

Nuclear parity- and time-reversal-symmetry violation in the ^{201}HgH molecule

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Investigation of the nuclear magnetic quadrupole moment (MQM) is an excellent way to reveal the new physics in the hadron sector of matter. Therefore, we investigate the violation of parity (\mathcal{P}) and time-reversal (\mathcal{T}) invariance induced by the MQM of the ^{201}Hg nucleus in the HgH molecule, which has been proposed as a very promising candidate for the experimental search of the electric dipole moment of electron [M. G. Kozlov and A. Derevianko, *Phys. Rev. Lett.* **97**, 063001 (2006)]. We report the precise value of the molecular parameter, W_M , associated with the \mathcal{P} , \mathcal{T} -odd nuclear MQM-electron interaction in ^{201}HgH using the four-component relativistic coupled-cluster method. This parameter is required to interpret the experimental \mathcal{P} , \mathcal{T} -odd frequency shift in terms of the MQM of nuclei. Furthermore, the magnetic hyperfine structure (HFS) constants of the molecule are computed at the same level of theory. We also study the role of core-correlating functions and the virtual energy functions in the calculations of the HFS constant and W_M . The most reliable value of W_M in HgH is obtained as $3.22 \times 10^{33} \text{ Hz}/e \text{ cm}^2$ with an uncertainty of around 6%.

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I. INTRODUCTION

The magnetic quadrupole moment (MQM) of nuclei arises due to the simultaneous violations of parity (\mathcal{P}) and time-reversal (\mathcal{T}) symmetry [1]. The \mathcal{PT} violations beyond the standard model can provide the insight to explain the dominance of matter over the antimatter in the known universe [2]. Thus, in recent times, symmetry-violating physics beyond the standard model, also known as “new physics,” is able to draw the attention of physicists. In addition to the nuclear MQM [1,3,4], the other symmetry-violating properties such as the intrinsic electric dipole moment of electron (eEDM) [3] and nucleon (nEDM) [3], scalar-pseudoscalar (S-PS) nucleus-electron coupling [3], and the Schiff moment (SM) of a nucleus [3,5] can contribute to the permanent atomic and molecular electric dipole moment (EDM). Measurement of this EDM can explore the new physics.

The property of our interest in this work is the nuclear \mathcal{P} , \mathcal{T} -odd effect induced by the MQM of nuclei. The possible sources of the nuclear MQM are the nEDM [6] and the \mathcal{P} , \mathcal{T} -odd forces inside a nucleus [4]. However, the \mathcal{P} , \mathcal{T} -odd internucleon interaction can induce larger MQM than the nEDM [4]. It is noteworthy that the nuclear EDM is screened by the electrons in neutral atoms and molecules. That is why it has a negligible contribution to the atomic and molecular EDM, and it is not possible to directly measure the nuclear EDM. Usually, in such a system, the nuclear SM

is mainly responsible for the observable EDM. On the other hand, the magnetic interaction between the nuclear moment and electrons is not screened. Thus, the interaction of nuclear MQM with electrons can significantly contribute to the EDM of atoms and molecules. The nuclear MQM is significantly enhanced in heavy deformed nuclei [7] and the effects associated with the MQM only exist for the nuclei having spin $I > 1/2$ in paramagnetic systems. It has been found that the nuclear MQM can generate larger EDM in paramagnetic systems than the nuclear SM [4]. Hence, the \mathcal{P} , \mathcal{T} -odd interaction of the nuclear MQM with the gradient of the magnetic field produced by electrons in a heavy paramagnetic atom or molecule is very important to explore the \mathcal{P} , \mathcal{T} -odd hadronic physics. In recent times, many groups theoretically investigated this effect in various heavy polar diatomic molecules such as ThF^+ [8], TaN [8–10], ThO [8,11], HgF [8,12], HfF^+ [8,13], YbF [8], and BaF [8]. The knowledge of nuclear MQM can help for establishing new limits on the quantum chromodynamics \mathcal{CP} -odd parameter $\tilde{\Theta}$ (\mathcal{C} means the charge conjugation symmetry), the EDM of u and d quarks, $d_{u,d}$, chromo-EDMs, $\tilde{d}_{u,d}$, and the nEDM [8,11]. Physicists are now taking interest in the experimental search for the nuclear MQM in the molecular system. But for the interpretation of the experimental data in terms of nuclear MQM, the accurate value of the MQM interaction constant (W_M) is required. However, the value of W_M cannot be measured from any experiment and, hence, it has to be calculated using an accurate *ab initio* method. It is worth mentioning here that the precise calculation of the “atom-in-compound” (AIC) [14] properties such as W_M and the magnetic hyperfine structure (HFS) interaction constant is very sensitive to the accuracy of the wave function near the core region of the heavy atom. Thus, an *ab initio* method, which can incorporate both the relativistic and correlation

