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Schiff moments of Xe isotopes in the nuclear shell model

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The existence of the permanent electric dipole moment of a fundamental particle implies violation of time reversal invariance. The electric dipole moment of a paramagnetic neutral atom is mainly induced by the nuclear Schiff moment. In this study the Schiff moments induced by the interaction which violates parity and time reversal invariance are calculated for various Xe isotopes using the shell-model wavefunctions. The contributions to the Schiff moment from one-particle and one-hole excitations turn out to be very different from orbital to orbital. It is also found that the contributions from the core excitations are larger than other particle-hole contributions.

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1. INTRODUCTION

The electric dipole moment (EDM) is a physical observable which violates time reversal symmetry. Through the CPT theorem stating that the simultaneous application of charge (C), parity (P) and time (T) reversal operators keeps the total symmetry of a system, violation of T reversal symmetry is equivalent to the violation of CP reversal symmetry. The Standard Model in particle physics violates CP invariance only through a single phase in the Kobayashi-Maskawa matrix that mixes quark flavors [1]. The resulting T reversal violation is therefore expected to produce only tiny EDMs.

At present the upper limit on the neutron EDM is experimentally $2.9 \times 10^{-26} e$cm [2]. However, the Standard Model predicts quite a small value, $10^{-32} e$cm [3, 4, 5]. Some theories beyond the Standard Model predict larger EDMs [3, 6, 7, 8]. Thus if an EDM is observed experimentally to be larger than those predicted by the Standard Model, it would provide evidence for physics beyond the Standard Model, and also places important constraints on the construction of a new physics.

EDMs originating from CP violation in the hadron sector are searched for in neutron and diamagnetic atoms such as ^{129}Xe, ^{199}Hg and ^{225}Ra. Measurements of EDMs for these atoms have been attempted and their upper limits are $4.1 \times 10^{-27} e$cm for ^{129}Xe [9], $7.4 \times 10^{-30} e$cm for ^{199}Hg [10], and $5.0 \times 10^{-22} e$cm for ^{225}Ra [11]. At present with new techniques, experimental efforts searching for EDMs of diamagnetic atoms are now in progress [12, 13, 14, 15].

The EDM of a neutral diamagnetic atom arises from the Schiff moment of the nucleus. The nuclear Schiff moment originates mainly from two different sources; from nucleon intrinsic EDMs, and from the two-body nuclear interaction which violates P and T invariance. In the latter case theoretical calculations have been carried out for Hg, Rn, and Ra isotopes using mean field theories [16, 17, 18, 19, 20, 21]. However, until recently not so many nuclei have been investigated theoretically.

In our previous study [22], the EDMs and Schiff moments of Xe, Ba and Ce isotopes arising from the nucleon intrinsic EDMs were calculated in terms of the nuclear shell model. The EDMs and Schiff moments of Xe isotopes which come from interactions violating P and T invariance were also calculated [23, 24].

In the present article the Schiff moments of the lowest $1/2^+$ states for ^{135}Xe, ^{133}Xe, ^{131}Xe, and ^{129}Xe nuclei are calculated assuming two-body interactions violating P and T invariance. Particularly effects of the particle-hole excitations from the core of the nucleus are considered, which were not considered in our previous study [23]. Furthermore, contributions to the Schiff moment from one orbital to another is individually calculated and analyzed.

2. Theoretical framework

The Schiff moment operator $\mathbf{S}$ coming from the asymmetric charge distribution in a nucleus [25] is expressed in terms of spherical tensors

$$S_{\mu}^{(1)} = \sum_{i=1}^{A} \frac{e_i}{10} \left(r_i^2 r_{i,\mu}^{(1)} - \frac{5}{3} \langle r^2 \rangle_{\mathrm{ch}} \, r_{i,\mu}^{(1)} + \frac{\sqrt{10}}{3} \left[Q_i^{(2)} \otimes r_i^{(1)} \right]_{\mu}^{(1)} \right), \tag{2.1}$$

