EDM OPERATOR FREE FROM SCHIFF’S THEOREM

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ABSTRACT

We present generalized Schiff’s transformation on electric dipole moments (EDM) in quantum field theory. By the unitary transformation, the time and parity violating interaction $i \frac{ge}{2} \bar{\psi} \sigma_{\mu\nu} \gamma_5 \psi F^{\mu\nu}$ is transformed into a new form, but its nonrelativistic reduction has a unique form, which is free from Schiff’s theorem. The relativistic corrections to the new EDM operator turn out to be a small increase to the EDM as given by $b_2 (\alpha Z)^2$ with $b_2 \simeq 2$. Therefore, the calculation of the EDM with nonrelativistic Hartree-Fock wave functions presents the most conservative but reliable estimation for the enhancement factor of the EDM in atoms.

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1. **Introduction**

Symmetries in physics are fundamental for understanding nature. The highest symmetry in quantum field theory is the CPT (charge conjugation, parity and time reversal) invariance. Any field theoretical models should be consistent with the CPT theorem. The next highest symmetry may be the time reversal invariance. Indeed, the T-invariance is also kept well in most of the field theoretical models.

It is of fundamental interest to find the T-violating interactions in nature. Electric dipole moments (EDM) of particles, nuclei and atoms in ground state reveal the violation of the T-invariance. Until now, the upper limit of the neutron EDM is around $-(3 \pm 5) \times 10^{-26}$ e · cm [1].

There have been many experimental efforts to measure the EDM of the atomic systems. The best example is found for the EDM of $^{199}$Hg [2]. In this case, however, one has to be careful for extracting the EDM of the electrons or nucleons from the measurement of the atomic EDM since there is Schiff’s theorem [3]. 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.

Due to the presence of Schiff’s theorem, people have long believed that the calculation of the enhancement factor in atomic systems should be carried out by employing the relativistic many body wave functions. However, it is not clear to what extent the Dirac Hartree-Fock method for the relativistic many body wave functions can be reliable. In fact, the Dirac Hartree-Fock method may well have some conceptual difficulties since the relativistic many body theory should be treated by field theories. The relativistic quantum mechanics is well defined only for the one body case.
In this sense, it is of particular importance to find a way to estimate the EDM enhancement factor which does not depend on the ambiguity arising from atomic wave functions.

In this paper, we present a generalization of Schiff’s transformation which is extended to the quantum field theory of electrodynamics. We show that the T and P-violating interaction \( ig e \bar{\psi} \sigma_{\mu\nu} \gamma_5 \psi F^{\mu\nu} \) is transformed into a new form which has a unique shape of the nonrelativistic reduction. For this operator, we can reliably calculate the EDM of the atomic system with nonrelativistic Hartree-Fock wave functions.

In particular, the estimation of the EDM with Dirac wave functions in hydrogen-like atoms shows that we can write the EDM \( d_Z \) of the atoms with \( Z \) in units of electric EDM \( d_e \) as

\[
d_Z = \frac{b_0 b_1}{\epsilon_0} (Z\alpha)^2 \left(1 + b_2 (Z\alpha)^2\right) d_e \tag{1.1}
\]

where \( b_0, b_1 \) and \( \epsilon_0 \) are dimensionless constants which are determined by the nonrelativistic wave functions. \( b_2 \) is a positive number around \( b_2 \simeq 2 \). Eq.(1.1) indicates that the relativistic corrections are of the order of \((\alpha Z)^2\), and therefore they cannot be very large. Further, the relativistic effects must be smaller for the Hartree-Fock case than the hydrogen-like atoms since the Hartree-Fock effects always push the electron of the last orbit outward and thus the relativity becomes less.

On the other hand, many body effects on the EDM are very large. This is mainly due to the fact that the EDM operator is, roughly speaking, proportional to \( \frac{1}{r^2} \), and thus the many body wave functions which are pushed outward due to electron electron repulsions reduce the EDM expectation values by an order of magnitude compared to the hydrogen-like wave function. Thus, the careful treatment of the many body effects is much more important than the relativistic corrections to the EDM.
In this paper, we calculate the EDM for the hydrogen, Li and Cs atoms as examples and estimate the EDM with the nonrelativistic Hartree-Fock wave functions. In particular, it is found that the enhancement factor of Cs atom in comparison with the electron EDM $d_e$ is 91.2, which should be compared with the previous estimations of 100-150 [4-10].

This paper is organized in the following way. In the next section, we explain briefly Schiff’s theorem in the nonrelativistic quantum mechanics. Then, section 3 treats the field theoretical version of the Schiff transformation. In section 4, we evaluate the Foldy-Wouthuysen transformation of the relativistic EDM operator and obtain a unique form of the EDM operator which has no influence from Schiff’s theorem. In section 5, we carry out the numerical evaluations of the EDM with the hydrogen-like wave functions. In particular, we compare the calculations with nonrelativistic and relativistic wave functions. In section 6, we present our calculations of the EDM with nonrelativistic Hartree-Fock wave functions. Section 7 summarizes what we have clarified in this paper.

