Electric dipole moments (EDM) of ionic atoms

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(Received 8 August 2009; published 17 March 2010)

Recent investigations show that the second-order perturbation calculations of electric dipole moments (EDM) from the finite nuclear size as well as the relativistic effects are all canceled out by the third-order perturbation effects and that this is due to electron screening. To derive the nucleon EDM from the nucleus, we propose to measure the EDM of an ionic system. In this case, it is shown that the nucleon EDM can survive by the reduction factor of $1/Z$ for the ionic system with one electron stripped off.

DOI: 10.1103/PhysRevC.81.038501 PACS number(s): 13.40.Em, 11.30.Er, 14.20.Dh, 21.10.Ky

I. Introduction. It is well known that the electric dipole moments (EDM) of the point nucleus can be completely canceled out because of Schiff's theorem [1,2]. In addition, the EDM of the nucleus with the finite size effects can be also canceled out by electron screening [3,4]. In electron screening, the second-order perturbation calculation is canceled out by the third-order perturbation estimation because of the difference in perturbative interactions between the nucleus and the electrons. That is, like in perturbation theory, the EDM interaction is always the first order in the EDM coupling constant, and in third-order perturbation calculations electron screening can become as large as the second-order effects of the nucleon EDM; therefore they can cancel each other out. This suggests that there is no way to measure any nucleon EDM in the neutral atomic systems.

However, there may well be some claim that nuclear EDM can be extracted from Schiff moments [5,6] using theoretical EDM calculations [7]. As we explain later, the physics of the Schiff moments originates from the EDM interactions between nucleons and atomic electrons, and the EDM energy can be obtained from the intermediate atomic excitation. However, the nucleon EDM from the Schiff moments vanishes when the nuclear state is in the s state, and if it is in the p state, the nuclear EDM d_A is suppressed as $d_A \leqslant 10^{-6} d_n$. Therefore, it is practically impossible to extract any nuclear EDM from Schiff moments.

Here, we first show that the nucleon EDM arising from any kind of nuclear EDM interactions is completely canceled out. In fact, the nuclear operator

$$\sum_i^Z e\boldsymbol{R}_i \cdot \boldsymbol{E}_{\rm ext} \tag{1.1}$$

can be canceled out completely by

$$\sum_n \langle \Psi_N \psi_0 | \sum_{i,j} \frac{e^2(\boldsymbol{r}_j \cdot \boldsymbol{R}_i)}{r_j^3} |\Psi_0 \psi_n\rangle \frac{1}{E_0 - E_n} \times \langle \Psi_0 \psi_n | \sum_i e\boldsymbol{r}_i \cdot \boldsymbol{E}_{\rm ext} |\Psi_0 \psi_0\rangle + \text{h.c.} = -\sum_i^Z e\boldsymbol{R}_i \cdot \boldsymbol{E}_{\rm ext}, \tag{1.2}$$

where Ψ_0 (Ψ_N) denote the nuclear ground (excited) states and ψ_0 (ψ_n) denote the atomic ground (excited) states, respectively, and hereafter, we denote $|\Psi_N \psi_n\rangle \equiv |N, n\rangle$. This is similar to the Schiff screening in which the nucleon EDM operator [2]

$$\sum_i^A \boldsymbol{d}_N^i \cdot \boldsymbol{E}_{\rm ext} \tag{1.3}$$

can be canceled out completely by

$$\sum_n \langle 0, 0| \sum_{i,j} \boldsymbol{d}_i^N \cdot \nabla_j \frac{e}{r_j} |0, n\rangle \frac{1}{E_0 - E_n} \times \langle 0, n| \sum_i e\boldsymbol{r}_i \cdot \boldsymbol{E}_{\rm ext} |0, 0\rangle + \text{h.c.} = -\sum_i^A \boldsymbol{d}_i^N \cdot \boldsymbol{E}_{\rm ext}. \tag{1.4}$$

This means that any nuclear operators that couple to the external electric field $\boldsymbol{E}_{\rm ext}$ should be canceled out by electron screening, and therefore there is no chance to observe the nuclear EDM in the neutral atomic system.

