Calculation of parity nonconservation in xenon and mercury

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We use configuration interaction technique to calculate parity nonconservation in metastable Xe and Hg [proposal of the experiment in L. Bougas *et al.*, Phys. Rev. Lett. **108**, 210801 (2012)]. Both nuclear-spin-independent and nuclear-spin-dependent (dominated by the nuclear anapole moment) parts of the amplitude are considered. The amplitudes are strongly enhanced by the proximity of states of opposite parity.

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I. INTRODUCTION

The study of parity nonconservation (PNC) in atoms is a low-energy, relatively inexpensive alternative to the high-energy search for new physics beyond the standard model (see, e.g., [1–3]). For example, PNC in cesium is currently the best low-energy test of the electroweak theory [1,3]. This is due to the high accuracy of the measurements [4] and their interpretation [5] (see also [6]). Since the cesium result is unlikely to be significantly improved, the focus of PNC study in atoms has shifted to two important areas: (i) PNC measurements for a chain of isotopes and (ii) measurements of the nuclear anapole moment (see, e.g., [3]). Most of current or planed PNC experiments in atoms consider both possibilities.

Experiments are in progress at Berkeley for Dy and Yb atoms [7,8], at TRIUMF for Rb and Fr atoms [9,10], and at Groningen (KVI) for Ra^+ ions [11]. There was an an interesting recent suggestion to measure PNC in metastable Xe and Hg [12]. In the present paper we support this proposal by atomic calculations.

The advantages of using Xe and Hg for measurements of PNC in a chain of isotopes and measurements of anapole moments include (i) the large number of stable isotopes of both atoms (maximal difference in number of neutrons is $\Delta N = 12$ for Xe and $\Delta N = 8$ for Hg); (ii) the presence of two stable isotopes for each of the atoms with nonzero nuclear spin (^{129}Xe, $I = 1/2$; ^{131}Xe, $I = 3/2$; ^{199}Hg, $I = 1/2$; ^{201}Hg, $I = 3/2$)—these isotopes are suitable for anapole moment measurements; and (iii) PNC amplitudes in Xe and Hg atoms are enhanced due to the high nuclear charge and strong mixing with close states of opposite parity.

An extra advantage comes from the fact that xenon and mercury nuclei with nonzero spin have a valence neutron, therefore nuclear anapole measurements will provide the strength constant for the neutron-nucleus PNC potential. The anapole moment so far has been measured only for ^{133}Cs [4], which has a valence proton. The data for xenon and mercury would be complementary to those obtained for cesium.

In the present work we use the configuration interaction (CI) technique to calculate the nuclear-spin-independent (SI) PNC amplitudes caused by the weak nuclear charge and nuclear spin-dependent (SD) PNC amplitudes dominated by nuclear anapole moments. The result is presented in a convenient form as the sum of two contributions for different hyperfine structure components. This would allow the extraction of both the value and the sign of anapole moments by comparing the measured amplitudes with the calculated ones.

II. GENERAL FORMALISM

The Hamiltonian describing parity-nonconserving electron-nuclear interaction can be written as the sum of the nuclear SI and nuclear SD parts (we use atomic units: $\hbar = |e| = m_e = 1$):

$$H_{\rm PNC} = H_{\rm SI} + H_{\rm SD} = \frac{G_F}{\sqrt{2}}\left(-\frac{Q_W}{2}\gamma_5 + \frac{\varkappa}{I}\boldsymbol{\alpha}\boldsymbol{I}\right)\rho(\boldsymbol{r}), \tag{1}$$

where $G_F \approx 2.2225 \times 10^{-14}$ a.u. is the Fermi constant of the weak interaction, Q_W is the nuclear weak charge, $\boldsymbol{\alpha} = \left(\begin{smallmatrix} 0 & \sigma \\ \sigma & 0 \end{smallmatrix}\right)$ and γ_5 are the Dirac matrices, $\boldsymbol{I}$ is the nuclear spin, and $\rho(\mathbf{r})$ is the nuclear density normalized to 1. The strength of the spin-dependent PNC interaction is proportional to the dimensionless constant $\varkappa$, which is to be found from the measurements. There are three major contributions to $\varkappa$, arising from (i) electromagnetic interaction of atomic electrons with the nuclear *anapole moment* [13], (ii) electron-nucleus SD weak interaction [14], and (iii) the combined effect of SI weak interaction and magnetic hyperfine interaction [15] (see also [1]). In this work we do not distinguish different contributions to $\varkappa$ and present the results in terms of total $\varkappa$, which is the sum of all possible contributions.

