lowest nonvanishing order of the perturbation theory in the residual Coulomb interaction the self-energy operator $\hat{\Sigma}$ is described by the two diagrams shown in Fig. 1. In the case of alkaline atoms the direct diagram [Fig. 1(a)] is approximately 10 times larger than the exchange one [Fig. 1(b)] and we use different techniques to calculate them. The direct diagram is calculated using the Green's functions and the Feynman diagram technique. This enables us to take into account the two dominating classes of higher-order correlations in the calculation of $\hat{\Sigma}$: (i) the hole-particle interaction in the polarization operator (Fig. 2) and (ii) the screening of the Coulomb interaction (Fig. 3). It was shown in [26,17,14,18] that these higher-order correlations are very important for accurate calculations.

The use of the Green's functions also provides better numerical accuracy than a direct summation over the intermediate states. This can be seen by comparing the values of the second-order correlation corrections for the energy levels of cesium obtained by different authors (see Table I). In our earlier work [27], the calculations were done via the direct summation over the intermediate states. The basis set used was restricted due to the limited computer power available at that time. The numerical accuracy in the calculation of the second-order correlation corrections was about 10%. In our later works ([17] and the present work), when the Green's functions and the Feynman diagram technique were used to calculate the direct diagram, the agreement between our results and those of Johnson *et al.* [28] and Liaw [29] is at a level of 1% of the correlation correction value, which corresponds to the accuracy of about 0.1% for the level energies. The slight difference between our results in the third and fourth columns of Table I may be attributed to a difference in the values of some numerical parameters (such as coordinate grid, etc.). This illustrates the stability of our results with respect to variation of the parameters. The contribution of higher-order correlation is not small and makes up about 10% of the correlation correction. Therefore, it is essential to calculate the second-order diagrams with high numerical accuracy when higher-order diagrams are also included.

There is no need to calculate the exchange diagram with very high numerical accuracy and we calculate it by means of direct summation over the intermediate states. The higher-order correlations are taken into account in



FIG. 3. Screening of the electron-electron interaction.

TABLE I. Second-order correlation corrections to the energy levels of cesium (cm^{-1}).

State	Dzuba <i>et al.</i> [27]	Dzuba <i>et al.</i> [17]	Present work	Johnson <i>et al.</i> [28]	Liaw [29]
6s	-3514	-3886	-3873	-3896	-3867
6p _{1/2}	-1413	-1533	-1510	-1517	-1508
6p _{3/2}	-1279	-1374	-1352	-1356	-1352

a semiempirical way by introducing the screening factors f_k in each Coulomb line (k is the multipolarity of the Coulomb interaction). The values of f_k are estimated from accurate calculations of the higher-order corrections to the direct diagram. We used the same set of values for both cesium and francium atoms: $f_0 = 0.67$, $f_1 = 0.62$, $f_2 = 0.82$, $f_3 = 0.87$, $f_4 = 0.95$, $f_5 = 1$, etc. Note that due to a small contribution of the exchange diagram, the final results are not sensitive to the method of its evaluation. The diagrams for the self-energy operator with screening of the Coulomb interaction and the hole-particle interaction taken into account are presented in Fig. 4.

When $\hat{\Sigma}$ has been calculated, the states of the external electron are found by solving Eq. (1) iteratively, starting from the Hartree-Fock orbitals. The iterations in Eq. (1) correspond to the summation of another infinite series of higher-order diagrams — the iterations of the self-energy operator (Fig. 5).

The one-electron wave functions in the Brueckner approximation and the energy levels are found by the procedure described above. In order to calculate the $E1$ transition amplitudes and the PNC effect the core polarization by the external fields should be taken into account. This is done by means of the time-dependent Hartree-Fock (TDHF) method (see [16] for details). Calculations of $E1$ amplitudes were carried out in “length” form, which was proved to be more stable for optical transitions when photon frequency is relatively small. The one-electron wave function in the electric field of ω frequency has the form

$$\tilde{\Psi}_k = \Psi_k + X_k e^{-i\omega t} + Y_k e^{i\omega t}, \quad (5)$$

where Ψ_k are the Hartree-Fock or Brueckner electron wave functions, and X_k, Y_k are the corrections due to the external electric field and the core polarization effect. The amplitudes of allowed $E1$ transitions are given by

$$E1(k \rightarrow n) = \langle Y_n | \Psi_k \rangle + \langle \Psi_n | X_k \rangle. \quad (6)$$

Whether this expression takes into account the correlation corrections depends on what sort of one-electron wave functions are substituted into it—the Hartree-Fock or the Brueckner ones. Note, however, that by proceeding this way one can take into account only the dominating, Brueckner-type correlation diagrams, while non-Brueckner corrections (the structural radiation, the renormalization of the wave function, etc.) require separate consideration (see [16] for a detailed discussion). The contribution of non-Brueckner diagrams was very small for cesium [14,18] and we do not calculate them for francium.

