Parity nonconservation in thallium

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We report a calculation of the parity nonconserving (PNC) $E1$ amplitude for the $6p_{1/2}\rightarrow 6p_{3/2}$ transition in ^{205}Tl. Our result for the reduced matrix element is $(E1)_{\rm PNC}=-(66.7\pm 1.7)\times i\,10^{-11}(-Q_W/N)$ a.u. Comparison with the experiment of Vetter *et al.* [Phys. Rev. Lett. **74**, 2658 (1995)] gives the following result for the weak charge of ^{205}Tl: $Q_W/Q_W^{\rm SM}=0.97(\pm 0.01)_{\rm expt}(\pm 0.03)_{\rm theor}$, where $Q_W^{\rm SM}=-116.7\pm 0.1$ is the standard-model prediction. This result confirms an earlier conclusion based on the analysis of a Cs experiment that atomic PNC experiments are in agreement with the standard model.

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I. INTRODUCTION

The thallium atom is the second simplest atom where parity nonconservation (PNC) has been observed [1,2]. The simplest and best understood such atom is cesium, where theory has the accuracy of 1% [3,4] (see also more-recent calculations [5,6,7]). That, together with the best experimental result for Cs [8] allowed one to obtain the most-accurate result for the weak charge of the cesium nucleus [6,7]:

$$Q_W(^{133}{\rm Cs})=-72.5(3)_{\rm expt}(7)_{\rm theor}, \tag{1}$$

$$Q_W^{\rm SM}(^{133}{\rm Cs})=-73.09(3), \tag{2}$$

where Eq. (2) is the standard model prediction given in Ref. [9]. Note, that these two values are in agreement with each other. Recently there has been some discussion on the accuracy of the theory for Cs; in Ref. [10] the accuracy of the theoretical amplitude in Cs was estimated to be 0.4%, but at present there seems to be a consensus that it is closer to 1%.

In this paper, we report a calculation of the PNC $E1$ amplitude for the $6p_{1/2}\rightarrow 6p_{3/2}$ transition in thallium. Combining this calculation with the most-accurate experiment [1], leads to a value of the weak charge of the ^{205}Tl nucleus that can also be compared with the standard-model prediction [9]:

$$Q_W(^{205}{\rm Tl})=-113(1)_{\rm expt}(3)_{\rm theor}, \tag{3}$$

$$Q_W^{\rm SM}(^{205}{\rm Tl})=-116.7(1). \tag{4}$$

Again, these two values are in agreement with each other. The atomic theory involved in both calculations is similar, as are the possible sources of theoretical uncertainty. That can possibly explain why the central values in Eq. (1) and Eq. (3) are shifted in the same direction from the standard-model predictions (note that in both cases the theoretical uncertainty dominates the experimental one).

The structure of this paper is as follows: In Sec. II we briefly describe the method of the calculation. More details can be found in Refs. [11–13]. Results of our calculation and a discussion of its accuracy are given in Sec. III. Our conclusions are summarized in Sec. IV.

II. CALCULATIONAL DETAILS

One important difference between thallium and cesium is that the former atom has three valence electrons above a relatively compact and rigid core, while the latter has only one. Correlations between three-valence electrons are not small and cannot be treated accurately by many-body perturbation theory (MBPT). In Ref. [11], it was suggested that MBPT be combined with the configuration interaction (CI) method for such atoms. The latter method is well suited to account for correlations between a few-valence electrons, while the former method allows one to treat core-valence and core-core correlations. This combined CI and MBPT method was first tested in calculations of energy spectra of Tl [11], then for Ca, Sr, Ba, and Yb [14]. Later it was extended to the calculations of observable such as hyperfine-structure constants [12] and polarizabilities [13].

There is a significant difference in MBPT for one-electron atoms, such as Cs, and three-electron atoms such as Tl. For one-electron atoms one has to calculate only MBPT diagrams with one external line, while for many-electron atoms there are also diagrams with two, three, and more external lines. For combinatorial reasons the number of such diagrams grows rapidly with the number of external lines, making calculations for many-electron atoms much-more complicated. Fortunately, the three-particle diagrams appear to be small for Tl [11]. If the three-particle diagrams are neglected, the effective Hamiltonian for valence electrons is a two-particle operator, which not only drastically reduces the number of diagrams at the MBPT stage of the calculation, but is also essential for the CI stage of the calculation because the Hamiltonian matrix remains sparse.