Within the standard model the weak nuclear charge Q_W is given by [16]

$$Q_W \approx -0.9877N + 0.0716Z. \tag{2}$$

Here N is the number of neutrons, and Z is the number of protons.

The PNC amplitude of an electric dipole transition between states of the same parity $|i\rangle$ and $|f\rangle$ is equal to

$$E1^{\rm PNC}_{\rm fi} = \sum_n \left[\frac{\langle f|\boldsymbol{d}|n\rangle\langle n|H_{\rm PNC}|i\rangle}{E_i - E_n} + \frac{\langle f|H_{\rm PNC}|n\rangle\langle n|d_q|i\rangle}{E_f - E_n}\right], \tag{3}$$

where $\boldsymbol{d} = -e\sum_i \boldsymbol{r}_i$ is the electric dipole operator. To extract from the measurements the parameter of the nuclear SD weak interaction $\varkappa$, one needs to consider PNC amplitudes in specific hyperfine structure components of the initial versus

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the final state. These amplitudes can be expressed as

$$E1_{\rm fi}^{\rm PNC} = (-1)^{F_f-M_f}\begin{pmatrix} F_f & 1 & F_i \\ -M_f & q & M_i \end{pmatrix}\langle J_f F_f||d_{\rm PNC}||J_i F_i\rangle. \tag{4}$$

Here $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{I}$, where I is nuclear spin. Detailed expressions for the reduced matrix elements of the SI and SD PNC amplitudes can be found, e.g., in Refs. [17] and [18]. For the SI amplitude we have

$$\begin{aligned}&\langle J_f, F_f||d_{\rm SI}||J_i, F_i\rangle \\ &= (-1)^{I+F_i+J_f+1}\sqrt{(2F_f+1)(2F_i+1)}\begin{Bmatrix} J_i & J_f & 1 \\ F_f & F_i & I \end{Bmatrix} \\ &\quad\times\sum_n\left[\frac{\langle J_f||\boldsymbol{d}||n,J_n\rangle\langle n,J_n||H_{\rm SI}||J_i\rangle}{E_i-E_n}\right. \\ &\quad\left.+\frac{\langle J_f||H_{\rm SI}||n,J_n\rangle\langle n,J_n||\boldsymbol{d}||J_i\rangle}{E_f-E_n}\right] \\ &\equiv c(F_f,J_f,F_i,J_i)E'_{\rm fi}.\end{aligned} \tag{5}$$

Here $c(F_f,J_f,F_i,J_i)$ is the angular coefficient and the sum over n, $E'_{\rm fi}$, does not depend on F_f or F_i:

$$\begin{aligned}E' = \sum_n\left[\frac{\langle J_f||\boldsymbol{d}||n,J_n\rangle\langle n,J_n||H_{\rm SI}||J_i\rangle}{E_i-E_n}\right. \\ \left.+\frac{\langle J_f||H_{\rm SI}||n,J_n\rangle\langle n,J_n||\boldsymbol{d}||J_i\rangle}{E_f-E_n}\right].\end{aligned} \tag{6}$$

For the SD PNC amplitude we have

$$\begin{aligned}&\langle J_f, F_f||d_{\rm SD}||J_i, F_i\rangle \\ &= \frac{G_F}{\sqrt{2}}\varkappa\sqrt{(I+1)(2I+1)(2F_i+1)(2F_f+1)/I} \\ &\quad\times\sum_n\left[(-1)^{J_f-J_i}\begin{Bmatrix} J_n & J_i & 1 \\ I & I & F_i \end{Bmatrix}\begin{Bmatrix} J_n & J_f & 1 \\ F_f & F_i & I \end{Bmatrix}\right. \\ &\quad\times\frac{\langle J_f||\boldsymbol{d}||n,J_n\rangle\langle n,J_n||\boldsymbol{\alpha}\rho||J_i\rangle}{E_n-E_i} \\ &\quad+(-1)^{F_f-F_i}\begin{Bmatrix} J_n & J_f & 1 \\ I & I & F_f \end{Bmatrix}\begin{Bmatrix} J_n & J_i & 1 \\ F_i & F_f & I \end{Bmatrix} \\ &\quad\left.\times\frac{\langle J_f||\boldsymbol{\alpha}\rho||n,J_n\rangle\langle n,J_n||\boldsymbol{d}||J_i\rangle}{E_n-E_f}\right].\end{aligned} \tag{7}$$

The PNC amplitude between different hfs components of the initial and final states can be presented in the form

$$E_{\rm PNC}(F_1,F_2) = c(F_1,F_2)E'Q_w[1+R(F_1,F_2)\varkappa], \tag{8}$$

where c is an angular coefficient and R is the ratio of SD-to-SI PNC amplitudes.

