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HfF$^+$ as a candidate to search for the nuclear weak quadrupole moment

L. V. Skripnikov,[1,2,*] A. N. Petrov,[1,2] A. V. Titov,[1,2,†] and V. V. Flambaum[3,4]
[1]*National Research Centre "Kurchatov Institute" B.P. Konstantinov Petersburg Nuclear Physics Institute, Gatchina, Leningrad District 188300, Russia*
[2]*Saint Petersburg State University, 7/9 Universitetskaya Naberezhnaya, St. Petersburg 199034, Russia*
[3]*School of Physics, The University of New South Wales, Sydney New South Wales 2052, Australia*
[4]*Johannes Gutenberg-Universität Mainz, 55099 Mainz, Germany*

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Nuclei with a quadrupole deformation, such as ^{177}Hf have enhanced weak quadrupole moment which induces the tensor weak electron-nucleus interaction in atoms and molecules. Corresponding parity-non-conserving (PNC) effect is strongly enhanced in the $^3\Delta_1$ electronic state of the ^{177}HfF$^+$ cation which has very close opposite parity levels mixed by this tensor interaction. In the present paper we perform relativistic many-body calculations of this PNC effect. It is shown that the tensor weak interaction induced by the weak quadrupole moment gives the dominating contribution to the PNC effects in ^{177}HfF$^+$ which significantly exceeds contributions of the vector anapole moment and the scalar weak charge. The anapole and the weak charge can contribute due to the nonadiabatic mechanism proposed here. Therefore, corresponding experiment will allow one to separate the tensor weak PNC effect from the other PNC effects and to measure the quadrupole moment of the neutron distribution which gives the dominating contribution to the weak quadrupole moment.

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I. INTRODUCTION

Parity-non-conserving (PNC) effects are a way to test the standard model as well as new physics outside it ([1,2]). They have been extensively studied theoretically and experimentally in atoms (see, e.g., Refs. [1–3]). Considerable resources were devoted to search for the weak scalar charge and vector anapole moment of nuclei.

In Ref. [4] the effect of the *tensor* contribution to the PNC electron-nucleus interaction was calculated in atoms. It was shown that corresponding experiments may allow one to investigate the quadrupole moment Q_n of neutrons in nuclei. Note that the nuclear *electric* quadrupole moment is induced by nonspherical distribution of charged particles and can be measured by investigating hyperfine splittings in atomic systems. However, no such methods are available for Q_n measurement. Previously, there were some studies devoted to the investigation of the spherical distribution of neutrons compared to protons, the neutron skin effect [5,6].

It was shown in Refs. [7,8] that PNC effects are enhanced within diatomic molecules as they have closely spaced rotational levels of opposite parity (e.g., in the HgH molecule [9]). Recently, the experimental progress in investigating systematic effect has been achieved on the ^{138}Ba ^{19}F molecule [10] where the vector weak interactions were considered. In the experiment, the external magnetic field has been applied to the molecules to Zeeman shift opposite parity levels up to almost degeneracy. Upper limit on the anapole moment of the ^{19}F atom has been obtained.

A significant progress has been also achieved in the measurement of effects of fundamental time-reversal and spatial parity symmetry violation $\mathcal{T},\mathcal{P}$-odd effects) using the ^{180}HfF$^+$ cation [11] (^{180}Hf has zero nucleus spin). The experimental data [11] combined with theoretical data [12–15] can be used to set the upper bound on the electron electric dipole moment (eEDM) and the constant of the scalar-pseudoscalar nuclear-electron interaction. It was shown in Refs. [16–18] that the ^{177}HfF$^+$ cation with the ^{177}Hf isotope having spin $I = 7/2$ can be used to search for the $\mathcal{T},\mathcal{P}$-odd nuclear magnetic quadrupole moment.

In the present paper, we calculate a tensor weak interaction effect in the ground rotational level of the first excited metastable electronic state $^3\Delta_1$ of the ^{177}HfF$^+$ cation. The attractive feature of the HfF$^+$ cation (which was exploited in the $\mathcal{T},\mathcal{P}$-odd experiment [11]) is that there are two opposite parity states with a very small energy interval (~10 MHz, see below) leading to the enhancement of the effect. This can be used also to search for the PNC effect induced by the tensor weak interaction [19]. We have not found previous calculations or estimations of the PNC tensor weak interaction effect in molecules in literature.

