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Enhancement of Parity and Time Invariance Violation in Heavy Atoms

Vladimir A. Dzuba, Victor V. Flambaum, Jacinda S. M. Ginges

School of Physics, University of New South Wales, Sydney 2052, Australia

Abstract. Parity (P) and time (T) invariance violating effects are enhanced in atoms with close states of opposite parity, large nuclear charge Z , and collective P, T -odd nuclear moments. We have performed calculations of the atomic electric dipole moment (EDM) induced in radium by the electron EDM and the nuclear magnetic quadrupole and Schiff moments. We have also calculated the effects of parity nonconservation in radium produced by the nuclear anapole moment and the nuclear weak charge. Our results show that the values of parity and time invariance violating effects in radium are much larger than those considered so far in other atoms.

INTRODUCTION

Atoms are very good objects to study when searching for parity and time invariance violating effects, as these effects can be strongly enhanced in heavy atoms. The enhancement occurs due to several mechanisms. The three main contributing mechanisms to the enhancement in atoms are close electronic levels of opposite parity, large nuclear charge, and deformation of the nucleus.

If an atom has energy levels, E_1 and E_2 , of opposite parity then the P - and T -odd effects associated with these levels are proportional to $1/(E_1 - E_2)$. So in the case when the energy interval $E_1 - E_2$ is very small the effect is strongly enhanced.

The matrix elements of P - and T -odd interactions increase with Z faster than $Z^2 R(Z)$, where Z is the nuclear charge and $R(Z)$ is a relativistic factor which also increases with Z . A large enhancement of P, T -odd effects can therefore occur in heavy atoms.

It has been demonstrated that deformed nuclei lead to enhanced nuclear moments compared to those associated with spherical nuclei [1-3]. A quadrupole deformed nucleus has a strongly enhanced magnetic quadrupole moment (MQM) [1]. The MQM is a P - and T -odd moment which can exist only if there are P - and T -odd interactions between nuclear particles. The parameter of enhancement is $A^{2/3}$, where A is the nuclear mass number. So effects in heavy atoms with nuclear quadrupole deformation can be enhanced by a factor ~ 10 . An octupole deformed

nucleus leads to strong enhancement of the nuclear Schiff moment (SM) [2,3], which is also P - and T -odd.

In the work of Flambaum [4] it was shown that radium is an excellent candidate for the study of P - and T -odd effects, and estimates for some of these effects were made. In the current work we make more accurate calculations of these and other effects. Below we present our results for the EDM induced in radium, ^{223}Ra and ^{225}Ra , by the electron EDM and the nuclear Schiff moment and MQM. We also present our results for the parity nonconserving electric dipole transition induced by the nuclear weak charge and that induced by the nuclear anapole moment.

P- AND T-ODD EFFECTS IN RADIUM

The radium atom satisfies all criteria listed above which lead to strong enhancement of P,T -odd effects: the states $7s7d\ ^3D_2$ and $7s7p\ ^3P_1$ with the respective energies $E = 13993.97\text{ cm}^{-1}$ and $E = 13999.38\text{ cm}^{-1}$ are separated by about $5\text{ cm}^{-1} \sim 10^{-3}\text{ eV}$ (it should also be noted that the states $7s7d\ ^3D_1$ and $7s7p\ ^3P_1$ are also quite close, $\Delta E \sim 283\text{ cm}^{-1}$); radium has a large nuclear charge ($Z = 88$); there is theoretical and experimental evidence that the odd isotopes of radium, e.g. ^{223}Ra with nuclear spin $I = 3/2$ and ^{225}Ra with $I = 1/2$, have nuclear octupole deformation, leading to enhanced Schiff moments [3]; and the isotope ^{223}Ra has nuclear quadrupole deformation which leads to an enhanced magnetic quadrupole moment (the MQM is zero for $I < 1$).

