Current trends in searches for new physics using measurements of parity violation and electric dipole moments in atoms and molecules

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We review current status of the study of parity and time invariance phenomena in atoms, nuclei and molecules. We focus on three most promising areas of research: (i) parity non-conservation in a chain of isotopes, (ii) search for nuclear anapole moments, and (iii) search for permanent electric dipole moments (EDM) of atoms and molecules which are caused by either, electron EDM or nuclear T, P-odd moments such as nuclear EDM and nuclear Schiff moment.

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I. INTRODUCTION

The study of the parity and time invariance violation in atoms, molecules and nuclei is a low-energy, relatively inexpensive alternative to high-energy search for new physics beyond the standard model (see, e.g. a review [1]). Until very recently the accurate measurements of the parity non-conservation (PNC) in atoms was one of the most promising ways of exploring this path. It culminated in very precise measurements of the PNC in cesium [2]. There were even indications that these measurements show some disagreements with the standard model and might indeed lead to new physics [3]. It took considerable effort of several groups of theorists to improve the interpretation of the measurements and resolve the disagreement in favor of the standard model. The disagreement were removed when Breit [4] and quantum electrodynamic corrections [5] were included and the accuracy of the treatment of atomic correlations were improved [6, 7].

In is unlikely that any new measurements of the PNC in atoms can compete with the cesium experiment in accuracy of the measurements and interpretation (the heavy alkaline atoms like Fr and Ra[+], where the PNC effect is 20 times larger than in Cs, may be exceptions). Therefore, the main interest in the area has shifted mostly to three other important subjects: (i) the PNC measurements for a chain of isotopes; (ii) the measurements of nuclear anapole moments; and (iii) the measurements of the P,T-odd permanent electric dipole moments of atoms and molecules. Below we will briefly review each of these subjects.

II. CHAIN OF ISOTOPES

The values measured in atomic PNC-experiments can be presented in a form

\[ E_{PNC} = k_{PNC}Q_W, \]

where \( k_{PNC} \) is an electron structure factor which comes from atomic calculations and \( Q_W \) is a weak nuclear charge. Very sophisticated calculations are needed for accurate interpretation of the measurements as has been discussed in introduction for the case of Cs. An alternative approach was suggested in Ref. [8]. If the same PNC effect is measured for at least two different isotopes of the same atom than the ratio

\[ R = \frac{E'_{PNC}}{E_{PNC}} = \frac{Q'_W}{Q_W} \]

of the PNC signals for the two isotopes does not depend on electron structure factor. It was pointed out however in Ref. [9] that possible constrains on the new physics coming from isotope ratio measurements are needed for accurate interpretation of the measurements as has been discussed in introduction for the case of Cs. An alternative approach was suggested in Ref. [8]. The authors of Ref. [10] argue that experimental data on neutron distribution, such as, e.g. the data from the experiments with antiprotonic atoms[12], can be used to reduce the uncertainty. In more general approach of Ref. [11] nuclear calculations are used to demonstrate that the neutron distributions are correlated for different isotopes which leads to cancelation of the relevant uncertainties in the ratio [2].

The parameter \( \mathcal{F} \) of the sensitivity of the ratio [2] to
new physics can be presented in the form

$$F = \frac{F_p}{F_0} = \left( \frac{R}{R_0} - 1 \right) \frac{N N'}{Z \Delta N},$$

(3)

where $F_p$ is the new physics coupling to protons ($\Delta Q_{\text{new}} = Z F_p + N h_n$), $F_0$ comes from the SM, $R_0$ is the ratio (2) assuming that each isotope has the same proton and neutron distribution (no neutron skin), $N$ and $N'$ are the numbers of neutrons in two isotopes, $Z$ is the number of protons and $\Delta N = N' - N$. The constrains on new physics parameter $h_p$ are affected by the experimental error $\delta R_{\text{exp}}$ and uncertainties in $R_0$ due to insufficient knowledge of nuclear distributions. The later, as is argued in Ref. [11], are correlated and strongly cancel each other. Estimations of Ref. [11] show that corresponding contribution to $\delta F$ is in the range $10^{-3} \div 10^{-2}$ which is about an order of magnitude smaller than the uncorrelated ones. In the end, the isotope-chain measurements are more sensitive to new physics than current parity-violating electron scattering measurements [13] (by a factor of 10 for such atoms as Cs, Ba and Dy).

