

Core-polarization studies of nuclear-Schiff-moment-induced permanent electric dipole moments of atomic ^{129}Xe , ^{171}Yb , and ^{225}Ra

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We have calculated the intrinsic electric dipole moments (EDMs) of ^{129}Xe , ^{171}Yb , ^{225}Ra atoms induced by the nuclear Schiff moment (NSM). We use the coupled perturbed Hartree-Fock [CPHF] framework to perform this calculation. In this work, the effects of electron correlation on atomic EDMs are studied in CPHF framework by gradual inclusion of virtual orbitals of higher symmetries. Individual orbital contributions to the final magnitude of the EDM are presented. The results for the NSM-induced EDM for these atoms show a trend similar to the electron-nucleon tensor-pseudotensor (T-PT)-induced EDM, the study of which was performed elsewhere. This behavior can be attributed to the fact that the influence of virtual orbitals of higher symmetry on the magnitude of EDM is essentially the same for both T-PT and NSM-induced atomic EDMs. However, we also report in this paper, that the most dominant contribution to the atomic EDM of ^{129}Xe , ^{171}Yb , ^{225}Ra atoms induced by the NSM arises from the $s_{1/2}$ - $p_{3/2}$ pairings rather than the $s_{1/2}$ - $p_{1/2}$ pairings, which were the dominantly contributing pairings for the electron-nucleon tensor-pseudotensor-induced atomic EDM.

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I. INTRODUCTION

Fundamental symmetry violation has received much attention among physicists after Lee and Yang proposed CP violation in weak interaction [1]. As long as the CPT theorem holds, one can expect time-reversal (T) violation. The permanent electric dipole moment (EDM) of a nondegenerate physical system is a direct evidence of time-reversal violation [2], which has been one of the most profound puzzles in elementary particle physics for more than four decades. For diamagnetic atoms, the dominant contribution to the EDM comes from the tensor-pseudotensor (T-PT) electron-nucleon interaction and the nuclear Schiff moment (NSM) whereas, for paramagnetic atoms the scalar-pseudoscalar electron-nucleon interaction and electron EDM produce dominant contributions [3]. According to Schiff theorem, when charged particles, treated as point charges, interact electrostatically with each other and with an arbitrary external electric field, in the nonrelativistic limit, the shielding effect is complete. But in relativistic case, the interaction between atomic electrons and the nuclear Schiff moment induces an atomic EDM [4]. Experiment on ^{199}Hg constrains the limit of the Schiff moment of the ^{199}Hg nucleus, which serves as best upper limit of nuclear Schiff moment to date [5]. High-precision atomic calculations are necessary for calculating the atomic EDMs that are parameterized in terms of the P and T violating coupling constants. Many attempts have been made in this direction [6,7]. The time-dependent Hartree Fock (TDHF) method, multiconfiguration Hartree Fock (MCHF) method, CI method, MBPT method, and combination of these were widely used by a number of authors for accurate calculation properties of many-electronic system. Recently the coupled-cluster (CC) method was employed for the calculation of the NSM-induced EDM in Xe [8] and earlier for the EDM of Hg [9]. Coupled perturbed Hartree-Fock (CPHF) has proved to

