Nuclear electric dipole moment with relativistic effects in Xe and Hg atoms

Sachiko Oshima,[1] Takehisa Fujita,[2,*] and Tomoko Asaga[1,2,†]
[1]*Department of Physics, Faculty of Science, Tokyo Institute of Technology, Tokyo, Japan*
[2]*Department of Physics, Faculty of Science and Technology, Nihon University, Tokyo, Japan*
(Received 4 August 2006; revised manuscript received 5 December 2006; published 29 March 2007)

The atomic electric dipole moment (EDM) is evaluated by considering the relativistic effects as well as nuclear finite size effects in Xe and Hg atomic systems. Due to Schiff's theorem, the first order perturbation energy of EDM is canceled out by the second order perturbation energy for the point nucleus. The nuclear finite size effects arising from the intermediate atomic excitations may be finite for deformed nucleus but it is extremely small. The finite size contribution of the intermediate nuclear excitations in the second order perturbation energy is completely canceled by the third order perturbation energy. As the results, the finite contribution to the atomic EDM comes from the first order perturbation energy of relativistic effects, and it amounts to around 0.3 and 0.4 percents of the neutron EDM d_n for Xe and Hg, respectively, though the calculations are carried out with a simplified single-particle nuclear model. From this relation in Hg atomic system, we can extract the neutron EDM which is found to be just comparable with the direct neutron EDM measurement.

DOI: 10.1103/PhysRevC.75.035501 PACS number(s): 21.10.Ky, 13.40.Em, 11.30.Er, 14.20.Dh

I. INTRODUCTION

The violation of the T-invariance can be measured by the electric dipole moments (EDM) of particles, nuclei and atoms in their ground states. Until now, the upper limit of the neutron EDM d_n is around [1]

$$d_n \simeq (0.19 \pm 0.54) \times 10^{-25}\, \mathrm{e} \cdot \mathrm{c.m.} \tag{1.1}$$

There have been many experimental efforts to measure the EDM of the atomic systems. The good examples are found for the EDM of ^{129}Xe [2,3] and ^{199}Hg [4,5]. In this case, however, one has to be careful for extracting the EDM of electrons or nucleons from the measurement of the atomic EDM since there is Schiff's theorem [6]. This theorem states that the EDM of the atom is canceled out due to the symmetry restoration mechanism as long as the constituents are interacting through the electromagnetic interactions with the nonrelativistic kinematics.

In order to obtain the EDM of atomic system, one has to find the relativistic effects in the EDM operators [7] since they are free from Schiff's theorem. In heavy atoms, electrons become relativistic, and therefore, the EDM of the atomic systems becomes larger than the electron EDM d_e due to a large enhancement factor [8–15]. In fact, the EDM of Cs atom has an enhancement as

$$d_{Cs} \simeq 91\, d_e \tag{1.2}$$

which is mainly because of the small energy difference between the ground state and the excited state with the opposite parity.

However, it is also believed that the electron EDM might well be rather small compared to the neutron EDM. This is based on the EDM operator which is derived from the supersymmetry model calculations [16–22]. The EDM interaction $\mathcal{H}_{\mathrm{edm}}$ is written for ψ_i fermion field with the EDM coupling constant d_i,

$$\mathcal{H}_{\mathrm{edm}} = -\frac{i}{2} d_i \bar{\psi}_i \sigma_{\mu\nu} \gamma_5 \psi_i F^{\mu\nu}, \tag{1.3}$$

where $F^{\mu\nu}$ denotes the electromagnetic field strength. Up to now, there are many efforts to determine the strength of the EDM coupling constant d_i from the supersymmetric model calculations.

At the present stage, however, it is not clear yet how large the electron EDM d_e and neutron EDM d_n should be. But most of the estimations of the EDM suggest that the electron EDM must be much smaller than the neutron EDM [7,23]. This means that it should be better if one can measure the neutron EDM from atomic systems.

Due to the presence of Schiff's theorem, the EDM of nuclear systems should be quite small, and one obtains the nuclear EDM from Schiff moments [6]. According to the definition of the Schiff moment by Khriplovich and Lamoreaux [7], the Schiff moment $\boldsymbol{S}$ is described in terms of the individual nucleon EDM $d_{p,n}$ as

$$\boldsymbol{S} \sim d_{p,n} R_0^2 \boldsymbol{I}, \tag{1.4}$$

where R_0 and $\boldsymbol{I}$ denote the radius and the total spin of the nucleus, respectively. However, the atomic EDM from the Schiff moment is normally very small.

In this paper, we present a new calculation of the nuclear EDM starting from the microscopic interactions in atomic and nuclear Hamiltonian. The EDM interactions are derived both from the nuclear finite size effects and the relativistic effects. In the nuclear finite size effects, there are two different types of the contributions for the second order perturbation energy of the EDM Hamiltonian. The first case is connected with the Schiff moment in which the intermediate atomic excitations are considered. In this case, the EDM energy is very small. In the second type, we consider the intermediate nuclear excitations in the second order perturbation theory while the atomic states are in the ground state. However, it

*Electronic address: fffujita@phys.cst.nihon_u.ac.jp
†Electronic address: asaga@phys.cst.nihon_u.ac.jp

turns out that the EDM contributions from this second order perturbation energy can be completely canceled out by the third order perturbation energy [24] and there is no effect left for the nuclear EDM from the nuclear finite size effects.