It was recently shown for Cs [5–7] that the Breit interaction correction is larger than earlier estimated [4]. For this reason, we have included the dominant magnetic part of the Breit interaction (the so-called Gaunt interaction) at all stages of the present calculation. The Dirac-Fock equations

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TABLE I. Spectrum of Tl for Coulomb and Coulomb-Gaunt potentials. The ground-state three-electron binding energy $|E_{\rm val}|$ corresponds to the sum of the first-three ionization potentials. For other levels, we give transition frequencies Δ. The effective Hamiltonian for valence electrons is calculated for the energy $E_{\rm val} = -1.64$ a.u.

		CI+MBPT		Experiment	
		C	C-G		
$6p_{1/2}$	$\lvert E_{\rm val}\rvert$ (a.u.)	2.0742	2.0720	2.0722	[22]
$6p_{3/2}$		7925	7836	7793	
$7s_{1/2}$		26583	26455	26478	
$7p_{1/2}$	Δ (1/cm)	34193	34087	34160	[23]
$7p_{3/2}$		35215	35098	35161	
$6d_{3/2}$		36363	36208	36118	
$6d_{5/2}$		36469	36321	36200	

were solved in the Coulomb-Gaunt approximation for the ground state of the Tl^+ ion (the V^{N-1} approximation) with the help of the code described in Ref. [15].

We used different basis sets for the CI and MBPT parts of the calculation. That enabled us to improve the CI convergence without having an enormous Hamiltonian matrix. The core and valence orbitals were taken from the numerical solution of the Dirac-Fock equations on a radial grid. The CI basis set included virtual orbitals formed using the method suggested in Ref. [16], while virtual states for the MBPT basis set were formed from *B* splines [17]. The Dirac-Fock Coulomb-Gaunt Hamiltonian was diagonalized on both sets. Two different variants of the MBPT basis set were used for calculating diagrams for the effective Hamiltonian and for solving the random-phase approximation (RPA) equations. The former included partial waves with $l=5$, while the latter included more orbitals but was restricted to $l \leqslant 4$.

We use the Brillouin-Wigner variant of MBPT. In this formalism, the effective Hamiltonian for the valence electrons is symmetric but energy dependent. It was shown earlier [18] that the accuracy of the theory can be improved by calculating the Hamiltonian at shifted energies. The optimal valence energy for Tl was found to be -1.64 a.u.

For some observables such as polarizabilities, Stark-induced amplitudes, and PNC amplitudes, one needs to sum over intermediate states or solve the corresponding inhomogeneous equations (Sternheimer [19] or Dalgarno-Lewis [20] method). Here we apply the Sternheimer-Dalgarno-Lewis method to the valence part of the problem as described in [13,21].

III. RESULTS AND DISCUSSION

A. Test calculations of the spectrum and observables

To control the accuracy of our calculation of the PNC amplitude, we calculated as many different observables as

TABLE II. Hyperfine constants for ^{205}Tl (MHz). First row gives Dirac-Fock values and the following rows give various corrections described in the text.

	$A_{6p_{1/2}}$	$A_{6p_{3/2}}$	$A_{7s_{1/2}}$	$A_{7p_{1/2}}$	$A_{7p_{3/2}}$	$A_{6d_{3/2}}$	$A_{6d_{5/2}}$
DF	17339	1291	7579	1940	187	21	9
CI	924	-1369	3799	-102	112	-185	391
$H_{\rm eff}$	3428	-45	765	331	-56	114	-226
$A_{\rm RPA}$	959	359	1031	103	73	5	15
A_{σ}	-1071	-31	-269	-92	-9	3	-5
$A_{\rm sbt}$	-1389	-161	-75	-113	-19	-19	-8
$A_{\rm tp}$	1731	120	-22	133	4	21	7
$A_{\rm SR}$	209	88	-29	14	6	-1	0
Norm.	-467	-4	-113	-20	-3	0	0
Total	21663	248	12666	2193	295	-41	183
Theor. [a]	21760	-1919	12470	2070	195		
Theor. [b]	21300	339	12760				
Theor. [c]	21623	264	12307	2157	315	-35	184
Expt.	21311	265	12297	2155	309	-43	229

[a]Reference [24].
[b]Reference [25].
[c]Reference [12].