be one of the robust methods for atomic and molecular property calculation, which correspond to one-electron perturbation operator [10]. This method was widely used in calculation of atomic polarizability of various atoms [11,12]. The effect of electron correlation in atoms causes a change in the value of the EDM compared to the Dirac-Fock contribution and can be attributed to the inclusion of a class of two-hole two-particle interactions, through the CPHF theory. In this paper, we have studied the effect of inclusion of virtual orbitals of various symmetries on the final magnitude of EDMs of ^{129}Xe , ^{171}Yb , ^{225}Ra . The CPHF theory is complete in itself and incorporates a class of important many-body correlation effects. This is evident from our results of the CPHF and the Dirac Hartree-Fock (DHF) contributions to the nuclear Schiff moment of atomic ^{225}Ra . The DHF contribution is $^{225}\text{Ra} = -1.842 \times 10^{-17} [\text{S}/(\text{e fm}^3)] \text{e cm}$ and the CPHF contribution is $^{225}\text{Ra} = -8.093 \times 10^{-17} [\text{S}/(\text{e fm}^3)] \text{e cm}$. This wide variation between CPHF and DHF values of EDM is due to incorporation of correlation effects arising from certain hole-particle and particle-hole kinds of excitations. The CPHF method includes the correlation effects substantially by its multi-iteration nature. This method is one of the best post-DHF methods, where certain class of correlation effects are taken into account [10,13]. Atomic ^{129}Xe , ^{171}Yb are also studied in this work. Our results are in good agreement with the previously reported values by Dzuba *et al.* [14]. The three atomic systems ^{129}Xe , ^{171}Yb , ^{225}Ra have half nuclear spin $I = 1/2$, therefore higher-order nuclear moment interactions could be avoided. In this work, we have presented calculation of atomic EDM arising from nuclear Schiff moment of ^{129}Xe , ^{171}Yb , ^{225}Ra . These atoms are of great experimental interest for detecting EDMs [15–17].

This paper is organized as follows. In Sec. I, we briefly present the CPHF equations for a general P and T violating potential. Section II contains the nuclear-Schiff-moment Hamiltonian H_{SM} due to interaction of Schiff moment with atomic electrons. Section III contains the tabulation of results followed by discussions and finally the conclusion.

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II. CPHF EQUATIONS

We consider a closed-shell N -electron system. The single-particle orbitals $|\psi_a^0\rangle$ are solutions of the relativistic Hartree-Fock equation.

$$(h^0 + g^0 - \varepsilon_a^0)|\psi_a^0\rangle = 0, \quad (1)$$

where h^0 and g^0 are the relativistic single-particle Hamiltonian and the Hartree-Fock potential, respectively. The system is perturbed by an EDM interaction Hamiltonian h_{int} , which is a one-body operator in nature. The set of coupled perturbed Hartree-Fock equations corresponding to one order in EDM interaction is [18]

$$(h^0 + g^0 - \varepsilon_a^0)|\psi_a^1\rangle = (-h_{\text{int}} - g^{(1)})|\psi_a^0\rangle, \quad (2)$$

where g^1 is perturbed Hartree-Fock potential [10]. The first-order perturbed state $|\psi_a^1\rangle$ can be expanded as $|\psi_a^1\rangle = \sum_p^{\text{unocc}} C_{ap}|\psi_p^0\rangle$, where $|\psi_p^0\rangle$ is the unperturbed virtual state. Equation (2) can be solved through iteration of the CPHF equations. The mixing coefficients of k th iteration are

$$C_{pa}^{(k,1)} = \frac{-B_{pa}}{\varepsilon_p^0 - \varepsilon_a^0} - \sum_b^{\text{occ}} \sum_q^{\text{unocc}} \times \left[\tilde{V}_{pqab} \frac{C_{qb}^{(k-1,1)}}{\varepsilon_p^0 - \varepsilon_a^0} + \tilde{V}_{pbaq} \frac{C_{qb}^{(k-1,1)}}{\varepsilon_p^0 - \varepsilon_a^0} \right], \quad (3)$$

where $B_{pa} = \langle \psi_p^0 | h_{\text{int}} | \psi_a^0 \rangle$ and $\tilde{V}_{pqab} = \langle \psi_p^0 \psi_q^0 | v | \psi_a^0 \psi_b^0 \rangle - \langle \psi_p^0 \psi_q^0 | v | \psi_b^0 \psi_a^0 \rangle$, $\tilde{V}_{pbaq} = \langle \psi_p^0 \psi_b^0 | v | \psi_a^0 \psi_q^0 \rangle - \langle \psi_p^0 \psi_b^0 | v | \psi_q^0 \psi_a^0 \rangle$, and v is the residual Coulomb interaction between electrons. In terms of the CPHF coefficients, atomic EDM is defined as in Refs. [10,13], $D_{\text{atom}} = \sum_a^{\text{occ}} \sum_p^{\text{unocc}} [\langle a | d | p \rangle C_{pa}^{(\infty,1)} + C_{pa}^{*(\infty,1)} \langle p | d | a \rangle]$, where d is the electric dipole operator and the single-particle orbitals i correspond to the wave function $|\psi_i\rangle$.