Experiments on isotope chains are in progress at Berkeley for Dy and Yb atoms [14, 15], at TRIUMF for Fr atoms [16], at Los Alamos for Yb+ ions [17], and at Groningen (KVI) for Ra+ ions [70].

III. ANAPOLE MOMENT

The notion of the anapole moment was introduced by B. Ya. Zeldovich [19]. Nuclear anapole moment (AM) is the magnetic $P$ and $C$-odd, $T$-even nuclear moment caused by the $P$-odd weak nuclear forces. Interaction of electrons with AM magnetic field (which may be called the PNC hyperfine interaction) dominates the nuclear-spin-dependent contribution to the atomic or molecular PNC effect.

First calculations of nuclear AM and proposals for experimental measurements were presented in Ref. [20–23]. Corrections to the AM interaction with electrons due to finite nuclear size were considered in Ref. [24]. The authors of [22, 23] (see also [24]) note in particular that the effect of AM is strongly enhanced in diatomic molecules due to mixing of the close rotational states of opposite parity including mixing of a $\Lambda$ or $\Omega$ doublet. The PNC effects produced by the weak charge are not enhanced. Therefore the AM effect dominates PNC in molecules. This greatly simplifies the detection of AM in diatomic molecules compared to atoms. In atoms the AM effect is 50 times smaller than the weak charge effect; AM effect is separated as a small difference of the PNC effects in different hyperfine transitions. A review of the parity and time invariance violation in diatomic molecules (including the AM effect) can be found in Ref. [25].

The idea of the AM contribution enhancement may be explained as follows. After the averaging over electron wave function the effective operator acting on the angular variables may contain three vectors: the direction of molecular axis $\mathbf{N}$, the electron angular momentum $\mathbf{J}$ and nuclear spin $\mathbf{I}$. Scalar products $\mathbf{N}\mathbf{I}$ and $\mathbf{N}\mathbf{J}$ are $T$-odd and $P$-odd. Therefore, they are produced by the $T, P$-odd interactions discussed in the next section. $P$-odd, $T$-even operator $V_P$ must be proportional to $N[I \times J]$. It contains nuclear spin $I$, therefore, the weak charge does not contribute. The nuclear AM is directed along the nuclear spin $I$, therefore, it contributes to $V_P$. The matrix elements of $\mathbf{N}$ between molecular rotational states are well-known, they produce rotational electric dipole transitions in polar molecules. Therefore, $V_P$ (induced by the magnetic interaction of the nuclear AM with molecular electrons) mixes close rotational-hyperfine states of opposite parity. The interval between these levels is five orders of magnitude smaller than the interval between the opposite parity levels in atoms (by the factor $m_e/M$ where $m_e$ and $M$ are the electron and reduced molecular masses), therefore PNC effects are five orders of magnitude larger. Further enhancement may be achieved by a reduction of the intervals by an external magnetic field [26].

The effect is further enhanced for heavy molecules. It grows with nuclear charge as $Z^2 A^{1/3} R(Z\alpha)$, where $R(Z\alpha)$ is the relativistic factor which grows from $R = 1$ at low $Z$ to $R \sim 10$ for $Z > 10$. Good candidates for the measurements include the molecules and molecular ions with $\Sigma_{1/2}$ or $\Pi_{1/2}$ electronic ground state [22, 23], for example, YbF, BaF, HgF, PbF, LaO, LuO, LaS, LuS, BiO, BiS, YbO+, PbO+, BaO+, HgO+, etc. Molecular experiments are currently in progress at Yale [27] and Groningen KVI [28]. An interesting idea of studying AM contribution to the NMR spectra of chiral molecules were discussed in Ref. [29].

So far the only nuclear AM which has been measured is the AM of the $^{133}$Cs nucleus. It is done by comparing PNC amplitudes between different hyperfine structure sublevels in the same PNC experiment which is discussed in the introduction [2]. Interpretation of the measurements [30] indicates some problems. For example, the value of Cs AM is inconsistent with the limit on the AM of Tl [31].

To resolve the inconsistencies and obtain valuable information about $P$-odd nuclear forces it would be extremely important to measure anapole moments for other nuclei. In particular, it is important to measure AM for a nucleus with an unpaired neutron (Cs and Tl have unpaired protons). AM of such nucleus depend on different combination of the weak interaction constants providing important cross-check. Good candidates for such measurements include odd isotopes of Ra, Dy, Pb, Ba, La, Lu and Yb. The Ra atom has an extra advantage because of strong enhancement of the spin-dependent PNC effect in the $^{1}S_{0} - ^{3}D_{2}$ transition due to proximity of the opposite-parity state $^{3}P_{1}^{0}$ ($\Delta E = 5 \text{ cm}^{-1}$) [32].

