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Relativistic many-body theory of the electric dipole moment of ^{129}Xe and its implications for probing new physics beyond the standard model

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We report the results of our theoretical studies of the time-reversal and parity violating electric dipole moment (EDM) of ^{129}Xe arising from the nuclear Schiff moment (NSM) and the electron-nucleus tensor-pseudotensor (T-PT) interaction based on the self-consistent and the normal relativistic coupled-cluster methods. The important many-body effects are highlighted and their contributions are explicitly presented. The uncertainties in the calculations of the correlation and relativistic effects are determined by estimating the contributions of the triples excitations and the Breit interaction, respectively, which together amount to about 0.7% for the NSM and 0.2% for the T-PT interactions. The results of our present work in combination with improved experimental limits for ^{129}Xe EDM in the future would tighten the constraints on the hadronic $\mathcal{CP}$ violating quantities, and this could provide important insights into new physics beyond the standard model of elementary particles.

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The observation of the electric dipole moment (EDM) of a nondegenerate system would be a signature of violations of both time-reversal ($\mathcal{T}$) and parity ($\mathcal{P}$) symmetries [1,2]. The $\mathcal{CPT}$ theorem implies that $\mathcal{T}$ violation amounts to $\mathcal{CP}$ violation [3]. The standard model (SM) of particle physics contains $\mathcal{CP}$ violation in the form of a complex phase in the Kobayashi-Maskawa matrix, which, however, cannot explain the large matter-antimatter asymmetry observed in the Universe [4]. This suggests [5,6] that although the SM predicts very small values for atomic EDMs, their actual sizes could lie close to the current experimental limits [7].

The EDMs of diamagnetic atoms have the potential to probe new physics at energy scales much higher than TeV [8]. They are primarily sensitive to the nuclear Schiff moment (NSM) and the tensor-pseudotensor (T-PT) electron-nucleus interaction [8]. The former arises due to $\mathcal{CP}$ violating nucleon-nucleon interactions and the EDMs of nucleons, which at the level of elementary particles arise from $\mathcal{CP}$ violating quark-quark interactions and the EDMs and chromo-EDMs of quarks [8]. On the other hand, the latter is due to the T-PT electron-nucleon interaction originating from the T-PT electron-quark interaction, which has been predicted by leptoquark models [9].

There have been important developments in the search for EDMs of elementary particles and composite systems in recent years. The most stringent EDM limit to date, $d_{\rm Hg} < 7.4\times10^{-30}e$ cm [95% confidence level (C.L.)], comes from the diamagnetic atom, ^{199}Hg [10]. This unprecedented precision has been achieved due to the steady improvements in the spin precession measurement for this atom over the past three decades. The first result for another diamagnetic atom, ^{225}Ra, for which the nuclear octupole deformation is expected to amplify its atomic EDM by about two to three orders of magnitude [11], was reported 3 years ago [12] to be $d_{\rm Ra} < 1.4\times10^{-23}e$ cm (95% C.L.). As for the ^{129}Xe diamagnetic atom, three experiments on its EDM are currently under way [13–15]. Among the above three diamagnetic species, ^{225}Ra is radioactive with a half-life of 14.9 d, while ^{199}Hg and ^{129}Xe are stable. Of the two stable atoms ^{199}Hg and ^{129}Xe, the latter is characterized by its exceptionally long transverse–spin relaxation times in a gas of atmospheric pressure [16]. The result for the first ^{129}Xe EDM measurement was published in 1984 [17]. In fact, two groups have reported improved measurements of EDM in ^{129}Xe recently [18,19]. One of these measurements gives its value as $(0.26 \pm 2.33_{\rm stat} \pm 0.72_{\rm sys})\times10^{-27}e$ cm (95% C.L.) [18], while the other measurement reports as $(-4.7 \pm 6.4)\times10^{-28}e$ cm (95% C.L.) [19] improving by factors of one-and-a-half and five times, respectively, than the previous measurement $(0.7 \pm 3.3_{\rm stat} \pm 0.1_{\rm sys})\times10^{-27}e$ cm (95% C.L.) [20]. It is still possible to improve its limit by carrying out measurement with a macroscopic number of confined atoms in a glass cell, enabling long spin coherence times and large spin precession signals. The theoretical foundations of the Xe EDM were laid in a series of seminal papers by Flambaum and co-workers [21–24]. There have been recent advances in the relativistic many-body calculations of the EDM of this atom [8,25]. The results of these calculations are necessary for extracting $\mathcal{CP}$ violating coupling constants from the measured values of the Xe EDM [8,25]. The relativistic coupled-cluster (RCC) theory, which is widely considered as the gold standard for the electronic structure of heavy atoms [26], was first applied to the ^{129}Xe EDM by Singh *et al.* by taking one particle–one hole (1p1h), two particle–two hole (2p2h), and partial three particle–three hole (3p3h) excitations [27]. In the present work, we overcome some of the limitations of the previous calculation by using two different variants of the RCC theory. Higher order excitations built from different powers of the 1p1h and 2p2h excitations are included in the first approach in a self-consistent manner in the evaluation of the EDM, which