The superscript in $C_{pa}^{(\infty,1)}$ refers to the order of the residual Coulomb interaction and h_{int} , respectively. Here, all orders in the Coulomb interaction associated with hole-particle interactions are taken into account.

III. NUCLEAR SCHIFF MOMENT

The nucleus with finite size has residual nuclear potential, though it is screened by atomic electrons. The asymmetry between charge and electric dipole moment distribution in the nucleus causes P, T violating nuclear potential, which interact with relativistic electrons and gives hadronic part of EDM to atomic EDM [4]. The Schiff moment is a nuclear moment produced by P, T violating nuclear potential. The Hamiltonian for the interaction of atomic electrons with the nuclear Schiff moment is as in Ref. [19],

$$H_{\text{SM}} = 3e \frac{S \cdot R}{B} \rho(R), \quad (4)$$

where $B = \int R^4 \rho(R) dR$ and R is the electron coordinate and \mathbf{S} is the Schiff moment vector defined as $\mathbf{S} = S(\frac{\mathbf{I}}{I})$ with S being the coupling constant and $\rho(R)$ is nuclear density, \mathbf{I} is nuclear spin. The term, H_{SM} plays the role of the term, h_{int} in the CPHF equations elaborated in Sec. II, for NSM-induced atomic EDM. The Schiff moment interaction Hamiltonian is dominant

TABLE I. All order contribution to Xe EDM arising from nuclear Schiff moment, in units of $[\text{S}/e \text{ fm}^3] e \text{ cm}$.

Pairings Occupied-Unoccupied	EDM $\times 10^{-17}$
$S_{1/2}$ - $P_{1/2}$	0.036
$P_{1/2}$ - $S_{1/2}$	0.138
$S_{1/2}$ - $P_{3/2}$	0.042
$P_{3/2}$ - $S_{1/2}$	0.268
Others	-0.106
Total	0.378

for s and p orbitals as these orbitals have nonzero density inside the nucleus. However, the EDM matrix element depends both on the matrix elements of P, T violating interaction Hamiltonian and the electric dipole operator.

IV. RESULTS AND DISCUSSION

The Gaussian basis set [20] is employed for all calculations. The basis set has been tested for completeness through the calculation of other experimentally determined properties like the hyperpolarizability.

A. Xenon

The complete basis set for the calculation of Xe atom is $(1-25)_{s_{1/2}}(2-25)_{p_{1/2}, p_{3/2}}(3-17)_{d_{3/2}, d_{5/2}}(4-8)_{f_{5/2}, f_{7/2}}(5-10)_{g_{7/2}, g_{9/2}}(6-8)_{h_{9/2}, h_{11/2}}$.

An atomic EDM is calculated by evaluating the expectation value of the electric dipole operator between the atomic states perturbed by a P and T violating interaction. In terms of the single-particle wave functions, the expectation value reduces to a product of matrix elements of h_{int} and the electric dipole operator, evaluated with respect to the single-particle occupied/unoccupied wave functions of opposite parity, followed by a summation over the entire single-particle basis as explained in the previous sections. In Table I, the notation S_i - P_j indicates that the pairings $\{a, p\}$ that contribute to the atomic EDM arise from the general S - P wave functions. The corresponding particular combinations of the S - P pairings are presented in the Table II. The same notation is carried over for all the tables presented in this paper. Total atomic EDM of ^{129}Xe induced by its nuclear Schiff moment, calculated in the Dirac-Fock and the CPHF framework are $0.289 \times 10^{-17} [\text{S}/e \text{ fm}^a] e \text{ cm}$ and $0.378 \times 10^{-17} [\text{S}/e \text{ fm}^3] e \text{ cm}$ respectively.

TABLE II. Dominant contributions to Xe EDM from the $P_{3/2}$ - $S_{1/2}$ pairing in units of $[\text{S}/e \text{ fm}^3] e \text{ cm}$.