If at least two PNC amplitudes E_1 and E_2 are measured, then the value of $\varkappa$ can be expressed via the measured ratio of the amplitudes E_1/E_2 and the calculated ratios R of the SD and SI PNC amplitudes.

$$E_1 = c_1E'Q_W(1+R_1\varkappa), \quad E_2 = c_2E'Q_W(1+R_2\varkappa), \tag{9}$$

$$\varkappa = \frac{c_1/c_2 - E_1/E_2}{R_2E_1/E_2 - R_1c_1/c_2}. \tag{10}$$

The ratios R_1 and R_2 are much less sensitive to numerical uncertainties than each of the SD and SI PNC amplitudes [19].

III. CALCULATIONS

Calculations for xenon and mercury were performed with the use of the CI method. We treat Hg as an atom with two valence electrons and Xe as an atom with six valence electrons. Calculations for Hg are very similar to what we did before for Hg [20] and Yb [21]. We use the V^{N-2} approximation in which the initial Hartree-Fock procedure is done for the Hg^{2+} ion. The complete set of single-electron orbitals is constructed using the B-spline technique [22]. Core-valence correlations are included by adding the second-order correlation potential $\hat{\Sigma}$ to the CI Hamiltonian in the framework of the CI + MBPT method [23]. The accuracy of the energies is further improved by rescaling the core-valence correlation operator Σ (see [20] and [21] for details). The rescaling coefficients are $\lambda_s = 0.82$ for s states and $\lambda_p = 0.9$ for p states. The calculated energies and g factors of mercury are presented in Table I together with the corresponding experimental numbers. The g factors are useful for the identification of states. The accuracy of the calculated energies is within 1% for the majority of states. It is not perfect in spite of the fitting because we use only two fitting parameters for all states.

A similar approach for xenon is problematic due to the larger number of valence electrons. We treat all $5p$ electrons as valence ones, so that the total number of valence electrons is six. Using the same technique as for Hg would lead to a very large CI matrix. It was suggested in [12] that the hole-particle formalism can be used for calculation of the electron structure of xenon. In this case only two active particles enter the CI calculations and the calculations might not be more complicated than for mercury. This assumes that only single excitations are allowed from the $5p$ subshell. However, in our experience double excitations are also important. Inclusion of double excitations within the hole-particle formalism hugely complicates the problem. Therefore, we use a simpler approach. We use standard CI technique for six valence electrons. The initial Hartree-Fock procedure is done for neutral xenon (the V^N approximation). Single-electron basis states above the core are calculated as the Hartree-Fock states in the V^{N-1} potential of the frozen core. Many-electron basis states for the CI calculations are formed by allowing single and double excitations from the $5p$ subshell to the states above the core.

Accurate treatment of the core-valence correlations for xenon within the CI + MBPT method is problematic due to

TABLE I. Energy levels (in cm^{-1}) and g factors of low states of mercury. States considered for PNC transitions are labeled A and B.

		Calculations		Experiment	
Configuration	State	Energy	g	Energy	g
$6s^2$	$^1S_0$	0	0.000	0	0.000
$6s6p$					
A_1	$^3P_0^o$	38 202	0.000	37 645	0.000
A_2	$^3P_1^o$	39 955	1.480	39 412	1.486
A_3	$^3P_2^o$	44 812	1.500	44 043	1.501
B	$^1P_1^o$	53 584	1.020	54 069	1.015
$6s7s$	$^3S_1$	61 879	2.000	62 350	2.003
	$^1S_0$	63 399	0.000	63 928	0.000

TABLE II. Energy levels (in cm^{-1}) and g factors of low states of xenon. States considered for the PNC transition are labeled A and B.

		Calculations		Experiment	
Configuration	J	Energy	g	Energy	g
$5p^6$	0	0	0.000	0	0.000
$5p^5 6s$					
A	2	64 680	1.500	67 068	1.501
	1	66 089	1.214	68 046	1.206
	0	74 844	0.000	76 197	0.000
B	1	75 999	1.314	77 186	1.321
$5p^5 6p$	1	76 083	1.853	77 270	1.852
	1	77 914	1.024	78 957	1.022

the large contribution of the subtraction diagrams [23]. On the other hand, the core-valence correlations are relatively small for xenon compared to the valence-valence correlations due to the large number of valence electrons. Therefore, they can be included approximately.