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forms a nonterminating series. The second approach, which is known as the relativistic normal coupled cluster (RNCC) theory, does not treat the bra and ket on the same footing and this enables the expectation value representing the EDM to terminate naturally [28]. We had recently performed ground state electric dipole polarizability calculations of ^{129}Xe using these two methods and obtained results that are in very good agreement with its measured value [29]. Given the similarities between the electric dipole polarizability and the EDM from the viewpoint of relativistic many-body theory, it is indeed appropriate to apply the two above-mentioned RCC methods to the ^{129}Xe EDM arising from the NSM and the T-PT electron-nucleus interaction.

The T-PT Hamiltonian is given by [30–32]

$$H_{\rm int}^{\rm T\text{-}PT} = i\sqrt{2}G_{\rm F}C_{\rm T}\sum_i(\boldsymbol{\sigma}_{\rm N}\cdot\gamma_i)\rho_{\rm N}(r), \tag{1}$$

where $G_{\rm F}$ is the Fermi constant, $C_{\rm T}$ represents the T-PT coupling constant, γ_i's are the Dirac matrices, $\boldsymbol{\sigma}_{\rm N} = (\sigma_x, \sigma_y, \sigma_z)$ where σ_x, σ_y, and σ_z are the Pauli spin operators for the nucleus with spin $I = 1/2$, and $\rho_{\rm N}(r)$ is the nuclear charge density.

The NSM interaction Hamiltonian in the atom is given by [31,32]

$$H_{\rm int}^{\rm NSM} = \frac{3\boldsymbol{S}\cdot\boldsymbol{r}}{B}, \tag{2}$$

where $\boldsymbol{S} = S\frac{\boldsymbol{I}}{I}$ is the NSM, and $B = \int_0^\infty dr\, r^4\rho_{\rm N}(r)$.

In this study, we only consider the first-order perturbation in the $\mathcal{P}$ and $\mathcal{T}$ violating interaction. Therefore, the total atomic Hamiltonian is expressed as

$$H = H_{\rm DC} + \lambda H_{\mathcal{P}\mathcal{T}_{\rm viol.}} \tag{3}$$

where $H_{\rm DC}$ is the Dirac-Coulomb (DC) Hamiltonian that is given by

$$H_{\rm DC} = \sum_i^{N_e}[c\boldsymbol{\alpha}\cdot\boldsymbol{p} + mc^2\boldsymbol{\beta} + V_{\rm N}(r_i)] + \frac{1}{2}\sum_{i,j}\frac{1}{r_{ij}}, \tag{4}$$

and $\lambda H_{\mathcal{P}\mathcal{T}_{\rm viol.}}$ corresponds to either of the $\mathcal{P}$ and $\mathcal{T}$ violating Hamiltonians given by Eqs. (1) and (2). Here we assume that the perturbation parameter λ is either S or $G_{\rm F}C_{\rm T}\langle\boldsymbol{\sigma}_{\rm N}\rangle$. The atomic wave function $|\Psi_0\rangle$ is written as

$$|\Psi_0\rangle \simeq \left|\Psi_0^{(0)}\right\rangle + \lambda\left|\Psi_0^{(1)}\right\rangle_\lambda, \tag{5}$$

where the superscripts (0) and (1) represent the unperturbed and the first-order perturbed wave functions due to $H_{\mathcal{P}\mathcal{T}_{\rm viol.}}$, respectively.

