Abstract

Highly correlated pure \textit{ab initio} relativistic configuration interaction theory is in the present paper applied to the calculation of the tensor-pseudotensor ($\mathcal{P}, \mathcal{T}$)-violating nucleon-electron interaction constant in the electronic ground states of atomic mercury and radium. The final best obtained results are $R_T(\text{Hg}) = -4.43 \times 10^{-20} \langle \sigma_N \rangle \text{ e cm}$ and $R_T(\text{Ra}) = -15.0 \times 10^{-20} \langle \sigma_N \rangle \text{ e cm}$. The accuracy of the employed electronic-structure models are confirmed by determining the static electric dipole polarizability $\alpha_d(\text{Hg}) = 35.7 \text{ a.u.}$ which is in accord with the experimental value to about 5%. $R_T(\text{Ra})$ will be useful for constraining (or obtaining) the ($\mathcal{CP}$)-violating parameter $C_T$ when combined with future measurements of the electric dipole moment of the radium atom.
I. INTRODUCTION

Charge-Parity ((CP))-violation has so far been observed in nature only in the decays of certain heavy mesons – such as the K and B mesons [1–3] – which are flavor-changing processes driven by the weak interaction. These sources of (CP)-violation have become an integral part of the Standard Model (SM) of particle physics through the Cabibbo-Kobayashi-Maskawa (CKM) quark-mixing matrix [4]. However, the observed disparity of matter and antimatter in the universe [5] which requires (CP) symmetry to be violated [6] cannot be explained solely through SM (CP)-violation. Additional sources of (CP)-violation are predicted by most theory models Beyond the SM [7], and they give rise to electric dipole moments (EDM) in atomic matter many orders of magnitude larger than the SM predictions [8].

If one accepts that CPT symmetry [9] is unbroken – and this is strongly suggested by its intertwining with Lorentz invariance – then (CP)-violation implies T-violation, which means that, e.g., an atomic energy shift would change sign if the laboratory were to travel backwards in time. The search for additional (CP)-violation in nature, therefore, can be carried out as search for EDMs of elementary particles and search for a T-violating piece of the weak interaction, for instance among the hadrons and leptons of an atomic system [10]. The latter can arise from the tree-level exchange of a BSM mediator particle such as in the framework of leptoquark scenarios [10, 11].

An important potential manifestation of (CP)-violation in atomic systems with closed electronic shells is an EDM due to the semi-leptonic spin-dependent nucleon-electron tensor-pseudotensor (Ne-TPT) interaction [12]. This is due to the zero total electronic angular momentum J in the closed-shell atomic ground state, and therefore the atomic EDM depending on nuclear angular momentum only. The Ne-TPT interaction is also present in open-shell systems, but there the scalar-pseudoscalar nucleon-electron interaction is by far dominant for heavier nuclei due to its scaling with nucleon number.

Experimental upper bounds to the EDMs of closed-shell atoms may therefore be used to constrain the possible value of the fundamental Ne-TPT coupling parameter CT. Such experiments have been carried out in the past in particular on the Hg atom [13, 14] and the Ra atom [15, 16], among others [17]. These measurements are subject to continued improvements, and the same should hold true for the electronic-structure calculations required to interpret them in terms of fundamental (CP)-violating parameters.

In the present paper I focus on the Ne-TPT atomic interaction constants of interest for the EDM measurements on 199Hg and 225Ra. The specific aims of the present work are threefold: First, a relativistic correlated electronic-structure method that has been applied earlier to the calculation of atomic [18] and molecular [19] EDMs and P, T-odd enhancements is made available for the calculation of the Ne-TPT
interaction in both atomic and molecular systems. The corresponding theory is outlined in the following section of the paper, sec. II. Second, the approach is put to the test on $^{199}$Hg where results for the Ne-TPT interaction constant have been obtained earlier using Coupled Cluster methods [20, 21]. Third, predictions for the Ne-TPT interaction constant in $^{225}$Ra are made using highly-correlated atomic wavefunctions which are compared with present theory results for this atom [22]. All applications are discussed in section III.