Experimental work is in progress for Rb and Fr at TRIUMF [16, 33], and for Dy and Yb at Berkeley [14, 15].
IV. ELECTRIC DIPOLE MOMENT

Permanent electric dipole moment (EDM) of a neutron, atom or molecule would violate both $P$ and $T$ invariance. Under conditions of the CPT-theorem this would also mean a CP-violation. The Kobayashi-Maskawa mechanism of the SM leads to extremely small values of the EDMs of the particles. It is also too weak to explain the matter-antimatter asymmetry of the Universe. On the other hand, most of the popular extensions to the SM predict much larger EDMs which are within experimental reach. The EDM of an atom or a molecule is mostly due to either electron EDM and $T,P$-odd electron-nucleon interactions in paramagnetic systems (with non-zero total momentum $J$) or to the $T,P$-odd nuclear forces in diamagnetic systems ($J = 0$; nuclear-spin-dependent e-N interaction contributes here too). The existence of $T,P$-odd nuclear forces leads to the $T,P$-odd nuclear moments in the expansion of the nuclear potential over powers of distance $R$ from the center of the nucleus. The lowest-order term in the expansion, the nuclear EDM, is unobservable in neutral atoms due to total screening of the external electric field by atomic electrons. It might be possible however to observe the nuclear EDM in ions (see below). The first non-vanishing term which survives the screening in neutral systems is the so called Schiff moment. Below we discuss the effects of nuclear and electron EDM and the Schiff moment.

A. Nuclear EDM

It was widely believed that one needs neutral particles (e.g., neutron, neutral atom or molecule) to study EDMs. This is because the EDM is expected to be very small and it would be very hard to see the effect of its interaction with external electric field on the background of the much stronger interaction with the electric charge. On the other hand, the EDM of neutral systems is very much suppressed by the effect of screening of the external electric field by atomic electrons (Schiff theorem). The Schiff theorem may be violated by the relativistic effect (which dominates in the case of the electron EDM), hyperfine interaction and finite size effect. For example, the lowest-order $T,P$-odd nuclear moment, the nuclear EDM is practically unobservable in the neutral systems (except for a small contribution due to the hyperfine interaction). First observable $T,P$-odd nuclear moment, the Schiff moment, is non-zero due to finite nuclear size.

It is important therefore to explore the possibility of studying EDMs of charged particles (e.g., muons or atomic ions). There are realistic suggestions of this kind in Refs. [34–36] based on the use of ion storage rings.

The external electric field is not totally screened on the nucleus of an ion. Its value is

$$E_N = \frac{Z_i}{Z} E_0,$$

where $E_0$ is external electric field, $E_N$ is electric field at the nucleus, $Ze$ is nuclear charge, $Z_i e$ is the charge of the ion, $e$ is proton charge. The formula (4) can be obtained in a very simple way. The second Newton law for the ion and its nucleus in the electric filed reads

$$M_i a_i = Z_i e E_0,$$

$$M_N a_N = Z e E_N,$$

where $M_i$ is the ion’s mass, $a_i$ is its acceleration, $M_N$ is nuclear mass ($M_N \approx M_1$), and $a_N$ is its acceleration. Since the ion and its nucleus move together, the accelerations must be the same ($a_i = a_N$), therefore

$$E_N = \frac{Z_i}{Z} E_0 \frac{M_N}{M_i} \approx \frac{Z_i}{Z} E_0.$$

Different derivation of this formula can be found in Ref. [37, 38]. Numerical calculations of the screened electric field inside an atomic ion were performed in a number of our works (see, e.g. Ref. [37]).

The Hamiltonian of the nuclear EDM ($d_N$) interaction with the electric field is given by

$$\hat{H}_d = d_N E_N = d_N \frac{Z_i}{Z} E_0.$$

Screening is stronger for diatomic molecules where we have an additional suppression factor in eq. (5), $M_N/M_i = M_1/(M_1 + M_2)$, where $M_1$ and $M_2$ are the masses of the first and second nucleus. For the average electric field acting on the first nucleus we obtain

$$E_{1N} = \frac{Z_i}{Z_1} \frac{M_1}{M_1 + M_2} E_0.$$

Note that the screening factor here contains both nuclear masses. This indicates that the nuclear motion can not be ignored and the screening problem is more complicated than in atoms. For example, in a naive model of a neutral polar molecule $A^+ B^-$, both ions $A^+$ and $B^-$ should be located in the area of zero (totally screened) electric field since their average acceleration is zero. This could make $A^+$ and $B^-$ EDM unobservable even if they are produced by a nuclear Schiff moment or electron EDM. In a more realistic molecular calculations the Schiff moment and electron EDM effects are not zero, however, they may be significantly suppressed (in comparison with a naive estimate of ionic EDM in a very strong field of another ion) and the results of the calculations may be unstable.