To calculate the PNC $E1$ amplitude the core polarization by an external electric field and by the weak interaction between the atomic nucleus and the electrons should be taken into account simultaneously. The corresponding expression has the form

$$E_{\text{PNC}}(k \rightarrow n) = \langle \delta Y_n | \Psi_k \rangle + \langle \delta \Psi_n | X_k \rangle + \langle Y_n | \delta \Psi_k \rangle + \langle \Psi_n | \delta X_k \rangle, \quad (7)$$

where δ stands for the corrections due to the weak interaction.

Here again one should substitute Brueckner orbitals into (7) to take into account dominating correlation corrections. However, we carried out calculations in a different way to include also dominating terms proportional to $\partial \hat{\Sigma} / \partial \epsilon$. All such terms were calculated for cesium [14] and it was shown there that the dominating contributions arise from the fact that the correlation potential $\hat{\Sigma}$ is different even for the states of equal symmetry due to their energies being different. The energy dependence of $\hat{\Sigma}$ is weak for the external electron and can be calculated in the leading, first order in $\hat{\Sigma}$ only. The corresponding expression for the correlation correction to the PNC amplitude of the $7s$ - $8s$ transition in francium has the form (see Fig. 6)

$$\begin{aligned} \Delta_{\text{corr}} E1_{\text{PNC}}(8s-7s) &= s_1 + s_2 + s_3 + s_4 \\ &= \langle \Psi_{8s} | \Sigma_s(\epsilon = \epsilon_{8s}) | \delta X_{7s} \rangle + \langle \delta \Psi_{8s} | \Sigma_p(\epsilon = \epsilon_{8s}) | X_{7s} \rangle \\ &\quad + \langle \delta Y_{8s} | \Sigma_s(\epsilon = \epsilon_{7s}) | \Psi_{7s} \rangle + \langle Y_{8s} | \Sigma_p(\epsilon = \epsilon_{7s}) | \delta \Psi_{7s} \rangle. \end{aligned} \quad (8)$$

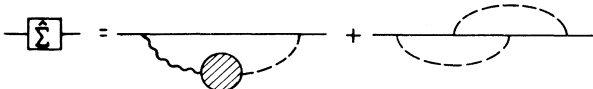


FIG. 4. Self-energy operator.

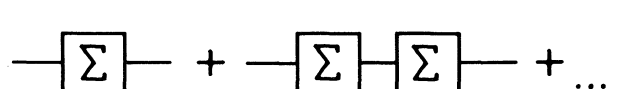


FIG. 5. Iterations of the self-energy operator.

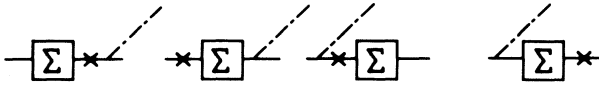


FIG. 6. Brueckner-type correlation corrections to the PNC $E1$ amplitude. The cross (\times) denotes the weak interaction and the dash-dotted line ($-\cdot-\cdot-$) denotes the electromagnetic field.

The contributions of higher orders in Σ to the PNC can be obtained from Eq. (7). This expression contains the terms of all orders in $\hat{\Sigma}$ including the linear one when Brueckner orbitals are used. The linear term should be eliminated from (7) to use the more accurate formula (8) instead. In order to do this, we introduce a numerical factor (say, a) before the correlation potential and examine the $E1_{\text{PNC}}$ dependence on the factor in the range $0 \leq a \leq 1$. When $a \ll 1$ the term linear in $\hat{\Sigma}$ dominates in (7) and its extrapolation to $a = 1$ yields the first order in Σ correlation correction to the PNC amplitude:

$$\frac{1}{a}[E1_{\text{PNC}}(V^{N-1} + a\hat{\Sigma}) - E1_{\text{PNC}}(V^{N-1})], \quad (9)$$

where $E1_{\text{PNC}}()$ is given by (7) with the one-electron wave functions calculated in the potential given in brackets. Formula (9) corresponds to (8) when the dependence of Σ on energy is neglected. Now the contribution of higher orders in $\hat{\Sigma}$ is given by

$$s_5 = [E1_{\text{PNC}}(V^{N-1} + \hat{\Sigma}) - E1_{\text{PNC}}(V^{N-1})] - \frac{1}{a}[E1_{\text{PNC}}(V^{N-1} + a\hat{\Sigma}) - E1_{\text{PNC}}(V^{N-1})]. \quad (10)$$

