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Atomic electric-dipole moments from Higgs-boson-mediated interactions

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Electric-dipole moments of paramagnetic atoms can provide important insights into a unique kind of CP violation involving Higgs-boson-mediated interactions between leptons and hadrons. We report a limit for the coupling constant of such an interaction by combining the results of our relativistic many-body calculations and experimental data on the electric-dipole moment of atomic thallium. The importance of electron correlation in determining this limit is highlighted and its significance in the context of particle physics and cosmology is pointed out.

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Atomic electric-dipole moments (EDMs) arising from the violations of parity (P) and time-reversal (T) symmetries can provide important information about physics beyond the standard model (SM) of elementary particle physics [1]. T violation implies CP violation via the CPT theorem [2,3]. The dominant sources of the EDM of a paramagnetic atom are the EDM of an electron and the scalar-pseudoscalar (S-PS) interaction between the electron and nucleus which violates P and T symmetries [4]. While the former has been dealt with extensively [5], the latter has received relatively little attention.

The S-PS electron-nucleus interaction originates from the S-PS electron-quark interaction. It could be mediated by a neutral Higgs (H) particle which has scalar and pseudoscalar components [6] as shown in Fig. 1. The SM of particle physics which contains only a single scalar Higgs particle rules out such an interaction. However, it is predicted by a number of multi-Higgs models including the minimal supersymmetric standard model (MSSM) [6,7]. The contribution of the S-PS electron-nucleus interaction to the atomic EDM can exceed that of the electron EDM for certain parameters of these models [6]. An interesting aspect of these models is that they also predict the baryonic asymmetry of the universe arising from the exchange of neutral Higgs particles [8].

In the present work, we use a relativistic many-body theory known as the relativistic coupled-cluster (RCC) method to determine the ratios of the atomic EDMs to the S-PS coupling constants for cesium (Cs) and thallium (Tl). Combining the result of our Tl calculation with the measured EDM value of that atom, we obtain a limit for the S-PS coupling constant (C_s), which, apart from having important implications for physics beyond the SM, could also enrich our understanding about a unique kind of CP violation involving the lepton and hadron sectors [1,4,6,7].

Following the EDM measurement of atomic Cs by Murthy *et al.* [9], a series of experiments were carried out by Commins and co-workers on atomic Tl [10,11]. Currently, the most accurate data on the measurement of the EDM of any paramagnetic atom comes from the experiment on Tl by Regan *et al.* [11]. New experiments on the EDM of atomic Cs using the techniques of laser cooling and trapping are in progress in three different laboratories [12–14]. They could improve the existing limit of the atomic EDM by two orders of magnitude.

The EDM of the ground state of an atom, D_a, can be written as

$$D_a = \frac{\langle \Psi_g | D | \Psi_g \rangle}{\langle \Psi_g | \Psi_g \rangle} = \frac{\langle \Psi_g^{(0)} | D | \Psi_g^{(1)} \rangle + \langle \Psi_g^{(1)} | D | \Psi_g^{(0)} \rangle}{\langle \Psi_g^{(0)} | \Psi_g^{(0)} \rangle}$$
$$= 2 \sum_{I \neq g} \frac{\langle \Psi_g^{(0)} | D | \Psi_I^{(0)} \rangle \langle \Psi_I^{(0)} | H_{\mathrm{EDM}}^{\mathrm{S\text{-}PS}} | \Psi_g^{(0)} \rangle}{(E_g^{(0)} - E_I^{(0)})(\langle \Psi_g^{(0)} | \Psi_g^{(0)} \rangle)}, \quad (1)$$

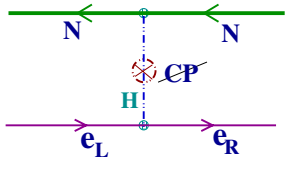

FIG. 1. (Color online) Scalar-pseudoscalar electron (e) and nucleus (N) interaction due to exchange of a Higgs (H) particle. Here e_L and e_R represent left- and right-handed electrons, respectively.