On the other hand, there is a finite contribution from the relativistic effects which are free from Schiff's theorem. The relativistic EDM Hamiltonian is usually written as

$$H_{\mathrm{edm}}^{(\mathrm{Rel})} = -d_n \gamma^5 \boldsymbol{\gamma} \cdot \boldsymbol{E} = -d_n \boldsymbol{\Sigma} \cdot \boldsymbol{E} - d_n(\gamma^0 - 1)\boldsymbol{\Sigma} \cdot \boldsymbol{E}, \tag{1.5}$$

where $\boldsymbol{\Sigma}$ is defined as

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix}.$$

The first term in the last equation corresponds to the nonrelativistic EDM operator, and the energy shifts in the presence of these operators will be calculated in Secs. II to V. As stated above, the contributions as the nuclear finite size effects are almost shielded. The second term is the relativistic EDM operator which is free from the Schiff shielding. In the atomic systems with odd numbers of electrons, the relativistic effect on the electron EDM is very large. In this calculation, the enhancement of the atomic EDM comes mainly from the intermediate atomic excited states in the second order perturbation EDM energy since the excitation energy with the opposite parity is quite close to the ground state. However, there is also the first order perturbation energy of the relativistic effect on the atomic EDM though it is of the order of 10% of the electron EDM d_e and therefore it is neglected in the Cs calculation [8].

In nucleus, we should consider the relativistic effects on the nuclear EDM even though the relativistic effects of nucleons are smaller than those of electrons. In particular, the second order perturbation EDM energy of the relativistic effect in the case of nucleus is negligibly small since the interaction is electromagnetic while the intermediate energy is due to the strong interaction, and thus there is no enhancement in nuclear EDM, contrary to the electron case. However, since the nuclear finite size effects are negligibly small, the first order perturbation EDM energy of the relativistic effect becomes important.

In this paper, we show that the first order relativistic effect amounts to around 0.4% of the neutron EDM d_n

$$d_A \simeq 0.004\, d_n \tag{1.6}$$

for the Hg system. As the result, this relativistic effect of the nuclear EDM is most important for the atomic system with even number of electrons in which there is no electron EDM contribution. Employing the above relation we can obtain the neutron EDM extracted from the Hg EDM measurement. Since the observed EDM of Hg atomic system is given as

$$d_{\mathrm{Hg}} \simeq -(1.06 \pm 0.49 \pm 0.40) \times 10^{-28}\, \mathrm{e \cdot c.m.}, \tag{1.7}$$

we find the neutron EDM from the Hg EDM measurement

$$d_n(\mathrm{Hg}) \simeq -(0.25 \pm 0.12 \pm 0.09) \times 10^{-25}\, \mathrm{e \cdot c.m.} \tag{1.8}$$

which should be compared to the direct neutron EDM measurement of Eq. (1.1). This shows that the Hg EDM measurement gives just the same level of constraint on the neutron EDM.

In the present paper, the shell model calculations are carried out with a simplified single particle model and the numerical estimations given here are only reliable up to a factor of two or so. Therefore, it is clear that the more elaborate numerical calculations are definitely needed in future together with the precise measurements of EDM.

This paper is organized in the following way. In the next section, we present a general formalism of the EDM in nuclear and atomic systems and show that the electric dipole operators with nuclear variables can contribute to the nuclear EDM in the second order perturbation theory where the electrons stay in its ground state. In Sec. III, we calculate the finite size effects of nuclear EDM which arises from the intermediate atomic excitation while the nucleus stays in the ground state. In Sec. IV, we evaluate the third order perturbation energy of the nuclear EDM and show that the third order EDM cancels out completely the second order nuclear EDM. Section V treats the relativistic effects of the nuclear EDM and we evaluate the first order perturbation energy of the relativistic nuclear EDM and find that it gives an appreciably large contribution to atomic EDM. Section VI summarizes what we clarify in this work.

II. EDM OF ATOMIC SYSTEMS

Now, we discuss the EDM arising from nuclear finite size effects and here we treat the Xe and Hg atomic systems since there are some measurements of the EDM in these atomic systems [2–5] and also there is a proposal to measure the EDM of the atomic and nuclear system [25].

The unperturbed Hamiltonian H_0 of the Xe system can be written

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

where $\boldsymbol{r}_i$, $\boldsymbol{p}_i$ denote the coordinate and the momentum of the electron while $\boldsymbol{R}_i$, $\boldsymbol{P}_i$ denote the nuclear variable and momentum, respectively.

On the other hand, the perturbed Hamiltonian coming from the EDM is written as

$$\begin{aligned} H_{\mathrm{edm}} & \\ = & - \sum_{i=1}^{Z} \sum_{j=1}^{Z} \frac{e\boldsymbol{d}_e^i \cdot (\boldsymbol{r}_i - \boldsymbol{R}_j)}{|\boldsymbol{r}_i - \boldsymbol{R}_j|^3} + \sum_{i=1}^{Z} \sum_{j \neq i}^{Z} \frac{e\boldsymbol{d}_e^i \cdot (\boldsymbol{r}_i - \boldsymbol{r}_j)}{|\boldsymbol{r}_i - \boldsymbol{r}_j|^3} \\ & - \sum_{i=1}^{Z} \sum_{j=1}^{A} \frac{e\boldsymbol{d}_N^j \cdot (\boldsymbol{r}_i - \boldsymbol{R}_j)}{|\boldsymbol{r}_i - \boldsymbol{R}_j|^3} - \sum_{i=1}^{A} \sum_{j \neq i}^{Z} \frac{e\boldsymbol{d}_N^i \cdot (\boldsymbol{R}_i - \boldsymbol{R}_j)}{|\boldsymbol{R}_i - \boldsymbol{R}_j|^3} \end{aligned}$$

$$- \sum_{i=1}^{Z} \boldsymbol{d}_e^i \cdot \boldsymbol{E}_{\rm ext} - \sum_{i=1}^{A} \boldsymbol{d}_N^i \cdot \boldsymbol{E}_{\rm ext} + e \sum_{i=1}^{Z} (\boldsymbol{r}_i - \boldsymbol{R}_i) \cdot \boldsymbol{E}_{\rm ext}, \quad (2.2)$$

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

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

A. Finite size of nucleus

Now, we evaluate the finite size effects on the second order EDM energy in heavy nucleus. The unperturbed Hamiltonian of the atomic and nuclear system becomes

$$H_0 = \sum_{i=1}^{Z}\left[\frac{\boldsymbol{p}_i{}^2}{2m} - \frac{Ze^2}{r_i}\right] + \frac{1}{2}\sum_{i\neq j}^{Z} \frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|} + \sum_{i=1}^{A} \frac{\boldsymbol{P}_i^2}{2M} + \frac{1}{2}\sum_{i\neq j}^{A} V_{NN}(|\boldsymbol{R}_i - \boldsymbol{R}_j|) + \frac{1}{2}\sum_{i\neq j}^{Z} \frac{e^2}{|\boldsymbol{R}_i - \boldsymbol{R}_j|}. \quad (2.3)$$

Here, we ignore the finite size effect of the unperturbed Hamiltonian.