2. Schiff’s theorem in quantum mechanics

Here, we first review the shielding mechanism which was initially found by Schiff [3]. We consider the hamiltonian $H_{0}^{NR}$ of the atomic system which is interacting through the Coulomb force as well as the external electric field $E^{ext}$,

$$H_{0}^{NR} = \sum_{i} \left( \frac{p_i^2}{2m_i} - eA_0(r_i) + e r_i \cdot E^{ext} \right)$$ (2.1)
where $A_0(r_i)$ is given as

$$A_0(r_i) = \frac{Ze}{r_i} - \frac{1}{2} \sum_{j \neq i} \frac{e}{|r_i - r_j|}. \quad (2.2)$$

To this system, we consider the T-and P-violating interaction $H_{edm}^{NR}$

$$H_{edm}^{NR} = -\sum_i d_i \cdot E_i \quad (2.3)$$

where $E_i$ is defined as

$$E_i = -\nabla_i A_0(r_i) + E^{ext} \quad (2.4)$$

d_i represents the EDM of the $i$-th particle and can be written as

$$d_i = ge\sigma_i \quad (2.5)$$

where $\sigma_i$ represents the spin operator of the $i$-th particle. $g$ is a constant and represents the strength of the T and P-violating interaction, and it has the dimension of the length.

Schiff’s theorem states that the total hamiltonian $H^{NR} = H_0^{NR} + H_{edm}^{NR}$ is related to the $H_0^{NR}$ by the unitary transformation (Schiff transformation) in the following way

$$H^{NR} = H_0^{NR} + H_{edm}^{NR} = \exp \left( -i \sum_i \frac{1}{e} p_i \cdot d_i \right) H_0^{NR} \exp \left( i \sum_i \frac{1}{e} p_i \cdot d_i \right) \quad (2.6a)$$

since we can easily evaluate the righthand side of eq.(2.6a)

$$\exp \left( -i \sum_i \frac{1}{e} p_i \cdot d_i \right) H_0^{NR} \exp \left( i \sum_i \frac{1}{e} p_i \cdot d_i \right) = H_0^{NR} - \sum_i d_i \cdot E_i + O(g^2). \quad (2.6b)$$

Therefore, up to the order of $g$, eq.(2.6a) holds. By the unitary transformation, one obtains the same energy spectrum between $H^{NR}$ and $H_0^{NR}$. Therefore, this means that the effect of the $H_{edm}^{NR}$ is absorbed into the original hamiltonian and thus cannot be observed at all. This is Schiff’s theorem.
In his paper, Schiff argued that the shielding of the EDM may be violated by the relativistic effects or some other effects like the addition of the strong interactions.

In what follows, we consider the Schiff transformation for the relativistic case.

3. Schiff transformation in QED

(a) Schiff transformation in lagrangian formulation

Now, we want to generalize Schiff’s theorem to the field theory. Here, we only consider the QED. The lagrangian density for fermions interacting with the gauge field can be written as

\[ \mathcal{L}_0 = \bar{\psi}(i\gamma_{\mu}D^\mu - m_0)\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu} \]  

(3.1)

where \( D_{\mu} \) and \( F_{\mu\nu} \) denote the covariant derivative and the field tensor, respectively and are given as

\[ D_{\mu} = \partial_{\mu} + ieA_{\mu} \]  

(3.2a)

\[ F_{\mu\nu} = \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu}. \]  

(3.2b)

In addition to the above lagrangian, we consider the T-and P-violating interaction which may presumably be induced by the supersymmetric model with some soft breaking interactions[11]. The T-and P-violating effective interaction can be given as

\[ \mathcal{L}_{edm} = -i\frac{ge}{2}\bar{\psi}\sigma_{\mu\nu}\gamma_{5}\psi F^{\mu\nu} \]  

(3.3)
where $\sigma_{\mu\nu}$ is defined as

$$\sigma_{\mu\nu} = \frac{i}{2}(\gamma_\mu \gamma_\nu - \gamma_\nu \gamma_\mu). \quad (3.4)$$

The corresponding Hamiltonian of eq.(3.3) which depends on the electric field can be written as

$$H_{edm}^{R_1} = -ge\gamma_0 \Sigma \cdot E \quad (3.5a)$$

where we define the relativistic spin operator $\Sigma$ as $\Sigma = \gamma^0 \gamma^5 \gamma$. Here, if we take a simple nonrelativistic limit of this operator, the Hamiltonian becomes

$$H_{edm}^{R_1} \simeq -ge\sigma \cdot E. \quad (3.5b)$$

Since the $d$ is written as $d = ge\sigma$, this just corresponds to the $H_{edm}^{NR}$. Now, we consider the following unitary transformation

$$\psi' = \exp(i g \gamma_5 p_\mu \gamma^\mu) \psi. \quad (3.6)$$

Under this transformation, the total lagrangian density $L = L_0 + L_{edm}$ becomes up to the order of $g$

$$L = L_0 - 2ig\bar{\psi}\gamma_5(p_\mu p^\mu - eA_\mu p^\mu)\psi. \quad (3.7)$$

This shows that the unitary transformation of eq.(3.6) completely cancels out the $L_{edm}$ term of eq.(3.3), but a new term $2ig\bar{\psi}\gamma_5 p_\mu p^\mu \psi$ appears.

