

# A new formulation of the relativistic many-body theory of electric dipole moments of closed shell atoms

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## Abstract.

The electric dipole moments of closed-shell atoms are sensitive to the parity and time-reversal violating phenomena in the nucleus. The nuclear Schiff moment is one such property, it arises from the parity and time reversal violating quark-quark interactions and the quark-chromo electric dipole moments. We calculate the electric dipole moment of atomic <sup>199</sup>Hg arising from the nuclear Schiff moment using the relativistic coupled-cluster theory. This is the most accurate calculation of the quantity to date. Our calculations in combination with the experiment data provide important insights to the P and T violating coupling constants at the elementary particle level. In addition, a new limit on the tensor-pseudo tensor induced atomic EDM, calculated using the relativistic coupled-cluster theory is also presented.

## 1. Introduction

The origin of parity violation can be explained within the frame work of the Standard Model (SM) of particle physics through the weak interactions, but there is no clear understanding of the origin of time-reversal violation in nature. The presence of a non-zero electric dipole moment of a non-degenerate physical system is a direct signature of parity ( $P$ ) and time-reversal ( $T$ ) symmetry violations [1, 2, 3]. In this paper we present a study of atomic EDMs of closed-shell atoms which arise mainly from the tensor-pseudo tensor (T-PT) electron-nuclear interactions and the nuclear Schiff moment (NSM). At the elementary particle level, the origin of closed-shell atomic EDMs is attributed to the  $P$  and  $T$  violating electron-quark interactions and quark-quark interactions which are predicted by the lepto-quark models, SUSY, etc [4]. The limits on the T-PT coupling constant ( $C_T$ ) has been obtained from the comparison of the most recent experimental result of <sup>199</sup>Hg atomic EDM [5, 6],  $|d(^{199}\text{Hg})| < 2.1 \times 10^{-28} \text{ ecm}$  and the enhancement factor (ratio of atomic EDM to the coupling constant of the interaction in question) calculated in [7]. The calculation uses Coupled-perturbed Hartree-Fock (CPHF)[8, 9] theory and the calculated value of the atomic EDM is  $d(^{199}\text{Hg}) = -6.0 \times 10^{-22} C_T \sigma_{Nem}$

combining with experimental result, a limit on  $C_T$  can be derived,

$$C_T < 3.26 \times 10^{-9} \sigma_N$$

where  $\sigma_N$  is the nuclear spin. A non-zero value of  $C_T$  would imply physics beyond the Standard Model. Improving the accuracy of the calculations would lead to a more stringent bound on  $C_T$ . The CPHF theory accounts for two-particle two-hole type of electron correlations to all orders in perturbation. In addition to this, for accurate atomic calculations[10], it is important to include other correlation effects which are absent in the CPHF theory. Coupled-cluster (CC) theory [11, 12] is one of the many-body methods which is non-perturbative and incorporates all forms of correlation effects [13, 14, 15]. CC theory with all levels of excitations is equivalent to all order Many-body Perturbation Theory. It has been successfully applied for calculation of a variety of atomic properties [14, 16, 17]. It has also been applied to atomic Hg for calculating transition energies [13].

The NSM(denoted by operator  $\vec{S}$ ) can originate from the nucleon-nucleon interactions or a nucleon EDM. At the elementary particle level it can arise from the interaction between the quarks and the chromo EDM of the quarks. The coupling constants associated with these interactions can be predicted by Multi-higgs, SUSY [4, 18] etc. The dependence of the T-PT and NSM interactions on the nuclear spin makes closed-shell atoms, in particular, those having non-zero nuclear spin the best candidates to look for EDMs sensitive to the nuclear sector. For  $^{199}\text{Hg}$ , the EDM induced by the NSM is calculated and parameterized in terms of the Schiff moment operator  $\vec{S}$ . The most recent calculation [19, 20] gives

$$d_{\text{Hg}} = -2.8 \times 10^{-17} \left( \frac{S_{\text{Hg}}}{\text{efm}^3} \right) \text{ ecm.}$$