with $r_{i,\mu}^{(1)} = r_i C_{\mu}^{(1)}(\theta_i, \varphi_i)$ and $Q_{i,\mu}^{(2)} = 2 r_i^2 C_{\mu}^{(2)}(\theta_i, \varphi_i)$, where $C_{\mu}^{(L)}$ represents the unnormalized spherical harmonics with rank L and its projection μ, and i represents the ith nucleon. Here A is the mass number of a specific nucleus, and $\mathbf{r}_i = (r_i, \theta_i, \varphi_i)$ indicates ith nucleon position. IIn this study the Schiff moments are calculated for the lowest states with spin $I = 1/2$. The third term in Eq. (2.1) vanishes for these states since there is no quadrupole moment for $I = 1/2$ states. Here e_i is the charge for the ith nucleon. $e_i = e$ is taken for a proton and $e_i = 0$ is assumed for a neutron. The $\langle r^2 \rangle_{\rm ch}$ is the mean squared radius of the nuclear charge distribution [23].

By perturbation theory, the expectation value of the Schiff moment operator is expressed as

$$S = \sum_{T=0,1,2} S_{(T)}, \tag{2.2}$$

$$S_{(T)} = \sum_k \frac{\langle I_1^+ | S_0^{(1)} | I_k^- \rangle \langle I_k^- | V_{\pi(T)}^{PT} | I_1^+ \rangle}{E_1^+ - \langle I_k^- | H_0 | I_k^- \rangle} + c.c., \tag{2.3}$$

where $V_{\pi(T)}^{PT}$ represents the isoscalar ($T = 0$), isovector ($T = 1$) or isotensor ($T = 2$) interactions between nucleons. Here $|I_1^+\rangle$ and E_1^+ represent the wavefunction and the eigen-energy of the lowest state with spin I and positive parity for the Hamiltonian H_0, respectively. $|I_k^-\rangle$ represents the kth intermediate state with spin I and negative parity. Note that this expression is valid as long as $|I_k^-\rangle$ forms an orthonormal complete system and each state $|I_k^-\rangle$ is not necessary to be the eigenstate of the Hamiltonian H_0. In the present study, only $I = 1/2$ states are considered. All these states have their projection (spin third component) $+1/2$.

The lowest positive parity state, $|I_1^+\rangle$, is calculated using the pair-truncated shell model (PTSM) [26, 27, 28]. The PTSM is one of the shell-model approaches, but a gigantic shell model space is restricted to the space mainly made of only low-spin collective pairs. For single particle energies, five orbitals between magic numbers 50 and 82 ($0g_{7/2}$, $1d_{3/2}$, $1d_{5/2}$, $2s_{1/2}$, and $0h_{11/2}$) are taken for neutrons and protons. The details of the framework and Hamiltonian for diagonalization are given in Ref. [28] in addition to the numerical results of the energy spectra and electromagnetic properties.

The P and T violating two-body interactions $V_{\pi(T)}^{PT}$ in Eq. (2.3) are considered as follows, which are explicitly written as [29, 30, 31],

$$V_{\pi(0)}^{PT} = F_0 (\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2)(\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2) \cdot \mathbf{r} f(r), \tag{2.4}$$

$$V_{\pi(1)}^{PT} = F_1 \left[(\tau_{1z} + \tau_{2z})(\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2) + (\tau_{1z} - \tau_{2z})(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \right] \cdot \mathbf{r} f(r), \tag{2.5}$$

$$V_{\pi(2)}^{PT} = F_2 (3\tau_{1z}\tau_{2z} - \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2)(\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2) \cdot \mathbf{r} f(r), \tag{2.6}$$

where

$$f(r) = \frac{\exp(-m_\pi r)}{m_\pi r^2} \left(1 + \frac{1}{m_\pi r} \right) \tag{2.7}$$

with $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$, and $r = |\mathbf{r}|$. The coefficients F_T ($T = 0, 1, 2$) are expressed as

$$F_0 = -\frac{1}{8\pi} \frac{m_\pi^2}{M_N} \bar{g}_{\pi NN}^{(0)} g_{\pi NN}, \tag{2.8}$$