Now, we want to make the corresponding Hamiltonian. In this case, we should make the conjugate momentum $\Pi_{A_0}$ for the $A_0$ and $\Pi_\psi$ for the $\psi$. It is clear that the terms proportional to the $p_0$ disappear from the Hamiltonian. Therefore, the new EDM Hamiltonian becomes

$$H_{edm}^{R_2} = 2ig\gamma_0 \gamma_5(p_0^2 - \mathbf{p}^2). \quad (3.8)$$
This is a new EDM hamiltonian which should be compared with the original one in eq.(3.5a). We should also note that the similar EDM hamiltonian is obtained in ref.[12]. In this case, the $p_0^2$ term is missing since they treat it in terms of the hamiltonian. Instead, we treat the problem in a covariant fashion. However, it is easy to see that the $p_0^2$ term does not contribute to the mixing of the wave functions since it does not depend on the coordinates. In this respect, we reproduce the result obtained in ref.[12] with the lagrangian formulation with the full relativistic covariance.

The important point is that the new EDM hamiltonian is free from Schiff’s theorem. Therefore, this term indeed contributes to the generation of the EDM.

Here, we should comment on the physical meaning of the unitary transformation of eq.(3.6). Under the transformation, we obtain a new lagrangian density which does not couple to the external electromagnetic field. This is just the statement which corresponds to Schiff’s theorem. Namely, the EDM can only be induced from the second order effect of the new hamiltonian as will be treated later in eq.(5.2).

(b) Schiff transformation in hamiltonian formulation

Next, we show here the same type of proof for the Dirac hamiltonian since the EDM leftover can be also obtained from the Dirac hamiltonian. This method is similar to the above proof of the field theory, but the transformation operator is different from the field theory treatment, but is the same as the nonrelativistic Schiff transformation.

The Dirac hamiltonian for fermions interacting with the Coulomb force
can be written as
\[ H_R^0 = \sum_i^N \left( p_i \cdot \alpha_i + m_i \gamma_i^0 - eA_0(r_i) + e r_i \cdot E_{\text{ext}} \right). \]  
(3.9)

In this case, the EDM hamiltonian which corresponds to \( L_{edm} \) can be written as
\[ H_{edm}^{R1} = -ge \sum_i^N \gamma_i^5 \gamma_i \cdot E_i. \]  
(3.10)

Here, we can rewrite the Hamiltonian \( H_{edm}^{R2} \) as
\[ H_{edm}^{R1} = -ge \sum_i^N \Sigma_i \cdot E_i - ge \sum_i^N (\gamma_i^0 - 1) \Sigma_i \cdot E_i. \]  
(3.11)

In this case, one can easily check that the first term of eq.(3.11) is canceled out by the Schiff transformation in the same way as the non-relativistic case of eq.(2.6a), and the following equation holds up to the order of \( g^{[13]} \).
\[ H_0^R - ge \sum_i^N (\gamma_i^0 - 1) \Sigma_i \cdot E_i = \exp \left( i \sum_i g p_i \cdot \Sigma_i \right) (H_0^R + H_{edm}^{R1}) \exp \left( -i \sum_i g p_i \cdot \Sigma_i \right). \]  
(3.12)

Therefore, the leftover is just the second term of eq.(3.11), and we define \( H_{edm}^{R3} \) as
\[ H_{edm}^{R3} = -ge \sum_i^N (\gamma_i^0 - 1) \Sigma_i \cdot E_i. \]  
(3.13)

In the next section, we will prove that the two terms (eq.(3.8) and eq.(3.13)) have the identical shape of the nonrelativistic reduction under the Foldy-Wouthuysen transformation. This nonrelativistic EDM operator is free from Schiff’s theorem.
4. **Nonrelativistic reduction of EDM operator**

When we want to evaluate operators which are expressed in the relativistic form, we should prepare wave functions which are obtained relativistically. In atomic systems with high Z, the lowest state is indeed quite relativistic. However, the system we are treating is not the hydrogen-like atom but real atoms. As an example, let us consider the Cs atom. In this case, there are many electrons around, and the state for the last electron in the ground state is 6s state which is far from relativistic. Therefore, we should rather obtain the EDM operator which is reduced to the nonrelativistic form. Since the EDM operators obtained in the last section are free from Schiff’s theorem, we should make the reliable nonrelativistic reduction of the operator.

Here, we employ the Foldy-Wouthuysen transformation which is a unitary transformation. It is here noted that the nonrelativistic reduction should be done at the last stage. Otherwise, one often makes mistakes since the Foldy-Wouthuysen transformation does not necessarily commute with other unitary transformation. Since the nonrelativistic reduction is an approximation, one has to do it after one has made other unitary transformations.

In the case of the EDM operator, we have obtained the two different Hamiltonians, eqs.(3.8) and (3.13). Here, we rewrite them again as the one body operators,

\[
H_{edm}^{R2} = 2i g \gamma_0 \gamma_5 (p_0^2 - \mathbf{p}^2) \tag{3.8}
\]

\[
H_{edm}^{R3} = -ge(\gamma^0 - 1) \Sigma \cdot \mathbf{E} \tag{3.13}
\]

They look very much different from each other. Now, we want to make the nonrelativistic reduction of the two operators.