According to the recent work [21] the expression for the P and T - odd nuclear potential arising from the nuclear Schiff moment

$$\Phi(\vec{R}) = -3 \frac{\vec{S} \cdot \vec{R}}{B} \rho(R), \quad (1)$$

where  $B = \int R^4 \rho(R) dR$  and  $R$  is the electron coordinate and  $\rho(R)$  is the nuclear density. The interaction Hamiltonian of electrons with this potential is

$$H_{\text{SM}} = 3e \frac{\vec{S} \cdot \vec{R}}{B} \rho(R) \quad (2)$$

where  $e$  is the charge of the electron. If  $\rho(R)$  is the normalized density function, which is 1 for  $R_N - \delta < R < R_N + \delta$ , where  $R_N$  is the nuclear radius and  $\delta$  is a small number. The single electron matrix elements of  $H_{\text{SM}}$  are

$$\langle \psi_{ks_{1/2}} | H_{\text{SM}} | \psi_{mp_{1/2}} \rangle = 3Se (-1/3) \int_0^\infty \left[ P_{ks_{1/2}}(r) P_{mp_{1/2}}(r) + Q_{ks_{1/2}}(r) Q_{mp_{1/2}}(r) \right] \frac{\rho(R)}{B} R dR. \quad (3)$$

where  $P_i$  and  $Q_i$  are the large and small components of the relativistic Dirac-wavefunctions  $|\psi_i\rangle$ . The matrix elements of  $H_{\text{SM}}$  between the states  $|\psi_{mp_{1/2}}\rangle$  and  $|\psi_{ks_{1/2}}\rangle$  is identical to the above expression.

## 2. Coupled-cluster theory for closed-shell atoms

The starting point of obtaining the coupled-cluster equations is the relativistic atomic Hamiltonian in the Dirac-Coulomb approximation in atomic units ( $m_e = 1$ ,  $|e| = 1$  and  $\hbar = 1$ )

$$H = \sum_i^N \left[ c\boldsymbol{\alpha}_i \cdot \mathbf{p}_i + (\beta_i - 1)c^2 + V_N(r_i) \right] + \sum_{i<j}^N \frac{1}{r_{ij}}, \quad (4)$$

where  $c$  is velocity of light,  $\alpha$  and  $\beta$  are the Dirac matrices,  $1/r_{ij}$  is the Coulomb potential energy between two electrons, and  $V_N(r_i)$  is the nuclear potential. In the above Hamiltonian, the rest mass energy is subtracted from the total energy eigen values. This is the Hamiltonian of an atomic system considering only the electrostatic interactions. The single particle equations are obtained by approximating the two-electron term in Eq.(4) by a central field potential  $U_{\text{DF}}(r)$ , known as the Dirac-Fock potential [22, 23], then

$$H_{\text{DC}} = \sum_i^N \left[ c\boldsymbol{\alpha}_i \cdot \mathbf{p}_i + (\beta_i - 1)c^2 + V_N(r_i) + U_{\text{DF}}(r_i) \right] + V_{\text{es}}. \quad (5)$$

The residual Coulomb interaction

$$V_{\text{es}} = \sum_{i<j}^N \frac{1}{r_{ij}} - \sum_i U_{\text{DF}}(r_i).$$

The non-central (or) correlation effects are included by treating  $V_{\text{es}}$  as a perturbation. The single electron wavefunctions  $|\psi_a\rangle$  satisfy the Schroedinger equation [22, 23]

$$\left[ c\boldsymbol{\alpha}_i \cdot \mathbf{p}_i + (\beta_i - 1)c^2 + V_N(r_i) + U_{\text{DF}}(r_i) \right] |\psi_a\rangle = \epsilon_a |\psi_a\rangle \quad (6)$$

and are expressed in the relativistic framework in terms of the two-component form discussed in succeeding sections. The Eq.(6) is obtained by variational extremization [22]. The perturbed equations are obtained by introducing the  $P$  and  $T$  violating tensor-pseudo tensor interaction Hamiltonian in addition to the residual Coulomb interaction. The exact atomic wavefunction in CC formalism  $|\Psi\rangle = e^T |\Phi_0\rangle$ , where  $|\Phi_0\rangle$  is the reference state,  $T = T_1 + T_2 + \dots + T_N$  is the cluster operator. In our calculations, we use the singles and doubles approximation  $T = T_1 + T_2$ , the second quantized form of the operators are

$$\begin{aligned} T_1 &= \sum_{a,p} a_p^\dagger a_a \mathbf{t}_a^p |\Phi_0\rangle \\ T_2 &= \sum_{a,p,b,q} \frac{1}{2!} a_p^\dagger a_q^\dagger a_b a_a \mathbf{t}_{ab}^{pq} |\Phi_0\rangle. \end{aligned} \quad (7)$$