II. THEORY

An atomic electric dipole moment (EDM) resulting solely from T-PT nucleon-electron interaction is defined as

$$d_a = R_T C_T$$

with $C_T$ the fundamental Ne-TPT coupling constant and $R_T$ the corresponding atomic interaction constant. The latter is determined in the framework of an effective field theory involving a neutral weak current between electrons and nucleons. This nucleon-electron tensor-pseudotensor interaction Hamiltonian has been given as [23]

$$\hat{H}_{Ne}^{T-PT} = i G_F \sqrt{2} 2 C_T \left( \gamma_e \cdot \sigma_N \right) \rho(r)$$

where $G_F$ is the Fermi constant, $\gamma$ is an electronic Dirac matrix, $\sigma_N = \langle \sigma_N \rangle_{\Psi_N} \frac{1}{I}$ with $\Psi_N$ a nuclear spinor, $\sigma_N$ a Pauli matrix, $I$ the nuclear spin, and $\rho(r)$ is the nuclear density at position $r$.

For convenience, the nuclear state is chosen as $|I, M_I = I\rangle$. From this it follows that $\langle I, M_I = I | (\sigma_N)_k | I, M_I = I \rangle = 0 \, \forall k \in \{1, 2\}$ where $k$ denotes cartesian components. Using the identity $\langle I, M_I = I | (\sigma_N)_3 | I, M_I = I \rangle = \langle \sigma_N \rangle_{\Psi_N}$ in a.u. the above Hamiltonian is rewritten as

$$\hat{H}_{Ne}^{T-PT} = i G_F \sqrt{2} 2 C_T \left( \gamma_e \right)_3 \langle \sigma_N \rangle_{\Psi_N} \rho(r).$$

where upper indices on four-tensors conventionally correspond to contravariant components.

The determination of the atomic EDM resulting from the corresponding T-PT interaction in first order in perturbation theory results calculation of the matrix element

$$M_{Ne}^{T-PT} = \langle \psi_e | (\gamma_e)^3 \rho(r) | \psi_e \rangle$$

where $\psi_e$ is the electronic wavefunction of the atomic state under consideration. The implementation of this matrix element has been carried out in a locally modified
version of the \textsc{dirac} program package \cite{24}, using the relation $(\gamma_e)^k = \gamma^0 \alpha_k = \beta \alpha_k$ where $\alpha, \beta$ are Dirac matrices.

The atomic EDM then results from the interaction constant

$$R_T = \sqrt{2} G_F \langle \sigma_N \rangle \Psi_N^T \langle \sigma_N \rangle \Psi_N$$

and Eq. (1).

\section{III. T-PT Interaction in $^{225}$Ra and $^{199}$Hg}

\subsection{A. Technical details}

Atomic basis sets of Gaussian functions are used, denoted valence quadruple-zeta (vQZ) and including all available polarizing and valence-correlating functions \cite{25, 26}. The complete sets amount to (38s,35p,24d,16f,3g) functions for Ra and (34s,30p,19d,13f,4g,2h) functions for Hg, respectively. Wavefunctions for the $^1S_0$ electronic ground state of the respective atoms are obtained through a closed-shell Hartree-Fock (HF) calculation using the Dirac-Coulomb Hamiltonian including the external electric field

$$\hat{H} = \hat{H}_{\text{Dirac-Coulomb}} + \hat{H}_{\text{Int-Dipole}}$$

$$= \sum_j c \alpha_j \cdot \mathbf{p}_j + \gamma_j c^2 + \frac{Z}{r_j} \mathbb{1}_4 + \sum_{j,k>j} \frac{1}{r_{jk}} \mathbb{1}_4 + \sum_j \mathbf{r}_j \cdot \mathbf{E}_{\text{ext}} \mathbb{1}_4 ,$$

where the indices $j,k$ run over $N$ electrons, $Z$ is the proton number ($N = Z$ for neutral atoms). Atomic units (a.u.) are used throughout ($e = m_0 = \hbar = 1$). This approach corresponds to what other authors \cite{22} call Random-Phase Approximation (RPA). The DCHF calculation is followed by linear expansion in the basis of Slater determinants formed by the occupied and virtual set of 4-spinors and diagonalization of the DC Hamiltonian including the external electric field in that basis (Configuration Interaction (CI) approach) \cite{27}. The resulting “correlated” wavefunctions $\psi_e$ – where the CI expansion coefficients are fully relaxed with respect to the external field – are then introduced into Eq. (4), and the resulting $\mathcal{P}$-odd expectation value gives the T-PT interaction constant via Eq. (5).