$$F_1 = -\frac{1}{16\pi} \frac{m_\pi^2}{M_N} \bar{g}_{\pi NN}^{(1)} g_{\pi NN}, \tag{2.9}$$

$$F_2 = -\frac{1}{8\pi} \frac{m_\pi^2}{M_N} \bar{g}_{\pi NN}^{(2)} g_{\pi NN}, \tag{2.10}$$

where M_N is mass of a nucleon, m_π is mass of a pion, and $g_{\pi NN}$ is the strong πNN coupling constant, and $\bar{g}_{\pi NN}^{(T)}$ is the strong πNN constant which violates P and T invariance with isospin T. In the following $\bar{g}_{\pi NN}^{(T)}$ and $g_{\pi NN}$ are denoted as $\bar{g}^{(T)}$ and g for short, respectively.

The total Schiff moment is the summation of three isospin components. In this study, Schiff moments are evaluated as coefficients in front of $\bar{g}^{(T)}g$,

$$S = a_{(0)}\,\bar{g}^{(0)}g + a_{(1)}\,\bar{g}^{(1)}g + a_{(2)}\,\bar{g}^{(2)}g. \tag{2.11}$$

Any intermediate state $\left|I_k^-\right\rangle$ in Eq. (2.3) is represented as a one-particle and one-hole excited state ($1p1h$-state) from the $\left|I_1^+\right\rangle$ state. Since the Schiff moment operator is a one-body operator working only on protons, it is enough to consider proton excited $1p1h$-states. To evaluate the Schiff moment in Eq. (2.3), kth intermediate $1p1h$-state is given as

$$\left|I_k^-\right\rangle = \left|(ij)K;I^-\right\rangle = N_{ij}^{(K)}\left[\left[c_{i\pi}^\dagger \tilde{c}_{j\pi}\right]^{(K)} \otimes \left|I_1^+\right\rangle\right]^{(I)}, \tag{2.12}$$

where $c_{i\pi}^\dagger$ ($c_{j\pi}$) represents the proton creation (annihilation) operator in the orbital i (j), with $\tilde{c}_{jm} = (-1)^{j-m}c_{j-m}$.

By nelecting the residual interaction, the energy denominator in Eq. (2.3) is approximately treated as $E_1^+ - \left\langle I_k^-\right|H_0\left|I_k^-\right\rangle \sim (-E_{ij})$ where $E_{ij} \equiv \varepsilon_i - \varepsilon_j$ represents the single particle-hole excitation energies from oribital j to i. Then Eq. (2.3) is written as

$$S_{(T)} = \sum_{Kij} \frac{\left\langle I_1^+\right|S_0^{(1)}\left|I_k^-\right\rangle\left\langle I_k^-\right|V_{\pi(T)}^{PT}\left|I_1^+\right\rangle}{(-E_{ij})} + c.c. \tag{2.13}$$

To calculate Eq. (2.13), three types of $1p1h$-excitations are considered. The first type is a set of excitations from an orbital between 50 and 82 to an orbital over 82. These excitations are called type-I excitations. The second type is a set of excitations from an orbital under 50 to an orbital between 50 and 82. These excitations are called type-II excitations. The third type is a set of excitations from an orbital under 50 to an orbital over 82. These excitations are called type-III excitations. Note that excitations among orbitals between 50 and 82 are vanished since these orbitals are not connected by the Schiff moment operator.