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effects of electrons in an intertwined manner, must be used to calculate these AIC properties. The reliable way to check the accuracy of the wave function (which can be used for the calculation of W_M) is to compare the theoretically calculated HFS constant with the available experimental value.

It is a well-known fact that a molecule with small rotational constant and large dipole moment is easily polarizable in a spectroscopic experiment. Notwithstanding the large value of rotational constant and small dipole moment of HgH, Kozlov and Derevianko recently suggested that it can be polarized easily in a matrix isolated solid-state nonspectroscopic experiment to measure the eEDM [15]. The theoretical study performed by Sasmal *et al.* [16] also proposed HgH as a potential candidate for eEDM experiments. Kozlov [17] and Sunaga *et al.* [18] also reported the \mathcal{P} , \mathcal{T} -odd S-PS nucleus-electron interaction constant and effective electric field of this molecule, respectively. Recently, Geddes *et al.* [19] studied the nuclear-spin-dependent parity-violation effects in the HgH molecule. However, the nuclear \mathcal{P} , \mathcal{T} -odd effect induced by the nuclear MQM in HgH has not been investigated to date. Thus, the aim of this paper is to provide the precise value of the \mathcal{P} , \mathcal{T} -odd nuclear MQM interaction constant, W_M , of ^{201}HgH in the ground electronic configuration ($^2\Sigma$) state using the expectation-value and the Z-vector methods in a relativistic coupled-cluster (CC) framework. The HFS constant of the said molecule is also computed at the same level of theory. The effects of basis sets, core-correlating functions, and virtual spinors on the computed properties of HgH are also discussed in this work. The highly correlated relativistic *ab initio* study of the nuclear \mathcal{P} , \mathcal{T} -odd MQM-electron interaction in the HgH molecule would be important in the search for the hadronic \mathcal{PT} -violating physics. The structure of the paper is as follows. The theory of the calculated properties and the employed methods (i.e., the expectation-value and the Z-vector approaches in the domain of the relativistic CC method) is discussed in Sec. II. Computational details are given in Sec. III. The findings of the our study are presented as well as discussed in Sec. IV, and then concluding remarks are given in Sec. V. Atomic units are used explicitly in the paper unless stated.

II. THEORY

The Hamiltonian of the interaction of nuclear MQM with the magnetic field produced by electrons is given by [13,20,21]

$$H^{\text{MQM}} = -\frac{M}{2I(2I-1)} T_{ik} \frac{3}{2} \frac{[\vec{\alpha} \times \vec{r}]_i r_k}{r^5}, \quad (1)$$

where M is known as the nuclear MQM with components

$$M_{ik} = \frac{3M}{2I(2I-1)} T_{ik}, \quad (2)$$

$$T_{ik} = I_i I_k + I_k I_i - \frac{2}{3} \delta_{ik} I(I+1). \quad (3)$$

As shown in Ref. [4], in the subspace of $\pm\Omega$, Eq. (1) becomes

$$H_{\text{eff}}^{\text{MQM}} = -\frac{W_M M}{2I(2I-1)} \vec{S}' \hat{T} \vec{n}, \quad (4)$$

