Enhanced effect of CP-violating nuclear magnetic quadrupole moment in a HfF$^+$ molecule

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The HfF$^+$ cation is a very promising system to use in the search for the electron electric dipole moment (EDM), and a corresponding experiment is carried out by JILA group [H. Loh, K. C. Cossel, M. C. Grau, K.-K. Ni, E. R. Meyer, J. L. Bohn, J. Ye, and E. A. Cornell, Science **342**, 1220 (2013); K.-K. Ni, H. Loh, M. Grau, K. C. Cossel, J. Ye, and E. A. Cornell, J. Mol. Spectrosc. **300**, 12 (2014). Here we theoretically investigate the cation to search for another effect which violates time-reversal (T) and spatial parity (P) symmetries—the nuclear magnetic quadrupole moment (MQM) interaction with electrons. We report an accurate *ab initio* relativistic electronic structure calculations of the molecular parameter $W_M = 0.494 \frac{10^{33}\,\mathrm{Hz}}{e\,\mathrm{cm}^2}$ that is required to interpret the experimental data in terms of the MQM of the Hf nucleus. For this we have implemented and applied the combined Dirac-Coulomb(-Gaunt) and relativistic effective core potential approaches to treat electron correlation effects from all of the electrons and to take into account high-order correlation effects using the coupled cluster method with single, double, triple and noniterative quadruple cluster amplitudes. We discuss interpretation of the MQM effect in terms of the strength constants of T,P-odd nuclear forces, proton and neutron EDMs, the QCD parameter θ, and quark chromo-EDMs.

I. INTRODUCTION

The HfF$^+$ cation is a very promising system to use in the search for the electron electric dipole moment (eEDM) [1–8] (see also Refs. [9–15]). At present JILA group prepares the ion trap experiment on the cation [2,16]. In contrast to the ^{232}ThO molecule which was used to obtain the best current limit on the eEDM [10], one can use the available stable isotope of Hf, e.g., ^{177}Hf, to search for the magnetic quadrupole moment of the ^{177}Hf nucleus in the ^{177}HfF$^+$ cation [11]. This is because the ^{177}Hf nucleus possesses a nuclear spin of $I > 1/2$ [17–19] while ^{232}Th has $I = 0$.

As was shown in Ref. [19], MQM can be strongly enhanced due to the collective nuclear effect. Below we study this effect for the case of the Hf nucleus.

The electronic structure of the HfF$^+$ cation has been previously studied in Refs. [1,3–5] for the eEDM problems—calculation of the effective electric field (E_{eff}) which is required to interpret the experimental energy shift in terms of the eEDM. In Refs. [3,4] the two-step relativistic effective core potential approach was used. In Ref. [5] a direct approach within the Dirac-Coulomb Hamiltonian was applied. In the present paper we follow the combined Dirac-Coulomb(-Gaunt) and two-step relativistic pseudopotential scheme [20] to study the electronic part of the problem of calculation of the interaction between the MQM of the Hf nucleus and electrons of HfF$^+$ in the first excited $^3\Delta_1$ state of the HfF$^+$ cation. This scheme allows one to treat all of the important effects including correlation of the inner-core electrons.

II. THEORY

Qualitatively the effect under consideration corresponds to the interaction of the nuclear magnetic quadrupole moment

with the gradient of the magnetic field produced by electrons. This is the time (T) reversal and spatial parity (P) violating interaction which mixes states of opposite parity in atoms and molecules [17,18]. The relativistic Hamiltonian of the interaction is given by the following expression [17,21,22]:

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

where Einstein's summation convention is implied, $\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}$ are the 4×4 Dirac matrices, $\boldsymbol{r}$ is the displacement of the electron from the Hf nucleus, $\boldsymbol{I}$ is the nuclear spin, M is the nuclear MQM,