Now, the perturbed Hamiltonian $H_{\rm edm}^{(0)}$ from the point charge and the Hamiltonian $H_{\rm edm}^{(fs)}$ with the finite size can be written up to the order of $(R_j/r_i)^2$

$$H_{\rm edm}^{(0)} = -\sum_{i=1}^{Z}\left[eZ\boldsymbol{d}_e^i \cdot \frac{\boldsymbol{r}_i}{r_i^3} + \left(\sum_{j=1}^{A} e\boldsymbol{d}_N^j\right) \cdot \frac{\boldsymbol{r}_i}{r_i^3} - \sum_{j\neq i}^{Z} \frac{e\boldsymbol{d}_e^i \cdot (\boldsymbol{r}_i - \boldsymbol{r}_j)}{|\boldsymbol{r}_i - \boldsymbol{r}_j|^3}\right] - \left(\sum_{i=1}^{Z} \boldsymbol{d}_e^i + \sum_{i=1}^{A} \boldsymbol{d}_N^i\right) \cdot \boldsymbol{E}_{\rm ext} + e\sum_{i=1}^{Z} \boldsymbol{r}_i \cdot \boldsymbol{E}_{\rm ext}, \quad (2.4a)$$

$$H_{\rm edm}^{(fs)} = \sum_{i=1}^{Z}\left[\boldsymbol{d}_e^i \cdot \boldsymbol{r}_i \sum_{j=1}^{Z} S_{ji} R_j^2 + \boldsymbol{r}_i \cdot \sum_{j=1}^{A} \boldsymbol{d}_N^j S_{ji} R_j^2\right] \frac{e}{r_i^5} - \sum_{i=1}^{A}\sum_{j\neq i}^{Z} e\boldsymbol{d}_N^i \cdot \frac{(\boldsymbol{R}_i - \boldsymbol{R}_j)}{|\boldsymbol{R}_i - \boldsymbol{R}_j|^3} - \frac{e}{2}\sum_{i=1}^{A}\left(1+\tau_i^z\right)\boldsymbol{R}_i \cdot \boldsymbol{E}_{\rm ext}, \quad (2.4b)$$

where S_{ji} in Eq. (2.4b) is defined as

$$S_{ji} = \tfrac{5}{2} - \tfrac{15}{2}\cos^2\Theta_{ji}, \quad (2.4c)$$

where Θ_{ji} denotes the angle between the electron coordinate $\boldsymbol{r}_i$ and the nucleon coordinate $\boldsymbol{R}_j$, and can be given as

$$\cos\Theta_{ji} = \sin\theta_j \sin\theta_i \cos(\phi_j - \phi_i) + \cos\theta_j \cos\theta_i.$$

B. Schiff shielding (point nucleus)

When we treat the nucleus as a point particle, the first order and the second order EDM energies cancel out each other, which is due to Schiff's theorem. Here, we show explicitly how the Schiff shielding occurs.

C. First order perturbation energy of EDM Hamiltonian

The first order perturbation energy of the EDM Hamiltonian can be easily evaluated as

$$\Delta E^{(1)} = -\left(\sum_{i=1}^{Z} d_e^i + \sum_{i=1}^{A} d_N^i\right) E_{\rm ext}. \quad (2.5)$$

D. Second order perturbation energy of EDM Hamiltonian

The second order perturbation energy of EDM Hamiltonian can be also calculated in the following way:

$$\Delta E_{PC}^{(2)} = -\sum_n \frac{1}{E_n - E_0} \times \langle\psi_e| \sum_{i=1}^{Z}\left(\left(\boldsymbol{d}_e^i + \frac{1}{Z}\sum_{j=1}^{A} \boldsymbol{d}_N^j\right) \cdot \nabla_i A_0(r_i)\right)|n\rangle \times \langle n|e\sum_{i=1}^{Z} \boldsymbol{r}_i \cdot \boldsymbol{E}_{\rm ext}|\psi_e\rangle + \text{h.c.}, \quad (2.6)$$

where $A_0(r_i) = \frac{Ze}{r_i}$ is introduced and E_0 denotes the energy eigenvalue of the ground state in the atomic system. Here, we should note that the nuclear part is always in the ground state and has no effect.

Now, we make use of the following identity:

$$\nabla_i A_0(\boldsymbol{r}_i) = i\,\boldsymbol{p}_i A_0(\boldsymbol{r}_i) = i[\boldsymbol{p}_i, A_0(\boldsymbol{r}_i)] = -\frac{i}{e}[\boldsymbol{p}_i, H_0], \quad (2.7a)$$

$$\sum_i^Z \nabla_i\left(\sum_j^Z \frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}\right) = 0, \quad (2.7b)$$

$$H_0|\psi_e\rangle = E_0|\psi_e\rangle, \qquad H_0|n\rangle = E_n|n\rangle, \quad (2.7c)$$

where the nucleus is assumed to stay in the ground state. Therefore, we can sum up all the intermediate states in Eq. (2.6) since the energy denominator $E_n - E_0$ cancels out, and thus obtain

$$\Delta E_{PC}^{(2)} = \left(\sum_{i=1}^{Z} d_e^i + \sum_{i=1}^{A} d_N^i\right) E_{\rm ext} \quad (2.8)$$

which is exactly the same as the first order perturbation result with the opposite sign, and thus it cancels out completely the first order perturbation result of the EDM. This is just the Schiff shielding.

