Electric dipole moment of $^{199}$Hg atom from P, CP-odd electron-nucleon interaction

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Abstract

We calculate the effect of the P, CP-odd electron-nucleon interaction on the electric dipole moment of the $^{199}$Hg atom by evaluating the nuclear spin matrix elements in terms of the nuclear shell model. It is found that the neutron spin matrix element of the $^{199}$Hg nucleus is $\langle \Psi | \sigma_p | \Psi \rangle$ with an errorbar of less than 20% and that of the proton is limited by $\langle \Psi | \sigma_p | \Psi \rangle < 0.01$, with a dominant configuration of $p_{1/2}$ orbital neutron. Combined with the results of the hadronic and atomic level calculations, the overall uncertainty of the relation between the CP-odd light quark-electron interaction renormalized at the TeV scale and the EDM of $^{199}$Hg atom is about 30%, which is the most accurately known for this system. We also derive constraints on the CP phases of Higgs-doublet models, supersymmetric models, and leptoquark models from the latest experimental limit $|d_{\text{Hg}}| < 7.4 \times 10^{-30} e$ cm.

1. Introduction

The baryon abundant Universe is realized if the fundamental theory fulfills Sakharov’s criteria [1]. One important issue is the lack of CP violation in the standard model (SM) of particle physics which generates a too small baryon number asymmetry, by ten orders of magnitude compared with the observed one [2, 3]. Motivated by this problem, the search for CP violation beyond the SM is nowadays an active area in particle physics.

One of the promising experimental approaches to unveil new sources of CP violation is the search for the electric dipole moment (EDM) [4, 5]. The EDM is an excellent probe of CP violation thanks to the small SM background [5, 6] and has been measured in many systems such as paramagnetic atoms [7], neutron [8], muon [9], and electron inside molecules [10, 11]. There are also many new experimental ideas to measure the EDM in other systems such as paramagnetic atoms using three-dimensional optical lattice [12, 13], proton and light nuclei using storage rings [14, 15, 16], strange and charmed baryons using bent crystals [17, 18], τ lepton from the precision analysis of collider experimental data [19, 20], electron using polar molecules and inert gas matrix [21], etc. The category of the most accurately measurable systems is the diamagnetic atom. The measured ones include $^{129}$Xe (current limit $|d_{\text{Xe}}| < 4.0 \times 10^{-27} e$ cm [22], prospective sensitivity $\sim 10^{-31} e$ cm), $^{225}$Ra (current limit $|d_{\text{Ra}}| < 1.5 \times 10^{-25} e$ cm [23], prospective sensitivity $\sim 10^{-28} e$ cm), and $^{199}$Hg which gives the current world record of the EDM upper limit $|d_{\text{Hg}}| < 7.4 \times 10^{-30} e$ cm [24].

Despite the exhaustive search in LHC experiments, their results are still consistent with the SM, and new approaches complementarily sensitive to new physics are now required. The EDM is actually an excellent alternative because it is more sensitive than the current reach of LHC (13 TeV) under the assumption of natural [O(1)] CP phases. The sensitivity of the EDM is so high that the detection of the Lorentz violation using this observable is also under discussion [25].

In the context of the atomic EDM, Schiff’s screening phenomenon [26] which cancels the EDM of nonrelativistic point-like constituent is well-known. The EDM of atoms is generated by three important mechanisms. These are (a) the relativistic enhancement of electron EDM, (b) the polarization of the atomic system by the P, CP-odd electron-nucleon (e-N) interaction, and (c) the nuclear Schiff moment which is the nonpointlike effect of the nucleus with an EDM. Among them, the atomic polarization due to the P, CP-odd e-N interaction is a purely atomic effect, and it can only be studied by measuring the EDM of heavy atoms [27, 28, 29]. The P, CP-odd e-N interaction is attracting attention, since it is generated in the two-Higgs doublet model (2HDM) at the tree level, and has extensively been discussed in the literature [30, 31]. This process is also interesting because of its specific sensitivity to several classes of models such as supersymmetric models with large tan $\beta$ [32, 33] or R-parity violation [34, 35], as well as to leptoquark models [36, 37, 38, 39] where the s-channel electron-quark interaction is relevant. Since atoms are one of the most accurately measurable systems and are now giving the world record in the EDM experiments, the study of the contribution of the CP-odd e-N interaction has an inevitable importance in the analysis of these models.

In the theoretical evaluation of the atomic EDM generated by new physics beyond the SM, hadronic, nuclear and atomic level calculations are required. In the context of the CP-odd e-N interaction, the results of the calculations at the hadronic level are already reaching a very good accuracy thanks to the progress of lattice QCD, currently being precise at the level of 10% [40, 41]. The atomic level calculations are also known to be very accurate, and the theoreti-
The CP-odd interaction, i.e. the extended Higgs models, supersymmetric framework of the calculation of the spin matrix elements of the EDM of \(^{199}\text{Hg}\), however, the nuclear spin matrix elements, which are the most important input, have never quantitatively been evaluated. An estimation using the simple shell model with only one valence nucleon is possible \([18, 19]\), but it is known in modern nuclear physics that this naive picture does not hold due to the configuration mixing, in particular for nuclei with nucleon numbers not close to magic numbers.