By the Foldy-Wouthuysen transformation which is the most reliable method
for the nonrelativistic reduction, we write the reduced hamiltonian after some repeated operations of the transformation [14],

$$H_{FW} = \gamma_0 \left( m + \frac{\mathcal{O}^2}{2m} - \frac{\mathcal{O}^4}{8m^3} \right) + \mathcal{E} - \frac{1}{8m^2}[\mathcal{O}, [\mathcal{O}, \mathcal{E}]]$$  \hspace{1cm} (4.1)

where $\mathcal{O}$ and $\mathcal{E}$ denote the odd and even operators in the gamma matrix space.

In the case of the EDM hamiltonian of eq.(3.8), the $\mathcal{O}$ and $\mathcal{E}$ can be written as

$$\mathcal{O} = \alpha \cdot \mathbf{p} - 2ig\gamma_0\gamma_5 \mathbf{p}^2$$  \hspace{1cm} (4.2a)

$$\mathcal{E} = -eA_0 + e\mathbf{r} \cdot \mathbf{E}^{ext}.$$  \hspace{1cm} (4.2b)

On the other hand, for the EDM hamiltonian of eq.(3.13), the $\mathcal{O}$ and $\mathcal{E}$ become

$$\mathcal{O} = \alpha \cdot \mathbf{p}$$  \hspace{1cm} (4.3a)

$$\mathcal{E} = -eA_0 - ge(\gamma^0 - 1) \Sigma \cdot \mathbf{E} + e\mathbf{r} \cdot \mathbf{E}^{ext}.$$  \hspace{1cm} (4.3b)

After some straightforward calculation, we obtain the nonrelativistic hamiltonian for both of the cases of eq.(3.8) and eq.(3.13),

$$V_{edm} = \frac{ge}{2m^2} \left[ (\mathbf{\sigma} \cdot \mathbf{E}) \nabla^2 - \rho(r)(\nabla \cdot \mathbf{\sigma}) - 2(\mathbf{E} \cdot \nabla)(\mathbf{\sigma} \cdot \nabla) \right]$$  \hspace{1cm} (4.4)

where $\rho(r)$ and $\mathbf{E}$ are defined as

$$\rho(r) = -\nabla^2 A_0(r),$$  \hspace{1cm} (4.5a)

$$\mathbf{E} = -\nabla A_0(r) + \mathbf{E}^{ext},$$  \hspace{1cm} (4.5b)

$$A_0(r) = \frac{Ze}{r} + \int \frac{\rho_0(r')}{|\mathbf{r} - \mathbf{r}'|} d^3 r'$$  \hspace{1cm} (4.5c)

with $\rho_0(r) = -e \sum_n |\psi_n(r)|^2$.

This is a proof that the apparent two different shapes of the relativistic hamiltonian eqs.(3.8) and (3.13) reduce to the identical and thus unique nonrelativistic hamiltonian.
As we stressed before, this hamiltonian is free from Schiff’s theorem. Therefore, there is definitely some mixture due to this operator between the opposite parity states like the 6s and 6p states.

5. **EDM with hydrogen-like wave functions**

Since we obtain the EDM operator which is free from Schiff’s theorem, we can now reliably calculate the EDM in actual cases. Before going to the calculations with the Hartree-Fock wave functions (in section 6), we first present our calculations with the hydrogen-like wave functions. The hydrogen-like wave functions are obviously far from reality in atoms since the interactions between electrons are very important, and thus the wave functions in the hydrogen-like atoms are quite different from the Hartree-Fock wave functions. But the use of the hydrogen-like wave functions helps us understand the basic structure of the EDM operator. This is quite important since we can evaluate all the matrix elements analytically. In addition, it turns out that the EDM evaluated by the hydrogen-like atom wave functions presents the upper limit of the enhancement factor even though the overestimation is quite significant.

Here, we should note that the energy eigenvalues are replaced by the estimation using Hartree-Fock wave function since otherwise it is in fact meaningless to use the energy eigenvalues of the hydrogen-like atoms which are degenerate between \( ns_{\frac{1}{2}} \) and \( np_{\frac{1}{2}} \) states.

Here, we consider the atomic systems in which one electron is found in the outer shell like Li or Cs cases.
Now, we prepare the $ns_{\frac{1}{2}}$ and $np_{\frac{1}{2}}$ state wave functions which can be written as

$$\psi_{ns_{\frac{1}{2}}}(r) = \frac{1}{\sqrt{4\pi}} R_{ns}(r) \xi_{\frac{1}{2}}, \quad (5.1a)$$

$$\psi_{np_{\frac{1}{2}}}(r) = R_{np}(r) \sigma \cdot \hat{r} \sqrt{\frac{4\pi}{4\pi}} \xi_{\frac{1}{2}}, \quad (5.1b)$$

where $R_{ns}(r)$ and $R_{np}(r)$ represent the radial part of the atomic wave functions. $\xi_{\frac{1}{2}}$ denotes the spin part.

In this case, we obtain the effective EDM $d_Z$ for $ns_{\frac{1}{2}}$ state in atoms as

$$d_Z = -2e \sum_{n'} \frac{<ns_{\frac{1}{2}}|z|np_{\frac{1}{2}}> <np_{\frac{1}{2}}|V_{edm}|ns_{\frac{1}{2}}>}{E_{ns_{\frac{1}{2}}} - E_{n'p_{\frac{1}{2}}}}. \quad (5.2)$$

Here, we only consider the $n' = n$ case since this gives a dominant contribution to the EDM. Further, we consider the atomic system when only one electron is found in the outer shell. Therefore, the summation over $i$ is just one single particle only. Also, we neglect the term which depends on the $\rho$ in eq.(4.4) since it vanishes for the hydrogen-like atoms.