TABLE III. Reduced matrix elements for $E1$ amplitudes in L gauge (a.u.).

	DF	CI	Total	Theor.	Expt.
$6p_{1/2}\rightarrow 7s_{1/2}$	2.049	1.863	1.77	1.72 [a]	1.81(2)[c]
				1.78 [b]	
$\rightarrow 6d_{3/2}$	2.722	2.454	2.30	2.39 [a]	2.30(9)[c]
$6p_{3/2}\rightarrow 7s_{1/2}$	3.966	3.466	3.35	3.18 [a]	3.28(4)[c]
				3.31 [b]	
$\rightarrow 6d_{3/2}$	1.633	1.472	1.40	1.39 [a]	1.38(7)[c]
$\rightarrow 6d_{5/2}$	4.840	4.292	4.08		4.0(2)[c]
					3.8(2)[d]
$7p_{1/2}\rightarrow 7s_{1/2}$	6.618	6.152	5.96		5.87(8)[e]
$\rightarrow 6d_{3/2}$	11.980	10.874	10.86		
$7p_{3/2}\rightarrow 7s_{1/2}$	8.794	8.252	7.98		7.88(11)[e]
$\rightarrow 6d_{3/2}$	5.395	4.887	4.90		
$\rightarrow 6d_{5/2}$	16.300	14.799	14.88		

[a]Reference [26].
[b]Reference [25].
[c]References [27,28].
[d]Reference [29].
[e]Reference [30].

possible. These results are presented in Tables I–IV. There are some differences with earlier calculations [11,12]. First, we use the Coulomb-Gaunt potential here instead of the Coulomb potential used in those earlier calculations. In Table I, we compare our theoretical Coulomb-Gaunt energies with the measured spectrum [22,23]. We also give Coulomb energies for comparison. One can see that the Gaunt correction to the fine structure is rather large, especially for the ground state. Both splittings $6p_{1/2}$-$6p_{3/2}$ and $7p_{1/2}$-$7p_{3/2}$ are significantly improved when the Gaunt interaction is included. The overall agreement with experiment is also improved, though not as dramatically.

Tables II and III present results of our calculations of hyperfine structure constants and $E1$ amplitudes. In Table II, we list all corrections to the initial Dirac-Fock values of hyperfine constants [24,25]. The CI correction accounts for mixing of configurations. The $H_{\rm eff}$ correction corresponds to the solution of the CI equations with the effective Hamiltonian and accounts for core polarization effects. The remaining corrections correspond to the different terms in the effective operator of the hyperfine interaction [12]. In this calculation we included the structural radiation (A_{SR}) correction [26], which was omitted in [12]. The most-important contributions are associated with the RPA and the Brueckner (A_σ) corrections to the effective operator. Two other large contributions from subtraction ($A_{\rm sbt}$) and two-particle corrections ($A_{\rm tp}$) almost cancel each other.

One can see that the Dirac-Fock approximation for the hyperfine constants works reasonably well only for $6p_{1/2}$ and $7p_{1/2}$ levels. For some of the other levels, even the sign and order of magnitude of the constants are wrong. That affects the final accuracy of the theory, which is better than 2% for the $np_{1/2}$ levels, about 3% for the $7s$ level, and worse for other small constants. It is actually quite surprising, that the CI and MBPT method gives rather accurate values even when the Dirac-Fock approximation fails completely.

The MBPT corrections to the $E1$ amplitudes in the length gauge are much smaller than for the hyperfine constants and the final values are closer to the initial Dirac-Fock ones. Usually, the V form of the $E1$ amplitude is less accurate for the optical transitions in neutral atoms. Therefore, we used the L form for the calculations presented in Table III. Accurate experimental results are available only for the $np_j\rightarrow 7s$

TABLE IV. Polarizabilities of the $6p_j$ levels of Tl in a.u.. Atomic polarizability includes valence and core contributions. The column δCore accounts for the change of the core polarization due to the fact that some valence orbitals are occupied.