where \vec{n} is the unit vector along the internuclear axis (z axis) of HgH, and \vec{S}' is known as the effective electron spin. If $I_z = I$ along \vec{n} , then $T_{zz} = \frac{I}{3}(4I-2)$ and $M_{zz} = M$. In such a case, the energy shift due to the nuclear MQM is $-\frac{1}{3}W_M M S'_z$ or $-\frac{1}{3}W_M M \Omega$. Ω is the projection of total electron angular momentum on the z axis. The value of Ω is 1/2 for the ground electronic state ($^2\Sigma$) of HgH. However, the nuclear spin is not quantized along the internuclear axis and this leads to the fact that the expression $-\frac{1}{3}W_M M \Omega$ provides only the order of the magnitude of real energy shift due to the nuclear MQM interaction. It is worth mentioning that Petrov *et al.* [22] recently discussed the MQM energy shift and its dependence on the hyperfine sublevel, which helps to distinguish the MQM shift from the shifts due to the electron EDM and the scalar-pseudoscalar nucleus-electron coupling.

Finally, W_M is defined by the following matrix element:

$$W_M = \left| \frac{3}{2\Omega} \langle \Psi_\Omega | \sum_i^n \left(\frac{\vec{\alpha}_i \times \vec{r}_i}{r_i^5} \right)_z r_z | \Psi_\Omega \rangle \right|. \quad (5)$$

Here Ψ_Ω is the wave function of the Ω state and n is the total number of electrons. The matrix element of the operator in Eq. (5) is heavily concentrated near the nuclear region of the heavy atom. This means W_M highly depends on the molecular wave function near the Hg nucleus. As the MQM of the nucleus is a second-rank tensor, the dominant contribution to the MQM interaction parameter comes from the matrix element between the $s_{1/2}$ and $p_{3/2}$ orbitals of the Hg atom.

The parallel (A_{\parallel}) and perpendicular (A_{\perp}) components of the magnetic hyperfine structure constant of a diatomic molecule can be defined as

$$A_{\parallel(\perp)} = \frac{\vec{\mu}_k}{I\Omega} \langle \Psi_\Omega | \sum_i^n \left(\frac{\vec{\alpha}_i \times \vec{r}_i}{r_i^3} \right)_{z(x/y)} | \Psi_{\Omega(-\Omega)} \rangle, \quad (6)$$

where $\vec{\mu}_k$ is nothing but the magnetic moment of the nucleus k .

The relativistic coupled-cluster singles and doubles (CCSD) wave function is used to calculate the properties defined in Eqs. (5) and (6). The form of the wave function is $|\Psi_{cc}\rangle = e^T |\Phi_0\rangle$, where Φ_0 is the four-component Dirac-Hartree-Fock (DHF) determinant and $T = T_1 + T_2$, is the excitation operator. The operator is defined as

$$T_m = \frac{1}{(m!)^2} \sum_{ij\dots ab\dots} t_{ij\dots}^{ab\dots} a_a^\dagger a_b^\dagger \dots a_j a_i, \quad (7)$$

Here i, j (a, b) indices refer to the hole (particle), a_p^\dagger (a_q) is the creation (annihilation) operator, and $t_{ij\dots}^{ab\dots}$ is the cluster amplitude of T_m . The amplitudes of T_1 and T_2 are obtained from the following equations:

$$\langle \Phi_i^a | (H_N e^T)_c | \Phi_0 \rangle = 0, \quad \langle \Phi_{ij}^{ab} | (H_N e^T)_c | \Phi_0 \rangle = 0, \quad (8)$$

where H_N is the normal ordered Dirac-Coulomb Hamiltonian and the subscript c suggests that the contracted terms between H_N and T are fully connected.

Now, one can calculate the desired properties using either the expectation-value or energy-derivative approach. The Z-vector method [23,24] is a well-known energy-derivative approach. Sasmal *et al.* [25] recently implemented the Z-vector method within the four-component relativistic CCSD

TABLE I. Basis and cutoffs for virtual spinors used in our calculation.