In Xe systems, the nuclear level inputs required in the analysis of the atomic EDM such as the contribution of the intrinsic nucleon EDM and the CP-odd nuclear force to the calculation of Xe systems, we expect that the application of the same framework to the analysis of the atomic EDM such as the contribution of the nuclear level inputs required in the calculation of Xe systems, we expect that the application of the same framework to the summary.

This paper is organized as follows. We first present in Section 2 the CP-odd e-N interaction and their relation with the EDM of \(^{199}\text{Hg}\) atom. We then give the detail of the framework of the calculation of the spin matrix elements of \(^{199}\text{Hg}\) and neighboring odd-nuclei in the shell model in Section 3 and show the result as well as the relation between the quark-gluon level CP-odd interaction and the EDM of \(^{199}\text{Hg}\). We then analyze in Section 4 the constraints on several candidates of new physics beyond the SM. The last section is devoted to the summary.

2. The P, CP-odd electron-nucleon interaction

The leading P, CP-odd electron-nucleon (e-N) interaction contributing to the atomic EDM is given by three types of dimension-six contact interactions \([8, 9, 10, 11]\):

\[
L_{eN} = -\frac{G_F}{\sqrt{2}} \sum_{N,p,a} \left[ C^{SP}_{N} \bar{N}\gamma_{5}e\bar{N}\gamma_{5}N\bar{e}e + C^{PS}_{N} \bar{N}\gamma_{\mu}N\bar{e}\gamma_{\mu}e + \frac{1}{2} C^{T}_{N} e^{\mu\nu\rho\sigma} \bar{N}\sigma_{\mu\rho}N\bar{e}\sigma_{\nu\sigma}e \right].
\]

(1)

Here we denote the first, second, and third terms by the scalar-pseudoscalar (SP), the pseudoscalar-scalar (PS), and the tensor (T) type interactions, respectively. Note the minus sign of \(C^{T}_{N}\) due to the convention.

The EDM of \(^{199}\text{Hg}\) atom is given by the leading order perturbation of the CP-odd electron-nucleus interaction

\[
H_{CP}:
\]

\[
d_{\text{Hg}} = 2 \sum_{m} \frac{\langle \psi_{a} | - e \sum_{m} r_{i} | \psi_{m} \rangle \langle \psi_{m} | H_{CP} | \psi_{a} \rangle}{E_{0} - E_{m}},
\]

(2)

where \(\psi_{m}\) labels the atomic eigenstates. From the nonrelativistic spin structure of the CP-odd e-N interaction \([12]\), it is possible to parametrize the EDM of \(^{199}\text{Hg}\) atom in the leading order of the CP-odd e-N couplings as

\[
d_{\text{Hg}} = R_{T} \left( C^{T}_{p} (\sigma_{p}^{\rho}, C^{T}_{n} (\sigma_{n}^{\rho}) \right)
+ R_{PS} \left( C^{PS}_{p} (\sigma_{p}^{\rho}, C^{PS}_{n} (\sigma_{n}^{\rho}) \right)
+ R_{SP} \left( 0.40 C^{SP}_{p} + 0.60 C^{SP}_{n} \right),
\]

(3)

where \((\sigma_{N}^{\rho}) \equiv \langle \text{Hg} | \sigma_{N}^{\rho} | \text{Hg} \rangle \), \((N = p, n)\) is the nuclear spin matrix element. We see that the T and PS type CP-odd e-N interactions depend on the nuclear spin matrix elements, and we therefore need their accurate value to quantitatively analyze the effect of new physics. The factors 0.40 and 0.60 are the fractions of the proton and neutron numbers over the total one, and are exact in the nonrelativistic limit. For the case of the SP type CP-odd e-N interaction, the calculation of nuclear matrix elements is therefore not required.

The atomic coefficient \(R_{T}\) was calculated in several atomic level approaches \([12, 13]\). Here we use the result of the calculation in the relativistic coupled-cluster method \(R_{T} \approx -3.4 \times 10^{-20} \text{cm} \), which is expected to be around 15%.

The PS type CP-odd e-N interaction is analytically related to the T type one with \([8, 11]\):

\[
\left( C^{PS}_{p} (\vec{\sigma}_{p}) + C^{PS}_{n} (\vec{\sigma}_{n}) \right) \leftrightarrow \frac{5 m_N R}{Z_{em}} \left( C^{T}_{p} (\vec{\sigma}_{p}) + C^{T}_{n} (\vec{\sigma}_{n}) \right),
\]

(4)

where \(R\) is the nuclear radius. From this relation we have \(R_{PS} \approx -1.2 \times 10^{-22} \text{cm}\).