To observe nuclear EDM, we propose measuring EDM in ionic systems in which one electron is stripped off. In this case, the nucleon EDM with finite size effects can be measured with a reduction factor of $1/Z$. Still, there is a good chance that nuclear EDM can be measured from the atomic system. The measurement of nuclear EDM in ionic systems is important, and the experimental proposal to measure EDM in ionic systems in storage rings may be interesting and promising [8]. Also, the experimental efforts to observe nuclear EDM in ionic systems must be related to the control of the ions in terms of the ion trap technique [9], and it should be a doable task.

This article is organized as follows. In Sec. II, we briefly discuss how the nucleon EDM in a neutral atomic system is shielded by electrons. In Sec. III, we discuss Schiff moments, and in Sec. IV, we evaluate the EDM of ionic systems in which one electron is stripped off.

II. Complete electron screening in a neutral atomic system. When experimental measurements of the EDM in neutral atomic systems are carried out, we should extract the nucleon EDM from the observed atomic EDM in order to compare it with the neutron EDM measurement. Theoretically, it seems to be quite possible that the nucleon EDM of a neutral atomic system is completely shielded by electrons in atoms and,

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therefore, any neutral atomic EDM cannot be observed. Later in this article, we see this in more detail. First, we discuss how the nucleon EDM of a neutral atomic system can be shielded by electrons. Before going to the discussion of electron shielding, we briefly describe the finite size effects of the atomic EDM; the detailed calculation can be found in Ref. [10].

A. Hamiltonian of atomic systems. We first write the Hamiltonian of the total atomic and nuclear systems. The unperturbed Hamiltonian H_0 of the neutral atomic system can be written

$$H_0 = \sum_{i=1}^{Z}\left[\frac{\boldsymbol{p}_i{}^2}{2m} - \sum_{j=1}^{Z}\frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{R}_j|}\right] + \frac{1}{2}\sum_{i\neq j}^{Z}\frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|} + \sum_{i=1}^{A}\frac{\boldsymbol{P}_i^2}{2M} + \frac{1}{2}\sum_{i\neq j}^{A}V_{NN}(\boldsymbol{R}_i, \boldsymbol{R}_j) + \frac{1}{2}\sum_{i\neq j}^{Z}\frac{e^2}{|\boldsymbol{R}_i - \boldsymbol{R}_j|}, \tag{2.1}$$

where $\boldsymbol{r}_i$ and $\boldsymbol{p}_i$ denote the coordinate and the momentum of the electron, respectively, while $\boldsymbol{R}_i$ and $\boldsymbol{P}_i$ denote the nuclear variable and the momentum, respectively. The perturbed Hamiltonian coming from the nucleon EDM is written as

$$H_{\rm EDM} = -\sum_{i=1}^{Z}\sum_{j=1}^{A}\frac{e\boldsymbol{d}_N^j\cdot(\boldsymbol{r}_i - \boldsymbol{R}_j)}{|\boldsymbol{r}_i - \boldsymbol{R}_j|^3} - \sum_{i=1}^{A}\sum_{j\neq i}^{Z}\frac{e\boldsymbol{d}_N^i\cdot(\boldsymbol{R}_i - \boldsymbol{R}_j)}{|\boldsymbol{R}_i - \boldsymbol{R}_j|^3} - \sum_{i=1}^{A}\boldsymbol{d}_N^i\cdot\boldsymbol{E}_{\rm ext} + e\sum_{i=1}^{Z}(\boldsymbol{r}_i - \boldsymbol{R}_i)\cdot\boldsymbol{E}_{\rm ext}, \tag{2.2}$$

where the summation over Z in the nucleus means that it should be taken over protons. The EDM of the nucleon can be expressed in terms of the nucleon isospin as

$$\boldsymbol{d}_N^i = \tfrac{1}{2}\left[\left(1+\tau_i^z\right)d_p\boldsymbol{\sigma}^i + \left(1-\tau_i^z\right)d_n\boldsymbol{\sigma}^i\right]. \tag{2.3}$$