Name	Nature	Basis		Virtual	
		Hg	H	Cutoff (a.u.)	Spinor
A	TZ	dyall.cv3z	cc-pCVTZ	500	369
B	TZ	dyall.ae3z	cc-pCVTZ	500	387
C	TZ	dyall.cv3z	cc-pCVTZ	1000	385
D	TZ	dyall.ae3z	cc-pCVTZ	1000	403
E	QZ	dyall.cv4z	cc-pCVQZ	500	477

framework for precise calculation of various AIC properties of molecules. The Z -vector energy derivative (i.e., desired property) is evaluated by

$$\Delta E' = \langle \Phi_0 | (O_N e^T)_c | \Phi_0 \rangle + \langle \Phi_0 | [\Lambda (O_N e^T)_c] | \Phi_0 \rangle. \quad (9)$$

Here, O_N is the property operator and Λ is known as the deexcitation operator (for more details see Refs. [23–25]). On the other hand, the expectation value of the property operator (O_N) of interest can be obtained using the following expression [26,27]:

$$\begin{aligned} \langle O_N \rangle &= \frac{\langle \Psi_{cc} | O_N | \Psi_{cc} \rangle}{\langle \Psi_{cc} | \Psi_{cc} \rangle} = \frac{\langle \Phi_0 e^{T^\dagger} | O_N | e^T \Phi_0 \rangle}{\langle \Phi_0 | e^{T^\dagger} e^T | \Phi_0 \rangle} \\ &= \langle \Phi_0 | (e^{T^\dagger} O_N e^T)_c | \Phi_0 \rangle. \end{aligned} \quad (10)$$

Although the above series is nonterminating, we adopt the linear approximation to get the expectation value, because the dominant contribution comes from the linear terms of the above expression (see Ref. [28]). The energy derivative in the nonvariational coupled-cluster method is nothing but the corresponding expectation value plus some other terms [24]. Thus, the property value obtained by the energy-derivative method is closer to that obtained by the full configuration interaction (FCI) method than the expectation-value approach. Also, the manual truncation considering only the linear terms in the expectation-value approach may yield some additional error. This means the Z vector is a better method than the expectation-value approach.

III. COMPUTATIONAL DETAILS

We use the locally modified version of DIRAC10 [29] to solve the DHF equation and to generate the one-body, two-body, and one-electron property integrals. The finite nucleus

described by the Gaussian charge distribution is considered in our calculation. The properties of interest are calculated using the locally developed expectation-value and Z -vector code. We consider the bond length of HgH as 1.766 Å [30]. We have used the following basis sets: in the triple-zeta (TZ) basis, dyall.cv3z [31] and dyall.ae3z [32] for Hg, and cc-pCVTZ [33] for H; in the quadruple-zeta (QZ) basis, dyall.cv4z [31] for Hg, and cc-pCVQZ [33] basis for H. Moreover, the double-zeta basis set (dyall.cv2z [31] for Hg, cc-pCVDZ [33] for H) is also used to see the effects of the virtual spinors in our calculations. None of the occupied spinors is frozen in our calculations. However, we have excluded the virtual functions having energy higher than a cutoff value. The details are given in Table I.

IV. RESULTS AND DISCUSSION

In Table II, we present the parallel and perpendicular components of the HFS coupling constant along with the nuclear MQM interaction parameter of ^{201}Hg in the HgH molecule using the expectation-value and the Z -vector methods. In the same table, we also compare our HFS results with the available experimental values [34]. It is clear from Table II that the expectation-value and the Z -vector results are in good agreement with the available experimental values. The HFS values gradually increase with the use of higher basis sets and higher cutoffs for the virtual spinors. This is because the addition of either higher angular momentum basis functions or higher virtual energy functions improves the configuration space. On the other hand, the role of core-correlating functions in our calculations can be understood by comparing the results obtained using the dyall.cvNz and dyall.aeNz (i.e., A with B and C with D) basis sets. This is because the dyall.aeNz basis contains some extra core-correlating basis functions, which is lacking in the corresponding dyall.cvNz basis. In Ref. [35], it was shown that the core-correlating functions can play a crucial role in the explicit treatment of the core polarization for the precise calculation of the HFS constants of atoms. However, in the present work, the contribution of the core-correlating functions to the HFS values is around 0.01%.

The values of W_M obtained using the expectation-value method in different basis sets varies from 3.17 to 3.19 in the units of 10^{33} Hz/e cm². On the other hand, the values of the same parameter calculated using the Z -vector method in those basis sets varies from 3.21 to 3.23 in the same units. As the Z -vector approach is a better method than the expectation-value approach in terms of accuracy, we consider

TABLE II. Magnetic HFS constants and the nuclear MQM interaction parameter (W_M) of ^{201}Hg in HgH (Expt. = experiment, Expect. = expectation value).