To simulate the effect of core-valence correlations we include in the CI Hamiltonian the core polarization potential

$$\delta V = -\frac{\alpha_c}{a^4 + r^4}, \tag{11}$$

where α_c is the polarizability of the core and a is a cutoff parameter. We use $a = a_B$ and treat α_c as a fitting parameter. This allows us to fit the energy interval $\Delta E = 84$ cm^{-1} between state B and a close state of the same total momentum J and opposite parity belonging to the $5p^5 6p$ configuration. This is important because the PNC amplitude is very sensitive to this energy interval. We use $\alpha_c = 0.554$ a.u. for s states of valence electrons and $\alpha_c = 0$ for other states.

The results for energies and g factors of xenon are presented in Table II. Note that the accuracy is similar to what we have for mercury. This is because the the core-valence correlations are strong for mercury; they are significantly stronger than the correlations between two valence electrons. This is a limitation factor for the accuracy of the calculation. In contrast, the core-valence correlations are low for xenon.

A. Dalgarno-Lewis method for matrix elements

To calculate PNC amplitude we need to calculate matrix elements between many-electron states and perform summation over the complete set of many-electron basis states [see, e.g., (6) and (7)]. We use the random phase approximation [24,25] for the matrix elements and the Dalgarno-Lewis method [26] for the summation.

Matrix elements are given by

$$E1_{vw} = \langle \Psi_v || \hat{f} + \delta V_f || \Psi_w \rangle, \tag{12}$$

where δV is the correction to the core potential due to the core polarization by an external field $\hat{f}$. In the present calculations $\hat{f}$ represents either the external electric field, SI weak interaction, or SD PNC interaction.

Summation over the complete set of many-electron states is reduced to calculation of the correction $\delta\Psi_v$ to the many-electron wave function of state v due to the weak interaction perturbation $H_{\rm PNC}$. Then the PNC amplitude is given by

$$A_{vw} = \langle \delta\Psi_v || \boldsymbol{d} || \Psi_w \rangle. \tag{13}$$

The correction $\delta\Psi_v$ is found by solving the system of linear inhomogeneous equations

$$(\hat{H}^{\rm eff} - E_v)\delta\Psi_v = -(\hat{H}_{\rm PNC} + \delta V_{\rm PNC})\Psi_v. \tag{14}$$

The proposal in [12] considers PNC transitions between the exited states A and B in Hg and Xe (see Tables I and II). The upper state B in both atoms is very close to another state of the same total momentum J but opposite parity. The interval is 8282 cm^{-1} for Hg and only 84 cm^{-1} in Xe. This is a strong advantage of using these transitions from the experimental point of view because the proximity of states of the same total angular momentum but opposite parity leads to strong enhancement of the PNC amplitude. On the other hand, this is a complication from the theoretical point of view. The PNC amplitudes are sensitive to small energy intervals where a small error in the calculated energy of the states can lead to a large error in the value of the PNC amplitude. To get around this problem we use a stabilizing procedure which consists of the following steps. First, we use the procedure described above [see Eqs. (13) and (14)] without modifications. Then we repeat the calculations applying the orthogonality conditions for $\delta\Psi_{\rm B}$ to a close state of the same J and parity. The contribution of the close state is found by comparing the two results. Finally, this contribution is added back to the PNC amplitude with the rescaling parameter $\Delta E_{\rm theor}/\Delta E_{\rm expt}$.

The procedure described above corresponds to the exact fitting of the energy denominators in (6) and (7). Therefore, the same results should be obtained if the important energy intervals are fitted exactly by rescaling the correlation potential $\hat{\Sigma}$ (for Hg) or polarization potential δV (for Xe). This is another important test which we used in the calculations.

B. Accuracy of the calculations

The accuracy of similar calculations for two-valence-electron atoms Hg and Yb were discussed in detail in our earlier works [20,21,27]. It was demonstrated that the accuracy for transition amplitudes and polarizabilities is on the level of 5%. Note that the PNC amplitude is a second-order effect similar to the polarizability but with one electric dipole operator replaced by a weak interaction. In the present work we assume the same 5% uncertainty for the PNC effect in mercury. This is supported by the study of the limitation factors which are discussed below.

The uncertainty for xenon is higher due to the larger number of valence electrons, which makes it difficult to saturate the basis. We assume a 10% uncertainty which comes from comparing the results obtained with two different basis sets, the B-spline basis set and the Hartree-Fock basis set.

