Atomic electric dipole moments of He and Yb induced by nuclear Schiff moments

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(Dated: February 1, 2008)

We have calculated the atomic electric dipole moments (EDMs) \(d\) of \(^{3}\text{He}\) and \(^{171}\text{Yb}\) induced by their respective nuclear Schiff moments \(S\). Our results are \(d(^{3}\text{He}) = 8.3 \times 10^{-28} \text{ e cm}\) and \(d(^{171}\text{Yb}) = -1.9 \times 10^{-28} \text{ e cm}\). By considering the nuclear Schiff moments induced by the parity and time-reversal violating nuclear-nucleon interaction we find \(d(^{171}\text{Yb}) \sim 0.6d(^{199}\text{Hg})\). For \(^{3}\text{He}\) the nuclear EDM coupled with the hyperfine interaction gives a larger atomic EDM than the Schiff moment. The result for \(^{3}\text{He}\) is required for a neutron EDM experiment that is under development, where \(^{3}\text{He}\) is used as a comagnetometer. We find that the EDM for \(^{3}\text{He}\) is orders of magnitude smaller than the neutron EDM. The result for \(^{171}\text{Yb}\) is needed for the planning and interpretation of experiments that have been proposed to measure the EDM of this atom.

PACS numbers: PACS: 32.80.Ys,31.15.Ar,21.10.Ky

I. INTRODUCTION

There are a number of experiments underway to measure the time-reversal violating electric dipole moment (EDM) of the neutron and of various atoms and molecules. The measurement of a non-zero EDM would signal the presence of new sources of CP violation beyond the standard model, standard model EDMs being undetectably small \([1]\).

The best limit on the neutron EDM is \(|d_n| < 2.9 \times 10^{-28} \text{ e cm (90\% c.l.)}\) \([2]\) and that on an atomic EDM has been obtained for \(^{199}\text{Hg}\), \(|d(^{199}\text{Hg})| < 2.1 \times 10^{-28} \text{ e cm (95\% c.l.)}\) \([3]\). The result for \(^{199}\text{Hg}\) constrains new physics scenarios largely in the nuclear sector, since \(^{199}\text{Hg}\) is a diamagnetic atom (total electronic angular momentum \(J = 0\)) and in lowest order the electric field couples to the nuclear spin.

The EDM in induced most efficiently from a nuclear Schiff moment; this is essentially a residual nuclear EDM (largely screened by atomic electrons) and is non-zero due to the finite size of the nucleus \([4]\).

In this work we calculate the atomic EDMs for \(^{3}\text{He}\) and \(^{171}\text{Yb}\) induced by their respective nuclear Schiff moments. The result for \(^{3}\text{He}\) is required for a neutron EDM experiment that is under development, where \(^{3}\text{He}\) is used as a comagnetometer \([5, 6]\). There are proposals to measure the time-reversal violating electric dipole operator. The \(P,T\)-odd interaction \(H_{PT}\) can be expressed as

\[
d = 2 \sum_M \frac{\langle M | D_z | N \rangle}{E_N - E_M},
\]

where the sum \(M\) runs over a complete set of many-body states, \(E_N\) and \(E_M\) are atomic energies, and \(D_z\) is the atomic electric dipole operator. The \(P,T\)-odd interaction Hamiltonian \(H_{PT}\) has the form

\[
H_{PT} = \sum_i h_{PT}^i = -e \sum_i \varphi(R_i),
\]

where \(\varphi\) is the electrostatic potential produced by the nuclear Schiff moment \(S\) which mixes states of opposite parity. The form for this potential that is suitable for relativistic atomic calculations is \([14]\)

\[
\varphi(R) = -\frac{3S \cdot R}{B} \rho(R),
\]

II. METHOD OF CALCULATION

The method we use in the current work is the same as one of the methods we used in our earlier work \([12]\).
where $B = \int \rho(R)R^4dR$ and $\rho(R)$ is the nuclear density.