Pairings Occupied-Unoccupied	EDM $\times 10^{-17}$
$5p_{3/2}$ - $6s_{1/2}$	0.011
$5p_{3/2}$ - $7s_{1/2}$	0.054
$5p_{3/2}$ - $8s_{1/2}$	0.105
$5p_{3/2}$ - $9s_{1/2}$	0.058
$4p_{3/2}$ - $10s_{1/2}$	0.013
$4p_{3/2}$ - $11s_{1/2}$	0.003

TABLE III. Gradual inclusion of virtual states (EDM in units of $10^{-17}[\text{S/e fm}^3]$ e cm and polarizability in a.u).

Virtual states	Xe EDM	α
Up to $p_{1/2}$	0.406	1.93
Up to $p_{3/2}$	0.486	6.83
Up to $d_{5/2}$	0.379	26.98
Up to $f_{7/2}$	0.378	27.03
Up to $g_{9/2}$	0.378	27.25
Up to $h_{11/2}$	0.378	27.28

The dominant contributions of individual orbital pairings to its atomic EDM are given in Table I. The contributions of higher symmetry to atomic EDM is given in the last row of Table I. The most dominant and the second most dominant contributions towards EDM comes from $P_{3/2}$ - $S_{1/2}$ and $P_{1/2}$ - $S_{1/2}$ combinations respectively. We also find that the non- (S, P) orbitals contribute almost the same magnitude as $P_{1/2}$ - $S_{1/2}$. This is a result of nontrivial summation over intermediate states as more orders of the Coulomb interaction are incorporated through the iteration and the interplay between the three terms involved in the summation, namely, the EDM matrix element, the dipole matrix element and the energy denominator. In Table II, the actual dominant single-particle transitions contributing to EDM are presented.

As shown in Table III, the value of the EDM of Xe saturates only after the inclusion of up to d virtual orbitals. The mixing of d and higher symmetry states with S and P , due to Schiff moment Hamiltonian is very small, because d and higher symmetries do not have nonzero density inside the nucleus. There is a 31% increase of the magnitude of the EDM of Xe in the CPHF framework compared to the Dirac-Fock value. Inclusion of d virtuals decreases the value of EDM by 28% as the residual Coulomb interaction taken to all orders, contributes with opposite sign to that of the S - P contribution.

B. Ytterbium

For the ^{171}Yb EDM calculation, the active orbitals are $(1 - 24)_{S_{1/2}}(2 - 17)_{P_{1/2}, P_{3/2}}(3 - 13)_{d_{3/2}, d_{5/2}}(4 - 8)_{f_{5/2}, f_{7/2}}(5 - 9)_{g_{7/2}, g_{9/2}}(6 - 9)_{h_{9/2}, h_{11/2}}$. The Tables IV and V show the dominant occupied-unoccupied orbital pairings and the single-particle transitions, respectively. The major contributions come from $S_{1/2}$ - $P_{3/2}$ and $S_{1/2}$ - $P_{1/2}$

TABLE IV. All order contribution to Yb EDM arising from the nuclear Schiff moment in units of $[\text{S/e fm}^3]$ e cm.

Pairings	EDM $\times 10^{-17}$
Occupied-Unoccupied	
$S_{1/2}$ - $P_{1/2}$	-1.058
$P_{1/2}$ - $S_{1/2}$	0.165
$S_{1/2}$ - $P_{3/2}$	-1.365
$P_{3/2}$ - $S_{1/2}$	0.296
Others	0.059
Total	-1.903

TABLE V. Dominant contributions to Yb EDM from the $S_{1/2}$ - $P_{3/2}$ pairing in units of $[\text{S/e fm}^3]$ e cm.

Pairings	EDM $\times 10^{-17}$
Occupied-Unoccupied	
$6s_{1/2}$ - $6p_{3/2}$	-0.347
$6s_{1/2}$ - $7p_{3/2}$	-0.723
$6s_{1/2}$ - $8p_{3/2}$	-0.339
$6s_{1/2}$ - $9p_{3/2}$	-0.033
$4s_{1/2}$ - $11p_{3/2}$	0.011

combinations. All the major excitations occur from the outermost $6s^2$ orbital. The Dirac-Fock contribution to the EDM of Yb atom is $-0.419 \times 10^{-17}[\text{S/e fm}^3]$ e cm and in CPHF theory is $-1.903 \times 10^{-17}[\text{S/e fm}^3]$ e cm. This change in the magnitude of EDM with respect to the Dirac-Fock contribution can be attributed to the two loosely bound $6s$ orbitals of Yb and also to the effects of core polarization.

