

Search for a permanent electric-dipole moment using atomic indium

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We propose indium (In) as a possible candidate for observing the permanent electric dipole moment (EDM) arising from violations of parity (P) and time-reversal (T) symmetries. This atom has been laser cooled and therefore the measurement of its EDM has the potential of improving on the current best EDM limit for a paramagnetic atom, which comes from thallium. We report the results of our calculations of the EDM enhancement factor due to the electron EDM and the ratio of the atomic EDM to the electron-nucleus scalar-pseudoscalar (S-PS) interaction coupling constant in In within the framework of the relativistic coupled cluster theory. It might be possible to get new limits for the electron EDM and the S-PS CP -violating coupling constant by combining the results of our calculations with the measured value of the EDM of In when it is available. These limits could have important implications for the standard model (SM) of particle physics.

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It is now widely recognized that atomic electric dipole moments (EDMs) arising from violations of parity (P) and time-reversal (T) symmetries can provide important information about new physics beyond the standard model (SM) [1,2]. T violation implies CP violation via the CPT theorem [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 the nucleus which violates P as well as T symmetries [4]. Atomic EDMs due to the electron EDM and the S-PS electron-nucleus interaction can shed light on CP violation in the leptonic and semileptonic sectors [1,5]. The origin of both of these kinds of CP violations is not well understood.

The best limit on the EDM of a paramagnetic atom currently comes from thallium (Tl) [6–9]. A new generation of EDM experiments on the alkali-metal atoms like rubidium [10], caesium [10–12], and francium [13] and based on the techniques of laser cooling and trapping is currently underway. These experiments have, in principle, the advantages of both the beam and the cell experiments [14]. In particular, it is possible to apply large electric fields and the coherence times are long in these experiments [14]. The projected precision of the current alkali-metal EDM experiments are about two orders of magnitude better than that of the Tl experiment [10–12]. Indium (In), which is homologous to Tl, appears to be an attractive candidate for the search of a permanent EDM for essentially two reasons: First, this atom has been laser cooled [15] and, second, the EDM enhancement factor due to the electron EDM and the ratio of the atomic EDM to the S-PS coupling constant can be calculated more accurately than that of Tl due to its relatively smaller size. To demonstrate this second point more elaborately, we carry out herein *ab initio* calculations for the corresponding factors due to the EDM of electron and the S-PS electron-nucleus interaction in In and discuss the role of different correlation effects in these properties.

Following the work of Sandars [4] and its extension [16–18], the effective atomic EDM Hamiltonian due to the electron EDM can be written as

$$H_{\text{EDM}}^e = 2icd_e \sum_j \beta_j \gamma_j^5 p_j^2, \quad (1)$$

and the S-PS interaction Hamiltonian is given by

$$H_{\text{EDM}}^{\text{S-PS}} = \frac{iG_F}{\sqrt{2}} C_S \sum_j \beta_j \gamma_j^5 \rho_n(r_j), \quad (2)$$

where d_e is the intrinsic electron EDM, γ^5 is a pseudoscalar Dirac matrix, C_S is the dimensionless S-PS constant, and $\rho_n(r_j)$ is the j th electron density over the nucleus.

The above interaction Hamiltonians mix atomic states of opposite parities but with the same angular momentum. They can be treated as first-order perturbations because their strengths are sufficiently weak. Therefore, any atomic state with a valence electron v can be expressed, after the inclusion of these interactions, as

$$|\Psi_v\rangle = |\Psi_v^{(0)}\rangle + \lambda |\Psi_v^{(1)}\rangle, \quad (3)$$

where $|\Psi_v\rangle$ is the modified wave function with respect to the original wave function $|\Psi_v^{(0)}\rangle$ by the first-order correction $|\Psi_v^{(1)}\rangle$. λ represents the weak-coupling parameter d_e for H_{EDM}^e or C_S for $H_{\text{EDM}}^{\text{S-PS}}$.