The main factor limiting the accuracy of the calculations of PNC amplitudes in xenon and mercury is the proximity of the levels of the same total momentum J and opposite parity. These states are mixed by weak interaction and the small energy interval between them leads to a stong enhancement of the PNC effect. This is one of the main reasons for the choice of atoms and transitions. However, it represents a challenge for the calculations. Even a small theoretical error in the

energies of the mixed states can lead to a large error in the PNC amplitude. There are two ways around this problem. One is to fit the energy interval exactly. Another is to isolate the resonant contribution from the rest of the amplitude and to rescale it to the correct energy interval. We did both things for xenon and found that they give the same results. Therefore, for mercury we just fit the energies. As long as the problem of small energy intervals is understood and properly dealt with, it does not contribute much to the uncertainty of the results.

Another important limitation factor for xenon, which is harder to deal with, is the large number of valence electrons. It was suggested in Ref. [12] that xenon can be treated as a system with one electron and one hole in the $5p$ subshell. This would make it a two-particle system similar to mercury. However, this approach assumes that only single excitations from the $5p$ subshell are considered. In our experience full saturation of the basis is not possible without the inclusion of double and maybe even triple excitations. This would lead to a CI matrix of extremely large size. Probably, this can be done with the use of supercomputers. Another open question for xenon is whether and how to include core-valence correlations. Incomplete saturation of the basis is the main source of the uncertainty of the present calculations for xenon.

Saturation of the basis is not a problem for mercury when it is considered as a system with two valence electrons. However, here we have another problem: strong core-valence correlations. The outermost subshell of the mercury core, $5d$, is strongly mixed with the valence $6s$ electrons. This is evident from the presence in the discrete spectrum of mercury states with excitations for the $5d$ subshell. The core-valence correlations are included in the present work with the use of the second-order correlation operator $\hat{\Sigma}$. Probably the correlations are too strong to be treated accurately within the second-order approach. The answer may come from the use of some all-order technique similar to what was recently developed in Ref. [28].

Even though some improvement in the accuracy of the calculations is possible, there is little chance that it will ever match the accuracy for cesium [5]. Therefore the main focus of the PNC study in Xe and Hg should be directed at measurements of the anapole moments and the study of the ratio of PNC effects in different isotopes.

IV. RESULTS AND DISCUSSION

The calculated nuclear SI PNC amplitude for Xe (z component) is

$$E_{\rm PNC}({\rm A} \to {\rm B}) = 1.76 \times 10^{-10}(-Q_W/N)iea_B. \qquad (15)$$

The SI PNC amplitudes for Hg are

$$\begin{aligned} E_{\rm PNC}({\rm A}_1 \to {\rm B}) &= 2.09 \times 10^{-10}(-Q_W/N)iea_B, \\ E_{\rm PNC}({\rm A}_2 \to {\rm B}) &= 1.77 \times 10^{-10}(-Q_W/N)iea_B, \\ E_{\rm PNC}({\rm A}_3 \to {\rm B}) &= 1.25 \times 10^{-10}(-Q_W/N)iea_B. \end{aligned} \qquad (16)$$

The difference in the value of the PNC amplitude for different isotopes is mostly due to the different value of the weak nuclear charge Q_W. Therefore, the amplitudes (15) and (16) may be used for any isotope.

Detailed data on both SD and SI PNC amplitudes for isotopes with nonzero nuclear spin are presented in Table III for Xe and Table IV for Hg.

A. $M1$ amplitudes

The experimental proposal [12] is aimed at the measurement of PNC optical rotation. The angle of rotation is proportional to the ratio $R = {\rm Im}(E_{\rm PNC}/M1)$. Therefore, we need to know the values of the magnetic dipole amplitudes for the transitions proposed for PNC measurements. The most accurate values of the $M1$ amplitudes can be found analytically using experimental values of the magnetic g factors to find the coefficients for configuration mixing.

This is especially important for the case of mercury, where numerical calculations of the $M1$ amplitudes give unstable results. The reason for this instability is easy to understand. The transitions considered for PNC measurements in mercury are between states of different spin ($S = 1$ for states $A_{1,2,3}$

TABLE III. PNC amplitudes (z components) for $|5p^5 6s^2\ ^2[3/2]^o_2, F_1\rangle \to |5p^5 6s\ ^2[1/2]^o_1, F_2\rangle$ transitions in ^{129}Xe and ^{131}Xe. I is the nuclear spin, $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{I}$. E' is given by (6).