Now, we first evaluate the angular parts of the matrix elements $<ns_{\frac{1}{2}}|z|np_{\frac{1}{2}}>$ and $<np_{\frac{1}{2}}|V_{edm}|ns_{\frac{1}{2}}>$, and obtain

$$<\psi_{ns}|z|\psi_{np}> = \frac{1}{3} <R_{ns}|r|R_{np}> \quad (5.3a)$$

$$<\psi_{np}|V_{edm}|\psi_{ns}> = \frac{g}{2m^2} Z \alpha \int_{0}^{\infty} R_{np}(r) \left[ \frac{1}{r^2} \left( \frac{2}{r} \frac{d R_{ns}(r)}{dr} - \frac{d^2 R_{ns}(r)}{dr^2} \right) \right] r^2 dr. \quad (5.3b)$$

Now, we want to make the matrix elements dimensionless and therefore we write them as

$$<ns_{\frac{1}{2}}|z|np_{\frac{1}{2}}> = b_0 \frac{a_0}{Z} \quad (5.4a)$$

$$<np_{\frac{1}{2}}|V_{edm}|ns_{\frac{1}{2}}> = b_1 \frac{g}{2m^2} (Z \alpha) \left( \frac{Z}{a_0} \right)^4 \quad (5.4b)$$

where $a_0$ denotes the Bohr radius in hydrogen atom and is written as

$$a_0 = \frac{\hbar^2}{me^2}. \quad (5.5)$$
Further, we write the energy difference $\Delta E = E_{np_{\frac{1}{2}}} - E_{ns_{\frac{1}{2}}}$ as

$$\Delta E = \epsilon_0 m(Z\alpha)^2. \quad (5.6)$$

In this case, we can write the EDM as

$$d_Z = \frac{b_0 b_1}{\epsilon_0} (Z\alpha)^2 d_e. \quad (5.7)$$

In what follows, we estimate the values of the $b_0$ and $b_1$ which depend on the states. Here, before doing so, we should make a comment concerning the first order contribution of the $V_{edm}$ term which couples directly to the external field of $E^{ext}$. This contribution is a few orders of magnitude smaller than that of eq.(5.2). However, in the case of hydrogen ground state, the contribution amounts to 17% of eq.(5.2). Therefore, we take into account the first order contribution to the hydrogen case.

(a) **Li (Z=3) : nonrelativistic case**

In this case, the electron is in the $2s_{\frac{1}{2}}$ orbit. For the $b_0$ and $b_1$, we can easily evaluate them and find

$$b_0 = -\sqrt{3} \quad (5.8a)$$

$$b_1 = -\frac{1}{2\sqrt{3}}. \quad (5.8b)$$

In this case, we can evaluate the EDM assuming the energy difference from the estimation using the Hartree-Fock wave functions

$$\Delta E = 0.135 \frac{m_0 \alpha^2}{2}. \quad (5.9a)$$

Thus, we obtain

$$\epsilon_0 = 7.5 \times 10^{-3}. \quad (5.9b)$$

Therefore, we finally obtain for the EDM value of Li case

$$d_{Li} = 0.032d_e. \quad (5.10)$$
This value should be compared with the one obtained by the Hartree-Fock calculation. The EDM expectation value with the hydrogen-like wave function overestimates the EDM value by a factor of 5 as we will see later.

(b) Li (Z=3) : relativistic case

Here, we evaluate the EDM matrix element using Dirac wave functions which are solved in a pure Coulomb potential \( V(r) = -\frac{Z\alpha}{r} \). In this case, the wave function is specified by the quantum number \( n \) and \( \kappa \). The \( ns_\frac{1}{2} \) state \( (\kappa = -1) \) can be written as

\[
\Psi_{ns_\frac{1}{2}} = \left( \frac{1}{\sqrt{4\pi}} G_{n,\kappa,\xi_\frac{1}{2}} + i \frac{1}{\sqrt{4\pi}} F_{n,\kappa,\xi_\frac{1}{2}} \right).
\]

(5.11a)

Also, the \( np_\frac{1}{2} \) state \( (\kappa = 1) \) can be written as

\[
\Psi_{np_\frac{1}{2}} = \left( \frac{1}{\sqrt{4\pi}} \tilde{G}_{n,\kappa,\xi_\frac{1}{2}} - i \frac{1}{\sqrt{4\pi}} \tilde{F}_{n,\kappa,\xi_\frac{1}{2}} \right).
\]

(5.11b)

The analytic expressions of the radial wave functions \( G_{n,\kappa} \), \( F_{n,\kappa} \), \( \tilde{G}_{n,\kappa} \) and \( \tilde{F}_{n,\kappa} \) are given in Appendix.