The enhancement factor due to the electron EDM and the ratio of the atomic EDM to the S-PS coupling constant, which is denoted here by $\mathcal{R} = \frac{D_a}{\lambda}$ for the atomic EDM D_a of a state $|\Psi_v\rangle$, is given by

$$\mathcal{R} = \frac{\langle \Psi_v^{(0)} | D | \Psi_v^{(1)} \rangle + \langle \Psi_v^{(1)} | D | \Psi_v^{(0)} \rangle}{\langle \Psi_v^{(0)} | \Psi_v^{(0)} \rangle}, \quad (4)$$

where D is the electric dipole ($E1$) operator. With the explicit form of $|\Psi_v^{(1)}\rangle$, we get

$$\mathcal{R} = \sum_{I \neq v} \frac{\langle \Psi_v^{(0)} | D | \Psi_I^{(0)} \rangle \langle \Psi_I^{(0)} | H_{\text{EDM}} | \Psi_v^{(0)} \rangle}{(E_v - E_I) \langle \Psi_v^{(0)} | \Psi_v^{(0)} \rangle} + \sum_{I \neq v} \frac{\langle \Psi_v^{(0)} | H_{\text{EDM}} | \Psi_I^{(0)} \rangle \langle \Psi_I^{(0)} | D | \Psi_v^{(0)} \rangle}{(E_v - E_I) \langle \Psi_v^{(0)} | \Psi_v^{(0)} \rangle}, \quad (5)$$

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where I represents the intermediate states and H_{EDM} is one of the EDM interactions given above.

The above expression depends explicitly on $E1$ matrix elements, excitation energies (EEs), and matrix elements of H_{EDM} . However, it is possible to consider only a finite number of excited states in the evaluation of this quantity if a sum-over-states approach is used. In order to circumvent this problem, we solve the first-order-perturbed wave function in a similar approach of

$$(H^{(0)} - E_v^{(0)})|\Psi_v^{(1)}\rangle = -H_{\text{EDM}}|\Psi_v^{(0)}\rangle. \quad (6)$$

In the above expression, $H^{(0)}$ is the atomic Hamiltonian and $E_v^{(0)}$ is the energy for the state $|\Psi_v^{(0)}\rangle$. It is possible to estimate the accuracy of the corresponding \mathcal{R} values by calculating the properties required to determine Eq. (5) for the dominant intermediate states.

We employ the coupled-cluster theory in the relativistic framework (RCC theory) to evaluate $|\Psi_v^{(0)}\rangle$ and $|\Psi_v^{(1)}\rangle$ as described in Refs. [8,9,17,18]. These wave functions can be expressed as

$$|\Psi_v^{(0)}\rangle = e^{T^{(0)}}\{1 + S_v^{(0)}\}|\Phi_v\rangle \quad (7)$$

$$\text{and } |\Psi_v^{(1)}\rangle = e^{T^{(0)}}\{T^{(1)}(1 + S_v^{(0)}) + S_v^{(1)}\}|\Phi_v\rangle, \quad (8)$$

where $|\Phi_v\rangle$ is the Dirac-Fock (DF) wave function obtained by appending the valence electron v to the closed-shell ($[4d^{10}]5s^2$ in the present case) reference wave function, $T^{(0)}$ and $S_v^{(0)}$ are the excitation operators for the core and valence electrons, respectively, in the unperturbed case, whereas $T^{(1)}$ and $S_v^{(1)}$ are their first order corrections. The atomic wave functions are calculated using the Dirac-Coulomb (DC) Hamiltonian, which is given by

$$H_0 = \sum_i \{c\alpha_i \cdot \mathbf{p}_i + (\beta_i - 1)m_i c^2 + V_n(r_i)\} + \sum_{i<j} V_C(r_{ij}), \quad (9)$$

where α and β are Dirac matrices, \mathbf{p} is the momentum operator, $V_n(r)$ is the nuclear potential, and $V_C(r)$ is the Coulomb potential.

We consider only single and double excitations in the expansion of the RCC wave functions (CCSD approximation) by defining

$$T = T_1 + T_2 \text{ and } S_v = S_{1v} + S_{2v} \quad (10)$$

for both the perturbed and unperturbed operators. Furthermore, we construct triple excitation operators for $S_v^{(0)}$ as

$$S_{vab}^{pqr,(0)} = \frac{\widehat{H}_0 T_2^{(0)} + \widehat{H}_0 S_{2v}^{(0)}}{\epsilon_v + \epsilon_a + \epsilon_b - \epsilon_p - \epsilon_q - \epsilon_r}, \quad (11)$$

which are used to evaluate the CCSD amplitudes iteratively. This is referred to as the coupled-cluster method with singles, doubles, and perturbative triples [CCSD(T)] approximation. Here, ϵ_i is the single-particle energy of orbital i .

