Shell model estimate of electric dipole moments in medium and heavy nuclei

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Abstract. Existence of the electric dipole moment (EDM) is deeply related with time-reversal invariance. The EDM of a diamagnetic atom is mainly induced by the nuclear Schiff moment. After carrying out the shell model calculations to obtain wavefunctions for Xe isotopes, we evaluate nuclear Schiff moments for Xe isotopes to estimate their atomic EDMs. We estimate the contribution from each single particle orbital for the Schiff moment. It is found that the contribution on the Schiff moment is very different from orbital to orbital.

1 Introduction

The electric dipole moment (EDM) of a fundamental particle violates time-reversal invariance. The finite value of the EDM gives crucial information on particle physics. Up to now neutron EDM has been searched to give its upper limit as 2.9 × 10⁻²⁶ ecm [1]. In contrast, the neutron EDM was estimated theoretically by the Standard Model to give its value around 10⁻³² ecm [2–4]. Thus if we observe a large value of EDM, we may conclude that we need a new extended model beyond the Standard Model, and experimental EDM values give a restriction on constructing new models. With this motivation in mind, experiments of searching EDMs have been performed in various systems. In the case of a diamagnetic atom, for example, in ¹²⁹Xe its upper limit is given as 4.1 × 10⁻²⁷ ecm [5]. In the case of ¹⁹⁹Hg, its upper limit is given as 3.1 × 10⁻²⁸ ecm [6]. This value is the smallest EDM upper limit measured at present.

Theoretical efforts of studying EDM of a diamagnetic atom have also been made. Its EDM is mainly induced by the nuclear Schiff moment [7]. Due to the Schiff theorem, other moments do not contribute to the atomic EDM. The Schiff moment originates mainly from two sources [8]. One comes from the intrinsic nucleon EDM. The other comes from the asymmetric nucleon charge distribution in a nucleus. Schiff moments in this kind are induced if we have two-body interactions which violate parity and time-reversal invariance. There are several theoretical studies of calculating nuclear Schiff moments in this context. For example, Ra and Hg isotopes were investigated using the quasiparticle random-phase approximation and Hartree-Fock-Bogoliubov method [8–10]. Nevertheless, all of them so far used mean field theories or collective models. In our group, we calculated nuclear Schiff moments and EDMs in medium and heavy nuclei using the pair-truncated shell model (PTSM) [11–13]. The PTSM is one of the shell model approaches that reduce the full shell model space by using the dominant collective pairs [14, 15]. In the present study we extend our previous studies to evaluate the nuclear Schiff moments for Xe isotopes using the nuclear shell model and estimate the upper limits of atomic EDMs. In this work we study the Schiff moments induced by the interactions which violate parity and time-reversal invariance.

2 Theoretical framework

The Schiff moment operator coming from the asymmetric nuclear charge distribution is written as

\[ S = \frac{1}{10} \sum_i^A e_i \left( r_i^2 - \frac{5}{3} \langle r_i^2 \rangle \right) r_i, \]  

where \( r_i \) is position of the \( i \)th nucleon and \( \langle r_i^2 \rangle \) means nuclear charge mean square radius. \( e_i \) is the effective charge of the \( i \)th nucleon and assumed to be zero for neutrons and \( e \) for protons. Using the nuclear wavefunction of spin \( I \) and parity \( \pi, |I \pi \rangle \), the Schiff moment is calculated as

\[ S = \langle I \pi | \hat{S} \rangle |I \pi \rangle. \]  