The \(^{199}\text{Hg}\) atom is a diamagnetic atom and has a closed electron shell, so the EDM is not generated by the SP type CP-odd e-N interaction. The CP-odd e-N interactions depend on the nuclear spin matrix elements, and we therefore need their accurate value to quantitatively analyze the effect of new physics. The factors 0.40 and 0.60 are the fractions of the proton and neutron numbers over the total one, and are exact in the nonrelativistic limit. For the case of the SP type CP-odd e-N interaction, the calculation of nuclear matrix elements is therefore not required.

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where $\tilde{G}_{\mu\nu}^a \equiv \frac{1}{v} \epsilon_{\mu\nu\rho\sigma} G_{\rho\sigma}^a$. Here note that $a \epsilon_{\mu\nu} G_{\mu\nu}^a$ and $a \tilde{G}_{\mu\nu}^a G_{\mu\nu}^a$ are renormalization group invariant in the leading order of the strong coupling $\alpha_s$. The sum over the quark flavor $q$ has to be taken up to that allowed by the renormalization scale $\mu$ (e.g. $q = u, d, s, c$ for $\mu = 2 \text{ GeV}$).

For the $T$ type CP-odd $e-N$ interaction, the couplings $C_T^u$ and $C_T^n$ are obtained by just multiplying the nucleon tensor charge $\delta q \equiv \sum p|\langle q | i \gamma_5 s \gamma_5 | p \rangle|$ to the quark level analogue $C_T^q$. By writing them explicitly, we have

$$C_T^u = C_T^u \delta u + C_T^u \delta d + C_T^u \delta s + C_T^u \delta c, \quad (6)$$

$$C_T^n = C_T^n \delta d + C_T^n \delta u + C_T^n \delta s + C_T^n \delta c, \quad (7)$$

where we assumed the isospin symmetry. The light quark contributions to the nucleon tensor charge are given by $\delta u = 0.8$ and $\delta d = -0.2$ from recent lattice QCD calculations in Refs. [74, 75, 76], with 10% of theoretical uncertainty, being conservative. They are also extracted from experimental data using perturbative QCD based frameworks [73, 74, 77, 80], but more accurate data with future experiments [78, 80] are required to perform quantitative analyses. For the strange quark contribution, previous works obtained $\delta s = 0.008(9)$ [73, 74, 79] and $\delta s = -0.0213(54)$ [80], which are marginally consistent within 2$\sigma$. The charm quark contribution is consistent with zero within the uncertainty $|\delta c| < 0.005$ [84].

We note that $C_T^u (q = u, d, s, c)$ calculated at the scale of the new physics (e.g. $\mu = 1 \text{ TeV}$) has to be renormalized down to the scale where the results of the calculations of the nucleon tensor charges are available ($\mu = 2 \text{ GeV}$ in most of the cases). The running of $C_T^u$ from $\mu = 1 \text{ TeV}$ down to $\mu = 2 \text{ GeV}$ brings a factor of about 0.8 [101, 103]. This suppression is intuitively understood by the radiative emission and absorption of the gluon, which flip the spin of the quark. A similar mechanism is also working at the level of the nucleon matrix element, attenuating the contribution of the quark to the nucleon tensor charge [104, 107].

For the $P$ type CP-odd $e-N$ interaction, we have to consider the gluonic contribution in addition to the CP-odd electron-quark interaction. The couplings are given by

$$C_P^{PS} = C_P^{PS}(p\tilde{u}\gamma_5 u|p) + C_P^{PS}(p\tilde{d}\gamma_5 d|p),$$

$$+ \sum_{q=u,c} C_P^{PS}(p\tilde{q}|i\gamma_5 q|p) + C_P^{PS} \frac{Q}{8\pi} \langle p|G_{\mu\nu}^a G_{\mu\nu}^a|p\rangle, \quad (8)$$

$$C_P^{PS} = C_P^{PS}(n\tilde{d}\gamma_5 d|n) + C_P^{PS}(n\tilde{u}\gamma_5 u|n),$$

$$+ \sum_{q=u,c} C_P^{PS}(n\tilde{q}|i\gamma_5 q|n) + C_P^{PS} \frac{Q}{8\pi} \langle n|G_{\mu\nu}^a G_{\mu\nu}^a|n\rangle, \quad (9)$$