For the type-I excitation, an intermediate state is explicitly written as

$$\left|I_k^-\right\rangle_{\text{type-I}} = N_{ph}^{(K)}\left[\left[a_{p\pi}^\dagger \tilde{c}_{h\pi}\right]^{(K)} \otimes \left|I_1^+\right\rangle\right]^{(I)}. \tag{2.14}$$

Here $a_{p\pi}^\dagger$ represents the proton creation operator in the orbital p, where p indicates an orbital over 82. $\tilde{c}_{h\pi}$ represents the proton annihilation operator in the orbital h, where h indicates an orbital between 50 and 82. For the type-II excitation, an intermediate state is written as

$$\left|I_k^-\right\rangle_{\text{type-II}} = N_{ph}^{(K)}\left[\left[c_{p\pi}^\dagger \tilde{b}_{h\pi}\right]^{(K)} \otimes \left|I_1^+\right\rangle\right]^{(I)}. \tag{2.15}$$

Here $c_{p\pi}^\dagger$ represents the proton creation operator in an orbital p, where p indicates an orbital between 50 and 82. $\tilde{b}_{h\pi}$ represents the proton annihilation operator in the orbital h, where h indicates an orbital under 50. For the type-III excitation, an intermediate state is written as

$$\left|I_k^-\right\rangle_{\text{type-III}} = N_{ph}^{(K)}\left[\left[a_{p\pi}^\dagger \tilde{b}_{h\pi}\right]^{(K)} \otimes \left|I_1^+\right\rangle\right]^{(I)}. \tag{2.16}$$

Table 1: Calculated results of $a^{\text{type-I}}_{(T)}(p)$ from each orbital p in the shell over 82 (type-I excitations) for ^{129}Xe (in units of 10^{-3}efm^3).

T	$1f_{7/2}$	$0h_{9/2}$	$0i_{13/2}$	$2p_{3/2}$	$1f_{5/2}$	$1p_{1/2}$	$1g_{9/2}$	$0i_{11/2}$
0	+0.107	+0.265	−0.007	+0.079	+0.385	+0.055	+0.018	+0.001
1	+0.047	+0.107	−0.005	+0.049	+0.153	+0.020	+0.008	+0.000
2	+0.176	+0.380	−0.025	+0.214	+0.531	+0.063	+0.027	+0.000
T	$1h_{9/2}$	$2f_{5/2}$	$2f_{7/2}$	$3p_{1/2}$	$3p_{3/2}$	$1i_{11/2}$	$1i_{13/2}$	$2g_{9/2}$
0	+0.406	−0.062	+0.076	−0.013	+0.002	+0.000	+0.010	−0.001
1	+0.184	−0.025	+0.050	−0.001	−0.007	+0.000	+0.007	−0.000
2	+0.699	−0.089	+0.222	+0.007	−0.045	+0.000	+0.032	−0.001

All orbitals under the magic number 50 are considered for core orbitals. However, $0d_{3/2}$, $1s_{1/2}$, and $0s_{1/2}$ orbitals are not connected by the Schiff moment operator.

3. NUMERICAL RESULTS

To analyze the contribution to the Schiff moments from each orbital, firstly a partial contribution of the excitation from any orbital (h) between 50 and 82 to a specific orbital (p) over 82 (type-I excitations) is defined as

$$s^{\text{type-I}}_{(T)}(p) = \sum_{Kh} \frac{\langle I_1^+|S_0^{(1)}|I_k^-\rangle\langle I_k^-|V^{PT}_{\pi(T)}|I_1^+\rangle}{(-E_{ph})} + c.c., \tag{3.1}$$

which is rewritten in terms of $\bar{g}^{(T)}g$ as, $s^{\text{type-I}}_{(T)}(p) = a^{\text{type-I}}_{(T)}(p)\ \bar{g}^{(T)}g$, where and $a^{\text{type-I}}_{(T)}(p)$'s are coefficients so determined in evaluating the partial Schiff moment $s^{\text{type-I}}_{(T)}(p)$.

Secondly, a partial contribution of the excitation to any orbital (p) between 50 and 82 from a specific orbital (h) under 50 (type-II excitations) is defined as

$$s^{\text{type-II}}_{(T)}(h) = \sum_{Kp} \frac{\langle I_1^+|S_0^{(1)}|I_k^-\rangle\langle I_k^-|V^{PT}_{\pi(T)}|I_1^+\rangle}{(-E_{ph})} + c.c., \tag{3.2}$$

which is rewritten in terms of $\bar{g}^{(T)}g$ as, $s^{\text{type-II}}_{(T)}(h) = a^{\text{type-II}}_{(T)}(h)\ \bar{g}^{(T)}g$.