The many-body Schroedinger equation of the Dirac-Coulomb Hamiltonian for an atomic system, in a state  $|\Psi\rangle$  in the CC formalism

$$H e^T |\Phi_0\rangle = E e^T |\Phi_0\rangle.$$

Operating from left side by  $e^{-T}$

$$e^{-T} H e^T |\Phi_0\rangle = E |\Phi_0\rangle.$$

Expressing  $H$  in normal ordered form,  $H = H_N + E_{DF}$ , where  $E_{DF} = \langle \Phi_0 | H | \Phi_0 \rangle - \langle \Phi_0 | H_N | \Phi_0 \rangle$  is the Dirac-Fock energy. Then,

$$e^{-T}(H_N + E_{DF})e^T|\Phi_0\rangle = E|\Phi_0\rangle \quad (8)$$

Projecting Eq.(8) with singly and doubly excited states  $\langle \Phi_a^r |$  and  $\langle \Phi_{ab}^{rs} |$  respectively, the single and double excitation cluster amplitude equations are [24]

$$\langle \Phi_a^r | \{ \overline{(H_N e^T)}_c \} | \Phi_0 \rangle = 0 \quad (9)$$

$$\langle \Phi_{ab}^{rs} | \{ \overline{(H_N e^T)}_c \} | \Phi_0 \rangle = 0. \quad (10)$$

### 2.1. EDM perturbed coupled-cluster equations

The  $H_{\text{EDM}}$  operator is the general EDM operator. In the present paper,  $H_{\text{EDM}}$  denotes  $H_{\text{SM}}$ , which is a single-particle operator. Consider the NSM perturbed Schroedinger equation

$$\tilde{H}|\tilde{\Psi}\rangle = E|\tilde{\Psi}\rangle \quad (11)$$

where  $\tilde{H} = H_{\text{DC}} + \lambda H_{\text{EDM}}$  and  $|\tilde{\Psi}\rangle = e^T|\Phi_0\rangle = e^{T^{(0)} + \lambda T^{(1)}}|\Phi_0\rangle$ . Taking upto one order in  $\lambda$  in the exponent,

$$\tilde{H}e^{T^{(0)}}(1 + \lambda T^{(1)})|\Phi_0\rangle = Ee^{T^{(0)}}(1 + \lambda T^{(1)})|\Phi_0\rangle.$$

Substituting for  $\tilde{H}$  in the above equation and comparing zeroth and first order terms of  $\lambda$  on both sides,

$$(H_{\text{DC}}e^{T^{(0)}})|\Phi_0\rangle = Ee^{T^{(0)}}|\Phi_0\rangle, \quad (12)$$

and

$$(H_{\text{DC}}e^{T^{(0)}}T^{(1)} + H_{\text{EDM}}e^{T^{(0)}})|\Phi_0\rangle = Ee^{T^{(0)}}T^{(1)}|\Phi_0\rangle. \quad (13)$$

Multiplying Eq.(12) by  $T^{(1)}$  on both sides and substitute  $H_{\text{DC}} = H_N + E_{DF}$

$$T^{(1)}H_Ne^{T^{(0)}}|\Phi_0\rangle = \Delta E_{\text{corr}}T^{(1)}e^{T^{(0)}}|\Phi_0\rangle. \quad (14)$$

and Eq.(13) can be written as

$$(H_Ne^{T^{(0)}}T^{(1)} + H_{\text{EDM}}e^{T^{(0)}})|\Phi_0\rangle = (\Delta E_{\text{corr}}e^{T^{(0)}}T^{(1)})|\Phi_0\rangle \quad (15)$$

since  $T^{(0)}$  and  $T^{(1)}$  commute and  $\Delta E_{\text{corr}} = E - E_{DF}$  is the correlation energy. Operate Eq.(15) on both sides by  $e^{-T^{(0)}}$

$$(\overline{H}_NT^{(1)} + \overline{H}_{\text{EDM}})|\Phi_0\rangle = \Delta E_{\text{corr}}T^{(1)}|\Phi_0\rangle \quad (16)$$