In Table VI, a dramatic increase in polarizability occurs when $p_{3/2}$ virtual orbitals are included.

C. Radium

The active orbitals used for calculation of nuclear-Schiff-moment-induced EDM of Ra atom is $(1 - 24)_{S_{1/2}}(2 - 18)_{P_{1/2}, P_{3/2}}(3 - 14)_{d_{3/2}, d_{5/2}}(4 - 9)_{f_{5/2}, f_{7/2}}(5 - 10)_{g_{7/2}, g_{9/2}}(6 - 8)_{h_{9/2}, h_{11/2}}$. The total EDM of atomic Ra in the Dirac-Fock and the CPHF framework are $-1.842 \times 10^{-17}[\text{S/e fm}^3]$ e cm and $-8.093 \times 10^{-17}[\text{S/e fm}^3]$ e cm respectively. The large magnitude of EDM in comparison with the Dirac-Fock result highlights the role of the electron-correlation effect in a heavy system such as radium. The sign of the final value of EDM is determined by that of the Dirac-Fock contributions.

The results in Table VII show the contributions of the orbital pairing where $S_{1/2}$ - $P_{3/2}$ and $S_{1/2}$ - $P_{1/2}$ orbital combinations are shown to contribute dominantly. Single-particle transition contributions to $S_{1/2}$ - $P_{3/2}$ combinations are given in Table VIII. From the Tables I, IV, VII, the non- S - P orbital pairings contribute with opposite sign to the S, P pairings. The core-polarization effect considerably increases the non- S - P contribution for Xe and Ra atoms. The effect of gradual inclusion of higher symmetry virtual orbitals on the values of EDM and polarizability are shown in Table IX.

TABLE VI. Gradual inclusion of virtual states (EDM in units of $10^{-17}[\text{S/e fm}^3]$ e cm and polarizability in a.u).

Virtual states	Yb EDM	α
Up to $p_{1/2}$	-0.884	82.07
Up to $p_{3/2}$	-1.88	173.02
Up to $d_{5/2}$	-1.903	175.99
Up to $f_{7/2}$	-1.901	176.00
Up to $g_{9/2}$	-1.901	176.16
Up to $h_{11/2}$	-1.903	176.16

TABLE VII. All order contribution to Ra EDM arising from nuclear Schiff moment in units of $[S/e \text{ fm}^3] \text{ e cm}$.

Pairings Occupied-Unoccupied	EDM $\times 10^{-17}$
$S_{1/2}$ - $P_{1/2}$	-5.279
$P_{1/2}$ - $S_{1/2}$	0.771
$S_{1/2}$ - $P_{3/2}$	-5.462
$P_{3/2}$ - $S_{1/2}$	1.288
Others	0.589
Total	-8.093

Higher symmetry or the non- S - P contributions to the atomic EDM for Xe are higher than that for Yb.

The CPHF effect increases the magnitude of the atomic EDM to about fivefold higher than the DF value, for atoms Yb and Ra. This dramatic variation is due to the presence of valence S electrons, that are easily excitable and have contributed dominantly. Hence, the core-valence interactions have played major role in determining the final magnitude of EDM. Contribution of d virtuals decreases the magnitude of atomic EDM for Xe atom but increases EDM value for Yb and Ra since the d orbitals contribute through the electric dipole matrix element with negative sign in the case of Yb and Ra and with a positive sign in the case of Xe.

The recent reported value for EDM of atomic Xe [8] is $0.337 \times 10^{17} \text{ S/e fm}^3$. This calculation was performed in the framework of the relativistic coupled-cluster method and the correlations not accounted for by the CPHF approach may amount to $\approx 10\%$ for atomic Xe.