In this case, we can first evaluate the angular parts of the EDM matrix elements as,

\[
< \Psi_{ns_\frac{1}{2}} | z | \Psi_{np_\frac{1}{2}} > = -\frac{1}{3} \int_{0}^{\infty} (G_{n,-1} \tilde{G}_{n,1} + F_{n,-1} \tilde{F}_{n,1}) r^3 dr
\]

(5.12a)

\[
< \Psi_{ns_\frac{1}{2}} | V_{edm} | \Psi_{np_\frac{1}{2}} > = -2gZ\alpha \int_{0}^{\infty} F_{n,-1} \tilde{F}_{n,1} dr.
\]

(5.12b)

Now, for Li case, the electron is in the \( n = 2 \) and \( \kappa = -1 \) state. After some calculations, we obtain for \( 2s_\frac{1}{2} - 2p_\frac{1}{2} \) case,

\[
< \Psi_{2s_\frac{1}{2}} | z | \Psi_{2p_\frac{1}{2}} > = -\sqrt{3} \left( 1 - \frac{5}{12}(\alpha Z)^2 \right) \left( \frac{a_0}{Z} \right)
\]

(5.13a)

\[
< \Psi_{2s_\frac{1}{2}} | V_{edm} | \Psi_{2p_\frac{1}{2}} > = -\frac{g}{2m^2}(\alpha Z) \left( \frac{Z}{a_0} \right)^4 \frac{1}{2\sqrt{3}} \left( 1 + \frac{13}{6}(\alpha Z)^2 \right).
\]

(5.13b)
Thus, we obtain the EDM with the relativistic wave functions as
\[
d_{R_{Li}} = 0.032 \left(1 + 1.75(\alpha Z)^2\right) d_e. \tag{5.14}
\]
Therefore, we can see that the relativistic correction to the EDM expectation value is of the order of \((\alpha Z)^2\), and thus it is quite small in this case.

(c) Cs (Z=55) : nonrelativistic case

In this case, the electron is in the \(6s_{\frac{1}{2}}\) orbit. For the \(b_0\) and \(b_1\), we can easily evaluate them and find
\[
b_0 = -3\sqrt{35} \tag{5.15a}
\]
\[
b_1 = -\frac{\sqrt{35}}{486}. \tag{5.15b}
\]
In this case, we can evaluate the EDM assuming the energy difference from the Hartree-Fock estimation
\[
\epsilon_0 = 1.31 \times 10^{-5}. \tag{5.16}
\]
Therefore, we finally obtain for the EDM value
\[
d_{Cs} = 2.66 \times 10^3 d_e. \tag{5.17}
\]
This value should be compared with the one obtained by the Hartree-Fock calculation. The EDM expectation value with the hydrogen-like wave function overestimates the EDM value by a factor of 30 as we will see later.

(d) Cs (Z=55) : relativistic case

In this case, the electron is in the \(n = 6\) and \(\kappa = -1\) states. After some calculations, we obtain for \(6s_{\frac{1}{2}} - 6p_{\frac{1}{2}}\) case.
\[
< \Psi_{6s_{\frac{1}{2}}} | z | \Psi_{6p_{\frac{1}{2}}} > = -3\sqrt{35} \left(1 - \frac{13}{84}(\alpha Z)^2\right) \left(\frac{a_0}{Z}\right) \tag{5.18a}
\]
Thus, we obtain the EDM with the relativistic wave functions as

\[ d_{Cs}^R = 2.66 \times 10^3 \left( 1 + 1.88(\alpha Z)^2 \right) d_e. \] (5.19)

Therefore, we can see that the relativistic correction to the EDM expectation value is again of the order of \((\alpha Z)^2\), and thus it is 30\% correction to the EDM. But we should note that the relativistic effect must be smaller for the relativistic Hartree-Fock case, and thus the relativistic correction to the EDM can be at most 30\%.

Here, we note that the contribution due to the next order term \((\alpha Z)^4\) is less than 10\%, and thus we do not have to worry about the higher order terms.

(e) **Hydrogen atom**

Finally, we want to present our calculation for the hydrogen atom. In this case, there is no stable \(2s_{1/2}\) state, and therefore there is no enhancement for the EDM. However, the hydrogen atom is best studied in many respects, and thus there might be some chance that one can observe the EDM for this case with very high precision.

Obviously, we have the wave functions analytically, and thus we can calculate the EDM in a closed form. Since the \(2s_{1/2}\) state is not stable, we consider the ground state \((1s_{1/2})\) which can be mixed with the \(2p_{3/2}\) state.

For the \(b_0\) and \(b_1\), we can easily evaluate them and find

\[ b_0 = \frac{128\sqrt{6}}{729}, \] (5.20a)

\[ b_1 = -\frac{16}{9\sqrt{6}}. \] (5.20b)
Since the energy difference is obtained as

\[ \Delta E = \frac{3}{8} m \alpha^2 \] (5.21a)

we obtain

\[ \epsilon_0 = \frac{3}{8}. \] (5.21b)

Finally we obtain the EDM for the hydrogen

\[ d_H = -5.32 \times 10^{-5} d_e. \] (5.22a)

which should be compared with Sandars calculation [5],

\[ d_H = -2\alpha^2 d_e = -10.7 \times 10^{-5} d_e. \] (5.22b)

The difference between them is due to the fact that Sandars took into account all of the \( np_{\frac{1}{2}} \) states while we consider only the first excited state of \( 2p_{\frac{1}{2}} \).

This is quite small and therefore it is not very clear whether one can choose the hydrogen atom for the EDM experiment.

6. EDM from Hartree-Fock wave functions

In the previous section, we have presented the EDM calculations with hydrogen-like wave functions. Now, we evaluate the EDM with the non-relativistic Hartree-Fock wave functions [15].