Operating by  $e^{-T^{(0)}}$  on Eq.14

$$T^{(1)}\overline{H}_N|\Phi_0\rangle = \Delta E_{\text{corr}}T^{(1)}|\Phi_0\rangle. \quad (17)$$

Subtracting Eq.(16) from Eq.(17)

$$[\overline{H}_N, T^{(1)}]|\Phi_0\rangle = -\overline{H}_{\text{EDM}}|\Phi_0\rangle, \quad (18)$$

where  $\bar{O} = e^{-T^{(0)}} \hat{O} e^{T^{(0)}}$  and  $\hat{O}$  is any operator. The equation for the  $H_{\text{EDM}}$  perturbed singles and doubles cluster amplitudes can be derived from the basic equation, Eq.(18) by projecting on both sides of the equation with singly and doubly excited determinantal states.

$$\begin{aligned} \langle \Phi_a^r | [\bar{H}_N, T^{(1)}] | \Phi_0 \rangle &= -\langle \Phi_a^r | \bar{H}_{\text{EDM}} | \Phi_0 \rangle \\ \langle \Phi_{ab}^{rs} | [\bar{H}_N, T^{(1)}] | \Phi_0 \rangle &= -\langle \Phi_{ab}^{rs} | \bar{H}_{\text{EDM}} | \Phi_0 \rangle \end{aligned} \quad (19)$$

which are equivalent to

$$\begin{aligned} \langle \Phi_a^r | \left\{ \overline{H_N T^{(1)}} \right\} | \Phi_0 \rangle &= -\langle \Phi_a^r | \bar{H}_{\text{EDM}} | \Phi_0 \rangle, \\ \langle \Phi_{ab}^{rs} | \left\{ \overline{H_N T^{(1)}} \right\} | \Phi_0 \rangle &= -\langle \Phi_{ab}^{rs} | \bar{H}_{\text{EDM}} | \Phi_0 \rangle. \end{aligned} \quad (20)$$

Further expanding  $T^{(1)} = T_1^{(1)} + T_2^{(1)}$ , these equations can be cast in the form of a system of linear matrix equations

$$\begin{aligned} H_{11} T_1^{(1)} + H_{12} T_2^{(1)} &= -H_{10}, \\ H_{21} T_1^{(1)} + H_{22} T_2^{(1)} &= -H_{20}, \end{aligned} \quad (21)$$

where  $H_{11}$ ,  $H_{12}$ ,  $H_{21}$ ,  $H_{22}$  are the sub blocks of the dressed  $H_N$  matrix elements and  $H_{10}$  and  $H_{20}$  are the sub blocks of the dressed  $H_{\text{EDM}}$  matrix elements.

## 2.2. Calculation of Atomic Electric Dipole moments

The EDM of the atom in the state  $|\tilde{\Psi}\rangle$  is

$$D_{\text{atom}} = \frac{\langle \tilde{\Psi} | D | \tilde{\Psi} \rangle}{\langle \tilde{\Psi} | \tilde{\Psi} \rangle} \quad (22)$$

where  $D$  is the electric dipole operator. Substituting the above expression for  $|\tilde{\Psi}\rangle$  and keeping terms only of order  $\lambda$ , we obtain the expression for EDM (the symbol of contraction appears using  $\overline{DT^{(1)}} = \overline{DT^{(1)}} + \{DT^{(1)}\}$ , where the curly brackets refer to normal ordering and the expectation value of normal ordered operator between the vacuum states is zero)

$$D_{\text{atom}} = \frac{\langle \Phi_0 | [\overline{DT^{(1)}} + T^{(1)\dagger} \overline{D}] | \Phi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}, \quad (23)$$

which can also be written as

$$D_{\text{atom}} = \frac{\langle \Phi_0 | [\overline{DT^{(1)}} + \overline{T^{(1)\dagger} D}] | \Phi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}, \quad (24)$$

