Probing CP violation with the electric dipole moment of atomic mercury

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The electric dipole moment of atomic ^{199}Hg induced by the nuclear Schiff moment and tensor-pseudotensor electron-nucleus interactions has been calculated. For this, we have developed and employed a novel method based on the relativistic coupled-cluster theory. The results of our theoretical calculations combined with the latest experimental result of ^{199}Hg electric dipole moment, provide new bounds on the T reversal or CP violation parameters $\theta_{\rm QCD}$, the tensor-pseudotensor coupling constant C_T and $(\widetilde{d}_u - \widetilde{d}_d)$. This is the most accurate calculation of these parameters to date. We highlight the the crucial role of electron correlation effects in their interplay with the P,T violating interactions. Our results demonstrate substantial changes in the results of earlier calculations of these parameters which can be attributed to the more accurate inclusion of important correlation effects in the present work.

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The existence of a nonzero permanent electric dipole moment of a non-degenerate physical system is a signature of the simultaneous violations of parity (P) and time-reversal (T) symmetries [1]. T violation implies the combined charge conjugation (C) and P violation ; i.e., CP violation via the CPT theorem [2]. The origin of CP violation is still not well understood. It has so far been observed only in the K [3] and B [4, 5] mesons and the results are essentially in agreement with the predictions of Kobayashi and Maskawa in the framework of the Standard Model [6]. However, this model cannot explain the matter-antimatter asymmetry [7] in the universe for which CP violation is a pre-requisite [8]. In addition, it predicts atomic EDMs several orders of magnitude below their current limits [9, 10]. Indeed, atomic EDMs are excellent probes of physics beyond the Standard Model [9, 10] and they provide important insights into a rich variety of CP violations–leptonic, semi-leptonic and hadronic sectors. Experimental searches are underway for the EDMs of para-magnetic (open-shell) and dia-magnetic (closed-shell) atoms [11, 12]. The results of the experiments can be combined with those of sophisticated atomic many-body calculations to determine various CP violating coupling constants at the atomic level which can ultimately be related to the CP violation parameters at the elementary particle level [13]. The EDM of dia-magnetic atoms arises predominantly from the nuclear Schiff moment (NSM) and/or the electron-nucleon tensor-pseudotensor interactions [13]. These in turn arise from the nucleon-nucleon interactions or the EDM of nucleons, which originate due to the quark-quark interactions, EDMs and chromo EDMs of quarks at the elementary particle level.

In the present work, we concentrate only on the EDM of mercury (^{199}Hg), a closed-shell atom. The present limits on important CP violation parameters like, $\theta_{\rm QCD}$ for strong interactions and the chromo EDMs of quarks have been obtained from the EDM of ^{199}Hg [11], which is the most accurate of all the data from atomic EDMs to date. The focus of our work in this Letter is to improve the current limits on the coupling constants associated with the electron-nucleon tensor-pseudotensor (T-PT) interaction (C_T) and the NSM(S). A nonzero value of C_T implies physics beyond the Standard Model. The dependence of the T-PT interactions and the NSM on the nuclear spin makes closed-shell atoms, in particular, those having nonzero nuclear spin the best candidates to measure EDMs sensitive to the nuclear sector.

For heavy atoms like mercury, it is customary to use the Dirac-Coulomb Hamiltonian $H_{\rm DC}$, in atomic units

$$H_{\rm DC} = \sum_i \left[c\boldsymbol{\alpha}_i \cdot \boldsymbol{p}_i + \boldsymbol{\beta}_i mc^2 + V_N(r_i) \right] + \sum_{i<j} \frac{1}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}, \quad (1)$$

where r_i refers to the electron coordinates, α and β, the Dirac matrices and $V_N(r_i)$, the nuclear potential, and the last term is the electron-electron Coulomb interaction. The key and the most challenging step in atomic many-body physics is to incorporate the effects of electron-electron Coulomb interaction, last term in Eq.(1), as accurately as possible. Under the independent particle and the central field approximations [14], with the introduction of the Dirac-Fock potential, the above Hamiltonian can be separated into an exactly solvable part (H_0) and a residual interaction part which consists of the Coulomb interaction and the Dirac-Fock potential [14]. The single particle wave functions are computed self-consistently from H_0 and the many particle wavefunctions are expressed as Slater determinants built out of the single particle wavefunctions. The effects of the residual Coulomb interaction are calculated with many-body methods. For this, finite order many-body perturbation theory (MBPT) and the configuration interaction (CI) approach are two widely used methods [14]. An even superior method, with strong theoretical many-body physics underpinnings is the coupled-cluster theory.