where the isospin symmetry was used. The nucleon matrix elements are phenomenologically derived from the anomalous Ward identity [102, 103, 108, 113], using the latest QCD level inputs [114, 115], we have $\langle p\tilde{u}\gamma_5 u|p \rangle = 180$, $\langle p\tilde{d}\gamma_5 d|p \rangle = -170$, $\langle N|\tilde{u}\gamma_5 u|N \rangle = -51$, $\langle N|\tilde{d}\gamma_5 d|N \rangle = -34$, and $\langle N|G_{\mu\nu}^a G_{\mu\nu}^a|N \rangle = -400 \text{ MeV} (N = p, n)$, with about 30% of theoretical uncertainty [17]. It is important to note that the $P$ type CP-odd $e-N$ interaction is enhanced, due to the pion pole contribution of the light quarks [108, 113]. We also point out that at a scale below the quark mass threshold, the $b$ and $t$ quarks contribute to $C_{PS}$ through quark loops, as $C_{PS} = \frac{1}{m_q} C_{PS}^q (Q = b, t)$, in the leading order in $\alpha_s$. For the case of $C_{PS}$, the renormalization grows the couplings when the scale decreases since the product of $(N|\tilde{q}\gamma_5 q|N)$ and the current quark mass form invariants. The running from $\mu = 1 \text{ TeV}$ to $\mu = 2 \text{ GeV}$ yields an enhancement of a factor of about two (this is also valid for $b$ and $t$ quark contributions since $C_{PS}^b = \frac{1}{m_q}$).

The SP type CP-odd $e-N$ interaction is derived in a similar way as the PS one:

$$C_P^{SP} = \frac{C_P^{SP}}{2} \left( \sigma_{\alpha N} \frac{\alpha_s}{m_u + m_d} + gs \right) + \frac{C_P^{SP}}{2} \left( \sigma_{\alpha N} \frac{\alpha_s}{m_u + m_d} - gs \right) + \sum_{q=u,c} \frac{C_P^{SP}}{2} \left( \sigma_{\alpha N} \frac{\alpha_s}{m_u + m_d} + gs \right),$$

$$+ \sum_{q=u,c} \frac{C_P^{SP}}{2} \left( \sigma_{\alpha N} \frac{\alpha_s}{m_u + m_d} - gs \right) + \sum_{q=u,c} \frac{C_P^{SP}}{2} \left( \sigma_{\alpha N} \frac{\alpha_s}{m_u + m_d} + gs \right), \quad (10)$$

$$C_{PS}^{SP} = \frac{C_{PS}^{SP}}{2} \left( \sigma_{\alpha N} \frac{\alpha_s}{m_u + m_d} - gs \right), \quad (11)$$

where we again used the isospin symmetry. Here the pion-nucleon sigma term is given by $\sigma_{\alpha N} = 40 \text{ MeV}$ [85, 83] and the isovector nucleon scalar charge is $g_s \approx 0.9$ at the scale $\mu = 2 \text{ GeV}$ [73, 74, 77, 79, 80], with errorbars of about 10%. We note here that $\sigma_{\alpha N}$ phenomenologically extracted from experimental data is around 60 MeV [122, 127]. The strange and charm contents of the nucleon are given by $\sigma_s \approx 40 \text{ MeV}$ [82, 83, 86, 89] and $\sigma_c \approx 80 \text{ MeV}$ [131, 133], respectively, with an uncertainty of about 50%. The gluonic condensate is derived from the trace anomaly as $a = (N|G_{\mu\nu}^a G_{\mu\nu}^a|N) = (-50 \pm 5) \text{ MeV} (N = p, n)$ [7]. As with the PS type one, the contribution from $b$ and $t$ quarks at a scale below the threshold is given by $C_{PS}^{SP} = \frac{1}{m_q} C_{PS}^b$. The renormalization of $C_{PS}^{SP}$ is exactly the same as that of $C_{PS}$ since the product of $(N|\tilde{q}\gamma_5 q|N)$ or $1/m_q (Q = b, t)$ with the current quark mass is invariant under the renormalization group evolution.

3. The nuclear shell-model calculation

The nuclear shell model is one of the most successful models to describe various properties of nuclear structure such as the energy spectra, the electromagnetic transitions, and the electromagnetic moments. In order to study the nuclear structure and calculate the nuclear spin matrix elements of $^{199}\text{Hg}$, it is preferable to exploit all the single-particle levels between magic numbers 82 and 126 for neutrons and those between magic numbers 50 and 82 for protons. It is, however, very hard to perform the full shell-model calculations for $^{199}\text{Hg}$ due to the large number of shell-model configurations. To get around this problem, the pair-truncated shell model (PTSM), where the full shell-model space is truncated within subspaces composed of collective pairs of nucleons, is utilized. The details of the PTSM framework are given in Ref. [133, 134].
For the single-particle orbitals in the shell-model space, we employ the six orbitals between magic numbers 82 and 126, \((0h_{11/2}, 1f_{5/2}, 0h_{11/2}, 0f_{7/2}, 1f_{5/2}, 2p_{1/2})\), for neutrons and the five orbitals between magic numbers 50 and 82, \((0g_{9/2}, 1d_{3/2}, 1d_{5/2}, 2s_{1/2}, 0h_{11/2})\), for protons. The single-particle energies listed in Table 1 are determined to reproduce some low-lying spectra in \(^{206}\text{Pb}\) and \(^{207}\text{Tl}\). Both neutrons and protons are considered as holes. The full shell-model space is truncated into the subspaces composed of collective pairs with angular momentum zero (S-pairs), two (D-pairs), and four (G-pairs) for protons, and S and D pairs for neutrons.

