Schiff moment of the Mercury nucleus and the proton dipole moment

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We calculated the contribution of internal nucleon electric dipole moments to the Schiff moment of $^{199}$Hg. The contribution of the proton electric dipole moment was obtained via core polarization effects that were treated in the framework of random phase approximation with effective residual forces. We derived a new upper bound $|d_p| < 5.4 \times 10^{-24}$ cm of the proton electric dipole moment.

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I. INTRODUCTION

The interest to electric dipole moments (EDM) of elementary particles and more complex systems like nuclei and atoms exists since 1950, when it was first suggested that there was no experimental evidence for symmetry of nuclear forces under parity transformation [1]. The interest was renewed after 1964 when it was discovered that the invariance under CP transformation, which combines charge conjugation with parity, is violated in $K$-meson decays. This provided a new incentive for EDM searches. Since the combined CPT transformation is expected to leave a system invariant, breakdown of CP invariance should be accompanied by T violation. Thus, there is a reason to expect that P and T violating EDMs should exist at some level.

The experimental upper limit on the neutron EDM is [2]

$$d_n < 0.63 \times 10^{-25} \text{ cm.}$$

The measured value for the proton EDM is [2]

$$d_p = (-4 \pm 6) \times 10^{-23} \text{ cm,}$$

and is compatible with zero. This corresponds to an upper limit which is three order of magnitude weaker than the one for the neutron.

The best upper limit on EDM ever obtained was in an atomic experiment with $^{199}$Hg [3]. The result for the dipole moment of this atom is

$$d(^{199}\text{Hg}) < 2.1 \times 10^{-28} \text{ cm}. \quad (3)$$

Unfortunately, the implications of this result are somewhat less impressive, due to the electrostatic screening of the nuclear EDM in this essentially Coulomb system. The point is that in a stationary state of such a system, the total electric field acting on each particle must vanish. Thus, an internal rearrangement of the system’s constituents gives rise to an internal field $E_{\text{int}}$ that exactly cancels $E_{\text{ext}}$ at each charged particle; the external field is effectively switched off, and an EDM feels nothing [1,4,5].

Still, some P and T odd component of the electrostatic potential survives due to final nuclear size. It is created by the next moment in the nuclear electric dipole density distribution. This is the Schiff moment defined as [6]

$$S = \frac{1}{10} \sum_q e_q \left( r_q^2 + \frac{5}{3} (r_q^2)_{\text{ch}} \right). \quad (4)$$

The Schiff moment generates a P and T odd electrostatic potential in the form

$$\phi(\mathbf{r}) = 4\pi S \cdot \nabla \delta(\mathbf{r}). \quad (5)$$

Interaction of atomic electrons with the potential given by Eq. (4) produces an atomic dipole moment

$$d_{\text{atom}} = \sum_n \langle 0 | - e \sum_i^Z \phi(\mathbf{r}_i) | n \rangle | n | - e \sum_i^Z z_i | 0 \rangle \frac{E_n - E_0}{E_n - E_0} + \text{H.c.} \quad (6)$$

Because of the contact origin of the potential, only the electrons in $s$ and $p$ atomic orbitals contribute to the dipole moment given by Eq. (6).

The Eq. (4) is valid for any system of point-like charges $e_q$. Let us split the sum in Eq. (4) into the sum over coordinates of nucleons and the sum over coordinates of charges inside the nucleons:

$$S = \frac{1}{10} \sum_N \sum_i e_i \left( (\mathbf{r}_N + \mathbf{p}_i)^2 - \frac{5}{3} (r_i^2)_{\text{ch}} \right) (\mathbf{r}_N + \mathbf{p}_i). \quad (7)$$

Here $\mathbf{r}_N$ is a nucleon position and $\mathbf{p}_i$ is the position of the $i$th charge inside the nucleon. Combining the terms of the zeroth and first order in $\mathbf{p}$ and using $\sum_i e_i = e_N$, $\sum_i e_i \mathbf{p}_i = \mathbf{d}_N$, we obtain an expression for the Schiff moment as a sum of two terms. The first of them is similar to [14]

$$S_1 = \frac{1}{10} \sum_N^A e_N \left( r_N^2 \mathbf{r}_N - \frac{5}{3} (r_N^2)_{\text{ch}} \mathbf{r}_N \right), \quad (8)$$

where $e_N$ is equal to $|e|$ for a proton and zero for a neutron. The mean value of this operator is nonzero only in the presence of the parity- and time-invariance violating nucleon-nucleon interaction.