III. RESULTS AND DISCUSSION

The energy levels of francium calculated in the RHF and Brueckner approximations are presented in Table II together with our earlier results [7] and experimental data. In [7] only second-order correlation corrections to the energy levels were taken into account. However, to improve the predictions of the energy level positions, further corrections were introduced based on the extrapolation of the theoretical error in similar calculations for cesium and on the known wavelength of the $7s-7p_{3/2}$ transition. Note that it was the only experimental energy interval available at the time of publication of [7].

TABLE II. Francium energy levels (cm^{-1}). The minus signs have been omitted. In the RHF + $\hat{\Sigma}_2$ calculation second-order correlations were included using Green functions and Feynman diagram techniques. Our predictions for the positions of unmeasured energy levels are based on the extrapolation of computational error from known levels.

State	Calculations				Experiment [1-6]
	Dzuba <i>et al.</i> [7]	RHF	RHF + $\hat{\Sigma}_2$	Brueckner orbitals	
$7s_{1/2}$	32841	28727	33406	32762	32849
$8s_{1/2}$	13136	12271		13082	13110
$9s_{1/2}$	7182	6854		7160	7171
$10s_{1/2}$	4540	4380		4534	4538
$11s_{1/2}$		3043		3123	3130
$12s_{1/2}$		2242		2290	2290
$7p_{1/2}$	20568	18855	20690	20654	20612
$8p_{1/2}$	9745	9240		9742	9736
$9p_{1/2}$	5754	5526		5736	
$7p_{3/2}$	18913	17652	18988	18926	18925
$8p_{3/2}$	9205	8810		9188	9191
$9p_{3/2}$	5505	5327		5485	
$6d_{3/2}$	16596	13837		16623	
$7d_{3/2}$	8614	7730		8663	
$8d_{3/2}$	5280	4860		5261	5248
$9d_{3/2}$		3326		3537	3532
$6d_{5/2}$	16446	13935		16423	
$7d_{5/2}$	8524	7751		8574	
$8d_{5/2}$	5230	4865		5218	5203
$9d_{5/2}$		3327		3513	3507
$5f$	6952	6866		6979	
$6f$	4439	4396		4469	

TABLE III. Francium fine structure intervals (cm^{-1}).

Level	Dzuba <i>et al.</i> [7]	RHF	RHF+ $\hat{\Sigma}_2$	Brueckner orbitals	Experiment
7p	1655	1203	1702	1728	1687
8p	540	430		554	545
9p	249	199		251	
6d	150	-97		200	
7d	90	-21		89	
8d	50	-5		43	45
9d		1		24	25

In spite of the poor numerical accuracy of the correlation correction calculations in [7] (see the discussion in Sec. II) the predicted positions of the francium energy levels proved to be very close to the values measured later (see Table II). This is a consequence of the similar electron structures of cesium and francium and is by no means fortuitous. With the present technique we calculate the correlation corrections with good numerical accuracy. When the second-order correlations are taken into account the agreement with the experimental data is about 0.5–1.5% (see the third column, Table II). On the other hand, when the higher-order correlations are also taken into account the discrepancy between the theoretical and the experimental data is reduced to 0.1–0.3%.

A PNC experiment is expected to be carried out on the 7s-8s transition. However, the position of the 8s level is still not measured. Thus it is very important to determine it as accurately as possible. Note that while in [7] we predicted the positions of the 7s and 10s levels with very good accuracy, we could not assume the same accuracy for the 8s and 9s levels. For the 10s state the accuracy was very high due to a small value of the correlation correction. As for the 7s state, the known value of the

wavelength of the 7s-7p_{3/2} transition was used to refine its energy. On the other hand, the calculations with the higher-order correlations taken into account give good accuracy systematically, for all levels. Therefore, further corrections can be made for the 8s and 9s levels based on the extrapolation of the theoretical error of our present calculations for the 7s and 10s levels. The new values, presented in the column 6 of Table II, agree with our previous predictions within the accuracy of our earlier calculations but hopefully are closer to the real positions of the levels.

In Table III we present the fine structure intervals for francium which were determined simply as the difference between the energies of the $j = l + \frac{1}{2}$ and $j = l - \frac{1}{2}$ levels. This table illustrates that the accuracy of the calculation is good for the fine structure intervals as well, in spite of the fact that the corrections are large and the RHF approximation fails to reproduce even the sign of the intervals for the d levels.