As a nuclear effective interaction, the so-called monopole plus quadrupole-quadrupole interaction is employed \([13]\). The Hamiltonian is written as

\[
\hat{H} = \hat{H}_n + \hat{H}_p + \hat{H}_{np},
\]

where \(\hat{H}_n\) and \(\hat{H}_p\) consist of the single-particle energies and the two-body interactions for neutrons and protons, respectively, and \(\hat{H}_{np}\) represents the quadrupole-quadrupole interaction between a neutron and a proton. The strength parameters of the effective two-body interactions in Eq. (12), which are listed in Table 2, are determined by performing a \(\chi^2\)-fit to the experimental spectra for some low-lying states in \(^{206}\text{Hg}\), \(^{198}\text{Hg}\), \(^{199}\text{Pt}\), and \(^{198}\text{Pt}\) nuclei. Figure 1 shows the energy spectrum for \(^{199}\text{Hg}\) in comparison with the experimental data.

In the simple shell model with one valence neutron, the nucleon spin matrix elements for the \(1/2^-\) state of \(^{199}\text{Hg}\) are

\[
\langle \sigma_{nc} \rangle = -0.3765,
\]

\[
\langle \sigma_{pc} \rangle = 0.0088.
\]

Although the optimized value of \(\chi^2 = 0.0979\) is obtained, these parameters are not so good with respect to the reproduction of the spin of the experimental ground state.

![Figure 1: Energy spectra for \(^{199}\text{Hg}\) with the optimized strength parameters of the effective two-body interactions (PTSM1) and the same parameters except for a single-particle energy \(\epsilon_n(1f_{5/2}) = -0.2\text{ MeV}\) (PTSM2). The experimental data (Expt.) is taken from Ref. \([13]\).](image)

The correct spin \(1/2^-\) for the ground state can be reproduced by artificially changing the single particle energy as \(\epsilon_n(1f_{5/2}) = -0.2\text{ MeV}\). In this case the results are

\[
\langle \sigma_{nc} \rangle = -0.3249, \quad \langle \sigma_{pc} \rangle = -0.0031.
\]

Thus, we estimate the systematic error of our calculation by the difference of these two sets of values. Our result for the nuclear spin matrix elements is therefore

\[
\langle \sigma_{nc} \rangle = -0.3249 \pm 0.0515, \quad \langle \sigma_{pc} \rangle = 0.0031 \pm 0.0118.
\]

In the simple shell model with one valence neutron, the nuclear spin matrix elements of \(^{199}\text{Hg}\) are given by \(\langle \sigma_{nc} \rangle = -\frac{1}{4}, \langle \sigma_{pc} \rangle = 0\). Our results for \(\langle \sigma_{nc} \rangle\) and \(\langle \sigma_{pc} \rangle\) are consistent with the simple estimations, which suggest that the one valence nucleon picture is relevant. Table 3 shows the results for odd-mass Hg isotopes. The results gradually approach the simple estimation as the number of valence neutrons decreased.

The above results provide us the relation between \(d_{1/2}\) and the CP-odd \(e-N\) couplings

\[
d_{1/2} = \left(1.1C_n^{-1} + 0.0040C_p^{SP}ight) \\
- 0.017C_n^{SP} - 0.011C_p^{SP} \times 10^{-20} \text{ e cm.} \quad (19)
\]

We neglected the effect from the proton spin matrix element since it is small and its theoretical uncertainty exceeds the
central value. We also display the relation between $d_{\text{HG}}$ and the CP-odd quark/gluon level interactions

$$d_{\text{HG}} = \left( -0.18 C_{0}^\nu + 0.73 C_{d}^\nu - 0.02 C_{t}^\nu - 1.2 C_{u}^\text{PS} + 1.3 C_{d}^\text{PS} - 0.04 C_{s}^\text{PS} - 0.002 C_{b}^\text{PS} - 0.0007 C_{b}^\gamma - 2 \times 10^{-3} C_{b}^\text{SP} + 2.9 \text{MeV}^{-1} C_{g}^\gamma - 0.14 C_{b}^\text{SP} - 0.15 C_{s}^\text{SP} - 0.02 C_{s}^\text{PS} - 0.003 C_{c}^\text{SP} - 8 \times 10^{-3} C_{b}^\gamma - 2 \times 10^{-6} e C_{g}^\gamma - 0.35 \text{MeV}^{-1} C_{g}^\gamma \right) \times 10^{-2} e \text{cm}, \quad (20)$$

with a conservative errorbar of 30% for the $u$- and $d$-quark contributions, and 60% for the others. Note that the CP-odd electron-quark/gluon couplings were renormalized at $\mu = 1$ TeV.