The second term in the operator (7) is related to the

$$S_2 = \frac{1}{10} \sum_N^A e_N \left( \frac{5}{3} (r_N^2)_{\text{ch}} - \mathbf{r}_N^2 \right) \mathbf{r}_N.$$
The effects of the core polarization for a single particle operator can be treated by introducing a renormalized operator $\tilde{S}$ satisfying the equation
\[ \tilde{S}_{\nu\nu} = S_{\nu\nu} + \sum_{\mu\mu'} \tilde{S}_{\mu\mu'} \epsilon_{\mu} - \epsilon_{\mu'} + \omega \langle \nu'\nu | F | \mu\mu \rangle, \tag{11} \]
where $S$ is the bare Schiff moment operator given by $\mu$, $S$ or $\tilde{S}$. $n_{\mu}$ and $\epsilon_{\mu}$ are single particle occupation numbers and energies. For static moments the external frequency $\omega \to 0$. The value of the Schiff moment is given by the diagonal matrix element of the $z$-component of the renormalized operator $\tilde{S}$ between mean field states of the last unpaired nucleon with a maximal angular momentum projection.

\[ S = \langle \mu j m = j | \tilde{S} | \mu j m = j \rangle. \tag{12} \]

For the residual interaction $F$ we use the phenomenological Landau-Migdal interaction that has the form
\[ F = C \chi_s(\sigma_1 \cdot \sigma_2) + g_s(\sigma_1 \cdot \sigma_2)(\tau_1 \cdot \tau_2) \delta(r_1 - r_2), \tag{13} \]
where $C = 300$ MeV fm$^3$. The values of the empirical interaction constants $g_s$ and $g'_s$ are crucial for our calculations. The proton contribution is proportional to the proton - neutron interaction $g_s - g'_s$. The constant $g'_s$ is determined from magnetic properties of nuclei and positions of Gamow-Teller resonances. Its adopted value varies between $g'_s = 0.9$–1 depending on details of the mean field potential used $[14, 15]$. The constant $g_s$ is not so well defined. The magnetic moments and M1 transitions are to large extent isovector and they do not fix $g_s$. An attempt to fix it from the structure of high spin states in $^{208}$Pb has been done in $[16]$. They found that $g_s = 0.25$ had to be used in order to reproduce the excitation energies of the M12 and M14 states. Another value $g_s = 0.19$ was quoted in the review paper $[17]$.

The Schiff moment operator can be presented in coordinate space in the form
\[ S_{1m} = \sum_{i=1}^{2} S^{i}(r) T_{1m}^{(i)}, \tag{14} \]
where we have introduced the set of linear independent tensor operators
\[ T_{JM}^{(1)} = \sigma \cdot Y_{JM}^{-1}(n), T_{JM}^{(2)} = \sigma \cdot Y_{JM}^{+1}(n), \tag{15} \]
where $Y_{JM}^{J}(n)$ is the vector spherical harmonic. For $J = 1$ we have $T_{1m}^{(1)} \sim \sigma_m$, and $T_{1m}^{(2)} \sim n_m (n \cdot \sigma) - \frac{1}{3} \sigma_m$. For a spherical nucleus we can separate the angular variables and solve the obtained equations in coordinate space. The equations are
\[ S^{ai}(r) = S_{0i}^{ai}(r) + \int_{0}^{\infty} A^{ai bj}(r, r') S_{b}^{bj}(r') \, dr', \tag{16} \]
where $a=p, n$ and $S_0^{ai}(r)$ is the radial part of the Schiff moment operator $\pi$ multiplied by $r$. The kernel of the integral equation $A^{ai bj}(r, r')$ was calculated by means of the Green functions of the radial Schrödinger equation.

$$
A^{ai bj}(r, r') = \frac{C g^{ab}}{3} \sum_{s,j} n^b_\kappa (ij||T_1^{(i)}||\kappa) (ij||T_1^{(j)}||\kappa) r R^b_\kappa (r)
$$

$$
\times r' R^a_\kappa (r') \left( G^{b}_{ji}(r, r'|\epsilon_\kappa + \omega) + G^{b}_{ji}(r, r'|\epsilon_\kappa - \omega) \right), \quad (17)
$$

where $g^{pp} = g^{nn} = g_s + g'_s$, $g^{pn} = g^{np} = g_s - g'_s$, $R^b_\kappa (r)$ are the radial wave functions, and $n^b_\kappa$ are the occupation numbers.