B. Nuclear EDM from nuclear excitation. The second-order EDM energy due to the intermediate nuclear excitations, keeping the atomic state in the ground state, can be written as [10–12]

$$\Delta E_{\rm fs}^{(2)} = -\sum_N\frac{e^2}{E_N - E_0}\langle 0,0|\sum_{i=1}^{A}\tau_i^z\boldsymbol{R}_i\cdot\boldsymbol{E}_{\rm ext}|N,0\rangle \times\langle N,0|\sum_{i\neq j}^{A}\frac{1}{2}\boldsymbol{d}_N^i\cdot\frac{\left(1+\tau_j^z\right)(\boldsymbol{R}_i - \boldsymbol{R}_j)}{|\boldsymbol{R}_i - \boldsymbol{R}_j|^3}|0,0\rangle + \text{h.c.}, \tag{2.4}$$

where E_0 and E_N denote the ground-state energy and the excitation energy of the nuclear states, respectively.

C. Third-order EDM energy. In the evaluation of the third-order perturbation EDM energy, we should consider the Hamiltonian of the finite size effects [3], which is written as

$$H_0^{(\rm fs)} = -\sum_{i,j=1}^{Z}\frac{e^2(\boldsymbol{r}_i\cdot\boldsymbol{R}_j)}{r_i^3}. \tag{2.5}$$

In this case, we can calculate the third-order perturbation energy of the EDM Hamiltonian where the two intermediate states $|\Psi_N\rangle$ and $|\psi_n\rangle$ are considered and obtain

$$\Delta E_{\rm fs}^{(3)} = -\sum_{N,n}\frac{2e^2}{(E_N - E_0)(E_n - E_0)}\langle 0,0|\sum_{i=1}^{Z}\boldsymbol{r}_i\cdot\boldsymbol{E}_{\rm ext}|0,n\rangle \times\langle 0,n|\sum_{i=1}^{Z}\sum_{j=1}^{Z}\frac{e^2(\boldsymbol{r}_i\cdot\boldsymbol{R}_j)}{r_i^3}|N,0\rangle \times\langle N,0|\sum_{i\neq j}^{A}\frac{1}{2}\boldsymbol{d}_N^i\cdot\frac{\left(1+\tau_j^z\right)(\boldsymbol{R}_i - \boldsymbol{R}_j)}{|\boldsymbol{R}_i - \boldsymbol{R}_j|^3}|0,0\rangle + \text{h.c.} \tag{2.6}$$

This can be calculated to be

$$\Delta E_{\rm fs}^{(3)} = \sum_N\frac{e^2}{E_N - E_0}\langle 0,0|\sum_{i=1}^{A}\tau_i^z\boldsymbol{R}_i\cdot\boldsymbol{E}_{\rm ext}|N,0\rangle \times\langle N,0|\sum_{i\neq j}^{A}\frac{1}{2}\boldsymbol{d}_N^i\cdot\frac{\left(1+\tau_j^z\right)(\boldsymbol{R}_i - \boldsymbol{R}_j)}{|\boldsymbol{R}_i - \boldsymbol{R}_j|^3}|0,0\rangle + \text{h.c.}, \tag{2.7}$$

which is just the same as the second-order perturbation energy of the EDM Hamiltonian of Eq. (2.4) with the opposite sign. Therefore, the second-order finite size effect that arises from the nuclear excitation is completely canceled out by the third-order effects.

Here, we note that the relativistic effects of nucleon EDM [13] free from Schiff shielding are also canceled out completely by electron screening as discussed in Ref. [4].

D. T-violating nucleon-nucleon interaction. The phenomenological nucleon-nucleon interactions [14,15] that violate the T invariance, such as

$$V_\pi^{\rm PT}(r_{12}) = \frac{1}{2M}\frac{g_\pi\bar{g}_\pi}{4\pi}(\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)(\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2)\nabla_1\frac{e^{-m_\pi r_{12}}}{r_{12}}, \tag{2.8}$$

can generate the second-order EDM energy as

$$\Delta E_{\rm PT}^{(2)} = -\sum_N\frac{e^2}{E_N - E_0}\langle 0,0|\sum_{i=1}^{Z}e\boldsymbol{R}_i\cdot\boldsymbol{E}_{\rm ext}|N,0\rangle \times\langle N,0|\sum_{i>j}^{A}V_\pi^{\rm PT}(r_{ij})|0,0\rangle + \text{h.c.} \tag{2.9}$$

However, this EDM energy can be canceled out completely by the third-order perturbation theory as shown in Eq. (1.1) in the Introduction.