The results of the calculations of the ordinary E1-transition amplitudes for francium are presented in Table IV in the form of the values of the corresponding radial integrals R . The radial integrals are formally de-

TABLE IV. Radial integrals for francium (in units of the Bohr radius). In column 5 non-Brueckner correlations are included (extrapolation from Cs). The last column gives our predictions (extrapolation of numerical error from Cs).

Transition	RHF	TDHF	Brueckner orbitals	Brueckner plus non-Brueckner	Prediction
7s-7p _{1/2}	-6.311	-5.851	-5.261	-5.241	-5.271
7s-7p _{3/2}	-6.153	-5.742	-5.124	-5.104	-5.133
7s-8p _{1/2}	-0.5558	-0.3508	-0.3355	-0.3568	-0.3684
7s-8p _{3/2}	-0.9459	-0.7478	-0.7560	-0.8004	
8s-7p _{1/2}	5.540	5.577	5.137	5.101	5.167
8s-7p _{3/2}	6.696	6.701	6.432	6.395	6.469
8s-8p _{1/2}	-13.23	-13.10	-12.46	-12.44	-12.25
8s-8p _{3/2}	-12.52	-12.42	-11.67	-11.65	-11.48
7p _{1/2} -6d _{3/2}	7.977	7.604	6.232		
7p _{1/2} -7d _{3/2}	-1.722	-1.855	-3.015		
7p _{3/2} -6d _{3/2}	8.282	7.947	6.411		
7p _{3/2} -6d _{5/2}	8.254	7.928	6.574		
7p _{3/2} -7d _{3/2}	-2.670	-2.791	-4.213		
7p _{3/2} -7d _{5/2}	-2.759	-2.850	-3.992		

finned as an amplitude divided by the angular matrix element $\langle \alpha | \mathbf{n} | \beta \rangle$ ($\mathbf{n} = \mathbf{r}/r$). The core polarization and the Brueckner-type correlations are both important, as can be seen from the table. The relative values of different contributions to the s - p $E1$ -transition amplitudes for francium are very close to the corresponding values for cesium [18]. This allowed us to make further corrections. The contributions of the non-Brueckner-type diagrams and the remaining discrepancy between the theoretical and experimental data were extrapolated from similar calculations for cesium [18] (fourth and fifth columns in Table IV). The agreement between the theoretical and the experimental values for the $E1$ amplitudes for cesium was about 0.5%. One should expect similar or even better accuracy for the corrected values of the s - p radial integrals for francium (Table IV, column 6). The accuracy of the calculation of the p - d radial integrals is probably a little worse due to huge correlation corrections to the d levels.

The values from Table IV can be used to obtain life-

TABLE V. Correlation-correction contributions to the E_{PNC} amplitude of the $7s$ - $8s$ transition in francium [in units $10^{-10}iea_B(-Q_W/N)$].

TDHF ^a	s_1^b	s_2^b	s_3^b	s_4^b	s_5^c	Sum
1.609	0.0927	0.3451	-0.1127	-0.3014	-0.04	1.59

^aThe polarization of the closed shells by the weak interaction and by the photon field is taken into account.

^bFormula (8).

^cFormula (10).

times of the francium excited states. The probability of the $E1$ transition from state i to state j ($p \rightarrow s$ transition) is given by (in atomic units)

$$W_{ji} = \frac{4}{9} \omega^3 \alpha^3 R_{ji}^2, \quad (11)$$

where ω is the frequency of the transition, $\alpha = 1/137.036$, and R is the radial integral. For example, for the $7p_{3/2}$

TABLE VI. Comparison of our calculations of the PNC effect in atoms with experiment.