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

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

In the subspace of $\pm\Omega$ states ($\Omega = \langle\Psi|\boldsymbol{J}\cdot\boldsymbol{n}|\Psi\rangle$, $\boldsymbol{J}$ is the total electronic momentum and Ψ is the *electronic* wave function for the considered $^3\Delta_1$ state of HfF$^+$), expression (1) is reduced to the following effective molecular Hamiltonian [17]:

$$H_{\mathrm{eff}}^{\mathrm{MQM}} = -\frac{W_M M}{2I(2I-1)}S'\hat{\boldsymbol{T}}\mathbf{n}, \tag{4}$$

where $\mathbf{n}$ is the unit vector along the molecular axis ζ directed from Hf to F, and S' is the effective electron spin [23] defined by the following equations: $\mathbf{S}'_\zeta|\Omega\rangle = \Omega|\Omega>$, $\mathbf{S}'_\pm|\Omega = \pm1\rangle = 0$ [21,24], and $S = |\Omega| = 1$. The W_M parameter is defined by the following equation:

$$W_M = \frac{3}{2\Omega}\langle\Psi|\sum_i\left(\frac{\boldsymbol{\alpha}_i\times\boldsymbol{r}_i}{r_i^5}\right)_\zeta r_\zeta|\Psi\rangle. \tag{5}$$

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As was shown in Ref. [25] for a completely polarized molecule the energy shift due to MQM interaction is

$$\delta_M(J,F) = (-1)^{I+F} C(J,F) M W_M \Omega, \qquad (6)$$

$$C(J,F) = \frac{(2J+1)}{2} \frac{\begin{pmatrix} J & 2 & J \\ -\Omega & 0 & \Omega \end{pmatrix}}{\begin{pmatrix} I & 2 & I \\ -I & 0 & I \end{pmatrix}} \begin{Bmatrix} J & I & F \\ I & J & 2 \end{Bmatrix}, \qquad (7)$$

where $(...)$ means elements with $3j$ symbols and $\{...\}$ are those with $6j$ symbols [26], F is the total angular momentum, and J is the number of the rotational level. Note that δ_M depends on J and F quantum numbers. Moreover, $H_{\text{eff}}^{\text{MQM}}$ has nonzero off-diagonal matrix elements on the J quantum number (between different rotational levels). This should be taken into account when mixing of different rotational levels becomes significant. In Eq. (6) this effect is neglected. For ^{177}HfF$^+$ $(I = 7/2)$ and the ground rotational level $J = 1$, Eq. (6) gives MQM energy shifts, $|\delta(J,F)|$, equal to $0.107 W_M M$, $0.143 W_M M$, and $0.05 W_M M$ for $F = 5/2, 7/2$, and $9/2$, correspondingly.

III. CALCULATION OF THE NUCLEAR MAGNETIC QUADRUPOLE MOMENT

The angular momentum I of a spherical nucleus is determined by a valence nucleon. In the single-valence-nucleon model the nuclear MQM is given by the following expression:

$$M = [d - 2 \times 10^{-21} \eta(\mu - q)(e\,\text{cm})]\lambda_p(2I-1)t_I, \qquad (8)$$

where $t_I = 1$ for $I = l + 1/2$ and $t_I = -I/(I+1)$ for $I = l - 1/2$, I and l are the total and orbital angular momenta of a valence nucleon, η is the dimensionless strength constant of the T,P-odd nuclear potential $\eta G/(2^{3/2} m_p)(\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} \rho)$ acting on the valence nucleon, ρ is the total nucleon number density, the nucleon magnetic moments are $\mu_p = 2.79$ for valence protons and $\mu_n = -1.91$ for valence neutrons, $q_p = 1$ and $q_n = 0$, and $\lambda_p = \hbar/m_p c = 2.1 \times 10^{-14}$ cm. The contribution of the valence nucleon EDM d was calculated in Ref. [18], the contribution of the T,P-odd nuclear forces was calculated in Ref. [17].

Using a natural assumption that in any model of CP violation the π-meson exchange gives significant contributions it was concluded in Ref. [17] that the contribution of the T,P-odd nuclear forces to any T,P-odd nuclear moment is 1–2 orders of magnitude larger than the contribution of the nucleon EDM [17].