The expectation value of the EDM in the ground state $|\Psi_0\rangle$ in an atom in our calculation is given by

$$d_{\rm a} = \frac{\langle\Psi_0|D|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}, \tag{6}$$

where D is the electric dipole moment operator. From Eqs. (5) and (6), we can equivalently express

$$d_{\rm a} = 2\lambda\frac{\left\langle\Psi_0^{(0)}\middle|H_{\mathcal{P}\mathcal{T}_{\rm viol.}}\middle|\Psi_0^{(1)}\right\rangle_g}{\left\langle\Psi_0^{(0)}\middle|\Psi_0^{(0)}\right\rangle}, \tag{7}$$

where $|\Psi_I^{(0)}\rangle_g$ is the first-order perturbed wave function due to the electric dipole, and it is written by

$$\left|\Psi_0^{(1)}\right\rangle_g = g\sum_I\left|\Psi_I^{(0)}\right\rangle\frac{\left\langle\Psi_I^{(0)}\middle|D_g\middle|\Psi_0^{(0)}\right\rangle}{E_0^{(0)} - E_I^{(0)}} \tag{8}$$

with $D_g = D/g$ for an arbitrary parameter g. In our calculation, we have used Eq. (7) for the calculation of an atomic EDM. We present our T-PT and NSM results in terms of $\eta = \frac{d_{\rm a}}{\langle\sigma_{\rm N}\rangle C_{\rm T}\times 10^{20}|e|{\rm cm}}$ and $\zeta = \frac{d_{\rm a}}{S\times 10^{17}|e|{\rm cm}/(|e|{\rm fm}^3)}$, respectively.

The ground state wave function of a closed-shell atom in the RCC theory is expressed as [33]

$$|\Psi\rangle = e^T|\Phi_0\rangle, \tag{9}$$

where $|\Phi_0\rangle$ is the Dirac-Fock (DF) wave function, the cluster operator T can be written as

$$T = \sum_{I=1}^N T_I = \sum_{I=1}^N t_I C_I^+, \tag{10}$$

where I is the index for the particle-hole excitation from the DF, closed-shell state, N is the maximum value for I, t_I is the excitation amplitude, and C_I^+ is a general I particle-hole excitation operator consisting of a string of creation and annihilation operators. In the singles and doubles approximation in the RCC theory (RCCSD method), the maximum value of I is restricted to 2; i.e., $T = T_1 + T_2$, where T_1 and T_2 are one particle–one hole and two particle–two hole excitation operators. We can express T as

$$T = T^{(0)} + gT^{(1)}, \tag{11}$$

where $T^{(1)}$ is the first-order excitation RCC operator due to D_g. Therefore, the total wave function is given by

$$|\Psi_0\rangle = e^{T^{(0)}+gT^{(1)}}|\Phi_0\rangle. \tag{12}$$

The amplitudes for $T^{(0)}$ can be obtained by solving the equation [34]

$$\langle\Phi_0|C_I^-\overline{H}_{\rm DC}|\Phi_0\rangle = 0, \tag{13}$$

where C_I^- referred to as the deexcitation operators, are the adjoint of C_I^+. From here onward, we use the notation $\overline{O} = e^{-T}Oe^T = (Oe^T)_{\rm c}$ for a general operator O and the subscript "c" stands for the connected terms [34]. Similarly, amplitudes of $T^{(1)}$ are obtained by

$$\langle\Phi_0|C_I^-(\overline{H}_{\rm DC}T^{(1)} - \overline{D}_g)|\Phi_0\rangle = 0. \tag{14}$$

Using Eqs. (7), (9), and (12), the expression for EDM in the RCCSD method can be written as [28]

$$\begin{aligned}\frac{d_{\rm a}}{\lambda} &= 2\langle\Phi_0|e^{T^{(0)\dagger}}H_{\mathcal{P}\mathcal{T}_{\rm viol.}}e^{T^{(0)}}T^{(1)}|\Phi_0\rangle_{\rm c}\\ &= 2\langle\Phi_0|\big[H_{\rm PTV} + \big(H_{\mathcal{P}\mathcal{T}_{\rm viol.}}T^{(0)} + {\rm c.c.}\big)\\ &\quad + \big(T^{(0)\dagger}H_{\mathcal{P}\mathcal{T}_{\rm viol.}}T^{(0)} + {\rm c.c.}\big)\\ &\quad + \big(\tfrac{1}{2}T^{(0)\dagger}H_{\mathcal{P}\mathcal{T}_{\rm viol.}}T^{(0)^2} + {\rm c.c.}\big) + \cdots\big]T^{(1)}|\Phi_0\rangle_{\rm c}.\end{aligned} \tag{15}$$