In the present work, the P and T violating interactions are treated perturbatively to first order in addition to the electron-electron residual Coulomb interaction within the framework of the relativistic coupled-cluster theory.

The wavefunction in coupled-cluster theory has an exponential structure, see [15] for a recent review of the method, to describe correlation effects in many-body systems. It is non-perturbative and defines atomic states as superposition of states of different levels of excitations, which arise from the residual Coulomb interaction, with respect to a reference state.

Mathematically, the coupled-cluster wavefunction can be expressed as

$$|\Psi_i\rangle = e^{T^{(0)}}|\Phi_i\rangle, \tag{2}$$

where $|\Phi_i\rangle$ is the reference state containing a fixed number of electrons and $T^{(0)}$ is an operator which excites electrons out of it, thereby giving rise to states with different levels of excitations corresponding to different many-body effects. In our calculations we use the coupled-cluster singles and doubles approximation, that is $T^{(0)} = T_1^{(0)} + T_2^{(0)}$. In second quantized form

$$T_1^{(0)} = \sum_{a,p} a_p^\dagger a_a t_a^p(0) \text{ and } T_2^{(0)} = \sum_{a,b,p,q} a_p^\dagger a_q^\dagger a_b a_a t_{ab}^{pq}(0),$$

excite one and two electrons respectively from the reference state. The equations that determine the amplitudes of $T^{(0)}$ are a set of coupled non-linear algebraic equations and these are solved iteratively till convergence.

For closed-shell atoms, as mentioned earlier, one prominent source of EDMs is the nuclear Schiff moment $\boldsymbol{S}$ (NSM), a P and T odd electromagnetic moment of the nucleus. For a finite size nucleus of radius R_N, the Schiff moment potential [16] is

$$\varphi(\boldsymbol{R}) = -\frac{3\boldsymbol{S}\cdot\boldsymbol{R}}{B}\rho(R), \tag{3}$$

where $B = \int \rho(R)R^4 dR$ and $\rho(R)$ is the nuclear density. This potential interacts electrostatically with the electrons, it mixes atomic states of opposite parities and generates a finite atomic EDM, d_A. Then, the atomic Hamiltonian is $H_{\rm atom} = H_{\rm DC} + \lambda H_{\rm PTV}$, where $H_{\rm PTV}^{\rm Schiff} = -\varphi(\boldsymbol{R})$ is the P and T violating interaction Hamiltonian and λ is a T or CP violation parameter which can be considered as perturbation parameter. The eigenstates of the $H_{\rm atom}$ are the mixed parity states $|\widetilde{\Psi}\rangle$. To incorporate $H_{\rm PTV}$ as a first order perturbation, the exponential operator in coupled-cluster theory is redefined as $e^{T^{(0)}+\lambda T^{(1)}}$. The cluster operator $T^{(1)}$ has one order of $H_{\rm PTV}$ and mixes the states of opposite parities. As a result of this, the ground state

$$|\widetilde{\Psi}_0\rangle = e^{T^{(0)}+\lambda T^{(1)}}|\Phi_0\rangle. \tag{4}$$

Then, unlike the $T^{(0)}$ equations, since $H_{\rm PTV}$ is considered to first order only, the equations for the amplitudes of $T^{(1)}$ are a set of linear algebraic equations,

$$\langle\Phi_0'|\left[\overline{H}_{\rm N}, T^{(1)}\right]|\Phi_0\rangle = -\langle\Phi_0'|\overline{H}_{\rm PTV}|\Phi_0\rangle \tag{5}$$

$\overline{O} = e^{T^{(0)\,\dagger}} O e^{T^{(0)}}$ where O is a general operator, $H_{\rm N}$ is the normal-ordered Hamiltonian and $|\Phi_0'\rangle$ are opposite parity Slater determinants. Further, like in the unperturbed cluster operators $T^{(0)}$, we use the approximation $T^{(1)} = T_1^{(1)} + T_2^{(1)}$. Then, the atomic EDM of the ground state is

$$d_A = \frac{\langle\widetilde{\Psi}_0|D|\widetilde{\Psi}_0\rangle}{\langle\widetilde{\Psi}_0|\widetilde{\Psi}_0\rangle}, \tag{6}$$

where D is the electric dipole operator. In the above expression, after expanding in terms of the cluster operators $T^{(0)}$ and $T^{(1)}$, only the terms first order in $T^{(1)}$ contribute. Often, $d_{\rm A}$ is computed perturbatively with the sum over states approach, which necessitates a truncation after the first few intermediate states. On the contrary, our relativistic coupled-cluster scheme doesn't involve summing over states and subsumes all possible intermediate states within the chosen configuration space.