### 4. Constraints on new physics beyond standard model

![Diagram](image)

Let us now discuss concrete constraints for several known models. The first candidate to be considered is the 2HDM. In the standard 2HDM, the CP phase appears in the mixing between two Higgs modes [138, 144]. This mixing generates SP and PS type CP-odd $e-N$ interactions at the tree level, as shown in Fig. 2(a). The experimental data of $d_{\text{HG}}$ yield the following constraints:

$$\frac{|(H_0 A)^\tan^2 \beta|}{m_{H_0}^2 m_{A}^2} < 64 \text{ TeV}^{-2}, \quad (21)$$

where we only considered the contribution from down-type quarks which is enhanced with $\tan \beta$. The mass of the lightest Higgs boson is $m_{H_0} = 125$ GeV [145, 147], but that of the CP-odd one A is undetermined. In the above discussion, we did not constrain the CP violation of the top quark sector [148, 149] because it is more tightly bounded by the analysis of the Barr-Zee type diagram [56, 158-178].

The supersymmetric models [179, 181] include the 2HDM as the limit of heavy sparticles. If the sfermions are relevant, additional contributions to the CP phase of the Yukawa coupling from loop diagrams are possible [182, 183]. The first effect we might consider is the squark loop induced the $HG_{\mu\nu} G_{a}^{\mu\nu}$ vertex which contributes to the SP type CP-odd $e-N$ interaction [see Fig. 2(c)] [54]. This contribution is, however, well below that given by the CP-odd electron-quark interaction, as we will see below.

The correction to the Yukawa vertex with intermediate sfermion propagation may be important in the case of large $\tan \beta$. This effect actually brings an additional $\tan \beta$ to the CP-odd $e-N$ interaction, resulting in a $\tan^3 \beta$ dependence [55, 59]. For large $\tan \beta$, we actually have

$$\begin{align*}
\frac{\tan^2 \beta (\sin \delta - \sin \delta_0)}{m_f^2 (1 - J_c \tan \beta) (1 - J_f \tan \beta)} &< 190 \text{ TeV}^{-2}, \quad (22) \\
\frac{\tan^2 \beta (\sin \delta - \sin \delta_0)}{m_f^2 (1 - J_c \tan \beta) (1 - J_f \tan \beta)} &< 330 \text{ TeV}^{-2}, \quad (23) \\
\frac{\tan^2 \beta (\sin \delta - \sin \delta_0)}{m_f^2 (1 - J_c \tan \beta) (1 - J_f \tan \beta)} &< 340 \text{ TeV}^{-2}, \quad (24)
\end{align*}$$

where $\sin \delta_i = \frac{\text{Im}(\lambda_{i+j}) \tan \beta}{\text{Re}(\lambda_{i+j})}$ ($i = e, d, s, b$). We note that for the bottom quark case, the contribution from the Barr-Zee type diagram is dominant, and other stronger constraints are available. Note that for the 2HDMs, interesting cancellations or fine-tunings may occur [183, 185], although we do not consider them in this work.

In the supersymmetric extension of the SM, $R$-parity violating (RPV) interactions [194, 195], which do not conserve lepton or baryon numbers, are also allowed. The relevant RPV interactions are given by

$$L_R = - \sum_{i,j,k} \left[ \begin{array}{c}
\frac{\lambda_{ij}}{2} \bar{\nu}_i \bar{P}_e P_L e_j + \bar{\nu}_i \bar{P}_\mu P_L \mu_j \\
\mp \frac{\lambda_{ij}}{\text{Re}(\lambda_{ij})} \bar{P}_\mu P_L e_j \mp (i \leftrightarrow j)
\end{array} \right]$$

$$+ \sum_{i,j,k} \left[ \begin{array}{c}
\bar{\nu}_i \bar{d}_i P_L d_j + \bar{d}_i \bar{d}_j P_L P_L + \bar{d}_i \bar{d}_j P_L P_L \\
- \bar{\nu}_i \bar{d}_i P_L u_j - \bar{u}_i \bar{d}_j P_L e_j \mp \bar{d}_i \bar{d}_j P_L P_L
\end{array} \right]$$