In the relativistic coupled-cluster self-consistent [RCC(SC)] approach, the combined power of $T^{(0)}$ and its adjoint $T^{(0)\dagger}$ increases in the successive terms in the above expression, and they are computed systematically avoiding double counting

TABLE I. Results for static dipole polarizability [ea_0^3], η, and ζ for ^{129}Xe using different theoretical methods. $\Delta_{\rm Breit}^{\rm CPDF}$ and $\Delta(T_3)$ are the corrections due to the Breit interaction at the CPDF method and the partial triple excitations, respectively.

	This work			Others		
Method	α_d	η	ζ	α_d	η	ζ
DF	26.87	0.45	0.29	26.87	0.45	0.26 [37]
				26.92	0.45	0.29 [27]
CPDF	26.97	0.57	0.38	26.98	0.56	0.37 [37]
				27.7	0.56	0.38 [27]
$\Delta_{\rm Breit}^{\rm CPDF}$		−0.001	−0.002			
RCCSD				27.74	0.50	0.34 [27]
RCCSD(SC)	28.12	0.48	0.32	28.13	0.47	0.33 [37]
$\Delta(T_3)$	−0.107	∼0	∼0			
RNCCSD	27.51	0.49	0.32			
Experiment				27.815(27) [36]		

until convergence is obtained. In the singles and double approximation, RCC(SC) will be referred to as RCCSD(SC).

In order to avoid the nontermination problem in the above expression of the RCC method, we use the RNCC method for the evaluation of the ^{129}Xe EDM. In this method the RCC bra state $\langle\Psi| = \langle\Phi_0|e^{T^\dagger}$ is replaced by

$$\langle\widetilde{\Psi}| = \langle\Psi|(1+\widetilde{T})e^{-T}, \tag{16}$$

where $\widetilde{T} = \sum_{I=1}^{N}\widetilde{T}_I = \sum_{I=1}^{N}\widetilde{t}_I C_I^-$ is a deexcitation operator with amplitude $\widetilde{t}_I$, similar to $T^\dagger = \sum_{I=1}^{N} T_I^\dagger = \sum_{I=1}^{N} t_I^* C_I^-$. The RNCC bra state should satisfy

$$\langle\widetilde{\Psi}|H = \langle\widetilde{\Psi}|E_0. \tag{17}$$

Furthermore,

$$\langle\widetilde{\Psi}|\Psi\rangle = \langle\Phi_0|(1+\widetilde{T})e^{-T}e^{T}|\Phi_0\rangle = 1, \tag{18}$$

since the DF state $|\Phi_0\rangle$ is normalized. Making use of this property, the expectation value of an operator O in the RNCC method can be expressed as

$$\langle O\rangle = \frac{\langle\widetilde{\Psi}|O|\Psi\rangle}{\langle\widetilde{\Psi}|\Psi\rangle} = \langle\Phi_0(1+\widetilde{T})\overline{O}|\Phi_0\rangle_{\rm c}. \tag{19}$$

The above expression terminates unlike its counterpart in the RCC.