Here, \( \hat{S} \) is the third component of the Schiff moment operator. If parity and time-reversal violating interaction \( V_{PT} \) exists, the Schiff moment for the first \( I = 1/2^+ \) state is calculated using first order perturbation theory as,

\[ S^{(I)} = \sum_k \left( \frac{1}{\varepsilon_k^{(I)} + |V_{PT}(T)|} \right) \langle \varepsilon_k^{(I)} + |V_{PT}(T)| \rangle |I \pi \rangle |I \pi \rangle + c.c., \]  

where \( V_{PT}(T) \) has three isospin components, isoscalar (\( T = 0 \)), isovector (\( T = 1 \)), and isotensor (\( T = 2 \)) components,
and they are explicitly written as [16–18]:

\[
V_{\pi(0)}^{PT} = \frac{mc^2q}{8\pi M_N} \left( \tau_1 \cdot \tau_2 \right) (\sigma_1 - \sigma_2) \cdot r f(r),
\]

\[
V_{\pi(1)}^{PT} = \frac{mc^2q}{10\pi M_N} \left[ \left( \tau_1 + \tau_2 \right) (\sigma_1 - \sigma_2) + \left( \tau_1 - \tau_2 \right) (\sigma_1 + \sigma_2) \right] \cdot r f(r),
\]

\[
V_{\pi(2)}^{PT} = \frac{mc^2q}{8\pi M_N} \left( 3\tau_1 \tau_2 - \tau_1 \cdot \tau_2 \right) \times (\sigma_1 - \sigma_2) \cdot r f(r),
\]

\[
f(r) = \frac{\exp(-mr^2)}{m r^2} \left( 1 + \frac{1}{m r^2} \right),
\]

where \(m_\pi\) and \(M_N\) are masses of pion and nucleon, respectively. Here \(r = r_1 - r_2\) and \(\tau = |r|\). The \(\sigma_i\) and \(\tau_i\) are the Pauli spin operator and the third component of isospin operator, respectively. \(q\) is the strong \(NN\) coupling constant, and \(g(T)\) is the strong \(NN\) constant violating time-reversal invariance for the isospin \(T\) component.

In the present study, we use a closure approximation to simplify our calculation. It was shown in Ref. [12] that this is a valid approximation. In the closure approximation, we set the energy denominator in eq. (3) \(\langle E \rangle = \langle E_{\pi(1)}^{\pm(1)} - E_{\pi(2)}^{\pm(1)} \rangle\) constant. Then the Schiff moment is now written as

\[
S^T = \frac{1}{\langle E \rangle} \langle \tau^+_{\pi(1)} | S, V_{\pi(2)}^{PT} | \tau^+_{\pi(2)} \rangle,
\]

where the relation \(\sum_{k=0}^{\infty} \left( \frac{1}{2k+1} \right) \frac{1}{2k+1} = 1\) is used.

For the calculation of shell model wavefunctions, we take the five single particle orbitals, \(0g_{7/2, 1d_{5/2, 1d_{3/2, 0h_{11/2, 2s_{1/2}}}}\) between the magic numbers 50 and 82 for both neutrons and protons. We first diagonalize a shell model Hamiltonian and obtain eigen-energies and eigenfunctions. The details of the shell model calculation are given in Ref. [19], but the strength of each individual interaction is changed a bit for a better description of energy spectra. In order to calculate Schiff moments, we need to consider one-proton excitations from the 50–82 shell to the outside of the shell, and also the excitations from the shell under 50 (core) to the 50-82 shell. We call excitations to the shell over 82, “over-shell excitations” and excitations from the shell under 50, “core excitations”. For over-shell excitations, we introduce eight orbitals, \(1f_{7/2, 0h_{9/2, 0I_{13/2, 1f_{5/2, 2p_{1/2}}}}\), and \(2s_{1/2} \). For core excitations, we take seven orbitals, \(0g_{9/2, 1p_{1/2, 1f_{5/2, 1p_{3/2, 0f_{7/2, 0p_{1/2, \text{and 0p}_{3/2}}} \). Orbitals unmentioned here for core excitations are not connected with the \(1/2^+\) states by the Schiff moment operator.