Besides the NSM, the other possible source of EDM in closed shell atoms is the tensor-pseudotensor electron-nucleus interaction

$$H_{\rm PTV}^{\rm T-PT} = \frac{iG_F C_T}{\sqrt{2}}\sum_i \boldsymbol{\sigma}_N\cdot\boldsymbol{\gamma}_i\rho_N(r), \tag{7}$$

where G_F is fermi constant, C_T is coupling constant, $\boldsymbol{\sigma}_N$ is nuclear spin and $\boldsymbol{\gamma}_i$ is Dirac matrix. It must be emphasized that, this form of interaction does not exist within the Standard Model of particle physics and C_T is zero. However, there are models which predict such an interaction [13].

To extract the T or CP violation parameters, the atomic theory calculations are combined with the experimental data. In this context it is appropriate to rewrite Eq.(6) as

$$d_A = \lambda\eta, \tag{8}$$

where η is the atomic enhancement factor. As defined earlier, the constant λ is a T or CP violation parameter considered as a perturbation parameter. It can for example be the nuclear Schiff moment $\boldsymbol{S}$ or the coupling constant C_T. A precision atomic many-body calculation, like the coupled-cluster calculation reported here, would provide the value for a particular η. Experimentally, the measured atomic EDM $d_{\rm A}$ is the sum total of contributions from all the P and T symmetry violating phenomena within the atom. A bound on $\lambda = d_{\rm A}/\eta$ is obtained by combining the results of atomic theory and experimental data. Depending on the choice of the atom, it is possible to identify the dominant sources of T or CP violation and derive tighter bounds.

For the present set of calculations, we employ the even-tempered Gaussian basis set expansion [17, 18]. The

orbital basis set consist of $(1-18)s$, $(2-18)p_{1/2,3/2}$, $(3-13)d_{3/2,5/2}$, $(4-11)f_{5/2,7/2}$, $(5-9)g_{7/2,9/2}$ and $(6-7)h_{9/2,11/2}$. This orbital basis set is considered complete for the coupled perturbed Hartree-Fock (CPHF) calculations. That is, further increase in the number of orbitals does not change the results. In addition, we compute the ground state dipole scalar polarizability for ^{199}Hg. We obtain a value $33.294ea_0^3$, where a_0 is the Bohr radius, which is in excellent agreement with its experimental value [19, 20, 21].

To date, among the closed-shell atoms, ^{199}Hg as mentioned earlier sets the standard for the most precise EDM results. In a recent paper [11], the new upper limit is reported as

$$|d(^{199}\text{Hg})| < 3.1 \times 10^{-29} e \text{ cm (95\% C. L.)}. \quad (9)$$

Our atomic calculation based on the relativistic coupled-cluster theory gives

$$d_A^{\text{Schiff}}(^{199}\text{Hg}) = -5.07 \times 10^{-17} \left(\frac{S}{e \text{ fm}^3}\right) e \text{ cm}. \quad (10)$$

This is the first ever relativistic coupled-cluster result for any atomic EDM calculation arising from the NSM. Combining with the experimental result, the limit on the NSM is

$$S(^{199}\text{Hg}) < 6.1 \times 10^{-13} e \text{ fm}^3. \quad (11)$$

There is a large change of 96% from the result of coupled perturbed Hartree-Fock calculation

$$d_A^{\text{Schiff}}(^{199}\text{Hg}) = 2.8 \times 10^{-17} \left(\frac{S}{e \text{ fm}^3}\right) e \text{ cm}, \quad (12)$$

reported earlier [22], which is in excellent agreement with the result of a similar calculation but in the framework of the relativistic coupled-cluster theory [23]. The large change in the two results demonstrates the importance of electron correlation effects and their interplay with the $H_{\text{PTV}}^{\text{Schiff}}$ interaction in determining the magnitude of the NSM.

It is possible to separate the contributions of individual terms in Eq.(6) and the many-body perturbation diagrammatic representation of the dominant terms are shown in Fig.1. These diagrams represent the excitations and de-excitations due to cluster operators and dressed dipole operator $\overline{D}$. Earlier calculations [22, 24] incorporate only a certain class of two-particle two-hole excitations which are subset of the correlation effects we have included through the cluster operator $T^{(0)}$ in the present calculation. The two most dominant terms are $T_1^{(1)\dagger}\overline{D}$ and $T_1^{(1)\dagger}DT_2^{(0)}$, in Eq.(10) these terms individually contribute $-5.40 \times 10^{-17}(S/(e \text{ fm}^3))e$ cm and $-0.17 \times 10^{-17}(S/(e \text{ fm}^3))e$ cm respectively. In Fig.1, the diagrammatic equivalent of these terms are (a) and (b) respectively.