Hence, \mathcal{R} in the RCC theory is given by

$$\mathcal{R} = \frac{\langle \Phi_v | \{1 + S_v^{(0)\dagger}\} \overline{D^{(0)}} \{T^{(1)}(1 + S_v^{(0)}) + S_v^{(1)}\} | \Phi_v \rangle}{\langle \Phi_v | e^{T^{(0)\dagger}} e^{T^{(0)}} + S_v^{(0)\dagger} e^{T^{(0)\dagger}} e^{T^{(0)}} S_v^{(0)} | \Phi_v \rangle} + \text{c.c.}, \quad (12)$$

TABLE I. Enhancement factor due to electron EDM and the ratio of the atomic EDM to the S-PS coupling constant denoted by \mathcal{R} to the ground state of In due to d_e (dimensionless) and S-PS (in $\frac{eE}{\sqrt{2}} C_S/A$; A is the ground state mass number) interactions obtained using DF and RCC methods.

Source	DF	CCSD	CCSD(T)
d_e	-49.53	-82.35	-82.37
S-PS	-31.10	-52.59	-52.60

where the dressed operator $\overline{D^{(0)}} = e^{T^{(0)\dagger}} D e^{T^{(0)}}$, $D = e\mathbf{r}$ is the $E1$ operator due to the applied electric field, and c.c. represents the complex conjugate terms. The procedure for the calculation of the above expression is discussed elsewhere [8,9,17,18].

The single-particle orbitals in our calculations are a linear combination of Gaussian-type orbitals (GTOs). They are optimized by comparing the energies and the radial integrals of these orbitals with those obtained numerically from GRASP2 [19]. We have allowed excitations from all the occupied orbitals to unoccupied bound and continuum orbitals with a maximum energy of 1500 a.u. This space is sufficiently large for the convergence of the results of our calculations. Orbitals up to $l = 4$ were included in the active space after observing that the contributions from orbitals with higher angular momenta were very small; inclusion of these orbitals would have been computationally expensive with little or no effect on the overall results.

In Table I, we present the \mathcal{R} values for both d_e and S-PS interactions at the DF, CCSD, and CCSD(T) levels. There is a significant difference between the DF and CCSD(T) results, highlighting the importance of strong correlation effects for the reported \mathcal{R} factors of this system. The small difference between the CCSD and CCSD(T) results suggests that the contributions from the triple excitations are small. We give below contributions from various CCSD(T) terms to understand the roles of different correlation effects in this property.

In Table II, we present the contributions from the core and the virtual orbitals to the factors \mathcal{R} at the DF level and individual contributions from different CCSD(T) terms. The CCSD(T) contributions in this table have been classified as important terms referring to terms whose contributions are large (Goldstone diagrams for these terms are shown in Fig. 1) and nonlinear terms whose contributions are relatively small. Figure 1(a), representing $\overline{D^{(0)}}T_1^{(1)}$, involves the lowest-order DF contributions due to the core orbitals [Fig. 1(i)] and some of the higher-order core-polarization correlation diagrams [Fig. 1(ii), 1(iii), and more]. By comparing the DF contributions from core orbitals and $\overline{D^{(0)}}T_1^{(1)}$, it is obvious that these core-polarization correlation effects contribute significantly; they are larger than the DF core contribution. The largest contributions come from the $\overline{D^{(0)}}S_{1v}^{(1)}$ term and, as shown in Fig. [1(b)], it contains the lowest-order DF contribution due to the virtual orbitals. It also includes many important core-polarization [Figs. 1(v) and 1(vi)] and pair-correlation [Fig. 1(vii)] diagrams. However, the net correlation contribution due to this diagram is not as large as it is from the higher-order diagrams in $\overline{D^{(0)}}T_1^{(1)}$. The other important term

TABLE II. Contributions to \mathcal{R} (with same units as in Table I) from different CCSD(T) terms. $\overline{D}_{\text{OB}}^{(0)}$ represents effective one-body terms from $\overline{D}^{(0)}$, terms containing the bare D operator are the effective two-body terms from $\overline{D}^{(0)}$, “Others” and “Norm” give contributions from other nonlinear terms and normalization of the wave function, respectively.