	Valence	Core	δCore	Total	Expt. [31]
$\alpha_0(6p_{1/2})$	43.47	6.23	−0.51	49.2	
$\alpha_0(6p_{3/2})$	73.79	6.23	−0.48	79.6	
$\alpha_2(6p_{3/2})$	−25.04	0	0.06	−25.0	−24.2(3)

TABLE V. $(E1_{\rm PNC})$ amplitude for $6p_{1/2}\rightarrow 6p_{3/2}$ transition in ^{205}Tl in the units $i\times 10^{-11}(-Q_w/N)$ a.u.

Right-hand side:	$H_P\|6p_{1/2}\rangle$	$H_P\|6p_{3/2}\rangle$
CI	−34.20	−29.88
$H_{\rm eff}$ & RPA	−7.26	+0.01
Brueckner	+1.29	+1.12
Subtraction	+1.03	+0.77
Two particle	−0.29	−0.53
Struc. Radiation	−0.04	−0.02
Core sum	−0.16	+0.06
Subtotal	−68.1	
Normalization	+1.4	
Total	−66.7	

amplitudes [27–30]. For these four amplitudes the difference between theory and experiment is within 2%. Taking into account the smallness of the MBPT corrections to the $E1$ amplitudes, we assume this to be the characteristic accuracy of the theory for $E1$ amplitudes.

As an additional test of the theory, we calculated the tensor polarizability of the $6p_{3/2}$ level, which was accurately measured by Gould [31] (see Table IV). The contribution to the polarizability was calculated by solving the inhomogeneous equation for the effective operators in the valence space. The core contribution was calculated as a direct sum of the RPA amplitudes over Dirac-Fock virtual orbitals. When calculating the polarizability of the core of the neutral atom, we should exclude occupied states from the sum over the intermediate states. The corresponding correction is given in the column δCore of Table IV. The 3.3% difference between theory and experiment for $\alpha_2(6p_{3/2})$ is consistent with our estimate of the theoretical accuracy of the $E1$ amplitudes, considering the fact that the experimental error is 1.2%. It should be noted, in regard to our error estimate for the PNC amplitude, that the tensor polarizability is a quadratic function of the electric field so errors in the component $E1$ amplitudes are doubled in polarizability calculations. The corresponding errors in the PNC sum over states from $E1$ and H_P matrix elements are anticorrelated since MBPT corrections to $E1$ and H_P matrix elements usually have opposite signs. Thus, for the PNC amplitude, the two errors can be added in quadrature.

We have omitted all-three-particle diagrams in the effective Hamiltonian. These diagrams are strongly suppressed by the small overlap between valence and core orbitals [11]. We calculated these diagrams for the small number of leading configurations and determined corrections to the energies and to the hyperfine constants. The valence energies changed by $\sim 10^{-4}$ a.u. and corrections to the hyperfine constants were on the order of a few MHz, confirming that three-particle corrections for Tl are well below the accuracy of the present calculation. We, therefore, neglected three-particle diagrams in all other calculations.

B. PNC amplitude

The PNC interaction of the electron with the weak charge of the nucleus has the form:

$$H_P = -\frac{G_F}{2\sqrt{2}} Q_W \gamma_5 \rho(\mathbf{r}), \tag{5}$$

where $G_F = 2.2225 \times 10^{-14}$ a.u. is the Fermi constant of the weak interaction, γ_5 is the Dirac matrix, and $\rho(\mathbf{r})$ is the neutron density of the nucleus. Calculation of the PNC amplitude is similar to calculation of polarizabilities. First, we must determine the effective operator $H_{P,\mathrm{eff}}$ for the PNC interaction of the valence electrons with the nucleus in the same way that we determined effective operators for the hyperfine interaction and the electric-dipole-moment operators. We must then solve the RPA equations for the operator (5), calculate the Brueckner $H_{P,\sigma}$, subtraction $H_{P,\mathrm{sbt}}$, two-particle $H_{P,\mathrm{tp}}$, and structural radiation $H_{P,\mathrm{SR}}$ corrections.