where  $\overline{D} = e^{T^{(0)\dagger}} D e^{T^{(0)}}$ . Using the fact that  $T^{(1)}$  and  $D$  operators are odd and  $T^{(0)}$  operator is even under parity, the bra and the ket vectors in the above expression must have the same parity. To simplify the calculations, we expand  $\overline{D}$  as [25, 24]

$$\overline{D} = \left( 1 + T^{(0)\dagger} + \frac{T^{(0)\dagger 2}}{2!} + \dots \right) D e^{T^{(0)}} = D e^{T^{(0)}} + \sum_{n=1}^{\infty} \frac{1}{n!} \left( T^{(0)\dagger} \right)^n D e^{T^{(0)}} \quad (25)$$

In Eq.(25), the one-body nature of the electric dipole operator  $D$  restricts the maximum possible contractions with  $T^{(0)}$  to just two. Define

$$|\Phi_1\rangle = T^{(1)}|\Phi_0\rangle = \left(T_1^{(1)} + T_2^{(1)}\right)|\Phi_0\rangle,$$

then

$$D_{\text{atom}} = \frac{\langle\Phi_0|\overline{D}|\Phi_1\rangle + \langle\Phi_1|\overline{D}|\Phi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} = 2\frac{\langle\Phi_1|\overline{D}|\Phi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}. \quad (26)$$

The last step follows as the two terms are the complex conjugates of each other and give equal contributions. Substituting the expanded form of  $\overline{D}$

$$\begin{aligned} D_{\text{atom}} &= 2\langle\Phi_1|\left[De^{T^{(0)}} + \sum_{n=1}^{\infty}\frac{1}{n!}\left(T^{(0)\dagger}\right)^n De^{T^{(0)}}\right]|\Phi_0\rangle/\langle\Psi_0|\Psi_0\rangle \\ &= 2\left[\langle\Phi_1|De^{T^{(0)}}|\Phi_0\rangle + \langle\Phi_1|\sum_{n=1}^{\infty}\frac{1}{n!}\left(T^{(0)\dagger}\right)^n De^{T^{(0)}}|\Phi_0\rangle\right]/\langle\Psi_0|\Psi_0\rangle \end{aligned} \quad (27)$$

The complexity of the above expression can be mitigated by exploiting the fact that not all the terms containing the  $T^{(0)\dagger}$  operators contribute to the infinite summation. In this scheme, the zeroth order  $D_{\text{atom}}$  consists of terms without  $T^{(0)\dagger}$  operator, first order  $D_{\text{atom}}$  consists of terms having one order of  $T^{(0)\dagger}$ , and so on. The unlinked terms of the numerator cancel with the denominator and only linked terms contribute in the numerator. At the linear level,

$$\begin{aligned} \overline{D} &= \left(1 + T^{(0)}\right)^\dagger D \left(1 + T^{(0)}\right) \\ &= D + DT^{(0)} + T^{(0)\dagger}D \\ &= D + DT_1^{(0)} + DT_2^{(0)} + T_1^{(0)\dagger}D + T_2^{(0)\dagger}D \end{aligned}$$

Following are the terms contributing to the EDM expectation value at the linear level :

$$D_{\text{atom}} = \langle\Phi_0|\overline{D}T^{(1)} + T^{(1)\dagger}\overline{D}|\Phi_0\rangle \quad (28)$$

The two terms in Eq.28 are complex conjugates of each other. Hence

$$D_{\text{atom}} = 2\langle\Phi_0|T^{(1)\dagger}\overline{D}|\Phi_0\rangle.$$

Substituting for  $\overline{D}$  the expression for the atomic EDM

$$D_{\text{atom}} = 2\langle\Phi_0|\left[T_1^{(1)\dagger}D + T_1^{(1)\dagger}DT_1^{(0)} + T_1^{(1)\dagger}DT_2^{(0)} + T_2^{(1)\dagger}DT_2^{(0)} + T_2^{(1)\dagger}DT_1^{(0)}\right]|\Phi_0\rangle \quad (29)$$