In a deformed nucleus the MQM in the "frozen" frame (rotating together with a nucleus) may be estimated using the following formula [19]:

$$M_{zz}^{\text{nucl}} = \sum M_{zz}^{\text{single}}(I,I_z,l)n(I,I_z,l), \qquad (9)$$

where the sum goes over occupied orbitals, $M_{zz}^{\text{single}}(I,I_z,l)$ is given by Eqs. (8) and (2), $T_{zz} = 2I_z^2 - \frac{2}{3}I(I+1)$, and $n(I,I_z,l)$ are the orbital occupation numbers, which may be found in Ref. [27]. The sum over a complete shell gives zero; therefore, for shells more than half filled, it is convenient to use hole numbers in place of particle numbers, using the relation $M_{zz}^{\text{single}}(\text{hole}) = -M_{zz}^{\text{single}}(\text{particle})$.

The nucleus ^{177}Hf has the following occupation numbers: 13 neutron holes in the orbitals $[\bar{l}_I, I_z] = [\bar{f}_{7/2}, -7/2]$,

$[\bar{l}_{13/2}, \pm 13/2, \pm 11/2, \pm 9/2]$, $[\bar{h}_{9/2}, \pm 9/2, \pm 7/2]$, and $[\bar{p}_{3/2}, \pm 3/2]$, and 8 proton holes in the orbitals $[\bar{d}_{3/2}, \pm 3/2]$, $[\bar{d}_{5/2}, \pm 5/2]$, and $[\bar{h}_{11/2}, \pm 11/2, \pm 9/2]$.

The MQM in the laboratory frame, $M \equiv M_{\text{lab}}$, can be expressed via the MQM in the rotating frame (9):

$$M^{\text{lab}} = \frac{I(2I-1)}{(I+1)(2I+3)} M_{zz}^{\text{nucl}}$$

$$= (1.5\eta_p - 1.1\eta_n) \times 10^{-33}(e\,\text{cm}^2)$$

$$- (4.0d_p + 2.9d_n) \times 10^{-13}\text{cm}, \qquad (10)$$

where $I = 7/2$ is the nuclear spin of ^{177}Hf.

The T,P-odd nuclear forces are dominated by the π_0-meson exchange [17]. Therefore, we may express the strength constants via strong πNN coupling constant $g = 13.6$ and T,P-odd πNN coupling constants corresponding to the isospin channels $T = 0, 1$, and 2: $\eta_n = -\eta_p = 5 \times 10^6 g(\bar{g}_1 + 0.4\bar{g}_2 - 0.2\bar{g}_0)$ (see details in Ref. [25]). As a result, we obtain

$$M(g) = -[g(\bar{g}_1 + 0.4\bar{g}_2 - 0.2\bar{g}_0) \times 1.0 \times 10^{-26} e\,\text{cm}^2. \qquad (11)$$

Possible CP violation in the strong interaction sector is described by the CP-violation parameter $\tilde{\theta}$. According to Ref. [28], $g\bar{g}_0 = -0.37\tilde{\theta}$. This gives the following value of the MQM for ^{177}Hf:

$$M(\theta) = -7 \times 10^{-28}\tilde{\theta} e\,\text{cm}^2. \qquad (12)$$

Almost the same final results for $M(\theta)$ can be obtained by using recently calculated relations of g_0 and g_1 constants by using lattice-QCD data for the proton-neutron mass splitting [29] which give updated values of gg_0: gg_0 is about twice smaller than the value obtained in Ref. [28] but an accounting of gg_1 [29,30] [which was omitted in Eq. (12)] gives additional contribution and the very close final value of $M(\theta)$.