Basis	A_{\parallel} (MHz)			A_{\perp} (MHz)			W_M (10^{33} Hz/e cm ²)	
	Expect.	Z vector	Expt.	Expect.	Z vector	Expt.	Expect.	Z vector
A	−2865.9	−3089.9	−2980(40) (in	−2161.3	−2393.0	−2380(30) (in	3.17	3.21
B	−2866.4	−3090.3	Ar matrix) [34]	−2161.6	−2393.2	Ar matrix) [34]	3.17	3.21
C	−2875.6	−3099.6		−2171.1	−2402.8		3.19	3.23
D	−2876.1	−3099.9	−2875(15) (in	−2171.4	−2402.9	−2275(10) (in	3.19	3.23
E	−2896.1	−3115.7	Ne matrix) [34]	−2200.6	−2427.1	Ne matrix) [34]	3.18	3.22

TABLE III. Molecular parameter W_M (in 10^{33} Hz/e cm²) for the heavy nucleus in various molecules.

Molecule	State	W_M
²⁰¹ HgH (This work)	$^2\Sigma_{1/2}$	3.22
²⁰¹ HgF [12]	$^2\Sigma_{1/2}$	3.59
^{177,179} HfF ⁺ [8]	$^3\Delta_1$	0.50
²²⁹ ThF ⁺ [8]	$^3\Delta_1$	1.70
²²⁹ ThO [8]	$^3\Delta_1$	1.90
¹⁸¹ TaN [9]	$^3\Delta_1$	0.74

3.22×10^{33} Hz/e cm², which is calculated using the E basis (QZ, cutoff = 500 a.u.), as the most reliable value of W_M in the present work. Thus, for the maximal nuclear spin projection along the molecular axis of HgH, the corresponding MQM energy shift would be $|\frac{1}{3}W_M M\Omega| = 0.536666667M \times 10^{33}$ Hz/e cm², where M is the MQM of ²⁰¹Hg nucleus. Our reported value of W_M in HgH is close to that in the HgF molecule, and is 6.5, 1.9, 1.7, and 4.3 times larger than that in HfF⁺, ThF⁺, ThO, and TaN, respectively (see Table III). Thus, the molecular parameter of HgH for the MQM interaction is significantly large, which implies that the interaction of the MQM of the ²⁰¹Hg nucleus with the magnetic field produced by the electron could be significant to induce a permanent EDM in the molecule. However, the energy shift due to the nuclear MQM-electron interaction also depends on the MQM of the nuclei. The nuclear quadrupole deformation enhances the nuclear MQM and this enhancement effect can be studied by *ab initio* nuclear structure calculation. But the nuclear structure calculations of the same are beyond the scope of our present work. Nevertheless, we believe that the contribution of the nuclear MQM interaction to the molecular EDM of HgH could be useful for the experimental search of the \mathcal{P} , \mathcal{T} -violating physics. Furthermore, the HgH molecule exhibits the quality of a potential candidate for eEDM search in nonspectroscopic solid-state experiments [15]. The molecule can be trapped in a cold matrix of inert-gas (Ar) atoms with a significant maximal number density due to its small dipole moment. In this proposed experiment, the authors of Ref. [15] argued that it has the potential of improving the present eEDM limit by at least one order of magnitude. Therefore, in addition to the eEDM, the nuclear MQM interaction in the ²⁰¹HgH molecule can also contribute to the \mathcal{P} , \mathcal{T} -odd frequency shift in the experiment. Thus, the investigated HgH molecule with stable isotope ²⁰¹Hg ($I = 3/2$) can probably be one of the candidates in search of the nuclear \mathcal{P} , \mathcal{T} -violating physics beyond the standard model.