### 3. Results

#### 3.1. Basis

The single particle orbitals for all calculations in the subsequent sections were generated using the Gaussian basis [17] set expansion whose salient features are presented in this section. In the central field approximation, the solution of the Dirac equation in terms of the four component spinors is given by

$$\psi_{n\kappa m}(r, \theta, \phi) = r^{-1} \begin{pmatrix} P_{n\kappa}(r) \chi_{\kappa m}(\theta, \phi) \\ iQ_{n\kappa}(r) \chi_{-\kappa m}(\theta, \phi) \end{pmatrix}$$

where  $P_{n\kappa}(r)$  and  $Q_{n\kappa}(r)$  are the large and the small components of the radial wavefunctions expanded in terms of the basis sets[26],

$$P_{n\kappa}(r) = \sum_p C_{\kappa p}^L g_{\kappa p}^L(r)$$

$$Q_{n\kappa}(r) = \sum_p C_{\kappa p}^S g_{\kappa p}^S(r)$$

where the summation over the index  $p$  runs over the number basis functions  $N$ ,  $g_{\kappa p}^L(r)$  and  $g_{\kappa p}^S(r)$  correspond to the large and small components and  $C_{\kappa p}^L$  and  $C_{\kappa p}^S$  are their expansion coefficients for each value of  $\kappa$ . The functions  $g_{\kappa p}^L(r)$  are chosen to be the two parameter Gaussian Type Orbitals (GTOs) [26] and large and small components are related by the condition of kinetic balance [27, 28]. The calculations presented in this paper correspond to the Even Tempered (ET) basis set. For the nuclear density we use the two parameter Fermi distribution

$$\rho_N(r) = \frac{\rho_0}{1 + e^{(r-c)/a}}$$

where  $r$  is the radial coordinate,  $a = 2.3/4\ln 3$  is the skin thickness parameter and  $c = \sqrt{(5r_{\text{rms}}^2/3 - 7a^2\pi^2/3)}$ , the half-charge radius [29]. In the expression of  $c$ , the  $r_{\text{rms}}$  is the nuclear mean-square radius. The quantity  $\rho_0$  is determined by normalising  $\rho_N(r)$  over a spherical volume. The radial grid has the form,  $r_k = r_0 \left( e^{(k-1)h} - 1 \right)$ ,  $k = 1, \dots, n_p$ ,  $n_p$  is the total number of grid points.

**Table 1.** No. of basis functions used to generate the even tempered Dirac-Fock orbitals and the corresponding value of  $\alpha_0$  and  $\beta$  used. The total number of active orbitals are shown in the brackets for Active holes.

	$s_{1/2}$	$p_{1/2}$	$p_{3/2}$	$d_{3/2}$	$d_{5/2}$	$f_{5/2}$	$f_{7/2}$	$g_{7/2}$	$g_{9/2}$
Number of basis	31	32	32	20	20	20	20	10	10
$\alpha_0 (\times 10^{-5})$	725	715	715	700	700	695	695	655	655
$\beta$	2.725	2.715	2.715	2.700	2.700	2.695	2.695	2.655	2.655
Active holes (36)	2	2	2	2	2	1	1	1	1
Active holes (39)	3	3	3	2	2	1	1	1	1
Active holes (43)	3	3	3	3	3	2	2	1	1
Active holes (45)	3	3	3	3	3	3	3	1	1
Active holes (51)	5	5	5	3	3	3	3	1	1
Active holes (57)	7	7	7	3	3	3	3	1	1
Active particles	6	4	4	3	3	1	1	0	0

For the present calculation, the details of the basis set used in generating the orbitals is shown in Table. 1. Using the above basis, the single particle orbitals have been generated. Next, an existing closed-shell coupled-cluster code developed inhouse has been used to generate the unperturbed cluster amplitudes [30]. The code for calculating the perturbed cluster amplitudes, and subsequently the atomic EDM was developed by our group [25, 24].