The nomenclature for CI models is defined as: S, D, T, etc. denotes Singles, Doubles, Triples etc. replacements with respect to the closed-shell DCHF determinant. The following number is the number of correlated electrons and encodes which occupied shells are included in the CI expansion. In the case of Hg we have $12 \equiv (5d,6s)$, $18 \equiv (5p,5d,6s)$, $32 \equiv (4f,5p,5d,6s)$, $34 \equiv (5s,4f,5p,5d,6s)$, $42 \equiv (4s,4p,5s,4f,5p,5d,6s)$, and $44 \equiv (4d,5s,4f,5p,5d,6s)$. In the case of Ra these are $10 \equiv (6s,6p,7s)$, $20 \equiv (5d,6s,6p,7s)$, $28 \equiv (5s,5p,5d,6s,6p,7s)$,
36 \equiv (4s, 4p, 5s, 5p, 6d, 6s, 7s), and 42 \equiv (4f, 5s, 5p, 6d, 6s, 7s). The notation type S8 SD36, as an example, means that the model SD36 has been approximated by omitting Double excitations from the (4s, 4p) shell.

The nuclear spin quantum number is \( I = 1/2 \) both for \(^{225}\text{Ra}\) and \(^{199}\text{Hg}\), respectively \[28\]. Atomic nuclei are described by Gaussian charge distributions \[29\] with exponents \( \zeta_{\text{Ra}} = 1.3101367628 \times 10^8 \) and \( \zeta_{\text{Hg}} = 1.4011788914 \times 10^8 \), respectively.

Atomic static dipole polarizabilities are obtained from fitting the total electronic energies using seven field points of strengths \( E_{\text{ext}} \in \{-1.2, -0.6, -0.3, 0.0, 0.3, 0.6, 1.2\} \times 10^{-4} \) a.u. For calculation of the T-PT interaction constant \( E_{\text{ext}} = 0.3 \times 10^{-4} \) a.u. and \( E_{\text{ext}} = 0.6 \times 10^{-4} \) a.u. for Hg and Ra, respectively.

**B. Results and discussion**

Results from a systematic study on Hg with different wavefunction models are compiled in Table I. For the T-PT interaction constant there is a general trend for absolute values, independent of basis set: Correlations among the valence electrons (5d and 6s) decreases \( R_T \) whereas inclusion of inner shells leads to an increase, the sole exception being the 5s shell which has a strong effect in the opposite direction. The net effect is an increase of about 5\% between RPA and SD34/50 in vTZ basis. Core-valence correlations among the inner (4s, 4p, 4d) electrons and valence and subvalence electrons adds another \( \approx 4\% \) to \( R_T \). To the contrary, replacements higher than Doubles (D) consistently decrease the T-PT interaction constant for all investigated shells. Up to Quadruple excitations from the valence (6s, 5d) shells have been considered in the model SDTQ12. The total effect of Triples and Quadruples for the considered atomic shells is a remarkable 18\%.

The final value for \( R_T \) is obtained from using the SD34/50 result in vTZ basis and by adding corrections to this value in the following manner:

\[
\Delta \rightarrow \Delta R_T = R_T(\text{vDZ}/S8, \text{SD42}/50) - R_T(\text{vDZ}/\text{SD34}/150) \\
+ R_T(\text{vDZ}/\text{S10, SD44}/50) - R_T(\text{vDZ}/\text{SD34}/150) \\
+ R_T(\text{vTZ}/\text{SDT12}/22) - R_T(\text{vTZ}/\text{SD12}/22) \\
+ R_T(\text{vDZ}/\text{SDTQ12}/22) - R_T(\text{vDZ}/\text{SDT12}/22) \\
+ R_T(\text{vDZ}/\text{SD12, SDT18}/22) - R_T(\text{vDZ}/\text{SD18}/22)
\]

\( \Delta R_T \) corrects for core-valence correlations from the (4s, 4p, 4d) shells and for higher excitations among the valence and the subvalence (5p) electrons.

