High-precision calculation of the parity-nonconserving amplitude in francium

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A high-precision calculation of the $7s$-$8s$ parity-nonconserving (PNC) transition amplitude in francium, based on a relativistic all-order method, is presented. Our values for the PNC amplitudes in ^{223}Fr and ^{210}Fr are $E_{\rm PNC}=15.41(17)$ and 14.02(15), respectively, in units $10^{-11}i|e|a_0(-Q_W/N)$, where Q_W is the weak charge and N is the neutron number. Spin-dependent contributions to the PNC amplitude are calculated for Fr isotopes with nucleon numbers $A=207$, 209, 211, and 213. To assess the accuracy of our calculations, we apply the present all-order method to the $6s$-$7s$ PNC amplitude in cesium and obtain a result in close agreement with previous high-precision calculations.

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Measurements of parity-nonconserving (PNC) amplitudes in francium, the heaviest alkali-metal atom, have been proposed [1], and considerable progress has been made recently in understanding the structure of the francium atom. On the experimental side, energies of the $8s$ and $9s$ levels, lifetimes of the $7p_{1/2}$ and $7p_{3/2}$ levels, and hyperfine constants of the $7p_{1/2}$ and $8s$ levels have been accurately measured [2–6]. On the theoretical side, calculations have been carried out for energies, transition rates, hyperfine constants, and the $7s$-$8s$ PNC amplitude [7–11]. With the possibility of new measurements of PNC in mind, we present a calculation of the $7s$-$8s$ PNC amplitude in francium accurate to 1%; our value for ^{223}Fr differs by 3% from the previous many-body value given in Ref. [9].

Measurements of the $6s$-$7s$ PNC amplitude in cesium [12,13], when combined with accurate many-body calculations, [14,15] provided a high-precision atomic-physics test of the standard model and yielded an experimental value for a nuclear anapole moment. Although precise measurements of PNC amplitudes have also been made for the $6p_{1/2}$-$6p_{3/2}$ transition in Tl [16] and the $6\,^3P_0$-$6\,^3P_1$ transition in Pb [17], the corresponding theoretical calculations are not sufficiently accurate to permit precise tests of the standard model to be made in these cases.

Recently, we carried out a systematic study of atomic properties of alkali-metal atoms using the relativistic single-double (SD) all-order method [7]. Our calculated energy levels, dipole matrix elements, and hyperfine constants in Fr were shown to be in excellent agreement with available measurements [2–6]. Furthermore, we made predictions of as yet unmeasured atomic data in francium including energies of the $9p$ and $10p$ levels, np-$n's$ dipole matrix elements, $8p_{1/2}$, $8p_{3/2}$ hyperfine constants, and polarizabilities. In this paper, we make use of the results of the SD calculations in [7] to evaluate the $7s$-$8s$ PNC amplitude in Fr.

The PNC amplitude in Fr can be represented as a sum over states:

$$E_{\rm PNC}=\sum_{n=2}^{\infty}\frac{\langle 8s|D|np_{1/2}\rangle\langle np_{1/2}|h_{\rm PNC}|7s\rangle}{E_{7s}-E_{np_{1/2}}}+\sum_{n=2}^{\infty}\frac{\langle 8s|h_{\rm PNC}|np_{1/2}\rangle\langle np_{1/2}|D|7s\rangle}{E_{8s}-E_{np_{1/2}}},\qquad(1)$$

where D is the dipole transition operator and $h_{\rm PNC}$ is the PNC Hamiltonian. In the present calculations, we evaluate this sum directly. The dominant part of the PNC interaction Hamiltonian is

$$h_{\rm PNC}=\frac{G_F}{2\sqrt{2}}Q_W\gamma_5\rho(r),\qquad(2)$$

where G_F is the universal Fermi coupling constant, Q_W is the weak charge [18], and γ_5 is the Dirac matrix associated with pseudoscalars. The quantity $\rho(r)$ is a nuclear density function, which is approximately the neutron density. In our calculations, we model $\rho(r)$ by the charge form factor, which is taken to be a Fermi distribution with 50% radius $c=6.83$ fm and 10–90 % thickness parameter $t=2.3$ fm for ^{223}Fr [19].