**Table 2.** Individual contributions

	Contributions in units of $e a_0 G_F C_T$
$T_1^{(1)\dagger} D$	-47.830
$T_1^{(1)\dagger} DT_1^{(0)}$	0.082
$T_1^{(1)\dagger} DT_2^{(0)}$	14.320
$T_2^{(1)\dagger} DT_2^{(0)}$	-0.386
$T_2^{(1)\dagger} DT_1^{(0)}$	-0.059
Total	-33.874

### 3.2. Results for Hg EDM induced by the $\hat{P}$ and $\hat{T}$ violating T-PT interaction

Contributions from each of the terms in Eq.(29) are shown in Table.2 for the basis with 57 active orbitals. The final result can be expressed in units of e-m

$$D_{\text{Hg}} = -1.125 \times 10^{-22} C_T e m \sigma_N.$$

The Dirac-Fock contribution is  $-2.45 \times 10^{-22} e m C_T \sigma_N$ . It can be noticed from the Table 2 that the largest contribution is from  $T_1^{(1)\dagger} D$ . This can be explained from the fact that it includes the Dirac-Fock effect, which is the most dominant contribution. The trend shown by the individual contributions in Table.2 is related to the fact that the  $T_1^{(0)}$  cluster amplitudes are smaller in magnitude compared to the  $T_2^{(0)}$  cluster amplitudes. In addition, the  $T_1^{(1)}$  amplitudes are larger in magnitude compared to the  $T_2^{(1)}$  amplitudes again due to the presence of the Dirac-Fock contribution in  $T_1^{(1)}$ . For example, from the above table, we see that the contribution of  $T_1^{(1)\dagger} DT_2^{(0)}$  is larger than that of  $T_1^{(1)\dagger} DT_1^{(0)}$ . Similarly, the contribution of  $T_2^{(1)\dagger} DT_2^{(0)}$  is greater than that of  $T_2^{(1)\dagger} DT_1^{(0)}$ . These arguments are equally valid for the atomic EDM induced by the nuclear Schiff moment shown in the next section, which follows the same trend as above. It is also interesting to note that in both cases contribution of the term  $T_1^{(1)\dagger} D$  is approximately 3 times larger in magnitude than that of the term  $T_1^{(1)\dagger} DT_2^{(0)}$ , which is the second largest contribution.

### 3.3. Results for Hg EDM induced by the $\hat{P}$ and $\hat{T}$ violating Nuclear Schiff moment

The  $^{199}\text{Hg}$  atomic EDM induced by the nuclear Schiff moment is calculated with the same basis given in the previous section. The methods of generating the perturbed and the unperturbed cluster amplitudes are the same as described earlier. The Dirac-Fock contribution is  $D_{\text{Hg}} = -0.546 \times 10^5 e a_0 S = -0.390 \times 10^{-17} e c m S (e f m^3)^{-1}$ . Contributions from each of the terms in Eq.29 is shown in Table.3. Again, the leading contribution is from  $T_1^{(1)\dagger} D$  and it can also be seen that the contribution of  $T_1^{(1)\dagger} D$  is approximately 3 times in magnitude of the contribution of  $T_1^{(1)\dagger} DT_2^{(0)}$ , which is also true for the results of the T-PT induced EDM.

**Table 3.** Individual contributions

	Contributions in atomic units of $S e \times a_0$
$T_1^{(1)\dagger} D$	$-0.177 \times 10^5$
$T_1^{(1)\dagger} DT_1^{(0)}$	$0.030 \times 10^3$
$T_1^{(1)\dagger} DT_2^{(0)}$	$0.525 \times 10^4$
$T_2^{(1)\dagger} DT_2^{(0)}$	$-14.258 \times 10^1$
$T_2^{(1)\dagger} DT_1^{(0)}$	$0.252 \times 10^{-4}$
Total	$-0.126 \times 10^5$

Our result is not in agreement with Dzuba et.al [19]. They have used CI + MBPT method for the generation of the orbitals. We have compared the Schiff moment interaction and the electric dipole matrix elements of the  $6s_{1/2}$  and the core  $p_{1/2}$  orbitals for  $^{199}\text{Hg}$  with the results obtained by the authors of Dzuba et al. at the Dirac-Fock level and found that the agreement was very good. This suggests that the discrepancy in our results could be majorly due to the different choices of the virtual orbitals in the two calculations.