The final value obtained in this way, \( \text{vTZ}/\text{SD34}/50 + \Delta R_T \), given in Table I lines up very well with the results of Singh et al. \[21\] (taken without the small Breit and QED corrections) and Latha et al. \[31\]. A conservative estimation of the uncertainty from atomic basis set, higher excitations, and inner-shell correlations yields a total
TABLE I. Ne-TPT interaction constant and static electric dipole polarizability for the Hg atom using different wavefunction models

| Model/virtual cutoff [a.u.] | α_d [a.u.] | R_T [10^{-20} \langle \sigma_N \rangle e cm] |
|-----------------------------|------------|------------------------------------------|
|                             | Basis set | Basis set |
|                             | vDZ vTZ   | vDZ vTZ |
| RPA/-                       |           |          |
| SD12/22                     | 44.5 45.5 | -4.70 -4.94 |
| SD18/22                     | 35.0 33.5 | -4.05 -4.25 |
| SD12,SDT18/22               | 30.7 34.2 | -5.52 -5.82 |
| SD32/50                     |           | -5.90   |
| SD34/22                     |           | -4.77 -5.16 |
| SD34/50                     | 30.0 34.8 | -4.95 -5.19 |
| S2,SD34/150                 |           | -4.97   |
| S8,SD42/50                  |           | -5.14   |
| S10,SD44/50                 |           | -5.00   |
| SDT12/22                    | 37.9 34.4 | -3.65 -3.71 |
| SDTQ12/22                   |           | -3.40   |
| vTZ/SD34/50 +Δ              | 35.7      | -4.43   |
| Singh et al.\footnote{a} CCSD$_p$T | 34.27 | -4.30 |
| Dzuba\footnote{b} RPA       | 44.9      |          |
| Latha et al.\footnote{c}    |           | -4.3    |
| Dzuba et al.\footnote{d}    |           | -5.1    |
| Experiment\footnote{e}      | 33.91     |          |

\footnote{a} Ref. \cite{21}
\footnote{b} Ref. \cite{30}
\footnote{c} Ref. \cite{31}
\footnote{d} Ref. \cite{22}
\footnote{e} Ref. \cite{32}

of 9% for $R_T$ by adding estimated individual uncertainties. The true uncertainty is likely to be significantly smaller because inner-shell effects and higher excitations generally act in opposite directions. This means that the result of Dzuba \textit{et al.} is outside of even the conservative uncertainty bar for the present result. The reason for this could be an incomplete treatment of higher excitations in the CI+MBPT approach of Dzuba \textit{et al.} since these lead to a large downward correction (on the absolute) of the T-PT interaction constant for atomic Hg.

For gauging the accuracy of the present electronic structure models the atomic static dipole polarizability is used for which experimental and other theory results...
are known. The RPA value of Dzuba (without correlations) is in excellent agreement with the present RPA value for $\alpha_d$ in Hg. However, and as expected, correlation effects are of major importance. As to be seen in Table II for the static electric dipole polarizability of Hg neither basis set effects nor electron correlation effects behave in a consistent manner, in contrast to those effects on $R_T$. It is, therefore, safer to derive the final value for $\alpha_d$ from the largest used basis set only. The correction is in this case calculated as follows:

$$\Delta \rightarrow \Delta \alpha_d = \alpha_d(\text{vTZ}/\text{SDT12}/22) - \alpha_d(\text{vTZ}/\text{SD12}/22)$$

The present final value of $\alpha_d = 35.7$ a.u. is more than 20% smaller than the RPA result and deviates from the experimental value by only about 5%. The final value for $R_T$ in Hg has been obtained using a similar computational protocol.