Once the effective operators are formed, we solve two inhomogeneous equations:

$$(E_{6p_{1/2}} - H_{\mathrm{eff}})\Psi^{(P)}_{6p_{1/2},m} = H_{P,\mathrm{eff}}|\Psi_{6p_{1/2},m}\rangle, \tag{6}$$

$$(E_{6p_{3/2}} - H_{\mathrm{eff}})\Psi^{(P)}_{6p_{3/2},m} = H_{P,\mathrm{eff}}|\Psi_{6p_{3/2},m}\rangle. \tag{7}$$

Afterward, the PNC amplitude $(E1)_{\mathrm{PNC}}$ for the $6p_{1/2} \to 6p_{3/2}$ transition can be readily calculated with the help of the (effective) electric-dipole-moment operator $\mathbf{D} = -e\mathbf{r}$:

$$(E1)_{\mathrm{PNC}} = \langle \Psi_{6p_{3/2}}||D_{\mathrm{eff}}||\Psi^{(P)}_{6p_{1/2}}\rangle + \langle \Psi^{(P)}_{6p_{3/2}}||D_{\mathrm{eff}}||\Psi_{6p_{1/2}}\rangle. \tag{8}$$

Alternatively, instead of Eqs. (6) and (7) we can solve inhomogeneous equations with the operator $D_{\mathrm{eff},0}$ on the right-hand side. The reduced matrix element of the PNC amplitude is then given by

$$E1_{\mathrm{PNC}} = (-1)^{(3/2)-m} \begin{pmatrix} \frac{3}{2} & 1 & \frac{1}{2} \\ -m & 0 & m \end{pmatrix}^{-1} \times (\langle \Psi^{(D)}_{6p_{3/2}}|H_{P,\mathrm{eff}}|\Psi_{6p_{1/2}}\rangle + \langle \Psi_{6p_{3/2}}|H_{P,\mathrm{eff}}|\Psi^{(D)}_{6p_{1/2}}\rangle). \tag{9}$$

Equations (8) and (9) should give identical results; a comparison of results obtained using the two equivalent methods can be used to check numerical accuracy of the calculations. On the other hand, it is easier to calculate the two-particle part of the operator $H_{P,\mathrm{eff}}$ using Eq. (9) and the two-particle part of the operator D_{eff} using Eq. (8). The results of the calculation based on Eqs. (6)–(8) are given in Table V. The inhomogeneous equations (6) and (7) do not account for the sum over intermediate core states. This sum was calculated explicitly in the RPA approximation and the corresponding results are also given in Table V.

1. Accuracy of the calculation

The principal theoretical uncertainty in calculations for atoms such as Tl is associated with higher orders in the residual two-electron interaction. The effective operator method accounts for some-important higher-order MBPT corrections. The valence-valence correlations are considered nonperturbatively within the CI method. In addition, by diagonalizing the effective Hamiltonian, we account for Brueckner and screening correction to all orders. The RPA equations for the PNC and the electric-dipole interactions effectively sum infinite chains of diagrams. However, already in third-order MBPT, there are diagrams that are neglected here.

It is known that for neutral atoms, the residual two-electron interaction is not small and it is very difficult to estimate the accuracy of different approximate methods. Therefore, we made a number of test calculations described above. We have seen that, even for hyperfine structure constants where the MBPT corrections are huge, the accuracy of the theory for the large constants is still about 2–3%, while

for the $E1$ amplitudes the accuracy is better than 2%. According to Table V, the MBPT corrections to the PNC amplitude are rather small. Therefore, we estimate the error caused by the neglect of the higher-order terms in the residual interaction to be about 2%.

The other possible sources of errors are QED corrections and the nuclear-size effects. Below, we discuss both of them in some detail.

2. QED corrections to PNC amplitude

The most-important radiative corrections to the PNC interaction given in Eq. (5) correspond to very-small distances and should be calculated within the electroweak theory. These corrections lead to scaling of the weak charge of the nucleus. The leading-order (tree-level) value of the weak charge for ^{205}Tl is

$$Q_W(0) = -N + Z(1 - 4\sin^2\theta_W) = -117.9, \qquad (10)$$

where N and Z are the numbers of neutrons and protons in the nucleus. The Weinberg angle θ_W here is taken at the energy of Z pole. Radiative corrections change $Q_W(0)$ by 1%; the resulting value, taken from Ref. [9], is given in Eq. (4).