$$(+ \text{h.c.}), \quad (25)$$

where field operators with tilde denote sparticles. The coupling constants $\lambda_{ij}$, $\lambda'_{ij}$ ($i, j, k = 1, 2, 3$ are the flavor indices) may have nonzero CP phases. In this case, a nonzero CP-odd $e-N$ interaction is generated through the $t$-channel process [see Fig. 2(a)]. Here we note that the pion pole effect enhances the contribution from the PS type CP-odd electron-quark interaction involving the $d$-quark. The constraints given from the experimental data of $d_{\text{HG}}$ are then

$$\begin{align*}
\sum_{i=2,3} \frac{\text{Im}(\lambda'_{3i+1})}{m_{\nu_i}^2} &< 1.2 \times 10^{-8} \text{ TeV}^{-2}, \quad (26) \\
\sum_{i=2,3} \frac{\text{Im}(\lambda'_{3i+2})}{m_{\nu_i}^2} &< 1.9 \times 10^{-6} \text{ TeV}^{-2}, \quad (27) \\
\sum_{i=2,3} \frac{\text{Im}(\lambda'_{3i+3})}{m_{\nu_i}^2} &< 2.6 \times 10^{-4} \text{ TeV}^{-2}. \quad (28)
\end{align*}$$

The coupling $\sum_{i=2,3} \frac{\text{Im}(\lambda'_{3i+1})}{m_{\nu_i}^2}$ [Eq. 26] can be specifically constrained by the EDM of $^{199}$Hg via the CP-odd $e-N$ interaction thanks to the pion pole enhancement. On
the other hand, heavier flavor contributions are more constrained by the analysis of the Barr-Zee type diagrams [14, 5, 19, 43, 195]. The analysis of the CP-odd e-N interaction also has an important impact on the CP violation of the leptoquark models [194, 195]. It is generated by the s-channel process, as shown in Fig. 1(c). We can conceive spin-1 and spin-0 leptoquarks, as given by the Lagrangian of Ref. [27]:

\[ \mathcal{L}_{LQ} = S_1 (g'_{L1} (\bar{u} P_L e - \bar{d} P_L \nu_e) + g'_{R1} (\bar{u} P_R e) - (R_2) \gamma \bar{d} P_L \mu + h_{S2} \bar{d} \gamma_\mu P_R e) + \text{h.c.}, \]

where \( S_1 \) and \( R_2 \) (\( U_1 \) and \( V_2 \)) are the spin-0 (spin-1) leptoquarks. The spin-1 leptoquarks can only generate SP and PS type CP-odd e-N interactions, whereas the spin-0 one also gives a T type one. We can then derive the following constraints from the experimental data of \( d_{\text{Hg}} \):

\[
\frac{\text{Im}(g'_{L1} g'_{R1})}{m_{S1}^2} < 2.8 \times 10^{-5} \text{eV}^{-2},
\]

\[
\frac{\text{Im}(h_{S1} h_{R1})}{m_{S1}^4} < 2.4 \times 10^{-5} \text{eV}^{-2},
\]

\[
\frac{\text{Im}(h_{S2} h_{R2})}{m_{S2}^4} < 6.1 \times 10^{-9} \text{eV}^{-2},
\]

\[
\frac{\text{Im}(g'_{L1} g'_{R1})}{m_{V1}^2} < 6.1 \times 10^{-9} \text{eV}^{-2},
\]

where \( m_{S1} \) and \( m_{R1} \) (\( m_{V1} \)) are the masses of the spin-0 (spin-1) leptoquarks. Here for simplicity, we only considered one leptoquark multiplet for each spin. In the general case with several leptoquark multiplets, there may be additional mixings [17]. For the exchange of spin-1 leptoquarks, the EDM of \( ^{199}\text{Hg} \) is dominantly generated by the PS type interaction, due to the pion pole enhancement. In the case of spin-0 leptoquark exchange, the contributions from the T and PS type CP-odd e-N interactions are comparable.

Let us also mention the SM contribution, generated by the CP phase of the CKM matrix. The current understanding is that its leading effect to the CP-odd e-N interaction is given by the pion-exchange process, via the SP type interaction \( (C_{S1}^\text{SP}) \) [5, 20, 22, 224]. The coupling is estimated to be

\[ C_{S1}^\text{SP} \sim 10^{-17}, \]

which gives a contribution of \( d_{\text{Hg}} \sim 10^{-39} \) e cm. In the diamagnetic atomic system, the contribution from the nuclear Schiff moment [153] is also relevant. From a model calculation, this contribution is given by \( d_{\text{Hg}} \sim 10^{-33} \) e cm [201], which is much larger than that of \( C_{S1}^\text{SP} \). We however have to note that the above analyses did not consider the dynamical nuclear effect of the intermediate hypernuclear state [222] and the neglect of it may introduce sizable systematics. This issue has to be inspected in future works.