Our calculation of $E_{\rm PNC}$ is divided into three parts: a main term $E_{\rm PNC}^{(1)}$ that contributes 97% of the total and consists of the sum over states with $n=7,\ldots,10$, a tail $E_{\rm PNC}^{(2)}$ that is the sum over states with $n=11,\ldots,\infty$, and the contribution $E_{\rm PNC}^{(3)}$ from autoionizing states given by the terms $n=2,\ldots,6$.

First, we discuss the calculation of the main term. As noted previously, the dipole matrix elements $\langle 8s|D|np_{1/2}\rangle$ and $\langle np_{1/2}|D|7s\rangle$ and removal energies E_{ns} and $E_{np_{1/2}}$ were calculated using the all-order SD method in [7]. Therefore, we only need to calculate $\langle 8s|h_{\rm PNC}|np_{1/2}\rangle$ and $\langle np_{1/2}|h_{\rm PNC}|7s\rangle$ to high accuracy to obtain an accurate value for the dominant part of the PNC amplitude. Since there are no data for matrix elements of $h_{\rm PNC}$ available for comparison in francium, we also calculate matrix elements of $h_{\rm PNC}$ in Cs using the present SD code and compare them with high-precision results in Ref. [15]. Our matrix elements of $h_{\rm PNC}$ in Cs, which include semiempirical corrections for triple excitations, agree with results from [15] to better then 0.5% for $\langle np_{1/2}|h_{\rm PNC}|6s\rangle$ transitions and to all digits quoted for $\langle 7s|h_{\rm PNC}|np_{1/2}\rangle$ transitions.

In Table I, we list zeroth-order Dirac-Hartree-Fock (DHF), all-order (SD), and scaled ($\rm SD_{sc}$) matrix elements of $h_{\rm PNC}$ in Fr. The $\rm SD_{sc}$ values are SD matrix elements scaled to include partial corrections for omitted triple excitations following the procedure given in [7]. As we see from the table, correlation corrections to the matrix elements of $h_{\rm PNC}$ are

TABLE I. Lowest-order (DHF) PNC matrix elements are compared with all-order (SD) and scaled (SD_{sc}) matrix elements in ^{223}Fr. Units: $10^{-11}i|e|a_0(-Q_W/N)$.

Term	DHF	SD	SD_{sc}
$\langle 7p_{1/2}\|h_{\rm PNC}\|7s\rangle$	0.6360	1.1689	1.1223
$\langle 8p_{1/2}\|h_{\rm PNC}\|7s\rangle$	0.3789	0.6449	0.6249
$\langle 9p_{1/2}\|h_{\rm PNC}\|7s\rangle$	0.2593	0.4313	0.4191
$\langle 10p_{1/2}\|h_{\rm PNC}\|7s\rangle$	0.1918	0.3160	0.3086
$\langle 8s\|h_{\rm PNC}\|7p_{1/2}\rangle$	0.3222	0.5348	0.5191
$\langle 8s\|h_{\rm PNC}\|8p_{1/2}\rangle$	0.1918	0.2944	0.2885
$\langle 8s\|h_{\rm PNC}\|9p_{1/2}\rangle$	0.1313	0.1967	0.1933
$\langle 8s\|h_{\rm PNC}\|10p_{1/2}\rangle$	0.0971	0.1441	0.1423

very large, ranging from 45% for the $7s$-$7p_{1/2}$ transition to 30% for the $8s$-$10p_{1/2}$ transition.