Unfortunately, we cannot obtain the Hartree-Fock wave functions analytically, and thus we have to carry out all of the calculations numerically. However, since the basic expressions are given in terms of the hydrogen-like wave functions, we can follow the same notations.
(a) Li (Z=3) : Hartree-Fock wave function

In this case, the electron is in the $2s_{\frac{1}{2}}$ orbit. For the $b_0$ and $b_1$, we can evaluate them and find

\[ b_0 = -4.17 \tag{5.23a} \]

\[ b_1 = -0.029. \tag{5.23b} \]

Now the energy difference between $2s_{\frac{1}{2}}$ and $2p_{\frac{1}{2}}$ states is calculated to be

\[ \Delta E = 0.135 \frac{ma^2}{2}. \tag{5.24a} \]

Therefore, we obtain

\[ \epsilon_0 = 7.5 \times 10^{-3}. \tag{5.24b} \]

Thus, we finally obtain

\[ d_{HF}^{Li} = 0.0077d_e. \tag{5.25} \]

This value should be compared with the EDM value calculated from the hydrogen-like wave function

\[ d_{Li} = 0.032d_e. \]

The absolute value of the EDM is smaller for the Hartree-Fock calculation than the hydrogen-like case by a factor of 5.

This is quite easy to understand since the wave function for the Hartree-Fock wave function should be pushed outward compared with the pure Coulomb case due to the electron-electron repulsion.

(b) Cs (Z=55) : Hartree-Fock wave function

In this case, the electron is in the $6s_{\frac{1}{2}}$ orbit. For the $b_0$ and $b_1$, we can evaluate them and find

\[ b_0 = -116 \tag{5.26a} \]
\[ b_1 = -6.39 \times 10^{-5}. \]  

(5.26b)

The energy difference between $6s_{1/2}$ and $6p_{1/2}$ states is calculated to be

\[ \Delta E = 0.025 \frac{m\alpha^2}{2}. \]  

(5.27a)

Thus, we obtain

\[ \epsilon_0 = 1.31 \times 10^{-5}. \]  

(5.27b)

Therefore, we finally obtain

\[ d_{Cs}^{HF} = 91.2d_e. \]  

(5.28)

This is the enhancement factor of the EDM in Cs atom from the nonrelativistic Hartree-Fock calculation. This should be compared with the EDM calculated by the Dirac Hartree-Fock wave function. They predict the EDM in Cs atom around $(100 - 150)d_e$ depending on the calculations [4-10]. This is slightly larger than the one calculated here. This is indeed reasonable since the relativistic effects in EDM must be of the order of $(\alpha Z)^2$ increase compared to the nonrelativistic evaluations.

In any case, it is now clear that the EDM in atoms is indeed enhanced compared with the electron EDM $d_e$ by a large enhancement factor for the atom with relatively high $Z$. Therefore, it would be better to use the atomic systems to observe the EDM.

7. Conclusions
We have presented the nonrelativistic reduction of the EDM operator which is free from Schiff’s theorem. This is important since we know definitely that the effect of the T-and P-violating interaction can be well observed in the atomic systems. Further, the enhancement factor is indeed quite large for the Cs atom. There are two reasons of the enhancement of the EDM in atoms. The first one is that the EDM operator is practically proportional to $\frac{1}{r^2}$ and thus the EDM expectation value become large for the large $Z$. As the second reason, the EDM becomes enhanced due to a very small energy difference between the ground state and the first excited state which has an opposite parity. Since the Hartree-Fock wave function is quite reliable in atomic systems, the estimated value of the EDM with the nonrelativistic reduction is indeed reliable. Here, we show that the relativistic correction to the EDM expectation value is of the order of $(Z\alpha)^2$ and therefore is not very large. Since the relativistic correction tends to increase the absolute value of the EDM, the nonrelativistic evaluation gives a conservative enhancement factor for the EDM in atoms.

Here, we should make comments as to what is the difference between the present approach and the Schiff’s calculation. The basic point is that the nonrelativistic reduction should be made at the last stage. For example, the simplest EDM operator is obtained when we make the nonrelativistic reduction at the lagrangian level. In this case, the EDM operator becomes eq.(3.5b) as discussed before. This is the worst case since there is no EDM operator left due to Schiff’s theorem.

The next level of the approximation which we have not presented in this paper is that we make the Foldy-Wouthuysen transformation before the Schiff transformation. Namely, we make the Foldy-Wouthuysen transformation for eq.(3.5a). In this case, we obtain the nonrelativistic EDM operator.
which is indeed different from eq. (4.4) after we remove the term described in eq. (2.3) by the Schiff transformation of eq. (2.6).

The procedure we employ in this paper is that we make the Schiff transformation at the lagrangian level and then make the Foldy-Wouthuysen transformation to the EDM operator. In this case, it is found that we obtain the unique nonrelativistic EDM operator which is free from Schiff’s theorem.

Therefore, as long as we employ the EDM operator of eq. (4.4), then we can estimate the EDM in atomic systems quite reliably with the Hartree-Fock wave functions.