III. Schiff moments. Schiff moments come from the EDM interaction between nucleons and electrons, and the interaction can be written as

$$H_{\rm EDM}^{eN} = -\sum_{i=1}^{Z}\sum_{j=1}^{A}\frac{e\boldsymbol{d}_N^j\cdot(\boldsymbol{r}_i - \boldsymbol{R}_j)}{|\boldsymbol{r}_i - \boldsymbol{R}_j|^3}. \tag{3.1}$$

This interaction can be rewritten as

$$H_{\rm EDM}^{eN} = \sum_{i=1}^{Z}e\langle\boldsymbol{d}_N\rangle\cdot\nabla_i\int\frac{\rho(\boldsymbol{R})}{|\boldsymbol{r}_i - \boldsymbol{R}|}d^3R, \tag{3.2}$$

which is just the interaction used in the Schiff moment calculations [5–7].

A. Finite size effect with atomic excitations. Now, we can carry out the microscopic calculation of the Schiff moments and consider the second-order perturbation energy with the finite size effects of the nucleus, and the EDM energy becomes

$$\Delta E_{\rm SM}^{(2)} = -\sum_n \frac{2eE_{\rm ext}}{E_n - E_0}\langle 0|H_{\rm EDM}^{eN}|n\rangle\langle n|\sum_{i=1}^{Z} z_i|0\rangle, \quad (3.3)$$

where the nuclear state is kept in the ground state. Further, $H_{\rm EDM}^{eN}$ can be rewritten as

$$H_{\rm EDM}^{eN} = \sum_{i=1}^{Z}\left[\boldsymbol{r}_i\cdot\sum_{j=1}^{A}\boldsymbol{d}_N^j S_{ji}R_j^2\right]\frac{e}{r_i^5}, \quad (3.4)$$

with S_{ji} defined as $S_{ji} = \frac{5}{2} - \frac{15}{2}\cos^2\theta_{ji}$. Now, we can calculate the expectation value of the $\boldsymbol{d}_N^j S_{ji}$ using a simple shell-model wave function, and as is well known, the spin expectation value of the shell-model calculation is normally larger than the one obtained by the realistic calculations.

B. Nuclear s and p states. Now we consider the s state case

$$\Psi_0 = |s_{\frac{1}{2}}\rangle \otimes |0\rangle, \quad (3.5)$$

where the state $|0\rangle$ denotes the core state of the nucleus with a spin and parity of 0^+. In this case, we find

$$\left\langle \sum_j \boldsymbol{d}_N^j S_{ji}\right\rangle = 0. \quad (3.6)$$

Therefore, there is no contribution from the s-state nucleus to the EDM of Schiff moments.

Next, we consider the p-state case,

$$\Psi_0 = |p_{\frac{1}{2}}\rangle \otimes |0\rangle, \quad (3.7)$$

and we can evaluate the expectation value as

$$\left\langle \sum_j \boldsymbol{d}_N^j S_{ji}\right\rangle = -\frac{4}{15}d_N. \quad (3.8)$$

In this case, we can make a rough estimation of the nuclear EDM d_A as

$$d_A \simeq \frac{2ea_0}{\Delta E}\times\frac{4d_N R_0^2}{15}\times\frac{e}{a_0^5}Z_{\rm eff}a_0 \simeq 2.4\times 10^{-6}d_N, \quad (3.9)$$

where we employed $R_0 \simeq 7$ fm and $a_0 \simeq 10^{-8}$ cm. Also, the value of ΔE is taken to be $\Delta E \simeq \Delta E_{\rm HF} \simeq 1$ eV, where $\Delta E_{\rm HF}$ denotes the prediction of the Hartree-Fock calculation. Further, the effective number $Z_{\rm eff}$ of electrons that contribute to the $E1$ excitation is taken to be $Z_{\rm eff} \simeq 30$. The estimation is optimistic for medium heavy atoms and nuclei of Z around 50, and therefore this gives the largest possible value of the nuclear EDM of the Schiff moments. However, despite the overestimation, we can see that the suppression factor is indeed severely small.