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where D is the electric-dipole ($E1$) operator and the ground state wave function ($|\Psi_g\rangle$) can be expressed as the sum of the unperturbed atomic wave function ($|\Psi_g^{(0)}\rangle$) with energy $E_g^{(0)}$ of the Dirac-Coulomb Hamiltonian ($H^{(0)}$) and the first-order correction ($|\Psi_g^{(1)}\rangle$) to it due to the S-PS electron-nucleus interaction Hamiltonian ($H_{\mathrm{EDM}}^{\mathrm{S\text{-}PS}}$). The first-order wave function $|\Psi_g^{(1)}\rangle$ has been expressed as a sum over intermediate ($|\Psi_I^{(0)}\rangle$) states with energies $E_I^{(0)}$'s.

The electron-nucleus S-PS interaction that violates P and T is given by

$$H_{\mathrm{EDM}}^{\mathrm{S\text{-}PS}} = \frac{G_F}{\sqrt{2}} C_s A \sum_e i\beta_e \gamma_e^5 \rho_N(r). \tag{2}$$

In the above expression G_F is the Fermi constant, C_s is the dimensionless S-PS constant which is given by $C_s=(ZC_{s,p}+NC_{s,n})/A$, where Z, N, and A are the atomic, neutron, and atomic mass numbers, respectively. It is a weighted average of the electron-neutron ($C_{s,n}$) and electron-proton ($C_{s,p}$) coupling constants with $C_{s,n} \approx C_{s,p}$. Again, $\rho_N(r)$ is the nuclear density function and $\gamma^5 (=i\gamma^0\gamma^1\gamma^2\gamma^3)$, which is a pseudoscalar, is the product of the four Dirac matrices. The matrix elements of the above Hamiltonian scale as Z^3; the reason for this is similar to the Z^3 scaling of the parity nonconserving neutral weak interaction matrix elements [15]. This suggests that the atomic EDM arising from the electron-nucleus S-PS interaction is large in heavy systems. This interaction is responsible for mixing states of opposite parities but with the same angular momentum (J). Its strength is sufficiently weak for it to be considered as a first-order perturbation.

In the RCC approach that we have used in the present work, the exact state $|\Psi_v\rangle$ for a single valence (v) open-shell system is given by [16,17]

$$|\Psi_v\rangle = e^T\{1+S_v\}|\Phi_v\rangle, \tag{3}$$

where $|\Phi_v\rangle=a_v^\dagger|\Phi_0\rangle$ and $|\Phi_0\rangle$ is the relativistic mean field [Dirac-Fock (DF)] wave function for a closed-shell system. Here T and S_v are the excitation operators; they act on the DF wave function to produce excitations of the core and valence electrons, respectively. We have considered all the single (T_1,S_{1v}) and double (T_2,S_{2v}) excitations involving all possible combinations of core and valence electrons and the most important subset of triple excitations which is known as the CCSD(T) method in the literature. One of the main virtues of the coupled-cluster (CC) theory is that it is equivalent to all order many-body perturbation theory at any level of excitation. Therefore, the residual Coulomb interaction (v_{es}) which is the difference of two-electron Coulomb potential and the one-electron DF potential has been incorporated in our calculation to all orders for the single, double, and leading triple excitations.

It is obvious from Eq. (1) that the accuracy of the calculation of D_a depends on the excitation energies of different intermediate states and the matrix elements of $H_{\mathrm{EDM}}^{\mathrm{S\text{-}PS}}$ and D. Equation (1) could, in principle, be used to calculate the atomic EDM. However, the accuracy of such an approach would be limited by the finite number of intermediate states that can be included in the summation. In order to avoid this problem, we obtain the first-order perturbed CC wave function as the solution of the following equation:

$$(H^{(0)}-E^{(0)})|\Psi_v^{(1)}\rangle = (E^{(1)} - H_{\mathrm{EDM}}^{\mathrm{S\text{-}PS}})|\Psi_v^{(0)}\rangle, \tag{4}$$

where $E^{(1)}$ vanishes in the present case since we are considering an odd parity perturbation. In this approach, $|\Psi_v^{(1)}\rangle$ implicitly contains all the intermediate states. It is a consequence of including the effects of the S-PS EDM interaction to first order in the cluster operators

$$T = T^{(0)} + G_F T^{(1)},$$

$$S_v = S_v^{(0)} + G_F S_v^{(1)}, \tag{5}$$

where $T^{(0)}$ and $S_v^{(0)}$ are the excitation operators in the absence of the S-PS interaction and $T^{(1)}$ and $S_v^{(1)}$ are the first-order corrections to these operators in the presence of this interaction. In our CCSD(T) method, we thus have $T^{(0)}=T_1^{(0)}+T_2^{(0)}$, $T^{(1)}=T_1^{(1)}+T_2^{(1)}$, $S_v^{(0)}=S_{1v}^{(0)}+S_{2v}^{(0)}$, and $S_v^{(1)}=S_{1v}^{(1)}+S_{2v}^{(1)}$.

We have presented our results for D_a/C_s in Table I and compared them with the previous relativistic atomic calculations in Table II. The dominant contributions for Cs and Tl are at the DF level. However, the contributions of the correlation effects beyond the DF approximation are significant.

TABLE I. Contributions from important RCC terms for D_a/C_s calculations of $6s\ ^2S_{1/2}$ and $6p\ ^2P_{1/2}$ states for Cs and Tl, respectively, in $\times 10^{-18}$ e cm.

Important terms	Cesium $6s\ ^2S_{1/2}$	Thallium $6p\ ^2P_{1/2}$
Contributions from DF		
$DH_{\mathrm{EDM}}^{\mathrm{S\text{-}PS}}+H_{\mathrm{EDM}}^{\mathrm{SPS}}D$	−0.597	5.023
Contributions from RCC		
$DT_1^{(1)}+T^{(1)^\dagger}D$	−0.035	3.056
$\overline{D^{(0)}}S_{1v}^{(1)}S_{1v}^{(1)^\dagger}\overline{D^{(0)}}$	−0.878	4.453
$\overline{D^{(0)}}S_{2v}^{(1)}+S_{2v}^{(1)^\dagger}\overline{D^{(0)}}$	0.043	−3.835
$S_{1v}^{(0)^\dagger}\overline{D^{(0)}}S_{1v}^{(1)}+S_{1v}^{(1)^\dagger}\overline{D^{(0)}}S_{1v}^{(0)}$	0.015	−0.304
$S_{2v}^{(0)^\dagger}\overline{D^{(0)}}S_{1v}^{(1)}+S_{1v}^{(1)^\dagger}\overline{D^{(0)}}S_{2v}^{(0)}$	0.041	0.174
$S_{1v}^{(0)^\dagger}\overline{D^{(0)}}S_{2v}^{(1)}+S_{2v}^{(1)^\dagger}\overline{D^{(0)}}S_{1v}^{(0)}$	0.004	0.023
$S_{2v}^{(0)^\dagger}\overline{D^{(0)}}S_{2v}^{(1)}+S_{2v}^{(1)^\dagger}\overline{D^{(0)}}S_{2v}^{(0)}$	−0.008	−0.036
Norm.	0.019	−0.032
Total	−0.801	4.056

TABLE II. Comparison of D_a/C_s results with others in $\times 10^{-18}$ e cm.