In the RNCC method, $\widetilde{T}$ is written as

$$\widetilde{T} = \widetilde{T}^{(0)} + g\widetilde{T}^{(1)}, \tag{20}$$

where $\widetilde{T}^{(0)}$ is the unperturbed deexcitation operator, and $\widetilde{T}^{(1)}$ is the first-order correction to it due to D_g. Then, the total bra state can be written as

$$\langle\widetilde{\Psi}_0| = \langle\Phi_0|(1+\widetilde{T}^{(0)}+g\widetilde{T}^{(1)})e^{-T^{(0)}-gT^{(1)}}. \tag{21}$$

From Eq. (17), the amplitudes for $\widetilde{T}^{(0)}$ are obtained from

$$\langle\Phi_0|(1+\widetilde{T}^{(0)})[\overline{H}_{\rm DC}, C_I^+]|\Phi_0\rangle = 0. \tag{22}$$

Similarly, the amplitudes for $\widetilde{T}^{(1)}$ are obtained from

$$\langle\Phi_0|[\widetilde{T}^{(1)}\overline{H}_{\rm DC}+(1+\widetilde{T}^{(0)})\{\overline{D}_g+(\overline{H}_{\rm DC}T^{(1)})_{\rm c}\}]C_I^+|\Phi_0\rangle = 0. \tag{23}$$

Adapting Eq. (6) to the case where D_g is a perturbation in the framework of RNCC, we get

$$\frac{d_{\rm a}}{\lambda} \equiv \frac{1}{g}\frac{\langle\widetilde{\Psi}_0|H|\Psi_0\rangle}{\langle\widetilde{\Psi}_0|\Psi_0\rangle} = \langle\Phi_0|\widetilde{T}^{(1)}\overline{H}_{\mathcal{P}\mathcal{T}_{\rm viol.}} + (1+\widetilde{T}^{(0)})\overline{H}_{\mathcal{P}\mathcal{T}_{\rm viol.}}T^{(1)}|\Phi_0\rangle_{\rm c}. \tag{24}$$

This expression terminates unlike Eq. (15) which corresponds to the RCC case. The RNCC method has the merit of satisfying the Hellmann-Feynman theorem [34] in contrast to that of the RCC method.

In the present study, we have used Gaussian type of orbitals (GTOs) to obtain the DF wave function. The details of the optimized parameters that are needed to define the GTOs are discussed in our previous work on the electric dipole polarizability (α_d) study on the ^{129}Xe atom [29]. Using these basis functions, we present our results for η and ζ at different levels of approximations of many-body methods in Table I. One of the methods that has been employed earlier [32,35] is the coupled-perturbed Dirac-Fock (CPDF) approximation, which takes into account the perturbation of the core to first order in the $\mathcal{T}$ and $\mathcal{P}$ violating interaction and all orders by the residual Coulomb interaction. We had also performed these calculations earlier using the RCCSD method, but considering only some lower order nonlinear terms in Eq. (15) in contrast to the self-consistent procedure in the present work. The DF contribution as expected is the largest. The CPDF contributions are over 20% of the DF results in both cases. Our DF and CPDF calculations are in good agreement with the previous calculations [32,35]. The correlation effects beyond CPDF, primarily those involving various classes of pair correlation, collectively reduce the values of η and ζ as reflected in the final results for the two versions of the RCC theory used in the present work. We have also given the α_d value obtained using our methods in the same table and compared with other available results. As can be seen, our RCCSD(SC) and singles and doubles approximation RNCC theory (RNCCSD method) calculations for α_d are close to its measured value [36]. Furthermore, our RCCSD(SC) results for this quantity as well as η and ζ are in good agreement with those of

TABLE II. Contributions for T-PT and NSM for ^{129}Xe from different terms in RCCSD(SC).

Leading RCC terms	η	ζ
$H_{\mathcal{PT}_{\rm viol.}} T_1^{(1)} + \text{H.c.}$	0.5387	0.3524
$T_1^{(0)\dagger} H_{\mathcal{PT}_{\rm viol.}} T_1^{(1)} + \text{H.c.}$	0.0023	0.0011
$T_1^{(0)\dagger} H_{\mathcal{PT}_{\rm viol.}} T_2^{(1)} + \text{H.c.}$	−0.0003	0.000036
$T_2^{(0)\dagger} H_{\mathcal{PT}_{\rm viol.}} T_1^{(1)} + \text{H.c.}$	−0.0610	−0.0354
$T_2^{(0)\dagger} H_{\mathcal{PT}_{\rm viol.}} T_2^{(1)} + \text{H.c.}$	0.0016	0.000789

other calculations of α_d and the two quantities related to the EDM, but with different GTO basis functions [27,37]. The values of the latter two quantities cannot be determined from experiments, but since the two $\mathcal{P}$ and $\mathcal{T}$ violating interactions related to them have the same rank and parity as the electric dipole operator, we expect our calculated values of η and ζ to be accurate.