The possible errors in our calculation may arise due to the following reasons: (i) exclusion of Breit and QED effects, (ii) missing higher-order electron correlation, (iii) basis set incompleteness, and (iv) restriction of correlation space. The error due to the exclusion of the Breit and QED effects is expected to be very small as the AIC properties are not very sensitive to these effects [36,37]. It is found that this error can be 0.5–1.0% [38–40]. The uncertainty that arises from the exclusion of the higher-order correlation effects can be assessed by comparing our values with the results obtained by the CCSDT method (where T means triple excitation) or

TABLE IV. Contribution of virtual spinors in our calculations. Basis used: dyall.cv2z for Hg and cc-pCVDZ for H (Expect. = expectation value).

Virtual		$A_{ }$ (MHz)		W_M (10^{33} Hz/e cm ²)	
Cutoff (a.u.)	Spinor	Expect.	Z vector	Expect.	Z vector
50	143	−2660.0	−2878.6	3.00	3.05
500	231	−2729.1	−2945.7	3.09	3.13
1000	239	−2742.5	−2959.0	3.11	3.15
No cutoff	355	−2762.2	−2978.7	3.13	3.17

the FCI method. But these calculations for the HgH molecule are extremely expensive and are just impossible to perform in the scope of the present work. Nevertheless, from our experience we expect an uncertainty of 3.0–3.5% due to the missing higher-order correlation effects in our calculation. On the other hand, the error due to the basis-set incompleteness can be estimated by comparing our results obtained with the A (TZ) and E (QZ) basis sets. It is seen from Table II that the basis-set incompleteness can yield an error of 0.3% in the W_M and 1.0–1.5% for the HFS constant. In other words, the contribution of the higher angular momentum basis functions to the HFS constant is more prominent than that to the MQM interaction parameter. Furthermore, the error caused by the restriction of correlation space can be assessed by comparing the property value at the cutoff of 500 a.u. for the virtual energy functions with that without any cutoff. We perform a series of calculations using the DZ basis (dyall.cv2z for Hg and cc-pCVDZ for H) at different cutoffs for virtual spinors and present the results in Table IV. From this table, it is seen that the virtual functions with energy higher than 500 a.u. contribute only 0.04 and 33 units, respectively, to the MQM interaction coefficient and the HFS constant. That means the error due to the restriction of correlation space is around 1.3% and 1.1% for the W_M and the HFS constant, respectively. It is noteworthy that the trends of the W_M and the HFS constant with the cutoffs for virtual spinors at a given basis set are found to be almost the same. On the contrary, our results are free from the error caused by the core-polarization effect because we have explicitly correlated all the electrons in our calculations. Thus, considering all the possible sources of error, we argue that the uncertainty in our most reliable result of W_M is around 6%.

It is well known that the accurate measurement of nuclear MQM can establish a new limit on the EDM of nucleons, quantum chromodynamics \mathcal{CP} -odd parameter, and EDM and chromo-EDM of u and d quarks, and that the precise value of W_M is necessary to measure the MQM from the experiment. Also, the electron correlation effects and the effect of relativistic motion of electrons play a significant role in the precise calculation of W_M of heavy molecules. We have employed two analytical methods (expectation value and Z vector) in the four-component relativistic CC framework, which incorporate both the relativistic and correlation effects of electrons in an intertwined manner to calculate the symmetry-violating nuclear MQM interaction constant in the HgH molecule. All the electrons are explicitly correlated and a sufficiently large relativistic basis is used in our calculation. Thus, the value

of W_M reported by us is expected to be quite reliable and accurate. This is evident from the observation that the HFS constant of HgH calculated in the present work at the same level of theory is in good agreement with the experimental value. Therefore, we argue that the present investigation of the symmetry-violating interaction induced by the nuclear MQM is important to explore the new physics in the hadron sector of matter using a paramagnetic molecular system.

V. CONCLUSION

In summary, we perform the precise relativistic coupled-cluster calculation of the parity- and time-reversal-symmetry-violating nuclear magnetic quadrupole moment interaction constant W_M in the ^{201}HgH molecule. Our most reliable value

of W_M is $3.22 \times 10^{33} \text{ Hz}/e \text{ cm}^2$, which is significantly large. Thus, ^{201}HgH exhibits the possibility to be a candidate for the experimental search of new physics in the hadron sector. The estimated uncertainty associated with our reported value is about 6%. Our study also infers that the higher-energy virtual functions play an important role in the calculations of the AIC properties of HgH.

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