Atom	Transition	Calculation		Experiment	
		$E1_{PNC}$ [$10^{-11}iea(-Q_W/N)$]	$10^8 R = \frac{\text{Im}(E1)}{M1}$	$E1_{PNC}$ [$10^{-11}iea(-Q_W/N)$]	$10^8 R = \frac{\text{Im}(E1)}{M1}$
¹³³ Cs	$6s$ - $7s$	0.88 ± 0.03^a		$0.89 \pm 0.10 \pm 0.07^d$	
		0.90 ± 0.02^b		0.90 ± 0.02^e	
		0.91 ± 0.01^c			
²⁰⁵ Tl	$6p_{1/2}$ - $7p_{1/2}$	$7.9(1 \pm 0.06)^b$		7.4 ± 1.4^f 11.4 ± 2.2^g	
	$6p_{1/2}$ - $6p_{3/2}$	$27.0(1 \pm 0.03)^b$	-14.0 ± 0.4^b		-12.5 ± 1.9^h $-14.73 \pm 0.06 \pm 0.15^i$
²⁰⁸ Pb	3P_0 - 3P_1 ($\lambda = 1279$ nm)		-10.4 ± 0.8^j		-9.9 ± 2.5^k $-9.86 \pm 0.04 \pm 0.11^l$
²⁰⁹ Bi	$^4S_{3/2}$ - $^3D_{3/2}$ ($\lambda = 876$ nm) $^4S_{3/2}$ - $^2D_{5/2}$ ($\lambda = 648$ nm)		-10.4 ± 1^j		-10.12 ± 0.20^m
			-7.5 ± 5^c		-20.2 ± 2.7^n -9.3 ± 1.4^o -7.8 ± 1.8^p -9.8 ± 0.9^q

^aReferences [30,31].

^bReference [32].

^cReference [14].

^dReference [33].

^eReference [10].

^fReferences [34,35].

^gRecalculation from measurements of $\text{Im}(E1/\beta)$ [34] using the new measured value of β [36].

^hReference [37].

ⁱReference [12].

^jReference [38].

^kReference [39].

^lReference [11].

^mReference [13].

ⁿReference [40].

^oReference [41].

^pReference [42].

^qReference [43].

state one should take, for the $7p_{3/2}$ - $7s$ transition, $R = 5.133a_B$ from Table IV and $\omega = 0.06344$ a.u. from Table II, which leads to $\tau = 2.082 \times 10^{-8}$ sec.

Table V presents our results for the calculation of the parity nonconserving $E1$ amplitude of the $7s$ - $8s$ transition in ^{223}Fr . As in the case of the ordinary $E1$ amplitudes, the relative values of different contributions to E_{PNC} for francium are very close to the corresponding values for cesium [14]. However, due to strong cancellations between different contributions to the correlation correction, the resulting value is quite different. The correlation correction to the PNC transition amplitude in Fr has opposite sign and its relative value is about two times smaller than the corresponding value for cesium (the absolute value is about ten times larger). So correlation corrections reduce the value of PNC amplitude in Fr by only 1.3%. This result is relatively stable with respect to variation of the numerical parameters. Since the relative values of the correlation corrections to energy levels, $E1$ transition amplitudes, and the PNC effect were very similar for francium and cesium, we believe that the accuracy of the calculation of the PNC transition amplitude for francium is about the same as for cesium (see [14]). Comparing the calculated energy levels with experimental data provides a good test of the numerical accuracy too because the same self-energy operator is used throughout all calculations [see formulas (1), (6), and (8)]. Note however, that we did not carry out such a careful analysis of the accuracy of PNC calculations for francium as we did it for cesium. Once there is progress in the measurements of francium the accuracy can be estimated more precisely by the calculation of hyperfine structure intervals, non-Brueckner-type correlation corrections, etc.

Our final result for E_{PNC} in ^{223}Fr has the form

$$^{223}\text{Fr} : E1(7s-8s) \\ = (1.59 \pm \sim 1\%) \times 10^{-10} iea_B (-Q_W/N), \quad (12)$$

where Q_W is the weak charge of the ^{223}Fr nucleus and $N=136$ is the number of neutrons. To obtain E_{PNC} for another francium isotope one should multiply (12) by the factor $N_i/136$, where N_i is the number of neutrons in this isotope. We have tested that a change in either the neutron or electric radius of the nucleus does not contribute at the present level of accuracy.

In conclusion, we would like to draw the reader's attention to the Table VI where we compare all our calculations of PNC in atoms with existing experimental data. The standard model of the electroweak interaction with $\sin^2 \theta_W = 0.23$ was used to recalculate the values in the table. Note the good agreement between our theoretical predictions and experimental data for all atoms. While for the heaviest atoms accuracy is restricted due to the complexity of their electron structure, the accuracy for cesium is very high. All our results for cesium agree with each other and with the result of Blundell, Johnson, and Sapirstein [15]. Their result is the only result other than our calculation which also claims an accuracy of 1%. Since our calculations of all PNC effects in all atoms were done before accurate measurements (and also before calculation [15] for Cs) one can consider an agreement as a very reliable test of our method of calculation. So, if we had 1% accuracy for cesium, our accuracy for francium should be as good due to similar electron structure and the very same approach to the PNC calculations.

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