To obtain $E^{(1)}_{\rm PNC}$, we substitute the single-double PNC matrix elements from Table I, together with previously calculated dipole matrix elements and removal energies from [7] into Eq. (1). The resulting *ab initio* value is $E^{(1)}_{\rm PNC}=15.08$ in units $10^{-11}i|e|a_0(-Q_W/N)$. (All subsequent data for contributions to PNC amplitude are in these units.) The corresponding value in the DHF approximation is 13.56, so the correlation correction is approximately 10%.

Including corrections from the Breit interaction, the value 15.08 above is reduced to $E^{(1)}_{\rm PNC}=14.93$. We evaluate the (lowest-order) Breit correction by modifying all wave functions in Eq. (1) using

$$|n\rangle \rightarrow |n\rangle + \sum_{k\neq n} \frac{|k\rangle\langle k|B|n\rangle}{\epsilon_n - \epsilon_k}, \tag{3}$$

where the summation ranges over both positive and negative energy states. In the above equation, $\langle k|B|n\rangle$ is the matrix element of the Breit Hamiltonian B. Only the one-body part of the Breit operator contributes in lowest order. To calculate the correction to the PNC amplitude, we use the substitution (3) to calculate corrections to individual matrix elements. The Breit corrections to energies in Eq. (1) are obtained using the prescription given in Ref. [20]. The resulting Breit correction to the *ab initio* PNC amplitude is -0.15. A more rigorous treatment of the Breit correction including contributions from the two-body part of the Breit Hamiltonian and accurate calculations of higher-order corrections is required before Breit correction to the PNC can be accurately determined. In Cs, the Breit contribution was found to be very small, $0.2(\pm 0.2)\%$ in Ref. [15]. In Fr, the Breit correction was recently estimated, including both one-body and two-body contribution, and found to contribute approximately -1.1% [21], in harmony with the present estimate.

In Table II, we list results for the main term $E^{(1)}_{\rm PNC}$ of the parity-nonconserving amplitude in ^{223}Fr obtained using various combinations of energies, dipole matrix elements, and PNC matrix elements. All entries in this table include Breit corrections. These values are used to check the stability of our calculation and to provide an estimate of the uncertainty. The *ab initio* single-double result for the main term is listed

TABLE II. Evaluation of $E^{(1)}_{\rm PNC}$. The entries under ''Energy,'' $\langle v\|D\|n\rangle$, and $\langle v\|h_{\rm PNC}\|n\rangle$ describe the sources used to determine energies, dipole matrix elements, and PNC matrix elements, respectively. The entry SD designates single-double all-order values and SD_{sc} designates scaled SD values. The entry BV designates ''best value'' dipole matrix elements obtained using the experimental dipole matrix element for the $7s$-$7p_{1/2}$ transition [4], SD_{sc} matrix elements for $7s$-$8p_{1/2}$, $7s$-$9p_{1/2}$, $8s$-$8p_{1/2}$, $8s$-$7p_{1/2}$ transitions [7], and SD matrix elements for the remaining transitions. Units: $10^{-11}i|e|a_0(-Q_W/N)$.

Energy	$\langle v\|D\|n\rangle$	$\langle n\|h_{\rm PNC}\|v\rangle$	$E^{(1)}_{\rm PNC}$
SD	SD	SD	14.93
Expt.	SD	SD	14.95
Expt.	BV	SD	14.93
Expt.	BV	SD_{sc}	14.81
Final			14.95(14)

in the first row. We give values for $E^{(1)}_{\rm PNC}$ using various combinations of experimental energies, scaled PNC matrix elements, and ''best-value'' dipole matrix elements in subsequent rows. The best-value matrix elements are defined here as the experimental dipole matrix element for the $7s$-$7p_{1/2}$ transition [4], scaled dipole matrix elements for the $7s$-$8p_{1/2}$, $7s$-$9p_{1/2}$, $8s$-$8p_{1/2}$, $8s$-$7p_{1/2}$ transitions [7], and SD matrix elements for the other transitions. This selection of best-value data is based on a comparison of the corresponding values for transitions in Cs with experiment and with other high-precision theoretical calculations [22,23]. Since the energies of the $9p_{1/2}$ and $10p_{1/2}$ states are not yet measured, we used our theoretical results for these levels [7] instead of experimental data.