		E'			PNC amplitude	
A	I	(units of $10^{-10}iea_0$)	F_1	F_2	(units of $E'Q_W$)	(units of $10^{-10}iea_0$)
129	1/2	3.16	3/2	1/2	$(1/3)(1+0.0387\varkappa)$	$1.05(1+0.0387\varkappa)$
			3/2	3/2	$-1/\sqrt{(50)}(1+0.010\varkappa)$	$-0.45(1+0.010\varkappa)$
			5/2	3/2	$\sqrt{(2/25)}(1-0.0226\varkappa)$	$0.89(1-0.0226\varkappa)$
131	3/2	3.25	1/2	1/2	$-1/\sqrt{18}(1+0.0345\varkappa)$	$-0.766(1+0.0345\varkappa)$
			1/2	3/2	$-1/\sqrt{90}(1+0.0252\varkappa)$	$-0.343(1+0.0252\varkappa)$
			3/2	1/2	$1/\sqrt{18}(1+0.0282\varkappa)$	$0.766(1+0.0282\varkappa)$
			3/2	3/2	$-\sqrt{8/125}(1+0.0189\varkappa)$	$-0.822(1+0.0189\varkappa)$
			3/2	5/2	$-1/\sqrt{375}(1+0.0034\varkappa)$	$-0.178(1+0.0034\varkappa)$
			5/2	3/2	$\sqrt{7/125}(1+0.0083\varkappa)$	$0.769(1+0.0083\varkappa)$
			5/2	5/2	$-\sqrt{3/70}(1-0.0072\varkappa)$	$-0.673(1-0.0072\varkappa)$
			7/2	5/2	$\sqrt{2/35}(1-0.0220\varkappa)$	$0.777(1-0.02204\varkappa)$

TABLE IV. PNC amplitudes (z components) for $|6s6p\ ^3\mathrm{P}^o_J, F_1\rangle \to |6s6p\ ^1\mathrm{P}^o_1, F_2\rangle$ transitions in ^{199}Hg and ^{201}Hg. I is the nuclear spin, $\boldsymbol{F} = \boldsymbol{J} + \boldsymbol{I}$. E' is given by (6).

			E'			PNC amplitude	
A	I	J	(units of $10^{-10} iea_0$)	F_1	F_2	(units of $E'Q_W$)	(units of $10^{-10} iea_0$)
199	1/2	0	3.41	1/2	1/2	$(1/3)(1+0.0084\varkappa)$	$1.14(1+0.0084\varkappa)$
				1/2	3/2	$-\sqrt{2/9}(1-0.0042\varkappa)$	$-1.61(1-0.0042\varkappa)$
		1	5.31	1/2	1/2	$\sqrt{2/27}(1+0.0538\varkappa)$	$1.44(1+0.0538\varkappa)$
				1/2	3/2	$\sqrt{1/27}(1-0.0860\varkappa)$	$1.02(1-0.0860\varkappa)$
				3/2	1/2	$\sqrt{1/27}(1+0.0308\varkappa)$	$1.02(1+0.0308\varkappa)$
				3/2	3/2	$1/\sqrt{6}(1-0.0105\varkappa)$	$2.17(1-0.0105\varkappa)$
		2	3.71	3/2	1/2	$(1/3)(1+0.0381\varkappa)$	$1.24(1+0.0381\varkappa)$
				3/2	3/2	$-1/\sqrt{50}(1+0.0471\varkappa)$	$-0.525(1+0.0471\varkappa)$
				5/2	3/2	$\sqrt{2/25}(1-0.0264\varkappa)$	$1.05(1-0.0264\varkappa)$
201	3/2	0	3.47	3/2	1/2	$(1/3)(1+0.0069\varkappa)$	$1.16(1+0.0069\varkappa)$
				3/2	3/2	$1/\sqrt{5}(1+0.0028\varkappa)$	$1.55(1+0.0028\varkappa)$
				3/2	5/2	$-\sqrt{2/15}(1-0.0041\varkappa)$	$-1.27(1-0.0041\varkappa)$
		1	5.40	1/2	1/2	$-1/\sqrt{54}(1+0.0171\varkappa)$	$-0.735(1+0.0171\varkappa)$
				1/2	3/2	$\sqrt{5/54}(1+0.00362\varkappa)$	$1.64(1+0.00362\varkappa)$
				3/2	1/2	$\sqrt{5/54}(1+0.0419\varkappa)$	$1.64(1+0.0419\varkappa)$
				3/2	3/2	$\sqrt{2/75}(1+0.0607\varkappa)$	$0.882(1+0.0607\varkappa)$
				3/2	5/2	$(1/5)(1-0.0515\varkappa)$	$1.08(1-0.0515\varkappa)$
				5/2	3/2	$(1/5)(1+0.0122\varkappa)$	$1.08(1+0.0122\varkappa)$
				5/2	5/2	$1/\sqrt{6}(1-0.0103\varkappa)$	$2.20(1-0.0103\varkappa)$
		2	3.78	1/2	1/2	$-1/\sqrt{18}(1+0.0385\varkappa)$	$-0.890(1+0.0385\varkappa)$
				1/2	3/2	$-1/\sqrt{90}(1+0.0414\varkappa)$	$-0.398(1+0.0414\varkappa)$
				3/2	1/2	$1/\sqrt{18}(1+0.0240\varkappa)$	$0.890(1+0.0240\varkappa)$
				3/2	3/2	$-\sqrt{8/125}(1+0.0269\varkappa)$	$-0.956(1+0.0269\varkappa)$
				3/2	5/2	$-1/\sqrt{375}(1+0.0318\varkappa)$	$-0.195(1+0.0318\varkappa)$
				5/2	3/2	$\sqrt{7/125}(1+0.00286\varkappa)$	$0.894(1+0.00286\varkappa)$
				5/2	5/2	$-\sqrt{3/70}(1+0.00774\varkappa)$	$-0.782(1+0.00774\varkappa)$
				7/2	5/2	$\sqrt{2/35}(1-0.0260\varkappa)$	$0.903(1-0.0260\varkappa)$