The final result is in the units where  $S$  is expressed in  $efm^3$

$$D_{\text{Hg}} = -0.126 \times 10^5 \times \frac{2 \times 10^{-23}}{0.529^2} \times \frac{S}{efm^3} \text{ecm}$$

$$D_{\text{Hg}} = -0.0901 \times 10^{-17} \text{ecm} \frac{S}{efm^3}$$

#### 3.4. Summary of the EDM results of $^{199}\text{Hg}$

The interaction Hamiltonian for the T-PT and the NSM are both dependent on the nuclear density  $\rho_N(r)$  and hence their matrix elements are sensitive to the  $s_{1/2}$  and the  $p_{1/2}$  orbitals, which have a non-zero probability density inside the nuclear radius. In addition, the NSM interaction Hamiltonian is proportional to the electron coordinate  $\vec{R}$ . In addition, the matrix elements of the atomic EDM contain the electric dipole operator  $\vec{D}$ . Hence the atomic EDMs arising from these interactions require the single particle orbitals to be very accurate at all radial ranges. The trend followed by the T-PT and NSM induced EDM shows that the atomic EDM is very sensitive to the inclusion of  $s_{1/2}$  and the  $p_{1/2}$  virtuals. On the other hand, there is not much variation in the polarizability as it is more sensitive to orbitals of higher orbital angular momenta. We have also performed linear CCEDM calculations without including any  $T^{(0)}$  cluster amplitudes. This in other words, amounts to the linear CCEDM calculation with the cluster amplitudes generated with the approximations  $\overline{H}_N \approx H_N$  and  $\overline{H}_{\text{EDM}} \approx H_{\text{EDM}}$  in Eq.(20). Hence all the correlation effects from  $T^{(0)}$  amplitudes are omitted. The results of this calculation for a basis of 39 active orbitals are discussed. The Dirac-Fock contribution for this basis is  $D_{\text{Hg}} = -3.17 \times 10^{-22} \text{em}$ . The total contribution is  $D_{\text{Hg}} = -5.77 \times 10^{-22} \text{em}$ , whereas the CPHF calculation gives  $D_{\text{Hg}} = -4.64 \times 10^{-22} \text{em}$ . Similar comparison can be made for a basis of 57 active orbitals, for which the Dirac-Fock contribution is  $D_{\text{Hg}} = -2.45 \times 10^{-22} \text{em}$ ,

**Table 4.** Summary of our results.

Basis size	In units of $10^{-22}C_{T\text{em}}$	In units of $10^{-17} \text{ e cm } \frac{S}{\text{efm}^3}$
36	-2.70	1.83
39	-2.97	-0.23
42	-2.21	-0.15
45	-1.41	-0.11
51	-1.40	-0.11
57	-1.13	-0.09

**Table 5.** P and T violating parameters

P and T violating parameter at the elementary particle level	Limits obtained from linear CCEDM
$\eta_{np}$	$< -1.6 \times 10^{-2}$
$\bar{g}_{\pi NN}$	$< 1.7 \times 10^{-10}$
$\theta_{\text{QCD}}$	$< 6.3 \times 10^{-9}$
$e(\bar{d}_u - \bar{d}_d)$	$< 0.86 \times 10^{-24} \text{ e cm}$

the bare-Coulomb calculation without  $T^{(0)}$  amplitudes gives  $D_{\text{Hg}} = -6.60 \times 10^{-22}\text{em}$ , the CPHF calculation gives  $D_{\text{Hg}} = -5.61 \times 10^{-22}\text{em}$ . This comparison helps in understanding the interplay between the various many-body effects : the the bare-Coulomb which contains all kind of correlation effects to one order in Coulomb interaction;the CPHF theory which contains the Coulomb effects only of the two particle-two hole kind; the linear CCEDM which subsumes the effects of the bare Coulomb, the CPHF and more.

Limits on the P and T violating parameters at the elementary particle level can be derived from the tensor-pseudo tensor coupling constant ( $C_T$ ) and the nuclear Schiff moment ( $S$ )[25, 24]. The results of various P and T violating parameters are shown in Table.5. A detailed discussion on the derivation of these parameters has been presented in [25]. Using these important parameters, the observable EDMs can be connected to the P and T violating coupling constants predicted by the underlying elementary particle theories. The bounds on these coupling constants can further be used to constrain various models of elementary particle physics.

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