III. FINITE SIZE EFFECT (ATOMIC EXCITATION)

Now, we consider the second order perturbation energy with the finite size effects of the nucleus. In order to evaluate the second order EDM energy, we first need to have the atomic and nuclear wave functions. We write the ground state wave functions by

$$|0\rangle \equiv \psi_A(\boldsymbol{R}_1, \cdots, \boldsymbol{R}_A) \otimes \phi_e(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_Z). \tag{3.1}$$

Here, we assume that the atomic state has the ground state with spin zero while the nuclear ground state has one outer neutron with spin $\frac{1}{2}$. This is mainly because we consider the ^{129}Xe and ^{199}Hg atomic systems in this paper.

The second order EDM energy with the finite size effect becomes

$$\Delta E_{fs}^{(2)} = -\sum_n \frac{2eE_{\rm ext}}{E_n - E_0} \langle 0|H_{\rm edm}^{(fs),0}|n\rangle\langle n|\sum_{i=1}^{Z} z_i|0\rangle, \tag{3.2}$$

where E_0 denotes the ground state energy of the whole system while the intermediate states $|n\rangle$ denote the atomic excited states and the nuclear state is kept in the ground state. Further, $H_{\rm edm}^{(fs),0}$ is defined as

$$H_{\rm edm}^{(fs),0} = \sum_{i=1}^{Z}\left[\boldsymbol{d}_e^i \cdot \boldsymbol{r}_i \sum_{j=1}^{Z} S_{ji} R_j^2 + \boldsymbol{r}_i \cdot \sum_{j=1}^{A} \boldsymbol{d}_N^j S_{ji} R_j^2\right] \frac{e}{r_i^5}. \tag{3.3}$$

Equation (3.2) can be evaluated by employing the closure approximation

$$\Delta E_{fs}^{(2)} \simeq -\frac{2e^2E_{\rm ext}}{\langle E_n - E_0\rangle}\langle 0|\sum_{i,k=1}^{Z}\left((\boldsymbol{d}_e^i\cdot\boldsymbol{r}_i)\sum_{j=1}^{Z} S_{ji}R_j^2 + \sum_{j=1}^{A}(\boldsymbol{d}_N^j\cdot\boldsymbol{r}_i)S_{ji}R_j^2\right)\frac{z_k}{r_i^5}|0\rangle. \tag{3.4}$$

This becomes

$$\Delta E_{fs}^{(2)} \simeq -\frac{2e^2ZE_{\rm ext}}{\langle E_n - E_0\rangle}\frac{d_n\langle S_{ji}\cos^2\theta_i\rangle\langle R^2\rangle}{a_0^3}, \tag{3.5}$$

where the first term in Eq. (3.4) vanishes since the spin of the atomic states is assumed to be zero. Here, a_0 denotes the Bohr radius of the atomic system and can be written as $a_0 = \frac{1}{Zme^2}$. Therefore, the nuclear EDM from the atomic excitations becomes

$$\begin{aligned} d_A &\simeq -\frac{2e^2Z}{mZ^2e^4}\frac{d_n\langle S_{ji}\cos^2\theta_i\rangle\langle R^2\rangle}{a_0^3} \\ &\simeq -9.9\times 10^{-10}\langle S_{ji}\cos^2\theta_i\rangle Z^2 A^{\frac{2}{3}} d_n, \end{aligned} \tag{3.6}$$

where we take $\langle E_n - E_0\rangle \simeq m(Ze^2)^2$ and $\langle R^2\rangle \simeq r_0^2 A^{\frac{2}{3}}$ with $r_0 = 1.2$ fm. $\langle S_{ji}\cos^2\theta_i\rangle$ is zero if we evaluate it for spherical nuclei such as ^{129}Xe and ^{199}Hg.

In the evaluation of the Schiff moments, people calculate them by assuming the T- and P-violating nucleon-nucleon interaction which is not connected to the individual EDM values of d_n or d_p. In this case, there may be some chance that the EDM value from the Schiff moments in heavy nucleus can be enhanced due to the nuclear collective motion [26,27].

IV. FINITE SIZE EFFECT (NUCLEAR EXCITATION)

Now, we consider the second order EDM energy due to the intermediate nuclear excitations, keeping the atomic state in the ground state. This process arises from the finite nuclear size effects in the EDM Hamiltonian. The second order EDM energy can be written as

$$\begin{aligned} \Delta E_{fs}^{(2)} = &-\sum_n \frac{e^2}{E_n - E_0}\langle 0|\sum_{i=1}^{A}\tau_i^z\boldsymbol{R}_i\cdot\boldsymbol{E}_{\rm ext}|n\rangle \\ &\times\langle n|\sum_{i\neq j}^{A}\frac{1}{4}\left[\left(1+\tau_i^z\right)d_p\boldsymbol{\sigma}^i + \left(1-\tau_i^z\right)d_n\boldsymbol{\sigma}^i\right] \\ &\times\frac{\left(1+\tau_j^z\right)(\boldsymbol{R}_i - \boldsymbol{R}_j)}{|\boldsymbol{R}_i - \boldsymbol{R}_j|^3}|0\rangle, \end{aligned} \tag{4.1}$$

where E_n denotes the excitation energy of the nuclear states. Here, we made use of the relation $\sum_{i=1}^{A}\boldsymbol{R}_i = 0$ since we set the center mass coordinate to zero.

However, it turns out that the nuclear finite size effects from the nuclear excitation can be completely canceled out by the third order perturbation energy of the EDM Hamiltonian. We will discuss it in the next section.