In Table X, the results of atomic EDM induced by the NSM from other methods are summarized. The differences between our results for the atomic EDM induced by the NSM when compared to MCHF results of Ref. [21] differ by about 13% for Yb and 6% for Ra. Apart from the method of generation of the single-particle orbitals and subsequently the perturbed orbitals, one reason for discrepancy might be due to the fact that in the CPHF approach, the entire space of core electrons participate in excitation. In Ref. [14], full CI was performed for valence electrons to incorporate valence-valence and core-

TABLE VIII. Dominant contributions to Ra EDM from $S_{1/2}$ - $P_{3/2}$ pairing in units of $[S/e \text{ fm}^3] \text{ e cm}$.

Pairings Occupied-Unoccupied	EDM $\times 10^{-17}$
$7s_{1/2}$ - $7p_{3/2}$	-1.703
$6s_{1/2}$ - $8p_{3/2}$	-0.014
$7s_{1/2}$ - $8p_{3/2}$	-2.705
$6s_{1/2}$ - $9p_{3/2}$	-0.026
$7s_{1/2}$ - $9p_{3/2}$	-1.014
$6s_{1/2}$ - $10p_{3/2}$	-0.057
$7s_{1/2}$ - $10p_{3/2}$	-0.098
$5s_{1/2}$ - $11p_{3/2}$	0.018

TABLE IX. Gradual inclusion of virtual states (EDM in units of $10^{-17}[S/e \text{ fm}^3] \text{ e cm}$ and polarizability in a.u).

Virtual states	Ra EDM	α
Up to $p_{1/2}$	-4.265	141.28
Up to $p_{3/2}$	-7.843	286.85
Up to $d_{5/2}$	-8.088	291.01
Up to $f_{7/2}$	-8.093	291.31
Up to $g_{9/2}$	-8.093	291.73
Up to $h_{11/2}$	-8.093	291.73

valence electron correlation effects in EDM calculations. In CPHF, the core and valence orbitals are treated on an equal footing and orbitals were generated under V^N approximation. The differences between our result and the results from MBPT + CI [14] may be due to valence-valence correlation effects. The differences between results of NSM-induced EDM in the TDHF and CPHF approaches, is less than 1% for Yb and is 1.7% for Ra.

V. CONCLUSION

The effect of all order of residual Coulomb interaction is studied in CPHF framework. The P , T violating Hamiltonian leads to excitation of valence electrons of opposite parity. Coulomb perturbed potential plays a major role for Yb and Ra atoms as these atoms have valence electrons. The CPHF method is computationally inexpensive. At the same time, we can attain good accuracy comparable to other MBPT based theories. In our work we are able to reproduce previously reported values of EDM by Dzuba *et al.* [14] with accuracy of 100% for Xe, 89% for Yb, and 91% for Ra. The difference in the results for Yb and Ra atoms may be due to the correlation effects of valence electrons that are missing in the CPHF framework. The S and P combinations of the occupied and unoccupied single-particle orbitals contribute more to atomic EDM since the Schiff moment produces a contact interaction only. The non- S - P pairings also contribute through residual Coulomb interaction and electric dipole operator but the contribution is to oppose the contribution of S - P combinations. At the CPHF level, for EDM, we find that the single-particle orbital

TABLE X. Nuclear-Schiff-moment-induced atomic EDMs of Xe, Yb, and Ra using CPHF method and comparison of the results with other methods (EDM in units of $10^{-17}[S/e \text{ fm}^3] \text{ e cm}$).

Methods	Atoms		
	Xe	Yb	Ra
MBPT + CI [14]		-2.12	-8.84
TDHF [14]	0.38	-1.95	-8.27
MCHF [21]		-2.15	-8.63
CCSD _p T [8]	0.337		
TDHF [6,22]	0.378	-1.91	-8.23
MBPT + CI [6]			-8.70
Our results	0.378	-1.903	-8.093

pairings ($s_{1/2}, p_{3/2}$) produce the most dominant contributions in Xe and Yb, though for Ra, the ($s_{1/2}, p_{1/2}$) pairings contribute comparably.

Our results will serve as an important benchmark for future accurate calculations based on coupled-cluster theory. Corrections beyond CPHF may change the magnitude of the EDM of xenon by about 10%.

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