The leading contributions from the terms in Eq. (15) are listed in Table II. The most important of these is $\langle\Phi_0|H_{\mathcal{PT}_{\rm viol.}} T_1^{(1)}|\Phi_0\rangle$, which we refer to as the $H_{\mathcal{PT}_{\rm viol.}} T_1^{(1)}$ term. It consists of the DF and certain classes of correlation effects to all orders in the residual Coulomb interaction such as those represented by the CPDF approximation [29]. In particular it subsumes an important correlation effect involving the simultaneous excitation of two core electrons [29]. Its magnitude is equal to that of its Hermitian conjugate (H.c.). The results of our RNCCSD calculations for η and ζ are given in Table I. The breakdown of the contributions from the individual terms are given in Table III. The leading contributors are $\langle\Phi_0|H_{\mathcal{PT}_{\rm viol.}} T_1^{(1)}|\Phi_0\rangle$ and $\langle\Phi_0|\widetilde{T}_1^{(1)} H_{\mathcal{PT}_{\rm viol.}}|\Phi_0\rangle$. The latter is the counterpart of the Hermitian conjugate (H.c.) of the former term. The two largest contributions in the case of RCCSD(SC), i.e., $\langle\Phi_0|H_{\mathcal{PT}_{\rm viol.}} T_1^{(1)}|\Phi_0\rangle$ and $\langle\Phi_0|T_2^{(0)\dagger} H_{\mathcal{PT}_{\rm viol.}} T_1^{(1)}|\Phi_0\rangle$, and their counterparts for RNCCSD are not very different. The final results for the two methods given in Table I differ by only 2.0% (T-PT) and are in complete agreement for the NSM case.

We have evaluated the numerical error in our RCC calculations by estimating the contributions from the leading electron correlation and relativistic effects that have been omitted in our calculations. The former is characterized by the 3p3h (triples) excitations and the latter by the Breit interaction, which is the leading relativistic correction to the electron-electron Coulomb interaction [38]. The error due to the first source has been estimated by calculating the perturbed triple excitation amplitudes [29] and the absolute values of this contribution for η and ζ in the present study is 3.9×10^{-5} and 1.3×10^{-4}, respectively. In this work, the Breit interaction contributions were found to be 0.6% and 0.9% of the total Dirac Coulomb contributions in the CPDF and RCCSD approximations, respectively. Our net estimate of the error in our calculations from these two sources are 1.1×10^{-3} for the T-PT interaction and 2.1×10^{-3} for the NSM.

TABLE III. Contributions for T-PT and NSM for ^{129}Xe from different terms in RNCCSD.

Leading RNCC terms	η	ζ
$H_{\mathcal{PT}_{\rm viol.}} T_1^{(1)}$	0.269	0.176
$\widetilde{T}_1^{(1)} H_{\mathcal{PT}_{\rm viol.}}$	0.256	0.169
$\widetilde{T}_1^{(1)} H_{\mathcal{PT}_{\rm viol.}} T_2^{(0)}$	−0.029	−0.017

The latest reported experimental result for the EDM of ^{129}Xe is $|d_{\rm a}| < 1.5\times10^{-27}|e|$cm with 95% C.L. [19]. Combining this result with our present RNCCSD calculations, $d_{\rm a} = 0.49\times10^{-20}\langle\sigma\rangle C_{\rm T} e\,$cm and $d_{\rm a} = 0.32\times10^{-17}\, S/(|e|\text{fm}^3)\,|e|$cm, and assuming that the EDM is due to a single source of either the NSM or the T-PT interaction, we obtain, respectively, the following upper limits:

$$|S| < 4.7\times10^{-10}|e|\text{fm}^3 \tag{25}$$

and

$$|C_{\rm T}| < 6.1\times10^{-7} \tag{26}$$

for the value $\langle\sigma_{\rm N}\rangle = 1/2$.