V. THIRD ORDER EDM ENERGY

In the evaluation of the third order perturbation EDM energy, we should consider the Hamiltonian of the finite size effects [24] which is written as

$$H_0^{(fs)} = \sum_{i,j=1}^{Z}\frac{e^2(\boldsymbol{r}_i\cdot\boldsymbol{R}_j)}{r_i^3}. \tag{5.1}$$

In this case, we can calculate the third order perturbation energy of the EDM Hamiltonian where the two intermediate states $|n\rangle$ and $|n'\rangle$ are considered. Here, $|n\rangle$ and $|n'\rangle$ correspond to the nuclear excitation with the atomic ground state and the atomic excitation with the nuclear ground state, respectively,

$$\begin{aligned} \Delta E_{fs}^{(3)} = &-\sum_{n,n'}\frac{2e^2}{(E_n - E_0)(E_{n'} - E_0)} \\ &\times\langle 0|\sum_{i=1}^{Z}\boldsymbol{r}_i\cdot\boldsymbol{E}_{\rm ext}|n'\rangle\langle n'|\sum_{i=1}^{Z}\sum_{j=1}^{Z}\frac{e^2(\boldsymbol{r}_i\cdot\boldsymbol{R}_j)}{r_i^3}|n\rangle \\ &\times\langle n|\sum_{i\neq j}^{A}\frac{1}{4}\left[\left(1+\tau_i^z\right)d_p\boldsymbol{\sigma}^i + \left(1-\tau_i^z\right)d_n\boldsymbol{\sigma}^i\right] \\ &\cdot\frac{\left(1+\tau_j^z\right)(\boldsymbol{R}_i - \boldsymbol{R}_j)}{|\boldsymbol{R}_i - \boldsymbol{R}_j|^3}|0\rangle + {\rm h.c.} \end{aligned} \tag{5.2}$$

Here, we rewrite $\frac{e^2(\boldsymbol{r}_i\cdot\boldsymbol{R}_j)}{r_i^3}$ in the following way:

$$\frac{e^2(\boldsymbol{r}_i\cdot\boldsymbol{R}_j)}{r_i^3} = -e^2\boldsymbol{R}_j\cdot\nabla_i\frac{1}{r_i} = -ie^2\boldsymbol{R}_j\cdot\boldsymbol{p}_i\frac{1}{r_i}. \qquad (5.3)$$

In addition, we define the unperturbed Hamiltonian for electron systems as

$$H_0^{(e)} = \sum_{i=1}^{Z}\left[\frac{\boldsymbol{p}_i{}^2}{2m} - \frac{Ze^2}{r_i}\right] + \frac{1}{2}\sum_{i\neq j}^{Z}\frac{e^2}{|\boldsymbol{r}_i-\boldsymbol{r}_j|}. \qquad (5.4)$$

Therefore, we can rewrite

$$\sum_i\left\{-ie^2\boldsymbol{R}_j\cdot\boldsymbol{p}_i\frac{1}{r_i}\right\} = \frac{i}{Z}\boldsymbol{R}_j\cdot\sum_i\left[\boldsymbol{p}_i,\sum_j\left(-\frac{Ze^2}{r_j}\right)\right]$$
$$= \frac{i}{Z}\boldsymbol{R}_j\cdot\sum_i\left[\boldsymbol{p}_i,H_0^{(e)}\right], \qquad (5.5)$$

where

$$\sum_i^Z\nabla_i\left(\sum_j^Z\frac{e^2}{|\boldsymbol{r}_i-\boldsymbol{r}_j|}\right) = 0 \qquad (5.6)$$

is employed. In this case, the summation over n' in Eq. (5.2) can be evaluated as

$$\sum_{n'}\frac{1}{(E_{n'}-E_0)}\langle 0|\sum_{i=1}^{Z}\boldsymbol{r}_i\cdot\boldsymbol{E}_{\rm ext}|n'\rangle\langle n'|$$
$$\times\sum_{i,j=1}^{Z}\frac{e^2(\boldsymbol{r}_i\cdot\boldsymbol{R}_j)}{r_i^3}|n\rangle + \text{h.c.}$$
$$= \sum_{n'}\frac{1}{(E_{n'}-E_0)}\langle 0|\sum_{i=1}^{Z}\boldsymbol{r}_i\cdot\boldsymbol{E}_{\rm ext}|n'\rangle$$
$$\times\ \langle n'|\sum_{i,j=1}^{Z}\frac{i}{Z}\boldsymbol{R}_j\cdot\left[\boldsymbol{p}_i,H_0^{(e)}\right]|n\rangle + \text{h.c.}$$
$$= \langle 0|\sum_{i,j=1}^{Z}\frac{i}{Z}\{(\boldsymbol{r}_i\cdot\boldsymbol{E}_{\rm ext})(\boldsymbol{R}_j\cdot\boldsymbol{p}_i)$$
$$-\ (\boldsymbol{R}_j\cdot\boldsymbol{p}_i)(\boldsymbol{r}_i\cdot\boldsymbol{E}_{\rm ext})\}|n\rangle$$
$$= -\langle 0|\sum_{j=1}^{Z}\boldsymbol{E}_{\rm ext}\cdot\boldsymbol{R}_j|n\rangle. \qquad (5.7)$$

Therefore, we obtain the third order perturbation energy as

$$\Delta E_{fs}^{(3)} = \sum_n\frac{e^2}{E_n-E_0}\langle 0|\sum_{i=1}^{A}\tau_i^z\boldsymbol{R}_i\cdot\boldsymbol{E}_{\rm ext}|n\rangle$$
$$\times\langle n|\sum_{i\neq j}^{A}\frac{1}{4}\left[(1+\tau_i^z)d_p\boldsymbol{\sigma}^i + (1-\tau_i^z)d_n\boldsymbol{\sigma}^i\right]$$
$$\times\frac{(1+\tau_j^z)(\boldsymbol{R}_i-\boldsymbol{R}_j)}{|\boldsymbol{R}_i-\boldsymbol{R}_j|^3}|0\rangle \qquad (5.8)$$

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

VI. RELATIVISTIC EDM ENERGY

It is well known that the atomic EDM is mostly shielded by Schiff's theorem, and a finite EDM term free from Schiff's theorem only comes from the relativistic effects [6–8]. There are two contributions of nucleon EDM in atomic systems, the finite nuclear size effects and the relativistic effects of EDM operators which are free from the Schiff shielding. In the previous sections, we have discussed the finite size effects on the EDM of nucleons in atomic systems. Now, we treat the relativistic effects of EDM of nucleons.