In the $V^N$ approximation, we can write the atomic EDM induced by the Schiff moment as

$$d = 2 \sum_n \langle \delta n_{PT}|d_z|n\rangle,$$

(4)

where the sum runs over the relativistic Hartree-Fock core states $|n\rangle$, $d_z$ is the single-particle dipole operator, and $\delta n_{PT}$ denotes the correction to the state $|n\rangle$ due to the $P,T$-odd Hamiltonian $h_{PT}$. The correction $|\delta n_{PT}|$ can be expressed as

$$|\delta n_{PT}| = \sum_\alpha \langle \alpha|h_{PT}|n\rangle/\epsilon_n - \epsilon_\alpha |\alpha\rangle,$$

(5)

where $|\alpha\rangle$ corresponds to an excited state. It is found by solving the equation

$$(h_0 - \epsilon_n)|\delta n_{PT}| = -h_{PT}|n\rangle.$$

(Equivalently, one may calculate the correction to $|n\rangle$ from the electric dipole (E1) field and take the matrix element of the weak Hamiltonian to obtain $d$.)

In the $V^N$ approximation, polarization of the core due to the fields $h_{PT}$ and $d_z$ is accounted for by including the polarization due to one field using the TDHF method, e.g., by replacing $h_{PT}$ in (4) by $\tilde{h}_{PT} = h_{PT} + \delta V_{PT}$, since $\sum_n \langle \delta n_{PT}|d_z|n\rangle = \sum_n \langle \delta n_{PT}|d_z + \delta V_d|n\rangle$.

As a test of our wave functions we have performed calculations for the ionization potentials and the scalar polarizabilities $\alpha$ of the ground-state for each atom and compared them with the available experimental data. The polarizability has the same form as the EDM, Eq.1

$$\alpha = -2 \sum_M |\langle N|D_z|M\rangle|^2/(E_N - E_M),$$

(7)

with the operator $H_{PT}$ in (1) replaced by the dipole operator $D_z$. So the scalar polarizabilities are calculated simply by replacing the correction $|\delta n_{PT}|$ due to the $P,T$-odd field by the correction $|\delta n_d|$ due the E1 field.

III. RESULTS OF ATOMIC CALCULATIONS

In Table I we present our results for the ionization potentials and scalar polarizabilities for He and Yb alongside the available experimental data. It is seen that the results for helium are in good agreement with experiment, while for Yb a deviation of about 15% is seen for the ionization potential.

Results for the atomic EDMs for He and Yb induced by their respective nuclear Schiff moments are listed in Table II. For comparison and easy reference we have also presented in the table the results from our previous work [12], calculated in the approximation $V^N$. The He EDM is very small, $\sim 10^{-21}(S/(e\text{ fm}^3))$ e cm, and is stable with inclusion of core polarization, the value changing by $\sim 10\%$.

As with Hg and Ra [12], the largest contribution to the atomic EDM for Yb comes from the outer $s$ electrons and this differs in sign to the overall contribution from the core. The final result for Yb is about 60% of the size of the Hg EDM (in terms of their Schiff moments). Our numerical result for Yb agrees with an estimate obtained by scaling the Hg result, $d(171\text{Yb}) \sim d(199\text{Hg})(SZ^2)^{Yb}/(SZ^2)^{\text{Hg}} \sim 1.65\text{(Yb)}/\text{S(Hg)}$, in the units of Table II $Z$ is the nuclear charge, and $R$ is a relativistic enhancement factor; see Refs. [18] and [19], respectively, where the parametric dependence was found and more recently applied.

One may be concerned about the huge corrections to Yb coming from inclusion of core polarization, the final value being over four times the HF value. We remind the reader that in our previous work [12] we also saw such corrections (for Ra and to a lesser extent Hg, see Table I). In Ref. [12] an entirely different method for the calculation of many-body corrections was also carried out and yielded results for the EDMs of Hg and Ra that differ from those obtained in the $V^N$ approximation by less than 10%.

We expect that the TDHF value for the EDM of Yb is accurate to about 20-30%, the result for He more accurate.

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### Table I: Ionization potentials (IP, in cm$^{-1}$) and scalar polarizabilities ($\alpha$, in $a_0^3$) for He and Yb

| Atom | HF | Exp. | TDHF | Exp. |
|------|----|------|------|------|
| He   | 201472 | 198311 | 0.997 | 1.32 |
| Yb   | 43130 | 50443 | 124 | 179 |

*Ref. [12]*

### Table II: Atomic EDMs $d$ induced by respective nuclear Schiff moments $S$ in the HF and TDHF approximations, units are $10^{-21}(S/(e\text{ fm}^3))$ e cm

| Z   | Atom | HF      | TDHF   |
|-----|------|---------|--------|
| 2   | He   | 0.743 $\times$ 10$^{-4}$ | 0.826 $\times$ 10$^{-4}$ |
| 54  | Xe   | 0.289   | 0.378  |
| 70  | Yb   | -0.416  | -1.91  |
| 80  | Hg   | -1.19   | -2.97  |
| 86  | Rn   | 2.47    | 3.33   |
| 88  | Ra   | -1.85   | -8.23  |