IV. Nucleon EDM in ionic systems. As we saw, it is almost impossible to extract the nucleon EDM from neutral atomic systems due to electron screening. However, we see below that the nucleon EDM with finite size effects can be extracted from ionic systems in which one electron is stripped off. In this case, we can prove that the nucleon EDM of ionic systems becomes $1/Z$ times the calculated nucleon EDM of the finite size effects. This means that electron screening occurs for the same numbers of electrons and protons and, therefore, if one electron is absent, then the electron screening is incomplete.

A. EDM in ionic systems. To see this effect explicitly, we calculate the third-order EDM energy with one electron stripped off as

$$\Delta E_{\rm fs}^{(3)} = -\sum_{N,n}\frac{2e^2}{(E_N - E_0)(E_n - E_0)}\langle 0,0|\sum_{i=1}^{Z-1}\boldsymbol{r}_i\cdot\boldsymbol{E}_{\rm ext}|0,n\rangle \times\langle 0,n|\sum_{i'=1}^{Z-1}\sum_{j=1}^{Z}\frac{e^2(\boldsymbol{r}_{i'}\cdot\boldsymbol{R}_j)}{r_{i'}^3}|N,0\rangle\langle N,0|\sum_{k\neq\ell}^{A}\frac{1}{2}\boldsymbol{d}_N^k \cdot\frac{(1+\tau_\ell^z)(\boldsymbol{R}_k - \boldsymbol{R}_\ell)}{|\boldsymbol{R}_k - \boldsymbol{R}_\ell|^3}|0,0\rangle + \text{h.c.} \quad (4.1)$$

Here, we first evaluate the electron part:

$$\sum_n \frac{1}{E_n - E_0}\langle 0,0|\sum_{i=1}^{Z-1}\boldsymbol{r}_i\cdot\boldsymbol{E}_{\rm ext}|0,n\rangle \times\langle 0,n|\sum_{i'=1}^{Z-1}\sum_{j=1}^{Z}\frac{e^2(\boldsymbol{r}_{i'}\cdot\boldsymbol{R}_j)}{r_{i'}^3}|N,0\rangle = \frac{Z-1}{Z}\langle 0|\sum_{j=1}^{Z}\boldsymbol{R}_j\cdot\boldsymbol{E}_{\rm ext}|N\rangle.$$

Therefore, we can express the third-order perturbation energy in terms of the second-order EDM energy as

$$\Delta E_{\rm fs}^{(3)} = -\frac{Z-1}{Z}\Delta E_{\rm fs}^{(2)}. \quad (4.2)$$

Thus, the cancellation is not complete, and after the electron screening, the nuclear EDM survives. However, it is reduced by a factor of $1/Z$,

$$\Delta E_{\rm fs}^{(2)} + \Delta E_{\rm fs}^{(3)} = \frac{1}{Z}\Delta E_{\rm fs}^{(2)}. \quad (4.3)$$

B. EDM measurements in storage rings. There is a proposal to measure the EDM of ions in storage rings [8]. This type of experiment should become very important in the future, though we cannot make any useful comments at present since there are no solid observations of EDM of ionic systems. The problem is of course related to the accuracy of the measurements whether the EDM measurement of ions can be better than that the neutron EDM experiment, and at the present stage one cannot claim that the EDM of ions can be measured very accurately. However, we believe that both of the experiments should be done in parallel in view of the importance of the EDM measurements.

C. Ion trap method. There may be a possibility to measure the EDM of ions by making use of the ion trap technique that has been greatly developed in recent years. In this case, however, it may be difficult to put a strong electric field on the ionic system since it is already trapped by the electric fields in the ion trap method. This is in contrast to the magnetic moment measurement where the interaction energy is proportional to the magnetic field [9].

Because there are some important experiments on the hyperfine structure measurement in terms of the ion trap technique, there may be similar experiments possible for the EDM measurements. This will be a difficult task, but it should be done in some way or other in the future.

The author is grateful to Professor K. Asahi, Professor T. Fujita, and Dr. A. Yoshimi for their helpful discussions and comments. This work is supported in part by the Japan Society for the Promotion of Science.

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