In the case of electron EDM, one finds a strong enhancement in the relativistic EDM of electrons due to the small energy difference between the ground state and the parity opposite first excited state in the second order perturbation calculations [7,8]. At the same time, however, it should be noted that there is a finite contribution of the relativistic EDM effects of electrons in the first order perturbation calculation even though the effects are rather small.

Clearly, there are relativistic EDM effects of nucleons in the first order perturbation calculation. Therefore, it is important to figure out the magnitude of the relativistic EDM effects of nucleons in nucleus.

The relativistic EDM Hamiltonian of nucleons can be written as

$$H_{\rm edm}^{(\rm Rel)} = -\sum_i^N d_N^i\gamma_i^5\boldsymbol{\gamma}_i\cdot\boldsymbol{E}_i$$
$$= -\sum_i^N d_N^i\boldsymbol{\Sigma}_i\cdot\boldsymbol{E}_i - \sum_i^N d_N^i\left(\gamma_i^0-1\right)\boldsymbol{\Sigma}_i\cdot\boldsymbol{E}_i, \qquad (6.1a)$$

where $\boldsymbol{\Sigma}_i$ is defined as

$$\boldsymbol{\Sigma}_i = \begin{pmatrix}\boldsymbol{\sigma}_i & 0\\ 0 & \boldsymbol{\sigma}_i\end{pmatrix}.$$

The first part of the last equation in Eq. (6.1a) [$\boldsymbol{\Sigma}_i\cdot\boldsymbol{E}_i$ term] corresponds to the nonrelativistic EDM operators. The energy shifts in the presence of these operators are already examined in Secs. II to V, and we have seen the contributions as the nuclear finite size effects are almost shielded, which corresponds to Schiff's theorem.

The last term in Eq. (6.1a) contributes to the EDM energy which is completely free from Schiff's theorem. We write the relativistic EDM operator which is free from the Schiff shielding

$$H_{\rm edm}^{(R)} = -d_n(\gamma^0-1)\boldsymbol{\Sigma}\cdot\boldsymbol{E}, \qquad (6.1b)$$

where $\boldsymbol{E}$ is written as

$$\boldsymbol{E} = -\nabla A_0(R) + \boldsymbol{E}^{\rm ext}. \qquad (6.1c)$$

$A_0(R)$ denotes a one body Coulomb potential which is produced by protons in nucleus and is written as

$$A_0(R) = \int\frac{\rho_0(R')}{|\boldsymbol{R}-\boldsymbol{R}'|}d^3R', \qquad (6.2)$$

where $\rho_0(R)$ denotes the charge distribution of protons in nucleus. In this case, it is easy to see that the EDM Hamiltonian of $H_{\rm edm}^{(R)}$ vanishes in the nonrelativistic limit since Eq. (6.1b) contains only the small components of Dirac wave functions.

Now, the relativistic EDM Hamiltonian $H_{\rm edm}^{(R)}$ can be transformed into the nonrelativistic reduction in terms of the Foldy-Wouthuysen transformation which is the unitary transformation to obtain the nonrelativistic form. Before going to the Foldy-Wouthuysen transformation, we first write the relativistic nucleon Hamiltonian which keeps the time reversal invariance

$$H_0^{(R)} = \boldsymbol{P}\cdot\boldsymbol{\alpha} + U_0(R) + M\gamma^0 + \frac{e}{2}(1+\tau^z)(A_0(R) + \boldsymbol{R}\cdot\boldsymbol{E}^{\rm ext}), \tag{6.3}$$

where $U_0(R)$ denotes the one body nuclear potential. Here, we assume that the nucleus is described by the single particle Hamiltonian with the one body nuclear and Coulomb potential. In this case, the EDM Hamiltonian after the Foldy-Wouthuysen transformation becomes

$$H_{\rm edm}^{FW} = \gamma_0\left(M + \frac{\mathcal{O}^2}{2M} - \frac{\mathcal{O}^4}{8M^3}\right) + \mathcal{E} - \frac{1}{8M^2}[\mathcal{O},[\mathcal{O},\mathcal{E}]], \tag{6.4}$$

where $\mathcal{O}$ and $\mathcal{E}$ denotes the odd and even operators in γ matrix space and here we can write

$$\mathcal{O} = \boldsymbol{\alpha}\cdot\boldsymbol{P}, \tag{6.5a}$$

$$\mathcal{E} = U_0(R) - d_n(\gamma^0 - 1)\boldsymbol{\Sigma}\cdot\boldsymbol{E} + \frac{e}{2}(1+\tau^z)(A_0(R) + \boldsymbol{R}\cdot\boldsymbol{E}^{\rm ext}). \tag{6.5b}$$

In this case, we obtain the nonrelativistic EDM operators which are free from Schiff's theorem

$$H_{\rm edm}^{FW} = \frac{d_n}{2M^2}\left[(\boldsymbol{\sigma}\cdot\boldsymbol{E})\nabla^2 - \rho(R)(\nabla\cdot\boldsymbol{\sigma}) - 2(\boldsymbol{E}\cdot\nabla)(\boldsymbol{\sigma}\cdot\nabla)\right]. \tag{6.6}$$