Method of Calculation

We used a relatively simple *ab initio* approximation which is a reasonable compromise between the simplicity of the calculations and the accuracy of the results. It is based on the relativistic Hartree-Fock (RHF) and configuration interaction (CI) methods. A minimum number of basis states were used at the CI stage of the calculations. However, important many-body effects, such as polarization of the atomic core by an external field and correlations between core and valence electrons, were included in the calculations of the single-electron matrix elements. These effects are important because core-valence correlations increase the electron density on the nucleus, strongly affecting the value of P,T -violating matrix elements, while core polarization makes $p - d$ single-electron matrix elements large due to the effective renormalization of the interaction of the external electron with the nucleus by the Coulomb field. To control the accuracy of the calculations we also calculated hyperfine structure intervals and lifetimes of the lower states of radium and its lighter analog barium. The accuracy for the energy is about 10% while the accuracy for the hfs and lifetimes is 10 - 30%.

Our calculations confirm the estimates done in the previous work [4] and show that the values of most P - and T -odd effects in radium are much higher than in other atoms considered before.

Atomic Electric Dipole Moment

The interaction of an electron EDM, d_e , with an atomic field mixes states with the same total electron momentum J and opposite parity. As a result, an atomic EDM, d_z , arises. The atomic EDM induced in radium by the electron EDM is strongly enhanced in the $7s7d\ ^3D_1$ state due to the admixture of the close opposite parity state 3P_1 . In an approximation where only this admixture to the contribution of the EDM is considered, the result is

$$d_z = 5370d_e. \quad (1)$$

This enhancement of the electron EDM is many times larger than corresponding values for the ground states of francium (910) and gold (260) [5].

The interaction of the atomic electrons with the nuclear Schiff moment produces an atomic EDM. In radium, the EDM arising due to the Schiff moment is strongly enhanced in the 3D_2 state. The results for the EDM of radium induced by the Schiff moment, in an approximation where only the admixture with the close opposite parity state 3P_1 is considered, are presented in Table 1. The results are presented in terms of the dimensionless constant of the P -, T -odd nucleon-nucleon interaction, η .

TABLE 1. EDM of the radium atom in the 3D_2 state induced by the nuclear Schiff moment

I	F^a	d_z (a.u.)	d_z (e cm)
0.5	1.5	$-0.94 \times 10^8 S$	$-0.19 \times 10^{-11} \eta^b$
1.5	0.5	$-0.16 \times 10^8 S$	$-0.36 \times 10^{-19} \eta$
1.5	1.5	$-0.30 \times 10^9 S$	$-0.80 \times 10^{-19} \eta$
1.5	2.5	$-0.28 \times 10^9 S$	$-0.15 \times 10^{-18} \eta$
			$-0.76 \times 10^{-11} \eta^c$
			$-0.14 \times 10^{-18} \eta$

^a F is the total atomic angular momentum, $\mathbf{F} = \mathbf{J} + \mathbf{I}$

^b Nuclear Schiff moment S is assumed to be $S = 400 \times 10^8 \eta \text{ e fm}^3$ [3]

^c $S = 300 \times 10^8 \eta \text{ e fm}^3$ [3]

An atomic EDM is also induced by the interaction of atomic electrons with the nuclear magnetic quadrupole moment. As with the Schiff moment, the EDM of radium induced by the MQM is strongly enhanced in the state 3D_2 by admixture with the state 3P_1 . It should be noted that the MQM of isotopes where the nuclear spin $I < 1$ (like ^{225}Ra where $I = 1/2$) is zero. Results for the leading contribution to the radium EDM in the state 3D_2 induced by the MQM are presented in Table 2.

The results for the EDM induced in radium due to the Schiff and magnetic quadrupole moments are of the same order of magnitude and are about 10^5 times larger than the EDM of the mercury atom, which currently gives the best upper limit on η [6].

The EDMs of some other heavy atoms have also been estimated. The results are presented in Table 3.

TABLE 2. EDM of the ^{223}Ra isotope ($I = 3/2$) in the 3D_2 state induced by the nuclear magnetic quadrupole moment

F	d_z^a	d_z^b
0.5	$1344Mm_e$	$7.4 \times 10^{-20}\eta \text{ e cm}$
1.5	$1292Mm_e$	$7.0 \times 10^{-20}\eta \text{ e cm}$
2.5	$-806Mm_e$	$-4.4 \times 10^{-20}\eta \text{ e cm}$

^a In terms of nuclear magnetic quadrupole moment M

^b M is assumed to be $M = 10^{-19}(\eta/m_p) \text{ e cm}$, [1] where m_p is the proton mass

Parity Nonconservation

We found that parity nonconserving (PNC) effects produced by the nuclear weak charge (nuclear spin-independent) and those produced by the nuclear anapole moment (nuclear spin-dependent) are also strongly enhanced.