Finally, we can express the MQM in terms of the quark chromo-EDMs $\tilde{d}_u$ and $\tilde{d}_d$ using the relations $g\bar{g}_1 = 4 \times 10^{15}(\tilde{d}_u - \tilde{d}_d)/$cm and $g\bar{g}_0 = 0.8 \times 10^{15}(\tilde{d}_u + \tilde{d}_n)/$cm [31]:

$$M(\tilde{d}) = -4 \times 10^{-11}(\tilde{d}_u - \tilde{d}_d)e\,\text{cm}. \qquad (13)$$

The contributions of d_p and d_n to the MQM in Eqs. (11)–(13) are from 1 to 2 orders of magnitude smaller than the contributions of the nucleon T,P-odd interactions.

IV. ELECTRONIC STRUCTURE CALCULATION DETAILS

It follows from Eq. (5) that the W_M parameter is mainly determined by the behavior of the electronic wave function in the region close to the heavy-atom nucleus. We call such parameters the atoms-in-compounds characteristics or properties [32–34]. Other examples are the hyperfine structure interaction constants, effective electric field, chemical shifts, etc. To compute such parameters we have previously developed the two-step method [32,35,36] which allows us to avoid direct four-component relativistic treatment. In the first stage, one considers the valence (and outer-core) part of the molecular wave function within the generalized relativistic effective core potential (GRECP) method [37–39]. The inner-core electrons are excluded from the explicit treatment. The feature of this stage is that the valence wave functions (spinors) are

smoothed in the spatial inner-core region of a considered heavy atom. This leads to considerable computational savings. Some technical advantage is that one can also use very compact contracted basis sets [20,40]. This is of crucial importance to treat high-order correlation effects. Besides, one can exclude the spin-orbit term of the GRECP operator and consider a scalar-relativistic approximation with a good nonrelativistic symmetry. Due to the corresponding savings one can use very large basis sets to consider basis set corrections and analyze their saturation. At the second step, one uses the nonvariational procedure developed in Refs. [32,35,36,41] to restore the correct four-component behavior of the valence wave function in the spatial core region of a heavy atom. The procedure is based on a proportionality of the valence and low-lying virtual spinors in the inner-core regions of heavy atoms. The procedure has been recently extended to consider not only the atomic and molecular systems but also three-dimensional periodic structures (crystals) in Ref. [42]. The GRECP and the restoration procedure were also successfully used for precise investigation of different diatomics [7,32,43–52]. The two-step method allows one to consider high-order correlation effects and large basis sets with rather modest requirements to computer resources in comparison to four-component approaches. However, some uncertainty remains due to the impossibility to consider the full version of the GRECP operator in the currently available codes and neglect of the inner-core correlation effects. In Refs. [20,53] we suggested to combine the two-step approach and the direct relativistic Dirac-Coulomb(-Gaunt) approach to take advantages of both approaches.

Computational scheme of the molecular W_M parameter (5) assumes evaluation of the following contributions: (i) the main correlation contributions within the 52-electron four-component Dirac-Coulomb coupled cluster with single, double, and noniterative triple cluster amplitudes [CCSD(T)] theory; (ii) the inner-core correlation contributions; (iii) correction on inclusion of the Gaunt interaction; (iv) the contribution of high-order correlation effects up to the coupled cluster with single, double, triple, and noniterative quadruple amplitudes [CCSDT(Q)] for the valence electrons within the two-component (with spin-orbit effects included) two-step approach; and (v) calculation of the basis set correction for 52 outer electrons of HfF$^+$ within the scalar-relativistic two-step approach.

For step (i) we used the CVQZ basis set for Hf [54,55] and the aug-ccpVQZ basis set [56,57] with two removed g-type basis functions for F. The inner-core electrons ($1s \ldots 3d$ of Hf) were excluded from the correlation treatment. For the correlation calculation we set the cutoff equal to 50 hartree for the virtual spinors. The inner-core correlation contribution was calculated at the CCSD level as the difference between the W_M values calculated with correlation of all 80 electrons of HfF$^+$ included in the correlation treatment and with 52 electrons as in stage (i). For these calculations we used the CVDZ [54,55] basis set on Th and the cc-pVDZ [56,57] basis set on F. We set the cutoff equal to 7000 hartree for virtual molecular spinors in these calculations to be sure that the necessary correlation functions were present in the one-electron spinor basis. Correction at step (iii) has been calculated at the Hartree-Fock level. In stage (iv) 20 electrons of HfF$^+$ were