A. Relativistic EDM of Xe atomic system

Now, we calculate the EDM which comes from the relativistic effects in nucleus. Since the contribution to the EDM in nucleus comes from the first order perturbation energy, the EDM operator for nucleus is written as

$$H_{\rm edm}^{FW} = \sum_i \frac{d_N^i}{2M^2}\left[(\boldsymbol{\sigma}_i\cdot\boldsymbol{E}_{\rm ext})\nabla_i^2 - 2(\boldsymbol{E}_{\rm ext}\cdot\nabla_i)(\boldsymbol{\sigma}_i\cdot\nabla_i)\right], \tag{6.7}$$

where the summation should be taken over all the nucleons in the nucleus. Here, the external electric field is chosen to be in z-direction

$$\boldsymbol{E}_{\rm ext} = (0, 0, E_{\rm ext}).$$

Now, we evaluate the first order EDM energy

$$\Delta E_{\rm edm}^{(R)}({\rm Xe}) = \langle {\rm Xe}^{({\rm g.s.})}|\sum_i \frac{d_N^i}{6M^2}(\sigma_z^i E_{\rm ext})\nabla_i^2|{\rm Xe}^{({\rm g.s.})}\rangle. \tag{6.8}$$

The EDM operators are composed of the spin part times the differential operators, and here, we employ the factorization ansatz between the spin operator and the differential operators ∇_i^2 [28]. In this case, Eq. (6.8) becomes

$$\Delta E_{\rm edm}^{(R)}({\rm Xe}) \simeq -\sum_i \frac{d_N^i}{3M} E_{\rm ext}\langle {\rm Xe}^{({\rm g.s.})}|\sigma_z^i|{\rm Xe}^{({\rm g.s.})}\rangle\langle {\rm Xe}^{({\rm g.s.})}|\frac{\boldsymbol{p}_i^2}{2M}|{\rm Xe}^{({\rm g.s.})}\rangle.$$

For the Xe wave function, we take a simple-minded shell model wave function as a guide

$$|{\rm Xe}^{({\rm g.s.})}\rangle = \left|\nu\left(3s_{\frac{1}{2}}\right)\otimes 0^+\right\rangle. \tag{6.9}$$

But the expectation value of the spin operator part should be corrected such that the expectation value of the spin operator is consistent with the observed magnetic moment. For the neutron odd nucleus, we may approximate the spin operator by the magnetic moment operator. Therefore, the expectation value of the spin operator can be described by the observed value of the Xe magnetic moment $\mu_{\rm Xe}^{\rm exp}$ in the following way:

$$\langle {\rm Xe}^{({\rm g.s.})}|\sigma_z|{\rm Xe}^{({\rm g.s.})}\rangle \simeq \left\langle 3s_{\frac{1}{2}}\middle|\sigma_z\middle|3s_{\frac{1}{2}}\right\rangle \times \frac{\mu_{\rm Xe}^{\rm exp}}{\mu_{\rm Xe}^{\rm s.p.}} = 0.203,$$

where $\mu_{\rm Xe}^{\rm s.p.}$ denotes the magnetic moment calculated by the single particle state.

For the expectation value of $\frac{\boldsymbol{p}^2}{2M}$, we employed the Virial theorem

$$\left\langle\frac{\boldsymbol{p}^2}{2M}\right\rangle_{3s} = \frac{1}{2}E_{3s} \tag{6.10}$$

and the energy of the $|3s_{\frac{1}{2}}\rangle$ state is taken to be

$$E_{3s} = 5.5\,\omega \simeq 45\,{\rm MeV}. \tag{6.11}$$

Therefore Eq. (6.8) becomes

$$\Delta E_{\rm edm}^{(R)}({\rm Xe}) \simeq -0.0032\,d_n E_{\rm ext}.$$

In this case, we can describe the EDM of Xe in terms of the neutron EDM as

$$d_{\rm Xe} \simeq -0.0032\,d_n. \tag{6.12}$$

Since the observed value of the Xe EDM is

$$d_{\rm Xe} = (0.7 \pm 3.3 \pm 0.1)\times 10^{-27}{\rm e}\cdot{\rm c.m.}$$

we find

$$d_n({\rm Xe}) \simeq -(2.2 \pm 10.2 \pm 0.3)\times 10^{-25}{\rm e}\cdot{\rm c.m.} \tag{6.13}$$

which should be compared to the direct neutron EDM measurement

$$d_n \simeq (0.19 \pm 0.54)\times 10^{-25}{\rm e}\cdot{\rm c.m.}$$

At present, the direct neutron EDM measurement gives stronger constraint on the neutron EDM.

It should be noted that the numerical calculations carried out here are obviously too much simplified as the shell model calculations and the numerical estimations given here are only reliable up to a factor of two or so. It is clear that the more elaborate calculations should be done in future [29].

B. Relativistic EDM of Hg atomic system

Now, we evaluate the Hg atomic system. For Hg nucleus, we take again a simple-minded shell model wave function

$$|\mathrm{Hg}^{(\mathrm{g.s.})}\rangle = |\nu(3p_{\frac{1}{2}}) \otimes 0^+\rangle. \qquad (6.14)$$

In this case, employing the following equation:

$$\langle \mathrm{Hg}^{(\mathrm{g.s.})}|\sigma_z|\mathrm{Hg}^{(\mathrm{g.s.})}\rangle \simeq \langle 3p_{\frac{1}{2}}|\sigma_z|3p_{\frac{1}{2}}\rangle \times \frac{\mu_{\mathrm{Hg}}^{\mathrm{exp}}}{\mu_{\mathrm{Hg}}^{\mathrm{s.p.}}} = -0.263$$

we obtain the first order perturbation energy of Hg EDM

$$\Delta E_{\mathrm{edm}}^{(R)}(\mathrm{Hg}) = \langle \mathrm{Hg}^{(\mathrm{g.s.})}| \sum_i \frac{d_i}{6M^2}\left(\sigma_z^i E_{\mathrm{ext}}\right)\nabla_i^2 |\mathrm{Hg}^{(\mathrm{g.s.})}\rangle$$
$$\simeq 0.0043\, d_n E_{\mathrm{ext}}, \qquad (6.15)$$