*Ref. [12]*

IV. ATOMIC EDMS IN TERMS OF THE $P,T$-ODD NUCLEON-NUCLEON INTERACTION

We’d like to express the atomic EDMs for He and Yb in terms of a more fundamental parameter, in particu-
lar, the parameter specifying the strength of the $P,T$-violating nucleon-nucleon interaction $\eta_{NN}$; we are interested in this interaction because it leads to the largest Schiff moments. This will give a better idea of the relative sensitivities of various atomic EDMs to fundamental physics. For instance, an order of magnitude enhancement of the nuclear Schiff moment may occur for deformed nuclei with close levels of opposite parity [18] (see also Refs. [20, 21] where nuclear EDM enhancement was considered); even more spectacular is the orders of magnitude enhancement that may arise in nuclei with octupole deformation [22, 23].

The ground state of $^{171}$Yb has quantum numbers $J^\pi = 1/2^-$ and the magnetic moment is very close ($\sim 10\%$) to that of the neutron; we consider that in the ground state there is an unpaired neutron in the state $s_{1/2}$. According to Ref. [18], the nuclear Schiff moment for $^3$He is $S(^3\text{He}) \sim 10^{-8} \eta_{np}$ cm. The Schiff moment scales with atomic mass $A$ as $A^{2/3}$. Scaling from $^{199}$Hg, $S(^3\text{He}) \sim S(^{199}\text{Hg}) \times (3/199)^{2/3} \sim 10^{-8} \eta_{np}$ cm, so the result of Ref. [18] looks reasonable. The induced atomic EDM will then be $d(^3\text{He}) \sim 10^{-30} \eta_{np}$ cm.

However, for very light atoms the finite size effect (Schiff moment) does not lead to the largest atomic EDMs. Another way to violate the screening of the nuclear EDM is to take account of magnetic fields. Considering the hyperfine interaction, an order of magnitude estimate for the atomic EDM arising from a nuclear EDM is [24]

$$d_{\text{atom}}(^3\text{He}) \sim Z \alpha^2 m_e d_{\text{nuc}}(^3\text{He}) ,$$

where $Z$ is the nuclear charge, $\alpha$ is the fine structure constant, $m_e$ and $m_p$ are electron and proton masses, and the nuclear EDM is denoted $d_{\text{nuc}}(^3\text{He})$. A more involved estimate was performed earlier by Schiff who obtained $|d(^3\text{He})| = 1.5 \times 10^{-7} d_{\text{nuc}}(^3\text{He})$ [4]. Using the value $d_{\text{nuc}}(^3\text{He}) \sim 10^{-21} \eta_{np}$ cm from Ref. [18], the size of the induced atomic EDM is then

$$|d(^3\text{He})| \sim 1.5 \times 10^{-28} \eta_{np} \text{ cm},$$

larger than that induced by the nuclear Schiff moment. The size of the neutron EDM induced by the nucleon-nucleon interaction is $d_n = 0.5 \times 10^{-23} \eta_{np}$ cm [18], and therefore it is seen that the atomic EDM of $^3\text{He}$ is negligibly small compared to the neutron EDM $d_n$.

$$d(^3\text{He}) \sim 3 \times 10^{-5} d_n .$$

V. SUMMARY

We have calculated the atomic EDMs for $^3\text{He}$ and $^{171}$Yb induced by their respective nuclear Schiff moments with the results $d(^3\text{He}) = 8.3 \times 10^{-5}$ and $d(^{171}\text{Yb}) = -1.9$ in units $10^{-17} (S/(e \text{ fm}^3))$ cm. The accuracy is about 20-30\% for Yb and is better for He. We also estimated the sizes of the nuclear Schiff moments induced by the $P,T$-violating nucleon-nucleon interaction. We find $d(^{171}\text{Yb}) \sim 0.6 d(^{199}\text{Hg})$. For $^3\text{He}$ the nuclear EDM coupled with the hyperfine interaction gives a larger atomic EDM than the Schiff moment. Nevertheless, the helium EDM is orders of magnitude smaller than the neutron EDM and therefore may be neglected in the neutron experiment [5, 6].

Acknowledgments

We thank B. Filippone for motivating our work for $^3\text{He}$. This work was supported by the Australian Research Council.

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