5. Conclusion

In summary, we evaluated the nuclear spin matrix elements of \( ^{199}\text{Hg} \), which are required in the evaluation of the atomic EDM generated by the PS and T type CP-odd e-N interactions, within the nuclear shell model. The \( ^{199}\text{Hg} \) nucleus has a dominant configuration with \( p_{1/2} \) orbital neutron, and the errorbar deduced is less than 20% for the neutron spin matrix element. For the proton one, the errorbar is larger than the central value, but its size is much smaller than the neutron one, so it can be neglected in the analysis of many candidates of new physics beyond the SM.

We also analyzed the contribution of the P, CP-odd e-N interaction to the EDM of the \( ^{199}\text{Hg} \) atom within 2HDMs, supersymmetric models, and leptoquark models. Thanks to the tight theoretical limit of the \( ^{199}\text{Hg} \) atom, we could set strong constraints on the semi-leptonic sector of these models. The CP-odd e-N interaction is therefore critically important to probe those specific candidates.

Before we obtained our result, the nuclear spin matrix elements of \( ^{199}\text{Hg} \) were the only missing link between the semi-leptonic CP violation and the experimental data of the EDM of \( ^{199}\text{Hg} \). Through our analysis, we could fill the gap, and combining with the accurate hadronic and atomic inputs, the CP-odd e-N interaction became the most accurately known CP-odd process of the EDM of \( ^{199}\text{Hg} \).

Our analysis using the nuclear shell model definitely has to be extended to the study of the nuclear Schiff moment generated by the intrinsic nucleon EDM and the CP-odd pion-nucleon interactions to reduce the theoretical uncertainty. We also expect our framework to be applicable in the evaluation of the spin matrix elements of other heavy nuclei such as \( ^{225}\text{Ra} \) which has already been measured in experiment [22].

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References

[1] A. D. Sakharov, Pisma Zh. Eksp. Teor. Fiz. 5, 32 (1967) [JETP Lett. 5, 24 (1967)].
[2] G. R. Farrar and M. E. Shaposhnikov, Phys. Rev. D 50, 774 (1994).
[3] P. Huef and E. Sather, Phys. Rev. D 51, 379 (1995).
[4] X.-G. He, B. H. J. McKellar, and S. Pakvasa, Int. J. Mod. Phys. A 4, 5011 (1989) [Erratum ibid. A 6, 1063 (1991)].
[5] W. Bernreuther and M. Suzuki, Rev. Mod. Phys. 63, 313 (1991).
[6] I. B. Khriplovich and S. K. Lamoreaux, CP Violation Without Strangeness, Springer, Berlin (1997).
[7] J. S. M. Ginnes and V. V. Flambaum, Phys. Rep. 397, 63 (2004).
[8] M. Pospelov and A. Ritz, Ann. Phys. 318, 119 (2005).
[9] M. Raidal et al., Eur. Phys. J. C 57, 13 (2008).
[10] O. Naviliat-Cuncic and R. G. E. Timmermans, Comptes Rendus Physique 13, 168 (2012).
[11] T. Fukuyama, Int. J. Mod. Phys. A 27, 1230015 (2012).
[186] S. Borowka, S. Paßehr and G. Weiglein, arXiv:1802.09886 [hep-ph].
[187] S. Heinemeyer and C. Schappacher, arXiv:1803.10645 [hep-ph].
[188] L. Bian, T. Liu, and J. Shu, Phys. Rev. Lett. 115, 021801 (2015).
[189] L. Bian and N. Chen, Phys. Rev. D 95, 115029 (2017).
[190] G. Bhattacharyya, arXiv:hep-ph/0709395.
[191] H. K. Dreiner, in Perspectives on Supersymmetry II, edited by G. L. Kane (World Scientific, Singapore, 1997), p. 565 [arXiv:hep-ph/9707435].
[192] M. Chemtob, Prog. Part. Nucl. Phys. 54, 71 (2005).
[193] R. Barbier et al., Phys. Rep. 420, 1 (2005).
[194] N. Yamanaka, T. Sato, and T. Kubota, Phys. Rev. D 85, 117701 (2012).
[195] N. Yamanaka, T. Sato, and T. Kubota, Phys. Rev. D 87, 115011 (2013).
[196] S. Davidson, D. Bailey, and B. A. Campbell, Z. Phys. C 61, 613 (1994).
[197] J. L. Hewett and T. G. Rizzo, Phys. Rev. D 56, 5709 (1997).
[198] P. Nath and P. Fileviez Perez, Phys. Rep.441, 191 (2007).
[199] I. Dor˘sner, S. Fajfer, A. Greljo, J. F. Kamenik, and N. Ko˘snik, Phys. Rep. 641, 1 (2016).
[200] M. Pospelov and A. Ritz, Phys. Rev. D 89, 056006 (2014).
[201] N. Yamanaka and E. Hiyama, J. High Energy Phys. 1602 (2016) 067.
[202] N. Yamanaka, Nucl. Phys. A 963, 33 (2017).