### 3 Numerical Results

We evaluate the nuclear Schiff moments considering both over-shell excitations and core excitations for the first \(1/2^+\) states of \(^{133}\text{Xe}\) and \(^{135}\text{Xe}\). Table 1 shows the numerical results for the Schiff moment in eq. (8). Here we take as an energy denominator, each single particle energy difference between one orbital in the 50–82 shell, and another orbital outside the 50–82 shell. If there are several orbitals that connect each other by the Schiff moment operator, we take the largest single particle energy difference for the energy denominator. The single-particle energy of each orbital is taken from the Nilsson model. As seen in Table 1, Schiff moments do not greatly differ in \(^{133}\text{Xe}\) and \(^{135}\text{Xe}\), and both of them have large contributions for the isotensor part.

Next we investigate the contribution from each excitation one by one. Table 2 shows the Schiff moment for \(^{135}\text{Xe}\) from each orbital excited to the shell over 82 (over-shell excitations). Schiff moments greatly change from orbital to orbital. The \(0h_{9/2, 1f_{5/2}}\) contributions are large and contributions from orbitals located at higher energy like \(1g_{9/2}\) and \(0i_{11/2}\) are small. The isospin dependence is similar from orbital to orbital, and the contribution from the isotensor component is the largest in most of the cases.

Table 3 shows the Schiff moment contributed from each orbital in the shell under 50 (core excitations). Similar to the over-shell excitations, they have orbital dependences. The \(0g_{9/2}\) contribution becomes the largest. Most core excitations have larger components compared to the over-shell excitations, and the \(0g_{9/2}\) contribution is almost ten times larger than the largest contribution of over-shell excitations. Since the sign of \(0g_{9/2}\) contribution is opposite to other contributions, this contribution cancels with a sum of other contributions. We do not show results for \(^{133}\text{Xe}\) here, but only to note that its Schiff moment is found to be similar to that of \(^{135}\text{Xe}\).

Next, we estimate the upper limit of the atomic EDM using the Schiff moment we have just calculated. The Schiff moment coming from the isoscalar component for...
$^{135}$Xe is given by (see Table 1)

$$S^{(0)}(^{135}\text{Xe}) = 1.79 \times 10^{-3} \, \tilde{g}^{(0)} \, g \, \text{efm}^3.$$  \hfill (9)

The relation between the Schiff moment and the atomic EDM for $^{129}$Xe is given as

$$d_{\text{Atom}}^{^{129}\text{Xe}} = 0.38 \times 10^{-17} \left( \frac{S}{\text{efm}^3} \right) \text{ cm}$$  \hfill (10)

in Ref. [20]. We assume that this estimation is also applicable for $^{135}$Xe. The upper limit of the coefficient $\tilde{g}^{(0)}$ for the parity and time-reversal violating interaction is estimated from the Hg experiment [6] as $|\tilde{g}^{(0)}g| < 1.1 \times 10^{-10}$. Using these relations, we estimate the upper limit of the atomic EDM for the spin $1/2^+$ state of $^{135}$Xe as

$$\left| d_{\text{Atom}}^{^{135}\text{Xe}(1/2^+)} \right| < 7.4 \times 10^{-31} \text{ cm.}$$  \hfill (11)

It should be noted that the observed EDM is a sum of all contributions such as other isospin components and the Schiff moment coming from the intrinsic nucleon EDM [8].

### 4 Summary

In this study we have evaluated nuclear Schiff moments for $^{133}$Xe and $^{135}$Xe nuclei using the nuclear shell model. We have calculated the contribution from each orbital to Schiff moments, and estimated the upper limit of the atomic EDM from the Schiff moment for $^{135}$Xe. We have found that the orbital dependence for the Schiff moment is large and the contributions of core excitations are one order of magnitude larger than those from the over-shell excitations. By analyzing the Schiff moments in more detail, we can find nuclei that have larger Schiff moments. As a future work, we will investigate $^{129}$Xe nucleus to estimate its Schiff moment without a closure approximation.

### References