Finally, we make a comment as to how the present calculation is related to the relativistic Hartree-Fock calculations. If we want to treat very high Z atoms, then we have to carry out the calculations relativistically. In this case, the direct evaluation of eq. (3.8) or (3.13) should be done if one obtains reliable wave functions with relativistic Hartree-Fock method [16]. However, if one really has to treat many body problems relativistically, then one has to carry out the calculations field theoretically. But this must be an extremely difficult task.

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Appendix

Here, we present the radial parts of the Dirac wave functions in a pure Coulomb potential $V(r) = -\frac{Z\alpha}{r}$.

1. $2s_{1/2}$ and $2p_{1/2}$ states

$$ G_{2,-1}(x) = \frac{m^{3/2}}{\Gamma(2\gamma + 1)} \sqrt{\frac{2\lambda^5(1 + W)\Gamma(2\gamma + 2)}{Z\alpha(Z\alpha + \lambda)}} x^{\gamma-1} e^{-x/2} \left[ -1 - \left( -1 - \frac{Z\alpha}{\lambda} \right) F(-1, 2\gamma + 1, x) \right] $$

$$ F_{2,-1}(x) = \frac{-m^{3/2}}{\Gamma(2\gamma + 1)} \sqrt{\frac{2\lambda^5(1 - W)\Gamma(2\gamma + 2)}{Z\alpha(Z\alpha + \lambda)}} x^{\gamma-1} e^{-x/2} \left[ 1 - \left( -1 - \frac{Z\alpha}{\lambda} \right) F(-1, 2\gamma + 1, x) \right] $$

and

$$ \tilde{G}_{2,1}(x) = \frac{m^{3/2}}{\Gamma(2\gamma + 1)} \sqrt{\frac{2\lambda^5(1 + W)\Gamma(2\gamma + 2)}{Z\alpha(Z\alpha - \lambda)}} x^{\gamma-1} e^{-x/2} \left[ -1 - \left( -1 - \frac{Z\alpha}{\lambda} \right) F(-1, 2\gamma + 1, x) \right] $$

$$ \tilde{F}_{2,1}(x) = \frac{-m^{3/2}}{\Gamma(2\gamma + 1)} \sqrt{\frac{2\lambda^5(1 - W)\Gamma(2\gamma + 2)}{Z\alpha(Z\alpha - \lambda)}} x^{\gamma-1} e^{-x/2} \left[ 1 - \left( -1 - \frac{Z\alpha}{\lambda} \right) F(-1, 2\gamma + 1, x) \right] $$

where

$$ \gamma = \sqrt{1 - (Z\alpha)^2} $$

$$ \lambda = \sqrt{1 - \left( \frac{E}{m} \right)^2} $$

$$ W = \frac{E}{m} = \frac{1}{\sqrt{1 + \left( \frac{Z\alpha}{1+\gamma} \right)^2}} $$

$$ x = 2m\lambda r $$

Here, the function $F(a, b, c)$ denotes the confluent hypergeometric function.
2. $6s_{\frac{1}{2}}$ and $6p_{\frac{1}{2}}$ states

\[ G_{6,-1}(x) = \frac{m^{3/2}}{\Gamma(2\gamma + 1)} \sqrt{\frac{2\lambda^5(1 + W)\Gamma(2\gamma + 6)}{5!Z\alpha(Z\alpha + \lambda)}} x^{\gamma-1} e^{-x/2} \]

\[ \times \left[ -5F(-4, 2\gamma + 1, x) - \left( -1 - \frac{Z\alpha}{\lambda} \right) F(-5, 2\gamma + 1, x) \right] \]

\[ F_{6,-1}(x) = \frac{-m^{3/2}}{\Gamma(2\gamma + 1)} \sqrt{\frac{2\lambda^5(1 - W)\Gamma(2\gamma + 6)}{5!Z\alpha(Z\alpha + \lambda)}} x^{\gamma-1} e^{-x/2} \]

\[ \times \left[ 5F(-4, 2\gamma + 1, x) - \left( -1 + \frac{Z\alpha}{\lambda} \right) F(-5, 2\gamma + 1, x) \right] \]

and

\[ \tilde{G}_{6,1}(x) = \frac{m^{3/2}}{\Gamma(2\gamma + 1)} \sqrt{\frac{2\lambda^5(1 + W)\Gamma(2\gamma + 6)}{5!Z\alpha(Z\alpha - \lambda)}} x^{\gamma-1} e^{-x/2} \]

\[ \times \left[ -5F(-4, 2\gamma + 1, x) - \left( 1 - \frac{Z\alpha}{\lambda} \right) F(-5, 2\gamma + 1, x) \right] \]

\[ \tilde{F}_{6,1}(x) = \frac{-m^{3/2}}{\Gamma(2\gamma + 1)} \sqrt{\frac{2\lambda^5(1 - W)\Gamma(2\gamma + 6)}{5!Z\alpha(Z\alpha - \lambda)}} x^{\gamma-1} e^{-x/2} \]

\[ \times \left[ 5F(-4, 2\gamma + 1, x) - \left( 1 - \frac{Z\alpha}{\lambda} \right) F(-5, 2\gamma + 1, x) \right] \]

where

\[ \gamma = \sqrt{1 - (Z\alpha)^2} \]

\[ \lambda = \sqrt{1 - \left( \frac{E}{m} \right)^2} \]

\[ W = \frac{E}{m} = \frac{1}{\sqrt{1 + (Z\alpha)^2}} \]