There is strong cancellation between the two sums in Eq. (1) and between $n=7$ and $n=8$ contributions in each sum. Therefore, it is important that the data for transitions to $7s$ and $8s$ states be of consistent accuracy. The results obtained using *ab initio* SD matrix elements treat correlation in a systematic way and are thus least effected by the cancellations. We believe that the calculation made using SD matrix elements and *experimental* energies $E^{(1)}_{\rm PNC}=14.95$ is the most reliable of those listed in the table, so we use this as our theoretical value for the PNC amplitude and we use the spread in values (0.14) to measure the uncertainty in the theoretical value.

We summarize our results for the PNC amplitude in ^{223}Fr in Table III. The main contribution $E^{(1)}_{\rm PNC}=14.95(14)$ is the final result given in Table II. The dominant correction $E^{(2)}_{\rm PNC}=0.49(10)$ is from excited $np_{1/2}$ states with $n>10$. We use the random-phase approximation (RPA) [15] to evaluate contributions from these states. Although we have no direct way to determine the accuracy of the RPA calculation, we assume that it is better than 20% based on comparisons with DHF calculations. Finally, we calculate the contribution of autoionizing states ($n=2,\ldots,6$) in the DHF pproximation using lowest-order values of matrix elements and energies. Since the resulting value is very small, $E^{(3)}_{\rm PNC}=-0.03$, more exact treatment of this correction is not warranted.

TABLE III. Contributions to the $7s$-$8s$ PNC amplitude in ^{223}Fr and comparison with the theory from Ref. [9]. Units: $10^{-11}i|e|a_0(-Q_W/N)$.

Term	Value
$E_{\mathrm{PNC}}^{(1)}$	14.95(14)
$E_{\mathrm{PNC}}^{(2)}$	0.49(10)
$E_{\mathrm{PNC}}^{(3)}$	−0.03(03)
E_{PNC}	15.41(17)
Ref. [9]	15.9(1%)

Our final result for the PNC amplitude in ^{223}Fr is $E_{\mathrm{PNC}}=15.41(17)$, where the number in parenthesis is the theoretical uncertainty. The estimated uncertainty does not include uncertainty in the nuclear parameters. We list the result of another high-precision calculation of PNC amplitude in ^{223}Fr [9] in the last row of Table III for comparison.

As an independent test of the accuracy of our calculation of the Fr PNC amplitude, we carried out an identical calculation for the $6s$-$7s$ transition in Cs. The result, which is listed in Table IV, is in excellent agreement with previous high-precision calculations [14,15].

We also investigate the dependence of the PNC amplitude on the parameters c and t of the nuclear distribution $\rho(r)$. It is sufficient to do so in the lowest order because this correction is expected to be small. In Table V, we list DHF results for the main term with different values of c and t. From Table V, we conclude that a 2.2% increase in c leads to a 1% decrease in the value of E_{PNC}; therefore, the parity-nonconserving amplitude is sensitive to the value of nuclear radii. The parameter t must be increased by 18% to decrease the value of E_{PNC} by 1%. The parameters used in the last line of Table V are those used by Dzuba *et al.* in [9] to calculate E_{PNC} in ^{223}Fr. The resulting value of lowest-order PNC amplitude is 0.6% higher than our lowest-order value, listed in the first row of Table V.

Our final value, $E_{\mathrm{PNC}}=15.41(17)$ for ^{223}Fr differs from the only other high-precision calculation of PNC amplitude in Fr [9] by $E_{\mathrm{PNC}}=15.9(1\%)$ by 3.1%. However, as noted above, 0.6% of this difference is due to the use of different parameters in the nuclear distribution. The calculation in Ref. [9] does not include Breit contribution, which accounts for another 1% of the difference. The remaining difference is

TABLE IV. Comparison of the calculation of the $6s$-$7s$ amplitude in Cs with other high-precision calculations. Units: $10^{-11}i|e|a_0(-Q_W/N)$.