In the case of monochromatic external electric field its frequency can be chosen to be in resonance with the atomic electron excitation energy. Then for the effective Hamiltonian we can have

$$\hat{H}_d = d_N E_N(t) \gg d_N E_0.$$
B. Electron EDM

Paramagnetic atoms and molecules which have an unpaired electron are most sensitive to the electron EDM. The EDM of such systems can be expressed in the form

\[ d = K d_e, \]  

where \( d \) is the EDM of an atom or molecule, \( d_e \) is electron EDM, and \( K \) is electron structure factor which comes from atomic calculations. The factor \( K \) increases with nuclear charge \( Z \) as \( Z^3 \) times large relativistic factor \( R(Z \alpha) \) which may exceed the value of 3 in heavy atoms. A rough estimate of the enhancement factor in heavy atoms with external atoms. A rough estimate of the enhancement factor in heavy atoms with external atoms. A rough estimate of the enhancement factor in heavy atoms with external atoms. A rough estimate of the enhancement factor in heavy atoms with external atoms.

Several orders of magnitude larger \( K \sim 10^7 \) exist in molecules due to the mixing of the close rotational levels of opposite parity (including \( \Lambda \)-doublets) \([22]\). Following Sandars this enhancement factor is usually presented as a ratio of a very large internal molecular field to the external electric field which polarizes the molecule.

The best current limit on electron EDM comes from the measurements of the thallium EDM \([41]\) and reads

\[ d_e = (6.9 \pm 7.4) \times 10^{-28} \text{e cm.} \]  

Here the value \( K = -585 \) \([42]\) were used for the interpretation of the measurements. The value of \( K \) for TI is very sensitive to the inter-electron correlations and two most complete calculations \([42, 43]\) give very close results.

In contrast to paramagnetic atoms the diamagnetic (closed shell) atoms are much less sensitive to electron EDM. This is because the only possible direction of the atomic EDM in this case is along nuclear spin and hyperfine structure interaction must be involved to link electron EDM to nuclear spin. For example, for the mercury atom \( K \sim 10^{-2} \) \([44, 45]\). However, due to very strong constrain on the mercury EDM \([46]\) the limit on electron EDM extracted from these measurements is competitive to the Tl result \([10, 46]\)

\[ d_e < 3 \times 10^{-27} \text{e cm.} \]  

New experiments are in progress to measure the electron EDM in Cs \([47]\), Fr \([48]\), YbF \([49]\), ThO \([50]\), PbO \([51]\) and in solid-state experiments \([52]\).

C. Schiff moment

Schiff moment is the lowest-order \( T, P \)-odd nuclear moment which appears in the expansion of the nuclear potential when screening of the external electric field by atomic electrons is taken into account. This potential can be written as (see the derivation, e.g. in \([53, 54]\)

\[ \phi(R) = \int \frac{e \rho(r)}{|R - r|} d^3r + \frac{1}{Z} (\mathbf{d} \cdot \nabla) \int \frac{\rho(r)}{|R - r|} d^3r, \]  

where \( \rho(r) \) is nuclear charge density normalized to \( Z \), and \( \mathbf{d} \) is nuclear EDM. The second term in \((12)\) is screening. Taking into account finite nuclear size the lowest-order term in the expansion of \((12)\) in powers of \( R \) can be written as \([55]\)

\[ \psi(R) = -\frac{3\mathbf{S} \cdot \mathbf{R}}{B} \rho(R), \]  

where \( B = \int \rho(R) R^4 d\mathbf{r} \) and

\[ S = \frac{e}{10} \left[ \langle r^2 \rangle - \frac{5}{32} \langle r^2 \rangle \right] \]  

is Schiff moment. The expression \((13)\) has no singularities and can be used in relativistic calculations. The Schiff moment is caused by the \( T, P \)-odd nuclear forces. The dominant mechanism is believed to be \( T, P \)-odd nucleon-nucleon interaction. Another important contribution comes from the EDMs of protons and neutrons.