The interaction of an electron with the nuclear weak charge Q_W mixes states of the same total momentum J and opposite parity. So electric dipole transitions between states of initially equal parity become possible. In particular, the transition between the ground state 1S_0 and the excited 3D_1 state of radium is enhanced due to the closeness of the opposite parity state 3P_1 . Taking into account only this dominating contribution to the PNC $E1$ transition, the results are:

$$^{225}\text{Ra} : E1_{PNC} = 0.77 \times 10^{-9}(Q_W/N)iea_0, \quad (2)$$

$$^{223}\text{Ra} : E1_{PNC} = 0.76 \times 10^{-9}(Q_W/N)iea_0. \quad (3)$$

The result for radium is about 100 times larger than the measured PNC amplitude in cesium [9], about 5 times larger than the corresponding amplitude in francium [10], and has the same order of magnitude as the PNC amplitude in ytterbium [11].

Similar to the spin-independent PNC interaction, the electron interaction with the nuclear anapole moment mixes states of opposite parity and leads to non-zero $E1$ transition amplitudes between states of initially equal parity. However, states with $\Delta J = 1$ can also be mixed and the interaction is dependent on the nuclear spin. The results for the dominating contributions to the transitions $^1S_0 - ^3D_1$ and $^1S_0 - ^3D_2$, due to admixture with $7s7p$, are presented in Table 4. The spin-dependent PNC transition amplitude $^1S_0 - ^3D_2$ is more than 1000 times larger than a similar amplitude in cesium [9].

TABLE 3. EDMs of some heavy atoms (in units $10^{-25}\eta \text{ e cm}$)

^{199}Hg	5.6 ^a	^{129}Xe	0.47 ^b	^{223}Rn	2000 ^c
^{221}Fr	240 ^c	^{223}Fr	2800 ^c	^{225}Ac	~1000 ^c

^a Calculated in Ref. [7]

^b Calculated in Ref. [8]

^c Calculated in Ref. [3]

TABLE 4. PNC E1 transition amplitude between different hyperfine structure components F and F' induced by the nuclear anapole moment; κ_a is a dimensionless constant proportional to the strength of the PNC nucleon-nucleon interaction

I	F	F'	$E1_{PNC}$ in units $10^{-10}\kappa_a i e a_0$	
			$^1S_0 - ^3D_1$	$^1S_0 - ^3D_2$
0.5	0.5	1.5	2.05	-20.3
1.5	1.5	0.5	-0.58	5.7
	1.5	1.5	-1.4	13.8
	1.5	2.5	1.3	-12.9

CONCLUSION

The radium atom turns out to be a very promising candidate for the study of parity and time invariance violating effects, as these effects are hugely enhanced.

The contribution of different mechanisms to the P - and T -odd effects can be studied separately if measurements are performed for different states and different isotopes of the radium atom. For example, the atomic EDM induced by the electron EDM is strongly enhanced in the 3D_1 state, while contributions of the nuclear Schiff and magnetic quadrupole moments are strongly enhanced in the 3D_2 state. Also, the magnetic quadrupole moment is zero for isotopes with nuclear spin $I = 1/2$, like ^{225}Ra , while the Schiff moment for these isotopes is not zero.

The contribution of the anapole moment to the measured PNC amplitude can be determined by comparing the amplitudes between different hyperfine structure components similar to what was done for cesium [9]. It would be more efficient to measure the effect of the anapole moment in the $^1S_0 - ^3D_2$ transition than the $^1S_0 - ^3D_1$ transition as it is about ten times larger and because the nuclear spin-independent PNC interaction does not contribute to this amplitude at all due to the large change of the total electron angular momentum $\Delta J = 2$.

Calculations of parity and time invariance violating effects in radium reveal the importance of relativistic and many-body effects. The accuracy achieved in the present work is probably 20-30 %. However, a further improvement in accuracy is possible if such a need arises from the progress in measurements.

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