Our result of ^{199}Hg EDM arising from the electron-nucleus tensor-pseudotensor interaction is

$$d_A^{\text{T-PT}} = -4.3 \times 10^{-20} C_T \sigma_N e \text{ cm}. \quad (13)$$

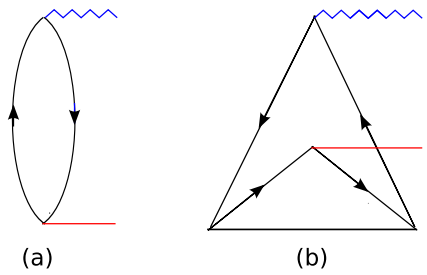

FIG. 1: Two of the dominant many-body perturbation diagrams of d_{A}. Diagrams (a) and (b) represent the terms $T_1^{(1)\dagger}\overline{D}$ and $T_1^{(1)\dagger}DT_2^{(0)}$ respectively. At the interaction vertices, the horizontal wavy blue, black and red lines represent the H_{PTV}, $T_2^{(0)}$ and the electric dipole operator D respectively.

Compared to the CPHF result $-6.19 \times 10^{-20} C_T \sigma_N e$ cm [23, 24], the change with the additional correlation effects is not so dramatic. There is a decrease of 31%, which is significant but not so spectacular as in $d_A^{\text{Schiff}}(^{199}\text{Hg})$. This comparison demonstrates, without any ambiguity, the importance of electron correlation effects in precision atomic EDM calculations. A closer examination of the structure of the two P and T violating Hamiltonians in the present work sheds some light on why the electron correlation effects are larger in the case of the NSM than the tensor-pseudotensor interaction. Both the $p_{1/2}$ and $p_{3/2}$ electrons are actively involved in the interplay of the H_{PTV} and electron correlation effects in the former, while the contribution of the $p_{3/2}$ electrons is negligible in the latter [22].

The individual contributions follow similar trend as in the case of NSM. The terms $T_1^{(1)\dagger}\overline{D}$ and $T^{(1)\dagger}\overline{D}T_2^{(0)}$ give the largest ($\approx 95\%$) and the second largest contributions to $d_{\text{A}}^{\text{T-PT}}$, $-4.8 \times 10^{-20} C_T \sigma_N e$ cm and $-0.27 \times 10^{-20} C_T \sigma_N e$ cm respectively. Then, a limit

$$C_T < 1.4 \times 10^{-9}, \quad (14)$$

is obtained after combining our results with the experimental data.

Assuming that the NSM arises from the nucleon-nucleon interactions with pions as the dominant mediators [25]

$$\boldsymbol{S}(^{199}\text{Hg}) = g_{\pi NN}\left[0.01\bar{g}_{\pi NN}^{(0)} + 0.07\bar{g}_{\pi NN}^{(1)} + 0.02\bar{g}_{\pi NN}^{(2)}\right] e \text{ fm}^3, \quad (15)$$

where $g_{\pi NN}$ and $\bar{g}_{\pi NN}^{(i)}$ are the CP conserving and CP violating pion-nucleon coupling constants respectively. Here, $i = 0, 1, \text{and } 2$ represent isoscalar, isovector and isotensor respectively. Considering $\bar{g}_{\pi NN}^{(1)}$ as the most dominant

$$\bar{g}_{\pi NN}^{(1)} < 6.4 \times 10^{-13}. \quad (16)$$

The coupling constant $\bar{g}^{(1)}_{\pi NN}$ is related to the chromo-EDMs of quarks [26], from the above result

$$(\widetilde{d}_u - \widetilde{d}_d) < 3.2 \times 10^{-27} e \text{ cm}. \quad (17)$$

Next, consider the maximum contribution to NSM arising from $\bar{g}^{(0)}_{\pi NN}$, then

$$\bar{g}^{(0)}_{\pi NN} < 4.5 \times 10^{-12}. \quad (18)$$

Since, $\bar{g}^{(0)}_{\pi NN} = 0.027\theta_{\rm QCD}$ [27], we get the bound

$$\theta_{\rm QCD} < 1.7 \times 10^{-10}. \quad (19)$$

The value we have obtained for the NSM is likely to give the most stringent bounds for supersymmetric CP violating phases [9, 10, 28]. In addition, from our results and the experimental data, it is also possible to set improved limits on the specific CP violating parameters predicted by various extensions of the Standard Model, $\epsilon_q^{\rm SUSY}$, $\epsilon^{\rm Higgs}$, $x^{\rm LR}$ [29].