where the energy of the $|3p_{\frac{1}{2}}\rangle$ state is taken to be

$$E_{3p} = 6.5\omega \simeq 46\,\mathrm{MeV}.$$

Therefore, we obtain the relation between the Hg EDM and the neutron EDM as

$$d_{\mathrm{Hg}} \simeq 0.0043\, d_n. \qquad (6.16)$$

Since the observed EDM of Hg atomic system is given as

$$d_{\mathrm{Hg}} \simeq -(1.06 \pm 0.49 \pm 0.40) \times 10^{-28}\,\mathrm{e\cdot c.m.}$$

we find the neutron EDM which is obtained from the Hg EDM experiment

$$d_n(\mathrm{Hg}) \simeq -(0.25 \pm 0.12 \pm 0.09) \times 10^{-25}\,\mathrm{e\cdot c.m.} \qquad (6.17)$$

This should be compared to the direct neutron EDM measurement

$$d_n \simeq (0.19 \pm 0.54) \times 10^{-25}\,\mathrm{e\cdot c.m.}$$

and we find that the neutron EDM from the Hg atomic system gives quite similar constraint on the neutron EDM.

VII. CONCLUSIONS

We have presented a new calculation of the atomic EDM in terms of the perturbative evaluations of the nuclear finite size effects as well as the relativistic effects. These effects are free from Schiff's theorem and contribute to the atomic EDM as physical observables. In this calculation, we show that the second order perturbation energy of EDM from the nuclear finite size effects are extremely small and there is practically no chance to extract the neutron EDM from the atomic EDM measurement. On the other hand, the relativistic effects of the nuclear EDM become around 0.3 and 0.4 % of the neutron EDM in Xe and Hg atomic systems, respectively, and therefore the neutron EDM extracted from the Hg atomic system is just comparable with the direct neutron EDM measurement at the present EDM accuracies for both of the observed values.

Since the shell model calculations in the present paper are carried out with a simplified single particle nuclear model, more reliable numerical calculations are necessary [29].

It seems that there are still many improvements in the atomic EDM measurements and, therefore, if the measurement accuracy of atomic EDM could be improved a great deal, there is a good chance that the finite EDM may be observed from the atomic EDM measurements.

ACKNOWLEDGMENTS

We thank K. Asahi and K. Muto for helpful discussions and comments.

[1] P. G. Harris *et al.*, Phys. Rev. Lett. **82**, 904 (1999).
[2] M. A. Rosenberry and T. E. Chupp, Phys. Rev. Lett. **86**, 22 (2001).
[3] T. G. Vold, F. J. Raab, B. Heckel, and E. N. Fortson, Phys. Rev. Lett. **52**, 2229 (1984).
[4] M. V. Romalis, W. C. Griffith, J. P. Jacobs, and E. N. Fortson, Phys. Rev. Lett. **86**, 2505 (2001).
[5] S. K. Lamoreaux, J. P. Jacobs, B. Heckel, F. J. Raab, and N. Fortson, Phys. Rev. Lett. **59**, 2275 (1987).
[6] L. I. Schiff, Phys. Rev. **132**, 2194 (1963).
[7] I. B. Khriplovich and S. K. Lamoreaux, *CP Violation Without Strangeness* (Springer, Berlin, 1997).
[8] T. Asaga, T. Fujita, and M. Hiramoto, Prog. Theor. Phys. **106**, 1223 (2001).
[9] P. G. H. Sandars, Phys. Lett. **14**, 194 (1965).
[10] P. G. H. Sandars, Phys. Lett. **22**, 290 (1966); J. Phys. B **1**, 511 (1968).
[11] A. C. Hartley, E. Lindroth, and A.-M. Martensson-Pendrill, J. Phys. B **23**, 3417 (1990).
[12] R. M. Sternheimer, Phys. Rev. **183**, 112 (1969).
[13] V. K. Ignatovich, Zh. Eksp. Theor. Fiz. **56**, 2019 (1969).
[14] W. R. Johnson, D. S. Guo, M. Idrees, and J. Sapirstein, Phys. Rev. A **32**, 2093 (1985).
[15] A.-M. Martensson-Pendrill and P. Öster, Phys. Scr. **36**, 444 (1987).
[16] Y. Kizukuri and N. Oshimo, Phys. Rev. D **46**, 3025 (1992).
[17] S. M. Barr and A. Zee, Phys. Rev. Lett. **65**, 21 (1990).
[18] A. Pilaftsis, Phys. Lett. **B435**, 88 (1998); Phys. Rev. D **58**, 096010 (1998).
[19] H. Georgi and S. Dimopoulos, Nucl. Phys. **B193**, 150 (1981).
[20] N. Sakai, Z. Phys. C **11**, 153 (1981).
[21] A. G. Cohen, D. B. Kaplan, and A. E. Nelson, Phys. Lett. **B388**, 588 (1996).
[22] T. Asaga and T. Fujita, "Possible suppression of neutron EDM", hep-ph/0202197.
[23] S. Oshima, T. Nihei, and T. Fujita, J. Phys. Soc. Jap. **74**, 2480 (2005).
[24] V. F. Dmitriev, I. B. Khriplovich, and R. A. Sen'kov, hep-ph/0504063.
[25] A. Yoshimi, K. Asahi, K. Sakai, M. Tsuda, K. Yogo, H. Ogawa, T. Suzuki, and M. Nagakura, Phys. Lett. **A304**, 13 (2002).
[26] V. Spevak, N. Auerbach, and V. V. Flambaum, Phys. Rev. C **56**, 1357 (1997).
[27] V. V. Flambaum and V. G. Zelevinsky, Phys. Rev. C **68**, 035502 (2003).
[28] T. Fujita and A. Arima, Nucl. Phys. **A254**, 513 (1975).
[29] K. Muto (private communications).