	E_{PNC}
Present	0.909(11)
Blundell *et al.*[a]	0.907(9)
Blundell *et al.*[b]	0.902(9)
Dzuba *et al.*[c]	0.908(10)

[a]Sum over state approach [15].

[b]Mixed-parity many-body perturbation theory [15].

[c]Mixed-parity many-body theory [14].

TABLE V. Dependence of the lowest-order PNC amplitude in ^{223}Fr on the parameters c and t of the nuclear distribution in units $10^{-11}i|e|a_0(-Q_W/N)$.

c (fm)	t (fm)	E_{PNC}
6.83	2.3	13.56
6.50	2.3	13.85
7.00	2.3	13.42
6.83	2.5	13.50
6.67	2.5	13.64

1.5%, which is consistent with the error estimates of our calculation and that of Ref. [9].

Since, in the present units, E_{PNC} is proportional to the neutron number N, it appears at first glance that the value of the PNC amplitude for any isotope could be obtained from the value for $A=223$, by scaling with N. Such scaling is of course only justified if the amplitude is insensitive to the parameters c and t in the nuclear distribution $\rho(r)$. The isotopes of Fr listed in [24] can be divided into two groups with $A=207-213$ and $A=220-228$, and the formula for the RMS radius $r_{\mathrm{rms}}=0.836A^{1/3}+0.570$ fm from [19] can be used to determine values of c for different isotopes with fixed $t=2.3$ fm. The maximum difference between c for ^{223}Fr and any other isotopes in the group $A=220-228$ is 0.7%, leading to a 0.3% correction to the PNC amplitude. Such a correction is negligible at the present level of accuracy. Therefore, the PNC amplitude for isotopes in the group $A=220-228$ can be obtained from the value for ^{223}Fr by scaling with the neutron number of the isotope. Scaling from the value for ^{223}Fr is not justified at the present level of accuracy for the isotopes in the group $A=207-213$, since differences in radii between isotopes in this group and ^{223}Fr lead to changes in the E_{PNC} at the 1% level. To obtain the value for the PNC amplitude in ^{210}Fr, we recalculate the total PNC amplitude, using parameters $c=6.72$ fm, $t=2.3$ fm, corresponding to the value $r_{rms}=5.560$ fm given in [5]. The resulting final value is $E_{\mathrm{PNC}}=14.02(15)$ for ^{210}Fr. The maximum difference between c for ^{210}Fr and c for any other isotope in the group $A=207-213$ is 0.5%, leading to a negligible effect on E_{PNC} at the present level of accuracy. Therefore, the PNC amplitude for isotopes with $A=207-213$ can be obtained by scaling the value for ^{210}Fr with the neutron number. In summary, the value of any Fr isotope (at the 1% level of accuracy) can be obtained from the values $E_{\mathrm{PNC}}=14.02(15)$ and 15.41(17) for ^{210}Fr and ^{223}Fr, respectively, by scaling with the number of neutrons; the first value should be used for the lighter isotopes and the second one for the heavier ones.

The PNC interaction given in Eq. (2) is obtained from the timelike part of the product of the vector nucleon current V_n and the axial vector electron current A_e; it does not depend on the nuclear spin I. The spacelike component of the product V_e and A_n leads to a nuclear spin-dependent interaction, which for the case of a single valence nucleon may be written

TABLE VI. Coefficients $A(F_F,F_I)$ for ^{133}Cs and ^{209}Fr, where F_F and F_I are final and initial total spin.