	Cesium D_a/C_s	Thallium D_a/C_s
Bouchiat [18]	−0.689	-
Venugopal [20]	−0.805	-
Mårtensson-Pendrill and Lindroth [19]	−0.72(103)	7(2)
Present	−0.801	4.06

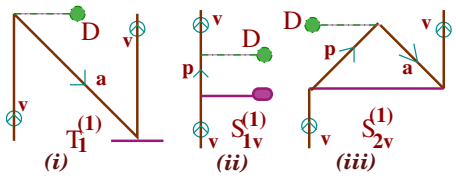

FIG. 2. (Color online) Important correlation diagrams for EDM. Dipole operator (D) is shown by the dotted line with a circle. $T_1^{(1)}$, $S_{1v}^{(1)}$, and $S_{2v}^{(1)}$ represent first-order S-PS EDM perturbed T_1, S_{1v}, and S_{2v} operators, respectively.

They are about 30% and 25% for Cs and Tl, respectively, and are characterized in the latter case by strong cancellations. It is therefore imperative to use an all order method such as the CC theory for an accurate quantitative description of these effects which embody the interplay of the residual Coulomb and the S-PS EDM interactions. The dominant correlation effects are represented diagrammatically in Fig. 2. They have been evaluated to all orders in the residual Coulomb interaction. The previous calculations were based on a semiempirical one electron theory [18], perturbed DF approach [19], and a method combining certain features of many-body perturbation theory and the multiconfiguration DF approach [20]. All these methods are approximations at different levels to the RCC theory that we have used in the present work. Our estimated error bars are just 0.004×10^{-18} e cm and 0.14×10^{-18} e cm (the procedure for estimating the errors will be explained later) which are about 115 and 10 times improvement over previous results [19] for Cs and Tl, respectively.

It is not straightforward to estimate the error associated with our RCC calculations. However, it is reasonable to assume that it would not exceed the contribution of the leading triple excitations, which we have taken as the upper bound of the error of our calculation. We have presented in Table III the results of our calculations of the properties that are related to the EDMs of the ground states of atomic Cs and Tl. Unlike the matrix elements of the electric-dipole operator and the excitation energies, the matrix elements of the $H_{\mathrm{EDM}}^{\mathrm{S\text{-}PS}}$ cannot be verified experimentally. However, it is possible to estimate the accuracies of these quantities from studies of hyperfine interactions as both the interactions involve the nuclear or the near nuclear regions. It is therefore reasonable to assume that the square root of the products of the magnetic dipole hyperfine structure constants (A) of the relevant states could be used to estimate the accuracies of the $H_{\mathrm{EDM}}^{\mathrm{S\text{-}PS}}$ matrix elements [15,21]. The good agreement of our Cs and Tl results, as shown in Table III, with measurements is a reflection of the high precision that we have achieved for our EDM calculations. We have followed two approaches to estimate the error bars mentioned above. First, we have taken the difference between D_a/C_s results obtained from the CCSD(T) method and by just taking single and double excitations (CCSD method). Second, we have considered the relative errors between the experimental and our theoretical results of the three properties presented in Table III and estimated the net error by combining the individual errors in quadrature. The larger of these two quantities is chosen as the upper limit of the error bars.

We obtain the following values for the S-PS coupling constant: $C_s = 2(7) \times 10^{-6}$ for Cs and $C_s = 1.0(18) \times 10^{-7}$ for Tl by combining our RCC results of D_a/C_s with the most accurate experimental data [9,11] available for the EDM (D_a) of these two atoms. The error bars are obtained by combining the theoretical and experimental uncertainties in quadrature. In this work, the theoretical uncertainties are three orders of magnitude smaller, and thus negligible. Different limits for

TABLE III. Excitation energies (cm^{-1}), $E1$ elements (a.u.), and magnetic dipole hyperfine structure constants (MHz) of important intermediate states in Cs and Tl.