Finally, a partial contribution of the excitation from a specific orbital (h) under 50 to any orbital (p) over 82 (type-III excitations) is also defined as

$$s^{\text{type-III}}_{(T)}(h) = \sum_{Kp} \frac{\langle I_1^+|S_0^{(1)}|I_k^-\rangle\langle I_k^-|V^{PT}_{\pi(T)}|I_1^+\rangle}{(-E_{ph})} + c.c., \tag{3.3}$$

which is rewritten in terms of $\bar{g}^{(T)}g$ as $s^{\text{type-III}}_{(T)}(h) = a^{\text{type-III}}_{(T)}(h)\ \bar{g}^{(T)}g$.

Table 1 shows calculated $a^{\text{type-I}}_{(T)}(p)$ for ^{129}Xe. The contributions from the $1f_{7/2}$, $0h_{9/2}$, $1f_{5/2}$ and $1h_{9/2}$ orbitals are large since the most orbitals are positive in the 50-82 major shell. Table 2

Table 2: Calculated results of $a^{\text{type-II}}_{(T)}(h)$ from each orbital h in the shell under 50 (type-II excitations) for ^{129}Xe (in units of $10^{-3}e\text{fm}^3$).

T	$0g_{9/2}$	$1p_{1/2}$	$0f_{5/2}$	$1p_{3/2}$	$0f_{7/2}$	$0p_{1/2}$	$0p_{3/2}$
0	−3.642	+0.621	+1.964	+1.443	+0.883	+0.648	+0.982
1	−2.022	+0.511	+0.867	+0.502	+0.473	+0.273	+0.536
2	−8.488	+2.444	+3.239	+1.568	+1.953	+0.988	+2.236

Table 3: Calculated results of $a^{\text{type-III}}_{(T)}(h)$ from each orbital h in the shell under 50 (type-III excitations) for ^{129}Xe (in units of $10^{-3}e\text{fm}^3$).

T	$0g_{9/2}$	$1p_{1/2}$	$0f_{5/2}$	$1p_{3/2}$	$0f_{7/2}$	$0d_{3/2}$	$1s_{1/2}$	$0d_{5/2}$
0	−0.090	−0.134	−0.008	−0.336	−0.029	+0.055	−0.416	−0.036
1	+0.007	+0.060	−0.028	−0.146	−0.018	+0.020	−0.389	−0.028
2	+0.134	+0.491	−0.015	−0.537	−0.076	+0.064	−1.918	−0.133

Table 4: Calculated results of $a_{(T)}$ for the lowest $1/2^+$ states (in units of $10^{-3}e\text{fm}^3$). Previous results ($a^{\text{prev}}_{(T)}$) are taken from Ref. [23].

	T	$a^{\text{type-I}}_{(T)}$	$a^{\text{type-II}}_{(T)}$	$a^{\text{type-III}}_{(T)}$	$a_{(T)}$	$a^{\text{prev}}_{(T)}$
^{135}Xe	0	+2.357	+0.670	−1.057	+1.969	+0.630
	1	+1.297	+1.693	−0.602	+2.389	+0.323
	2	+5.427	+9.490	−2.554	+12.363	+1.31
^{133}Xe	0	+1.812	+1.716	−1.047	+2.481	+0.464
	1	+0.949	+1.510	−0.578	+1.882	+0.285
	2	+3.982	+7.343	−2.419	+8.906	+1.24
^{131}Xe	0	+1.575	+2.097	−0.968	+2.704	+0.514
	1	+0.787	+1.282	−0.530	+1.539	+0.352
	2	+3.145	+5.596	−2.177	+6.564	+1.60
^{129}Xe	0	+1.322	+2.897	−0.978	+3.242	+0.507
	1	+0.586	+1.140	−0.522	+1.204	+0.399
	2	+2.192	+3.940	−1.961	+4.172	+1.89

shows calculated $a^{\text{type-II}}_{(T)}(h)$ for ^{129}Xe. The contribution from the $0g_{9/2}$ orbital becomes the largest. The $0g_{9/2}$ orbital is connected to the $0h_{11/2}$ orbital by the Schiff moment operator. The orbitals which demand large $1p1h$-excitation energies (like $0p_{3/2}$ and $0p_{1/2}$ orbitals) also have considerable contributions. Table 3 shows calculated $a^{\text{type-III}}_{(T)}(h)$ for ^{129}Xe. These contributions are not so large compared to results in Table 2.