It is important to notice here that the status of nuclear structure calculations for ^{129}Xe is far more satisfactory than that for ^{199}Hg. The first calculation of the Schiff moment for ^{129}Xe [39] was carried out by taking into full account core-polarization effects in the single neutron outside a core approximation of an even-even nucleus. More recently, a substantially improved large-scale calculation based on the pair-truncated shell model approach [6] has been reported. Results of this calculation are of the same sign and of the same order of magnitude as the previous calculation, unlike the case of ^{199}Hg [8,11]. Thus, both the atomic and the nuclear calculations are now more reliable for ^{129}Xe than those for ^{199}Hg. Turning to the cases of nuclei exhibiting octupole deformation and vibration collectivities, theoretical calculation of the Schiff moment for ^{129}Xe could be even more reliable. The isotopes of such kind, however, are all found (at least until present) to be unstable, radioactive ones, for which experimental precision is largely limited and therefore, reaching the sensitivities to $\mathcal{CP}$ violating coefficients of levels achieved by ^{199}Hg and ^{129}Xe requires a long journey of technical developments. Thus, the EDM of the ^{129}Xe atom would be among the leading probes of $\mathcal{CP}$ violating fundamental parameters for the diamagnetic atoms that are under experimental consideration.

It is obvious from the above discussions that the EDM of ^{129}Xe depends on two coupling constants $\bar{g}^{(0)}$, $\bar{g}^{(1)}$ (note that the $\bar{g}^{(2)}$ term is expected to be negligible) and one T-PT electron-nucleus coupling constant, $|C_{\rm T}|$ [40]. The predictions for the relative strengths of these three coupling constants vary for different models proposed for new physics. Limits for these three coupling constants have been obtained by considering the EDM results for three different systems, one of them being ^{129}Xe [40,41]. Clearly when the sensitivity of the ^{129}Xe EDM experiment improves, the former two limits in tandem with quantum chromodynamics [42–44] will give improved limits for $|\bar{d}_u - \bar{d}_d|$, $|\bar{d}_u + \bar{d}_d|$, and $|\bar{\theta}|$, where $\bar{d}_u$ and $\bar{d}_d$ are the up- and down-quark chromo-EDMs and $\bar{\theta}$ is a parameter associated with $\mathcal{CP}$ violation in quantum chromodynamics. These new limits are likely to provide useful information on the character of new physics beyond the standard model [8]. In

addition, as mentioned earlier, three experiments on the ^{129}Xe EDM are in progress, and improved limits for this quantity are expected in the near future [13–15]. These experiments aim to improve the current limit, which is of the order of $10^{-27}|e|$cm, by as much as three orders of magnitude [15]. If that comes to fruition, then the sensitivity of the ^{129}Xe EDM experiment could match or even surpass that of the Hg experiment, for which the upper limit ($7.4\times10^{-30}|e|$cm [10]) is currently the best that has been obtained for any elementary particle or composite systems. It is necessary to emphasize that the theoretical results for ^{129}Xe EDM reported in the present work are more accurate and reliable than those obtained for ^{199}Hg EDM [45]. The contributions of the higher-order many-body effects are not as large for the former as they are for the latter. This is evident from the distinctly smaller differences between the EDM results of the lowest-order and self-consistent RCCSD levels for ^{129}Xe (see Table I) compared to those of ^{199}Hg [45]. Furthermore, the latter result is in excellent agreement with that of the RNCCSD method. Therefore based on both experimental and theoretical considerations, it appears that the ^{129}Xe EDM has the potential to be a more promising candidate for probing new physics beyond the standard model than the ^{199}Hg EDM.

The self-consistent and the normal versions of the relativistic coupled cluster singles and doubles method have been employed to calculate the ratios of the atomic EDM of ^{129}Xe to the T-PT interaction coupling constant η and the Schiff moment ζ. The results from the two methods disagree only by 2% for the former and are in perfect agreement for the latter. A comparison of these results with that of the lowest-order relativistic coupled-cluster singles and doubles method show that the higher-order many-body effects converge rapidly, unlike in the case of the ^{199}Hg EDM. For the ^{129}Xe EDM, the estimated errors are 0.2% for the T-PT interaction and 0.7% for the NSM. The high accuracy that has been achieved in the present calculations of η and ζ for ^{129}Xe suggests that the results of these quantities in combination with the improved results of the future EDM experiments on ^{129}Xe could serve as a reliable probe for new physics beyond the standard model of elementary particle physics.

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