In addition to these radiative corrections, there are the QED radiative corrections specific to heavy atoms [32,33]. These corrections are dominated by vacuum-polarization effects and for hydrogen-like ions with $Z \approx 80$ were calculated to be 0.9% [33]. For the valence electron of a neutral atom, screening of the vacuum-polarization potential by relaxation of the core should be taken into account. It was recently shown that for the Breit interaction this screening significantly reduces corrections to the valence amplitudes [6,7,34]. Thus, the actual radiative corrections to the PNC amplitude in Tl could be few-times smaller.

Finally, there is the Breit correction to the PNC amplitude. The magnetic part of the Breit interaction (the Gaunt interaction) is known to be larger than the neglected retardation part of the Breit operator [34] by a factor of three or more. As we pointed out above, the Gaunt interaction should be included self-consistently at all stages of calculations. It is difficult to isolate the Gaunt correction in the self-consistent approach. To do that, one must repeat all calculations in the Coulomb approximation and take a difference. The calculations for Tl are rather time consuming, so for the Coulomb case we did only the CI calculation. At that level of approximation, the Gaunt correction to the PNC amplitude was about -0.5%. We think that the overall Gaunt correction may be up to two-times larger. The retardation correction, which is neglected here, should be at least few-times smaller than the Gaunt correction and the total uncertainty from QED effects should be within 1%.

3. Nuclear-size effects

The PNC amplitude is sensitive to both proton and neutron distributions: the former determines electronic-wave function inside the nucleus and the latter determines the weak-charge distribution in Eq. (5). In our calculations we approximate the nucleus ^{205}Tl by a uniform ball of the radius 0.1334×10^{-3} a.u. This value corresponds to a root-mean-square charge radius $r_N = 5.470(5)$ fm [35].

This model assumes that (i) proton and neutron radii of the nucleus are the same: $r_N^{(p)} = r_N^{(n)} = r_N$, and (ii) the nucleus has a sharp edge. Generally speaking, both assumptions are incorrect. Therefore, it is important to estimate the errors associated with each of them. That was recently done in Refs. [36,37]:

$$\frac{\delta(E1)_{\rm PNC}}{E1_{\rm PNC}} \approx -0.39\,\frac{\delta r_N}{r_N} - 0.14\frac{r_N^{(n)} - r_N^{(p)}}{r_N} + 0.03\,\eta, \qquad (11)$$

$$\eta = \frac{21}{25}\,\frac{\langle r_N^4\rangle}{\langle r_N^2\rangle^2} - 1. \qquad (12)$$

The first two terms in Eq. (11) give the dependence of the PNC amplitude on the nuclear radius r_N and on the difference $r_N^{(n)} - r_N^{(p)}$. At present there are no accurate experimental data on neutron radii. However, theory predicts that for heavy nuclei $r_N^{(n)} - r_N^{(p)} \approx 0.1 - 0.3$ fm [37]. The parameter η is defined so that it vanishes for a uniform distribution [36], therefore, the last term in Eq. (11) describes the dependence of the PNC amplitude on the details of the nuclear distribution. For a real nucleus, η is about 0.1 [37].

Substituting into Eq. (11), we find that the correction to the PNC amplitude from the details of the nucleon distribution is

$$\frac{\delta(E1)_{\rm PNC}}{(E1)_{\rm PNC}} \approx -0.003(2). \qquad (13)$$

This correction is seen to be small in comparison with other ones.