The solutions of Eq. (14) for $S^{ai}(r)$ are shown in Fig. 1 and 2. Figure 1 demonstrates the magnitude of the core polarization effects. Repulsive residual interaction [14] leads to not very significant decrease of the mean value of the Schiff moment. Figure 2 shows the radial dependence of the proton contributions induced by the core polarization. Note 1 order of magnitude difference in the scales in Fig. 1 and 2. The full curve in Fig. 2 is the radial dependence at the first operator $T_{1m}^{(1)}$ and the dashed curve is the radial dependence at the second operator $T_{1m}^{(2)}$. $S^{p1}(r)$ changes sign inside the nucleus, therefore its mean value is smaller than the mean value of $S^{p2}(r)$ which is mostly negative inside the nucleus.

### III. RESULTS

The value of the Schiff moment of $^{199}$Hg can be presented as a sum of proton and neutron contributions

$$
S = s_p d_p + s_n d_n.
$$

In Table I we list the values $s_p$ and $s_n$ calculated for different combinations of $g_s$ and $g'_s$. From Table I one can see that the uncertainties in $s_p$ and $s_n$ due to uncertainties in $g_s$ and $g'_s$ are

$$
s_p = 0.20 \pm 0.02 \text{ fm}^2, \quad s_n = 1.895 \pm 0.035 \text{ fm}^2. \quad (18)
$$

The main contribution to $s_p$ and $s_n$ comes from the second term in Eq. (14). The contribution of the first term is only $0.7 \text{ fm}^2$ in $s_n$ and $0.006 \text{ fm}^2$ in $s_p$.

The constraint for the Schiff moment of Mercury nucleus from the experiment [2] can be obtained using the results of Ref. [10]. They calculated EDM of an atom created by the nuclear Schiff moment. For $^{199}$Hg they found

$$
d = -2.8 \times 10^{-17} S \text{ [e fm}^3].
$$

From Eq. (19) we obtain the following upper bound for the Schiff moment

$$
|S(199 \text{Hg})| < 0.75 \times 10^{-11} \text{ e fm}^3, \quad (19)
$$

From Eq. (19) we can give the following constraints for EDM of nucleons:

$$
|d_p| < 3.8 \times 10^{-24} \text{ cm}, \quad |d_n| < 4.0 \times 10^{-25} \text{ cm}. \quad (20)
$$

The constraint for the neutron EDM is worse than the existing result $d_n < 0.63 \times 10^{-25} \text{ e cm}$ [2], therefore, we shall not discuss it below. For proton EDM the estimate (20) is 1 order of magnitude lower than the existing experiment $d_p = (-4 \pm 6) \times 10^{-23} \text{ e cm}$. In these

| Table I: Values of $s_p$ and $s_n$ for different $g_s$ and $g'_s$. |
|------------------|-------|------|------|
| $s_p$            | $s_n$ | $g_s$| $g'_s$|
| 0.18             | 1.89  | 0.25 | 0.9  |
| 0.19             | 1.86  | 0.25 | 1.0  |
| 0.20             | 1.93  | 0.19 | 0.9  |
| 0.22             | 1.90  | 0.19 | 1.0  |
circumstances the question about a real theoretical accuracy of our approach becomes important. It is clear that the value \( \pm 0.02 \) cited in Eq.\( (18) \) does not reflects the real accuracy of the theory. It just came from the difference in adopted values of \( g_s \) and \( g'_s \). The theoretical uncertainty appears from two sources. First, it is an uncertainty in the atomic calculations that couple the nuclear Schiff moment and EDM of an atom. We shall not discuss it here referring to the work \([10]\). Second, it is an uncertainty in calculations of the core polarization effects using RPA with effective forces. The latter can be estimated from the following considerations. Using RPA with the effective forces we can fit different nuclear moments in one nucleus. Then, in neighbor nuclei the calculated moments will differ from the data. This difference can be regarded as an uncertainty in the theory. In our experience this difference is of the order of 20\% on the average, reaching sometimes the value of 30\% \([17]\). To be safe, we can adopt a conservative 30\% uncertainty in calculations of \( s_p \). Therefore, instead of \((18)\) we would prefer to write for \( s_p \)

\[
    s_p = 0.2 \pm 0.06 \text{fm}^2. \tag{21}
\]

Since the error in \((21)\) is not statistical, we can not give a probability distribution for \( s_p \). If one takes 0.14 fm\(^2\) as a minimal value of \( s_p \), then it gives the following value for the proton EDM upper bound

\[
    |d_p| < 5.4 \times 10^{-24} \text{e} \cdot \text{cm}. \tag{22}
\]

In summary, we calculated the contributions of the proton and neutron EDM to the Schiff moment of \( ^{199}\text{Hg} \). The effects of core polarization were accounted for in the scope of RPA with the effective residual forces. A new upper bound of the proton EDM has been obtained from the upper bound on the atomic EDM of \( ^{199}\text{Hg} \) atom.

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