and $S = 0$ for state B). This means that the $M1$ amplitudes between these states vanish in the nonrelativistic limit. In relativistic calculations the amplitudes are not 0, but low. These small values are obtained as a result of strong cancellation between different contributions. This stong cancellation leads to unstable results.

On the other hand, analytical evaluation of the $M1$ amplitudes is simple and produces very accurate results. The operator of the magnetic dipole transition $[M_z = (L_z + 2S_z)\mu_B]$ has no radial part and cannot change a principal quantum number in the nonrelativistic limit. Therefore, the magnetic g factors and $M1$ amplitudes are mainly sensitive to the mixing of states belonging to the same configuration. Mixing with other configurations normally produces corrections at the 10^{-3} level [29]. We can see this in Tables I and II, where g factors of "pure" sp states with $J = 2$ and the sum of the g factors for mixed states $J = 1$ differ from the experimental values by less than 0.1%. Therefore, the mixing coefficients for states belonging to the same configuration and $M1$ amplitudes can be found almost exactly from the known values of the g factors. Note that we use the calculated value of the overlap between the radial wave functions $p_{1/2}$ and $p_{3/2}$, which is close, but not equal, to 1. For Hg it is 0.988.

We get, for states A and B of xenon,

$$\Psi_A = |5p_{3/2}6s\rangle,$$
$$\Psi_B = 0.05|5p_{3/2}6s\rangle + 0.999|5p_{1/2}6s\rangle. \qquad (17)$$

This leads to the $M1$ amplitude

$$M1_{AB} = 1.22\mu_B = 0.00446ea_B. \qquad (18)$$

Using E' from Table III we get $R = 7.1(7)(35) \times 10^{-8}$ for ^{129}Xe and $R = 7.3(7) \times 10^{-8}$ for ^{131}Xe. Here we assume a 10% uncertainty as discussed above. These values of $M1$ and R are close to, but not in perfect agreement with, what was found in Ref. [12]: $M1 = 0.0042ea_B$, $R = 11(3) \times 10^{-8}$. The reason for the difference in $M1$ is not clear. The authors of Ref. [12] use slightly different coefficients of configuration

TABLE V. Magnitudes of the $M1$ and PNC amplitudes (reduced matrix elements) and ratios $R \equiv \mathrm{Im}(E_{\mathrm{PNC}}/M1)$ for ^3P_J–$^1P_1$ transitions in mercury. Values for $M1$ from Ref. [12] are also presented for comparison.

	$M1$ amplitude				$\mathrm{Im}(E_{\mathrm{PNC}})$		R	
	This work		Ref. [12]		^{199}Hg	^{201}Hg	^{199}Hg	^{201}Hg
Transition	(units of $10^{-4}ea_B$)	μ_B	(units of $10^{-4}ea_B$)	μ_B	(units of $10^{-10}ea_B$)		(units of 10^{-7})	
$^3P_0^o$–$^1P_1^o$	8.37	0.229	14	0.384	3.4(2)	3.5(2)	4.1(2)	4.2(2)
$^3P_1^o$–$^1P_1^o$	7.26	0.199	42	1.15	5.3(3)	5.4(3)	7.3(4)	7.4(4)
$^3P_2^o$–$^1P_1^o$	9.94	0.272	57	1.56	3.7(2)	3.8(2)	3.7(2)	3.8(2)

mixing in (17). Their values are 0.062 and 0.998. However, if we use these coefficients, we get $M1 = 0.00444ea_B$, which is different from the value $M1 = 0.0042ea_B$ presented in Ref. [12].