Table 4 shows the calculated results of $a_{(T)}$ for the lowest $I = 1/2$ states of Xe isotopes. Here, using Eqs. (3), (3), and (3), $a_{(T)}$ is given by

$$a_{(T)} = a^{\text{type-I}}_{(T)} + a^{\text{type-II}}_{(T)} + a^{\text{type-III}}_{(T)}, \tag{3.4}$$

with $a^{\text{type-I}}_{(T)} = \sum_p a^{\text{type-I}}_{(T)}(p)$, $a^{\text{type-II}}_{(T)} = \sum_h a^{\text{type-II}}_{(T)}(h)$, and $a^{\text{type-III}}_{(T)} = \sum_h a^{\text{type-III}}_{(T)}(h)$. The contributions of the core excitations are a few times larger than those from the over-shell excitations for most of

Table 5: The comparison of $a_{(T)}$'s for ^{129}Xe between present results (This work), our previous results (prev.) [23], and the results by Dmitriev *et al.* with core polarization (core) and without core polarization (bare) [21] in units of $10^{-3}e\text{fm}^3$. The isotensor ($T = 2$) component in [21] is changed from its original sign in accordance with the different sign definition of the isotensor ($T = 2$) interaction in the present study.

T	This work	prev. [23]	bare [21]	with core [21]
0	+3.242	+0.507	+60	+8
1	+1.204	+0.399	+60	+6
2	+4.172	+1.89	+120	+9

the isospin components. The isotensor ($T = 2$) components are largest for all nuclei. The previous results [23] are also shown in Table 4. By comparing the present results with the previous ones, some contributions of Schiff moments are found to be nearly one order of magnitude larger than the previous ones (for examples, isotensor components of ^{135}Xe and ^{133}Xe). The isoscalar component for ^{129}Xe becomes 6.4 times larger than the previous one.

The present results, our previous results [23] and results by Dmitriev *et al.* [21] are compared for ^{129}Xe in Table 5. The present result is summarized as $S = 3.24\ \bar{g}^{(0)}g + 1.20\ \bar{g}^{(1)}g + 4.17\ \bar{g}^{(2)}g$ (in units of $10^{-3}e\text{fm}^3$) for ^{129}Xe. In the previous work [23], the Schiff moment of ^{129}Xe was calculated as $S = 0.51\ \bar{g}^{(0)}g + 0.40\ \bar{g}^{(1)}g + 1.89\ \bar{g}^{(2)}g$ (in units of $10^{-3}e\text{fm}^3$). The difference between the present study and the previous one is due to improvement of the model space adopted in the calculation.

4. SUMMARY

In the present study the nuclear Schiff moments induced by the interaction which violates parity and time reversal invariance are calculated for the lowest $1/2^+$ states of Xe isotopes. The wavefunctions of Xe isotopes are calculated in terms of the nuclear shell model approach. Excitations from orbitals between the magic numbers 50 and 82 to orbitals over 82 (type-I excitations), the excitations from orbitals under 50 to orbitals between the magic numbers 50 and 82 (type-II excitations), and the excitations from orbitals under 50 to orbitals over 82 (type-III excitations) are considered for the one-particle and one-hole excitations. It is found that the contributions of type-II excitations are a few times larger than those from the type-I and type-III excitations. The contribution of excitation from the $0g_{9/2}$ orbital to the $0h_{11/2}$ orbital is the largest. It is also found that the excitations which require large excitation energies have negligible contributions.

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