correlated. Correction was estimated as the difference in the calculated values of W_M within the CCSDT(Q) versus the CCSD(T) method. For Hf we used a slightly reduced version [12,16,16,10,8]/(6,5,5,1,1) of the basis set which was used in Refs. [3,4,7]. For F the ANO-I basis set [58] reduced to [14,9,4,3]/(4,3,1) was used. In stage (v) we considered the influence of additional $7g-$, $6h-$ and $5i-$ basis functions on Hf [with respect to the basis functions of these types included in the CVQZ basis set, used in step (i)]. For stages (iv) and (v) we used the semilocal versions of 12-electron and 44-electron GRECP operators [3,4,7,38,39].

In all the calculations the Hf-F internuclear distance in the $^3\Delta_1$ state was set to 3.41 bohr [1].

For the Hartree-Fock calculations and integral transformations we used the DIRAC12 code [59]. Relativistic correlation calculations were performed within the MRCC code [60]. For scalar-relativistic calculations we used the CFOUR code [61–64]. The code to compute matrix elements of the MQM Hamiltonian has been developed in the present paper.

V. RESULTS AND DISCUSSION

The final value of W_M is 0.494 $\frac{10^{33}\,\mathrm{Hz}}{e\,\mathrm{cm}^2}$.

The inner-core contribution to the final value of W_M is about 3%. The Gaunt contribution is about -1.6%. High-order correlation effects give -0.3%. This means that the convergence with respect to correlation effects is achieved. The basis set correction on high-order harmonics is negligible (in contrast to the ThO case [20]). We estimate the uncertainty of the final value of W_M to be lower than 4%. The main uncertainty is due to omitting the "interference" of the Gaunt interaction and correlation effects. Interestingly, the estimate of Ref. [11] appears to be rather close to our value though for the other considered systems the uncertainty is rather large; e.g., for ThF$^+$ the estimate from Ref. [11] differs from that of *ab initio* correlation calculations [32] by about 3 times [65]

The obtained W_M in HfF$^+$ is very close to the value of W_M in ThF$^+$ [32] and slightly smaller than that in TaN [66,67]. Note, however, that the HfF$^+$ cation is already under active investigation for the other T, P-odd effects and similar experimental techniques may be used to search for the nuclear MQM.

One can express the MQM energy shift, $(-1)^{I+F} C (J, F) M W_M \Omega$, in terms of the fundamental CP-violating physical quantities d_p, d_n, $\tilde{\theta}$, and $\tilde{d}_{u,d}$ using Eqs. (10), (12), and (13). For the lowest rotational level, for which the coefficient $|C(J = 1, F = 7/2)| = 0.143$ reaches a maximum value, we have

$$0.143 W_M M = -\frac{10^{25}(2.8d_p + 2.0d_n)}{e\,\mathrm{cm}}\,\mu\mathrm{Hz}, \quad (14)$$

$$0.143 W_M M = -5.0 \times 10^{10}\tilde{\theta}\,\mu\mathrm{Hz}, \quad (15)$$

$$0.143 W_M M = -2.8\frac{10^{27}(\tilde{d}_u - \tilde{d}_d)}{\mathrm{cm}}\,\mu\mathrm{Hz}. \quad (16)$$

The current limits on d_p, $|\tilde{\theta}|$, and $|\tilde{d}_u - \tilde{d}_d|$ ($|d_p| < 2.0 \times 10^{-25}e$ cm, $|\tilde{\theta}| < 1.5 \times 10^{-10}$, $|\tilde{d}_u - \tilde{d}_d| < 5.7 \times 10^{-27}$ cm [68]) correspond to the shifts $|0.143\ W_M M| < 6$, 7, and 16 μHz, respectively.

ACKNOWLEDGMENTS

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