**TABLE II. Ne-TPT interaction constant for the Ra atom using different wavefunction models**

| Model/virtual cutoff [a.u.] | $R_T$ | $10^{-20} \langle \sigma_N \rangle$ e cm | Basis set |
|-----------------------------|-------|----------------------------------------|-----------|
|                             |       |                                        | vDZ       | vTZ       | vQZ       |
| RPA/-                       | -14.5 | -14.7                                  | -14.7     |
| SD10/23                     | -12.5 | -13.6                                  | -13.7     |
| SD10/50                     | -12.5 |                                        |           |
| SD20/23                     | -13.6 | -13.9                                  | -14.0     |
| SD28/23                     | -14.7 | -15.0                                  | -14.9     |
| SD28/50                     | -14.9 |                                        |           |
| S8_SD36/50                  | -15.4 |                                        |           |
| S14_SD42/50                 | -15.1 |                                        |           |
| SDT10/23                    | -11.3 | -13.1                                  | -13.2     |
| SDTQ10/23                   | -10.7 |                                        |           |
| vTZ/SD12/50 +$\Delta R_T$  |       |                                        | -15.0     |
| Dzuba et al.$^a$           |       |                                        | -18       |

$^a$ Ref. [22]

The general trends for the T-PT interaction constant in Ra, displayed in Table II, are qualitatively the same as in the Hg atom. Valence correlations and higher excitations than Doubles diminish $R_T$, inner-shell correlations increase $R_T$, on the absolute. However, in Ra a large basis set effect of nearly 16% on higher excitations is observed. In the mercury atom the corresponding basis set effect is less than 2%, considering only the change from vDZ to vTZ. For this reason the effect of Triples is evaluated with the vQZ basis set for Ra where it is only about a fourth of that effect.
with the vDZ basis. Accordingly, the effect of Quadruples will be overestimated in the vDZ basis, and this correction is, therefore, scaled to the expected value in vQZ basis.

The correction $\Delta R_T$ of the base value for $R_T$ in atomic Ra is obtained from

$$
\Delta R_T = R_T(vTZ/SD836/50) - R_T(vTZ/SD28/50) \\
+ R_T(vTZ/SD14/SD42/50) - R_T(vTZ/SD28/50) \\
+ R_T(vQZ/SDT10/23) - R_T(vQZ/SD10/23) \\
+ [R_T(vDZ/SDTQ10/23) - R_T(vDZ/SDT10/23)]_{\text{scaled to vQZ}}.
$$

The estimated uncertainty of the final result for $R_T$ in atomic Ra is around 8%, using the same approach as for the Hg atom. Again, the result of Dzuba et al. is larger than the upper bound to the present result.

IV. CONCLUSIONS

The present result for the NeTPT interaction constant can be combined with the recent atomic EDM measurement of the Argonne group on $^{225}$Ra of $|d_{225}^{Ra}| < 1.4 \times 10^{-23}$ ecm \(13\) to yield a limit on the $(CP)$-violating parameter $C_T$, supposing a single-source interpretation of the atomic measurement. From Eq. (1)

$$
|C_T| < \left| \frac{d^{225}_{Ra}}{R_T} \right| = 9.3 \times 10^{-5} \frac{1}{\langle \sigma_N \rangle} \tag{7}
$$

The determination of $\langle \sigma_N \rangle$ via a simple spherical shell model of the Ra nucleus, following Ref. \[22\], is not attempted here due to the known strong deformation of the $^{225}$Ra nucleus. However, it can be assumed that since $I(^{225}Ra) = 1/2$, $\langle \sigma_N \rangle$ is on the order of $\{0.1, \ldots, 1\}$. The resulting bound for the $(CP)$-odd parameter is then

$$
|C_T| < 10^{-3} \tag{8}
$$

This limit is still about seven orders of magnitude weaker than the corresponding limit from measurements \[13\] and calculations (see Table \[1\]) on atomic Hg. However, the envisaged experimental improvements on the Ra EDM measurement laid out in Ref. \[15\] hold the promise to close this gap in future work.

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