	Cs		Tl			
Initial state →Final state	$6s_{1/2} \rightarrow 6p_{1/2}$		$6s_{1/2} \rightarrow 7p_{1/2}$	$6p_{1/2} \rightarrow 7s_{1/2}$		$6p_{1/2} \rightarrow 8s_{1/2}$
Excitation energy	11229.38		21796.31	26038.62		10462.32
Experiment	11177.84[a]		21765.30[a]	26477.50[a]		10520.01[a]
$E1$ transition amplitude	4.53		0.292	1.84		0.57
Experiment	4.5013(13)[b]		0.284(2)[c]	1.81(2)[d]		-
Atomic state	$6s_{1/2}$	$6p_{1/2}$	$7p_{1/2}$	$6p_{1/2}$	$7s_{1/2}$	$8s_{1/2}$
Hyperfine constant (A)	2292.32	284.86	94.67	21025.98	11992.11	4118.57
Experiment	2298.16[c]	291.90(9)[e]	94.35(4)[e]	21311[d]	12297[d]	-

[a]Reference [22].
[b]Reference [23].
[c]Reference [24].
[d]References [26,27].
[e]Reference [25].

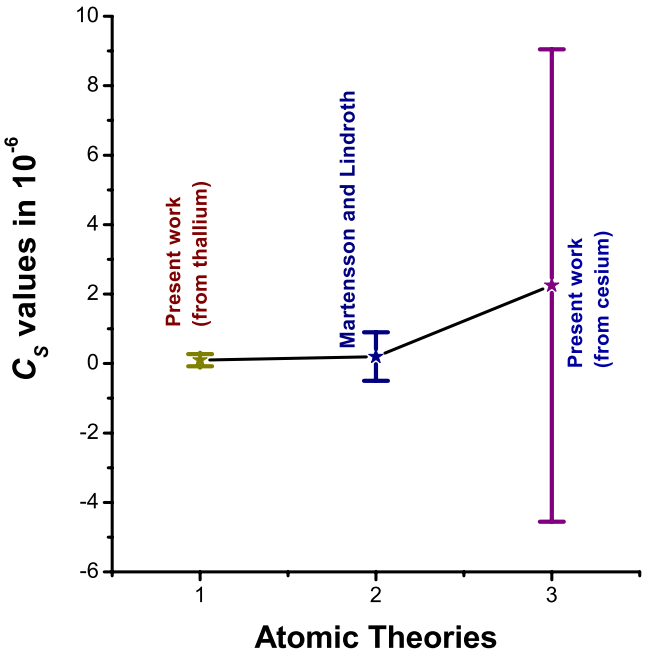

FIG. 3. (Color online) Limit of the C_s values obtained from different atomic theories.

C_s derived from various theoretical approaches are given in Fig. 3. The limit for Tl present here is a significant improvement over the previous limit [19] $C_s=2(7)\times10^{-7}$. This new limit can be used in the framework of different multi-Higgs models to extract a wealth of information about physics beyond the SM [1,7]. In particular, it can constrain the masses of the scalar Higgs bosons in certain ranges of some of the model parameters [1] and also the baryonic asymmetry of the universe [7,8]. Furthermore in the MSSM, it can constrain CP violation in the Higgs sector generated by radiative corrections [7]. This would have important implications for the searches of CP violating Higgs bosons using colliders such as LEP2, Tevatron, and the Large Hadron Collider (LHC) [7,8]. It would indeed be possible to improve the limit we have obtained for C_s even further if the new generation of EDM experiments using cold Cs atoms reach their expected levels of accuracy [12–14]. The results of these experiments could then be combined with our calculation of D_a/C_s for Cs (0.5% accuracy) to yield this new limit.

In summary, we have calculated D_a/C_s for Cs and Tl using the RCC theory with accuracies of 0.5% and 3.3%, respectively. Many-body effects were found to be significant in both cases. Our calculated value of D_a/C_s for Tl in combination with the experimental result of D_a for the same atom gives the most accurate limit for the S-PS coupling constant to date. This limit has the potential to provide important insights into physics beyond the SM, particularly the Higgs sector and electroweak baryogenesis. It is indeed remarkable that a table-top experiment to observe the EDM in a paramagnetic atom and its associated theory can throw light on profound questions in particle physics and cosmology.

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