Term	From d_e	From S-PS
	From DF	
$(DH_{\text{EDM}})_c + \text{c.c.}$	-17.56	-11.03
$(DH_{\text{EDM}})_v + \text{c.c.}$	-31.98	-20.07
	Important RCC terms	
$\overline{D}_{\text{OB}}^{(0)}T_1^{(1)} + \text{c.c.}$	-39.79	-25.33
$\overline{D}_{\text{OB}}^{(0)}S_{1v}^{(1)} + \text{c.c.}$	-44.59	-28.24
$\overline{D}_{\text{OB}}^{(0)}S_{2v}^{(1)} + \text{c.c.}$	10.10	6.39
	Nonlinear RCC terms	
$T_1^{(1)\dagger}\overline{D}_{\text{OB}}^{(0)}S_{2v}^{(0)}$	-4.12	-2.62
$S_{1v}^{(1)\dagger}\overline{D}_{\text{OB}}^{(0)}S_{1v}^{(0)} + \text{c.c.}$	3.55	2.27
$S_{2v}^{(0)\dagger}\overline{D}_{\text{OB}}^{(0)}S_{1v}^{(1)} + \text{c.c.}$	-2.06	-1.29
$T_1^{(1)\dagger}DT_2^{(0)} + \text{c.c.}$	-4.74	-3.02
$T_2^{(0)\dagger}DT_1^{(1)}S_{2v}^{(0)}$	-1.24	-0.78
$T_2^{(0)\dagger}DS_{2v}^{(1)} + \text{c.c.}$	0.86	0.56
$S_{2v}^{(0)\dagger}DS_{2v}^{(1)} + \text{c.c.}$	-0.97	-0.61
Others	0.21	0.17
Norm	0.83	0.52

that has been considered is $\overline{D}^{(0)}S_{2v}^{(1)}$ and it accounts mainly for a particular class of core polarization effects.

We now consider some of the quantitative aspects of the correlation effects in the above electron EDM enhancement factor and the ratio of the atomic EDM to the S-PS coupling

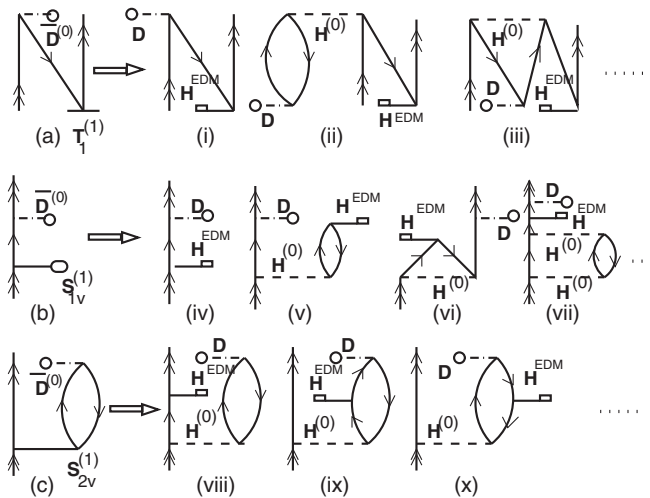


FIG. 1. Break down of important perturbed CCSD(T) diagrams into lower-order many-body perturbation diagrams. Lines with a single arrow pointing upward and downward represent the occupied and unoccupied orbitals, respectively. Lines with a double arrow represent the valence orbital.

constant. These effects in In are significantly larger than those in the alkali-metal atoms, but their cancellations are not as severe as in the case of Tl. The correlation effects for both the above quantities are one and a half times the total DF results. The core correlation effects are very strong, because of the large overlap between the wave functions of the valence $5p_{1/2}$ and the outermost core $5s$ orbitals and the small energy difference between them. At the DF level, the contributions from the virtual orbitals are larger than those of the core orbitals. The total contributions from both $\overline{D}^{(0)}T_1^{(1)}$ and $\overline{D}^{(0)}S_{1v}^{(1)}$ are comparable. The contribution from $\overline{D}^{(0)}S_{2v}^{(1)}$ is significant, but with opposite sign. These contributions are from the singly excited perturbed states; mainly from the $[4d^{10}]5s5p^2$ state. There are also some significant contributions from the higher-order RCC terms; especially $T_1^{(1)\dagger}DT_2^{(0)}$, $S_{1v}^{(1)\dagger}\overline{D}^{(0)}S_{1v}^{(0)}$, $S_{2v}^{(0)\dagger}\overline{D}^{(0)}S_{1v}^{(1)}$, and $T_1^{(1)\dagger}\overline{D}^{(0)}S_{2v}^{(0)}$ through some of the core-polarization and pair-correlation effects. Contributions due to the normalization of the wave function (norm) and terms containing nonlinear terms in $T^{(0)}$ and $T^{(1)}$ are small.

It is possible to get a sense of the accuracies of the individual quantities that appear in Eq. (5) by comparing their calculated values with their corresponding experimental results. Experimental values for the EEs are available up to very high accuracy [21] and experimental values of the $E1$ matrix elements can be extracted from the lifetime measurements of the available s states. The matrix elements of H_{EDM} cannot be measured directly. However, the accuracy of this quantity can be indirectly estimated from the square root of the product of the magnetic dipole hyperfine structure constants (A_{hyp}) of the appropriate states [8,9].