^{133}Cs			^{209}Fr		
F_F	F_I	$A(F_F,F_I)$	F_F	F_I	$A(F_F,F_I)$
3	3	0.0286	4	4	0.0171
3	4	0.0477	4	5	0.0287
4	3	−0.0413	5	4	−0.0256
4	4	−0.0223	5	5	−0.0140

$$h_{\rm PNC}^{(2)}=\frac{G_F}{\sqrt{2}}K_2\frac{\kappa-1/2}{I(I+1)}\alpha\cdot\mathbf{I}\rho_v(r) \tag{4}$$

where $\rho_v(r)$ is the valence nucleon density and where $\kappa=\mp(I+1/2)$ for $I=L\pm1/2$, L being the orbital angular momentum of the valence nucleon. The spin-dependent interaction that arises from the electromagnetic coupling of the atomic electrons to the nuclear anapole moment [25] is given by

$$h_{\rm PNC}^{(a)}=\frac{G_F}{\sqrt{2}}K_a\frac{\kappa}{I(I+1)}\alpha\cdot\mathbf{I}\rho_v(r). \tag{5}$$

The two spin-dependent terms (4) and (5) can be treated together, replacing K_a by $K=K_a-K_2(\kappa-1/2)/\kappa$ in Eq. (5). The PNC amplitude is then modified as

$$E_{\rm PNC}\rightarrow E_{\rm PNC}\left[\left(\frac{Q_W}{-N}\right)+KA(F_F,F_I)\right], \tag{6}$$

where $E_{\rm PNC}$ is the spin-dependent PNC amplitude in the units $i|e|a_0$ and F_F and F_I are angular momenta of the final and initial atomic hyperfine levels, respectively. We calculate spin-dependent PNC effects for light Fr odd-A isotopes with $A=207$, 209, 211, and 213, all of which have a single $h_{9/2}$ valence proton [24]. For these cases, the nuclear spin is $I=9/2$, $\kappa=5$, and angular momenta of the atomic hyperfine levels are $F_{I,F}=4$ or 5. We carried out the calculation of $A(F_F,F_I)$ in lowest-order approximation including weak core-polarization corrections [26]. We found that despite the fact that weak core-polarization modifies both the contributions from both spin-independent and spin-dependent terms by about 20%, it has a negligible (less then 0.5%) effect on the values of the ratio $A(F_F,F_I)$. Calculations of $A(F_F,F_I)$ were carried out using a Fermi distribution for $\rho(r)_v$ and a crude shell model; negligible differences in the results were found. The values of $A(F_F,F_I)$ are also insensitive to the parameters of the nuclear Fermi distribution: a 10% change in the parameter c or a 20% change in the parameter t results in a 0.1% change in the values of $A(F_F,F_I)$. Since there are no comparison values available for spin-dependent PNC effects in Fr, we also carried out similar calculations in ^{133}Cs, which has a single valence $g_{7/2}$ proton. Our results for Cs are in precise agreement with previously published data [15]. The values of $A(F_F,F_I)$ for ^{209}Fr as well as the comparison values for ^{133}Cs are given in Table VI. The values are given for only one of the isotopes, namely, ^{209}Fr; corresponding values for ^{207}Fr, ^{211}Fr, and ^{213}Fr are obtained by scaling ^{209}Fr values by $122/N$, where N is the number of neutrons in the corresponding isotope. The spin-dependent amplitude is needed to extract $E_{\rm PNC}$ from experimental measurements and to determine the value of K and, correspondingly, nuclear anapole moment K_a.

In summary, we have presented a calculation of the parity-nonconserving amplitude in Fr at the 1% level of accuracy. To estimate the accuracy, we investigated the stability of the final result by using various sets of data (SD, SD$_{sc}$, or experimental) for energies and matrix elements. As an independent test of the accuracy, we applied our method to ^{133}Cs and found excellent agreement with other high-precision calculations. The dependence of the PNC amplitude on the parameters of nuclear distribution was investigated. Spin-dependent PNC effects were evaluated for four light odd-A isotopes. The resulting values can be used in conjunction with measurements for future atomic-physics tests of the standard model.

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