The situation is more complicated for mercury. All the $M1$ transitions of interest happen between states with different total spins and vanish in the nonrelativistic limit since the operator $L_z + 2S_z$ conserves the total spin. This leads to strong suppression. The values of $M1$ amplitudes presented in Ref. [12] are too large for the spin-forbidden transitions. No choice of the configuration mixing coefficients can reproduce them.

The wave functions for states $\mathrm{A}_{1,2,3}$ and B for Hg have the form

$$\begin{aligned}
\Psi_{\mathrm{A}_1} &= |6p_{1/2}6s\rangle,\\
\Psi_{\mathrm{A}_2} &= 0.432|6p_{3/2}6s\rangle - 0.902|6p_{1/2}6s\rangle,\\
\Psi_{\mathrm{A}_3} &= |6p_{3/2}6s\rangle,\\
\Psi_{\mathrm{B}} &= 0.902|6p_{3/2}6s\rangle + 0.432|6p_{1/2}6s\rangle.
\end{aligned} \tag{19}$$

The coefficients 0.902 and 0.432 are chosen to fit the experimental g factors of states A_2 and B. When projections are included, all $|^{2S+1}P_{JJ_z}\rangle$ states of the $6s6p$ configuration can be written as

$$\begin{aligned}
\left|\mathrm{A}_1\colon {}^3P_{00}^o\right\rangle &= -\frac{1}{\sqrt{2}}\left[\left|6s_{\frac12\frac12}6p_{\frac12-\frac12}\right\rangle - \left|6s_{\frac12-\frac12}6p_{\frac12\frac12}\right\rangle\right],\\
\left|\mathrm{A}_2\colon {}^3P_{11}^o\right\rangle &= -0.216\left|6s_{\frac12\frac12}6p_{\frac32\frac12}\right\rangle\\
&\quad + 0.374\left|6s_{\frac12-\frac12}6p_{\frac32\frac32}\right\rangle + 0.902\left|6s_{\frac12\frac12}6p_{\frac12\frac12}\right\rangle,\\
\left|\mathrm{A}_3\colon {}^3P_{22}^o\right\rangle &= \left|6s_{\frac12\frac12}6p_{\frac32\frac32}\right\rangle,\\
\left|\mathrm{B}\colon {}^1P_{11}^o\right\rangle &= -0.451\left|6s_{\frac12\frac12}6p_{\frac32\frac12}\right\rangle\\
&\quad + 0.781\left|6s_{\frac12-\frac12}6p_{\frac32\frac32}\right\rangle - 0.432\left|6s_{\frac12\frac12}6p_{\frac12\frac12}\right\rangle.
\end{aligned} \tag{20}$$

Here we use (19) for the expansion. The results for $M1$ amplitudes obtained with the use of these formulas are presented in Table V together with the values from Ref. [12]. Note that there must be $M1 \ll \mu_B$ for spin-forbidden transitions. This holds for the results of the present work but not for the results in Ref. [12]. Table V also presents the PNC amplitudes and the ratios $R = \mathrm{Im}(E_{\mathrm{PNC}}/M1)$. The numbers include 5% error bars according to the estimated uncertainty of the calculations discussed in Sec. III B. Note that the values of the $M1$ amplitudes obtained in the present work are practically exact due to the fitting of the experimental g factors.

The values of the ratios R are larger than in Ref. [12] due to the lower $M1$ amplitudes. The values of R for mercury are about an order on magnitude larger than those for xenon (see above) and about an order of magnitude larger than those for Tl, Pb, and Bi [30–32].

B. Optical rotation

The angle of optical rotation is given by [33]

$$\phi_{\mathrm{PNC}} = -\frac{4\pi l}{\lambda}\,[n(\omega) - 1]\,R, \tag{21}$$

where l is the path length in vapor, λ is the wavelength of laser light, ω is its frequency, and $n(\omega)$ is the refractive index due to absorption. Although the angle is proportional to the ratio $R = \mathrm{Im}(E_{\mathrm{PNC}}/M1)$, the low values for the $M1$ amplitudes do not necessarily translate into a large angle of rotation. This is because the refractive index also depends on the $M1$ amplitude, $n(\omega) - 1 \sim |M1|^2$, which leads to $\phi \sim M1E_{\mathrm{PNC}}$. However, the suppression due to the low $M1$ amplitude can be compensated at a sufficiently high vapor pressure by the appropriate choice of the path length l. These questions are discussed in detail in Ref. [33]. Here we just note that the angle of rotation per unit length is $\phi \sim M1E_{\mathrm{PNC}}$. However, the angle of rotation per absorption length $\phi \sim R$ and it is large for small $M1$.

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