IV. CONCLUSION

Our final value for the PNC amplitude of the $6p_{1/2} \to 6p_{3/2}$ transition is in good agreement with the most-accurate previous calculation of Dzuba *et al.* [26] (the references to earlier calculations can be found in [38]):

$$\frac{(E1)_{\rm PNC}}{i\,10^{-11}(-Q_{\rm w}/N)} = \begin{cases} -(66.7 \pm 1.7) & \text{this work,} \\ -(66.1 \pm 2.0) & \text{Dzuba } \textit{et al.} \end{cases} \qquad (14)$$

In the experiment the following ratio is measured:

$$\mathcal{R} \equiv {\rm Im}\left(\frac{(E1)_{\rm PNC}}{M1}\right), \qquad (15)$$

where $M1$ is the $6p_{1/2} \to 6p_{3/2}$ magnetic-dipole transition amplitude. We have calculated this amplitude in two different ways. First, we did the CI and MBPT calculation using the effective Hamiltonian. Second, we did a third-order MBPT calculation in which Tl was treated as a one-electron atom:

$$M1 = \begin{cases} 4.145\times10^{-3} \text{ a.u.} & \text{CI+MBPT-II,} \\ 4.149\times10^{-3} \text{ a.u.} & \text{MBPT-III.} \end{cases} \qquad (16)$$

These two calculations account for different correlation effects, but give very close results. In general, the amplitudes for the allowed $M1$ transitions are very stable and can be calculated quite reliably. The experimental value of this amplitude follows from the measurements of the quadrupole amplitude $E2$ [39] and the ratio $\chi \equiv [\omega/(2\sqrt{3}c)](E2)/(M1)$ [40]:

$$\left.\begin{aligned} E2 &= 13.29(3) \\ \chi &= 0.2387(40) \end{aligned}\right\} \Rightarrow M1 = 4.16(7)\times 10^{-3}, \qquad (17)$$

which is in agreement with theoretical results of Eq. (16).

Using the theoretical value for the $M1$ amplitude (16) and the standard-model value of the weak charge (4), we get the following result for the PNC rate $\mathcal{R}$:

$$\mathcal{R}(Q_W = -116.7) = -15.2(4)\times 10^{-8}. \qquad (18)$$

The experimentally measured PNC rate for the $6p_{1/2} \rightarrow 6p_{3/2}$ transitions is

$$\mathcal{R} = \begin{cases} -14.68(17), & \text{Vetter } \textit{et al.} \quad [1], \\ -15.68(45), & \text{Edwards } \textit{et al.} \quad [2]. \end{cases} \qquad (19)$$

These experimental results formally contradict one another. Recently, Majumder and Tsai suggested [40] that the discrepancy could be due to the different values of the parameter χ used in the analysis by two groups. They accurately measured χ (17) and used their value to rescale the experimental result from Ref. [2] to find

$$\mathcal{R} = -14.71(45), \quad \text{Majumder and Tsai } [40]. \qquad (20)$$

This scaled value is in agreement with the measurement [1], where a nearly identical value of χ was used, and all three values are in agreement with the theoretical result (18) for the $Q_W = Q_W^{\rm SM}$. We use the best experimental result [1] together with our calculation (18) to derive the experimental value of the weak charge for ^{205}Tl:

$$Q_{\rm W}(^{205}{\rm Tl}) = -113(1)_{\rm expt}(3)_{\rm theor}. \qquad (21)$$

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[1] P. A. Vetter, D. M. Meekhof, P. M. Magumder, S. K. Lamoreaux, and E. N. Fortson, Phys. Rev. Lett. **74**, 2658 (1995).
[2] N. H. Edwards, S. J. Phipp, P. E. G. Baird, and S. Nakayama, Phys. Rev. Lett. **74**, 2654 (1995).
[3] V. A. Dzuba, V. V. Flambaum, and O. P. Sushkov, Phys. Lett. A **141**, 147 (1989).
[4] S. A. Blundell, J. Sapirstein, and W. R. Johnson, Phys. Rev. D **45**, 1602 (1992).
[5] A. Derevianko, Phys. Rev. Lett. **85**, 1618 (2000).
[6] M. G. Kozlov, S. G. Porsev, and I. I. Tupitsyn, Phys. Rev. Lett. **86**, 3260 (2001).
[7] V. A. Dzuba, C. Harabati, W. R. Johnson, and M. S. Safronova, Phys. Rev. A **63**, 044103 (2001).
[8] C. S. Wood, S. C. Bennett, D. Cho, B. P. Masterson, J. L. Roberts, C. E. Tanner, and C. E. Wieman, Science **275**, 1759 (1997).
[9] D. E. Groom *et al.*, Eur. Phys. J. C **15**, 1 (2000).
[10] S. C. Bennett and C. E. Wieman, Phys. Rev. Lett. **82**, 2484 (1999).
[11] V. A. Dzuba, V. V. Flambaum, and M. G. Kozlov, Phys. Rev. A **54**, 3948 (1996).
[12] V. A. Dzuba, M. G. Kozlov, S. G. Porsev, and V. V. Flambaum, Zh. Eksp. Teor. Fiz. **87** 1636 (1998) [JETP **87**, 885 (1998)].
[13] M. G. Kozlov and S. G. Porsev, Eur. Phys. J. D **5**, 59 (1999).
[14] M. G. Kozlov and S. G. Porsev, JETP **84**, 461 (1997).
[15] V. F. Bratsev, G. B. Deyneka, and I. I. Tupitsyn, Bull. Acad. Sci. USSR, Phys. Ser. (Engl. Transl.) **41**, 173 (1977).
[16] P. Bogdanovich and G. Žukauskas, Sov. Phys. Collect. **23**(5), 18 (1983).
[17] J. Sapirstein and W. R. Johnson, J. Phys. B **29**, 5213 (1996).
[18] M. G. Kozlov and S. G. Porsev, Opt. Spectrosc. **87**, 352 (1999).
[19] R. M. Sternheimer, Phys. Rev. **80**, 102 (1950).
[20] A. Dalgarno and J. T. Lewis, Proc. R. Soc. London **223**, 70 (1955).
[21] M. G. Kozlov, S. G. Porsev, and V. V. Flambaum, J. Phys. B **29**, 689 (1996).
[22] A. A. Radzig and B. M. Smirnov, *Reference Data on Atoms, Molecules and Ions* (Springer-Verlag, Berlin, 1985).
[23] C. E. Moore, *Atomic Energy Levels*, Natl. Bur. Stand. (U.S.), Circ. No. 467 (U.S., GPO, Washington, D.C., 1958), Vol. 1–3.
[24] V. A. Dzuba, V. V. Flambaum, P. G. Silvestrov, and O. P. Sushkov, Phys. Lett. A **20**, 1399 (1987).
[25] A.-M. Mårtesson-Pendrill, Phys. Rev. Lett. **74**, 2184 (1995).
[26] V. A. Dzuba, V. V. Flambaum, P. G. Silvestrov, and O. P. Sushkov, J. Phys. B **20**, 3297 (1987).
[27] J. C. Hsieh and J. C. Baird, Phys. Rev. A **6**, 141 (1972).
[28] A. Gallagher and A. Lurio, Phys. Rev. **136**, A87 (1964).
[29] N. P. Penkin and L. N. Shabanova, Opt. Spectrosc. **14**, 87 (1963).
[30] J. V. James, C. C. Wang, and C. Doty, Phys. Rev. A **34**, 1117 (1986).
[31] H. Gould, Phys. Rev. A **14**, 922 (1976).
[32] B. W. Linn and P. G. H. Sandars, J. Phys. B **27**, 1469 (1994).
[33] I. Bednyakov *et al.*, Phys. Rev. A **61**, 012103 (2000).
[34] E. Lindroth, A.-M. Mårtensson-Pendrill, A. Ynnerman, and P. Öster, J. Phys. B **22**, 2447 (1989).
[35] H. De Vries, C. W. De Jager, and C. De Vries, At. Data Nucl. Data Tables **36**, 495 (1987).

[36] J. James and P. G. H. Sandars, J. Phys. B **32**, 3295 (1999).
[37] C. J. Horowitz *et al.*, Phys. Rev. C **63**, 025501 (2001); e-print nucl-th/9912038.
[38] I. B. Khriplovich, *Parity Non-Conservation in Atomic Phenomena* (Gordon and Breach, New York, 1991).
[39] P. Vetter *et al.*, *E2-amplitude* $6p_{1/2} \rightarrow 6p_{3/2}$ *transition in Tl* (1995), cited in [25].
[40] P. K. Majumder and L. L. Tsai, Phys. Rev. A **60**, 267 (1999).