Schiff moment is the dominant nuclear contribution to the EDM of diamagnetic atoms and molecules. The best limit on the EDM of diamagnetic atoms comes from the measurements of the EDM of mercury performed in Seattle \([46]\)

\[ |d^{199}\text{Hg}| < 3.1 \times 10^{-29} e \text{cm.} \]  

Interpretation of the measurements requires atomic and nuclear calculations. Atomic calculations link the EDM of the atom to its nuclear Schiff moment. Nuclear calculations relate Schiff moment to the parameters of the \( T, P \)-odd nuclear interactions. Summary of atomic \([56, 58]\) and nuclear \([59, 60]\) calculations for diamagnetic atoms of experimental interest is presented in Table \(I\). To compare the EDM of different atoms we present only the results of our nuclear calculations which all were performed by the same method. For Hg and Ra there are several recent nuclear many-body calculations available (see references in the most recent calculation \([61]\)) and new calculations are in progress.

The dimensionless constant \( \eta \) characterizes the strength of the \( P, T \)-odd nucleon-nucleon interaction which is to be determined from the EDM measurements. Using \((15)\) and the data from the Table one can get

\[ S^{199}\text{Hg} = (-1.8 \pm 4.6 \pm 2.7) \times 10^{-13} \text{e cm} \]  

and for the \( T, P \)-odd neutron-proton interaction

\[ \eta_{np} = (1 \pm 3 \pm 2) \times 10^{-5}. \]  

a. Nuclear enhancement. It was pointed out in Ref. \([60]\) that Schiff moment of nuclei with octupole deformation can be strongly enhanced. This can be explained in a very simple way. Nuclear deformation creates an intrinsic Schiff moment in the nuclear reference frame

\[ S_{\text{intr}} \approx \epsilon Z R_N^3 \frac{9\beta_2\beta_3}{2\pi \sqrt{35}}, \]  

where
TABLE I: EDMs of diamagnetic atoms of experimental interest.

| Z  | Atom | $Z/(\epsilon\text{ fm}^3)$ | $\eta\epsilon\text{ cm}$ | $\times10^{-17}\epsilon\text{ cm}$ | $\times10^{-25}$ | Experiment |
|----|------|-------------------------|-------------------------|-------------------------------|----------------|------------|
| 2  | $^4\text{He}$ | $8 \times 10^{-17}$ | 5 | $\times10^{-4}$ | Seattle [63], Ann Arbor [64], Princeton [65] |
| 54 | $^{128}\text{Xe}$ | 0.38 | 0.7 | | |
| 70 | $^{171}\text{Yb}$ | -1.9 | 3 | | |
| 80 | $^{199}\text{Hg}$ | -2.8 | 4 | | |
| 86 | $^{223}\text{Ra}$ | 3.3 | 3300 | TRIUMF [68] |
| 88 | $^{223}\text{Ra}$ | -8.2 | 2500 | Argonne [69], KVI [70] |
| 88 | $^{223}\text{Ra}$ | -8.2 | 2500 | |

where $R_N$ is nuclear radius, $\beta_2 \approx 0.2$ is the parameter of quadrupole deformation, and $\beta_3 \approx 0.1$ is the parameter of octupole deformation. The intrinsic Schiff moment ([18]) does not violate $T$ or $P$ invariance and, if no $T, P$-odd interaction present, it averages to zero in the laboratory reference frame due to nuclear rotation. However, when $T, P$-odd interaction is included, it can mix close rotational states of opposite parity. Small energy interval between these states leads to strong enhancement of the nuclear Schiff moment in the laboratory reference frame

$$S_{\text{lab}} \sim \frac{\langle H_{PT} \rangle}{E_+ - E_-} S_{\text{intr}} \sim$$

$$0.05e\beta_2^2 Z A^{2/3} \eta r_0^3 \frac{E_+ - E_-}{eV} \sim 700 \times 10^{-8} \eta e\text{ fm}^3,$$

where $r_0 = 1.2$ fm is the inter-nucleon distance $|E_+ - E_-| \sim 50$ keV. The estimate ([19]) is about 500 times larger than the Schiff moment of a spherical nucleus like Hg.

It was pointed out in Ref. [62] that octupole deformation doesn’t need to be static. Soft octupole vibrations lead to similar enhancement. Large values of the Schiff moment for Ra and Rn (see Table II) are due to nuclear octupole deformation.

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