We present the results for the EEs, $E1$ matrix elements, and the hyperfine structure constants of the ground and excited s states in Table III that contribute significantly to \mathcal{R} .

TABLE III. Comparison of the excitation energies (in cm^{-1}), $E1$ matrix element, and hyperfine structure constants of low-lying states in In with the available experimental results and all-order SD calculations. Uncertainties from our calculations are given in the parentheses.

Transition	This work	All-order SD [20]	Experiment
	Excitation energies		
$6s \rightarrow 5p_{1/2}$	24 290 (80)	23 747	24 372.956 [21]
$7s \rightarrow 5p_{1/2}$	36 217 (90)	35 808	36 301.84 [21]
$8s \rightarrow 5p_{1/2}$	40 552 (100)	40 126	40 637.0 [21]
$9s \rightarrow 5p_{1/2}$	42 640 (115)	42 238	42 719.0 [21]
	$E1$ matrix elements		
$6s \rightarrow 5p_{1/2}$	1.91 (1)	1.91	1.92 (8) [22]
$7s \rightarrow 5p_{1/2}$	0.56 (2)	0.54	
$8s \rightarrow 5p_{1/2}$	0.31 (2)	0.09	
$9s \rightarrow 5p_{1/2}$	0.19 (2)		
	A_{hyp} of ^{115}In		
$5p_{1/2}$	2256 (30)	2306	2282 (40) [23]
$6s$	1611 (50)	1812	1687.2 (6) [24]
$7s$	516 (30)	544.5	541.1 (3) [24]
$8s$	234 (20)	240.8	
$9s$	106 (10)	128.1	

Experimental values for the EEs are available for most of the excited states, but the hyperfine structure constants are experimentally known only for the $5p_{1/2}$, $6s$, and $7s$ states. We find the $E1$ matrix element of the $6s \rightarrow 5p_{1/2}$ transition to be 1.92(8) a.u. by combining the experimental values of the lifetime of the $6s$ state [7.5(7) s] [22] and considering the branching ratio to be 2:3 of the $6s \rightarrow 5p_{1/2}$ and $6s \rightarrow 5p_{3/2}$ transitions [25] (refer to Ref. [26] for a detailed discussion of these results). For EEs, the largest uncertainty comes from the Breit interaction followed by the neglected basis orbitals and triple excitations. However, most of the uncertainties to the $E1$ matrix elements and A_{hyp} s come from the latter. All our results are in good agreement with the experimental results. Our calculated results have been compared with those obtained by the all-order SD method [20] and with the RCC method containing only the linear terms of our CCSD approach in the above table. Our EE results are in better agreement with accurate experimental data than those using the all-order SD method for all the excited states relevant for our present work. The corresponding DF results are given elsewhere (see Ref. [26]), and it is found in Ref. [20] that the Breit interaction contributes very little to this property in this atom. Therefore, the discrepancies between the results reported in Ref. [20] and in the present work could be due to the nonlinear terms of the CCSD(T) method. Our A_{hyp} for the $6s$ state, the most important excited state in the calculation of \mathcal{R} , is also more accurate than the all-order-SD result. Our results for the other quantities agree reasonably well with available experimental data. The

uncertainties in various quantities are estimated by considering the differences between the results of the CCSD(T) and CCSD methods as the upper limits to the contributions due to the triple excitations, neglecting relativistic effects (particularly the Breit interaction) and omitting higher angular momentum symmetry orbitals in the present calculations. After considering all possible uncertainties, the enhancement factor due to the electron EDM and the ratio of the atomic EDM to the S-PS coupling constant for In are estimated to be $-82(5)$ and $-53(3)$, respectively. These results are almost five and one and a half times smaller than those in Tl [9] and Cs [18], respectively, but three times larger than those in Rb [18]. Their accuracies can be further improved by using the general RCC theory [27].

In conclusion, we propose In as a suitable candidate for the search of a permanent EDM. Our theoretical studies show that accurate calculations of the electron EDM enhancement factor and the ratio of the atomic EDM to the S-PS coupling constant of this atom are possible. The limits for the electron EDM and the S-PS coupling constants that can be extracted by combining these factors with the measured value of the EDM of this atom, when it is available, could provide important information about the validity of the SM of particle physics.

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