In conclusion, we have developed a unique relativistic coupled-cluster based many-body method that takes into account the physical effects arising from the interplay of two very different kinds of fundamental interactions–the CP conserving electron-electron Coulomb and CP violating electron-nucleus interactions. The results obtained for the EDM of ^{199}Hg by the application of this method and the latest experiment on this atom [11] yield the most accurate limits to date on some important CP violating parameters. The electron correlation effects play a critical role in improving the existing limit on these parameters. These limits constrain the possible extensions to the Standard Model, thereby enhancing our current knowledge of the intriguing phenomenon of CP violation.

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[1] L. D. Landau, Sov. Phys. JETP **5**, 336 (1957).
[2] G. Luders, Ann. Phys. (N.Y.) **281**, 1004-1018 (2000).
[3] J. H. Christenson, J. W. Cronin, V. L. Fitch and R. Turlay, Phys. Rev. Lett. **13**, 138 (1964).
[4] K. Abe, et al. Phys. Rev. Lett. **87**, 091802 (2001).
[5] B. Aubert, et al. Phys. Rev. Lett. **87**, 091801 (2001).
[6] T. Ibrahim and P. Nath, Rev. Mod. Phys. **80**, 577 (2008) and references therein.
[7] M. Dine, and A. Kusenko, Rev. Mod. Phys. **76**, 1 (2004).
[8] M. B. Gavela, P. Hernandez, J. Orloff, O. Pene and C. Quimbay, Nucl. Phys. B **430**, 382 (1994).
[9] M. Pospelov, and A. Ritz, Ann. Phys. (N.Y.) **318**, 119 (2005).
[10] S. M. Barr, Int. J. Mod. Phys. A, **8**, 209 (1993).
[11] W. C. Griffith, M. D. Swallows, T. H. Loftus, M. V. Romalis, B. R. Heckel, and E. N. Fortson, arXiv:0901.2328 , 2009.
[12] J. M. Amini, C. T.Jr. Munger and H. Gould, Phys. Rev. A, **75**, 063416 (2007).
[13] S. M. Barr, Phys. Rev. D **45**, 4148 (1992).
[14] I. Lindgren and J. Morrison, *Atomic Many-Body Theory*, Springer-Verlag (1982), Berlin;New York.
[15] T. J. Bartlett and M. Musial, Rev. Mod. Phys. **79**, 291 (2007).
[16] V. V. Flambaum and J. S. M. Ginges, Phys. Rev. A **65**, 032113 (2002).
[17] A. K. Mohanty and E. Clementi, Chem. Phy. Lett., **157**, 348 (1989).
[18] R. K. Chaudhuri, P. K. Panda and B. P. Das, Phys. Rev. A **59**, 1187 (1999).
[19] T. M. Miller and B. Bederson, Adv. At. Mol. Phys. **13**, 1(1977).
[20] A. A. Radtsig and B. M. Smirnov, *References Data on Atoms, Molecules, and ions* Springer, Berlin, (1985).
[21] D. Goebel and U. Hohm J. Phys. Chem, **100**, 7710 (1996).
[22] V. A. Dzuba, V. V. Flambaum and J. S. M. Ginges, Phys. Rev. A **66**, 012111 (2002).
[23] K. V. P. Latha, D. Angom, R. K. Chaudhuri and B. P. Das, J. Phys. B **41**, 035005 (2008).
[24] A. Martensson-Pendrill, Phys. Rev. Lett. **54**, 11 (1985).
[25] J. H. de Jesus and J. Engel, Phys. Rev. C **72**, 045503 (2005).
[26] M. Pospelov, Phys. Lett. B **530**, 123 (2002).
[27] R. J. Crewther, P. Di Vecchiaa, G. Venezianoa and E. Witten, Phys. Lett. B **88**, 123 (1979).
[28] K. A. Olive, M. Pospelov, A. Ritz, and Y. Santoso, Phys. Rev. D **72**, 075001 (2005).
[29] M. V. Romalis, W. C. Griffith, J. P. Jacobs and E. N. Fortson, Phys. Rev. Lett. **86**, 2505-2508 (2001).