II. THEORY

PNC Hamiltonian is given by [20]

$$h_{\mathrm{PNC}} = -\frac{G_F}{2\sqrt{2}}\gamma_5[Zq_{w,p}\rho_p(\mathbf{r}) + Nq_{w,n}\rho_n(\mathbf{r})], \qquad (1)$$

where Z is the nuclear charge, N is the neutron number, γ_5 is the Dirac matrix, $G_F \approx 2.2225 \times 10^{-14}$ a.u. is the Fermi constant, $\rho_p(r)$ and $\rho_n(r)$ are the density distribution of protons and neutrons normalized to unity; $q_{w,p}$ and $q_{w,n}$ are the

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[*] leonidos239@gmail.com
[†] http://www.qchem.pnpi.spb.ru

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weak charges of the proton and neutron, respectively,

$$q_{w,p} \approx 1 - 4\sin^2\theta_W \approx 0.08, \tag{2}$$

$$q_{w,n} = -1. \tag{3}$$

Following Ref. [4] one can assume $\rho_p(\mathbf{r}) \approx \rho_{0p}(r) + \rho_{2p}(r)Y_{20}(\theta,\phi)$, $\rho_n(\mathbf{r}) \approx \rho_{0n}(r) + \rho_{2n}(r)Y_{20}(\theta,\phi)$ (it is taken into account that if the nuclear spin has fixed projection on the z axis the quadrupole part of the density is proportional to Y_{20}). Assuming also $\rho_{0p}(r) = \rho_{0n}(r) = \rho_0(r)$ and proportionality between $\rho_{2n}(r)$ and $\rho_0(r)$, one obtains the following expression for the tensor part of the PNC interaction [4],

$$h_{\mathrm{Q}} = -\frac{5G_F}{2\sqrt{2}\langle r^2\rangle}\Sigma_q(-1)^q T_q^{(2)} Q_{-q}^{TW}, \tag{4}$$

where $T_q^{(2)} = C_q^{(2)}\gamma_5\rho_0(r)$ is the electronic part of the operator,

$C_q^{(2)} = \sqrt{4\pi/5}Y_{2q}$, $\langle r^2\rangle = 4\pi\int\rho_0 r^4 dr \approx 3R_N^2/5$ is the mean squared nuclear radius, R_N is the nuclear radius. Here, the weak quadrupole moment $Q^{TW} = q_{w,n}Q_n + q_{w,p}Q_p = -Q_n + 0.08Q_p$ is introduced.

For the case of the considered ${}^3\Delta_1$ state, we introduce the molecular constant,

$$W_q = \langle {}^3\Delta_{+1}|\frac{5G_F}{2\sqrt{2}\langle r^2\rangle}C_2^{(2)}\gamma_5\rho_0(r)|{}^3\Delta_{-1}\rangle. \tag{5}$$

This constant is the analog of the W_a constant that is required for the interpretation of molecular experiments in terms of the nuclear anapole moment [21–24] (see below).

$\mathcal{P}$-odd interaction with the nuclear anapole moment is given by the following effective Hamiltonian [21]:

$$h_A = (W_a\kappa)\mathbf{n}\times\mathbf{S}'\cdot\mathbf{I}, \tag{6}$$

where $\mathbf{n}$ is the unit vector directed from the heavy nucleus to the light one, κ is the dimensionless constant determined by the nuclear anapole moment, $\boldsymbol{S}'$ is the effective electron spin [22], and W_a is the parameter determined by the electronic structure of a molecule. The Hamiltonian (6) couples electronic states with $\Delta\Omega = \pm 1$ (Ω is the projection of the total electronic angular momentum on the internuclear axis). For example, for $\Omega = 1/2$ states (e.g., the BaF molecule in the ground electronic state), W_a is defined by the following expression:

$$W_a = \frac{G_F}{\sqrt{2}}\langle\Psi_{\Omega=1/2}|\rho_0(r)\alpha_+|\Psi_{\Omega=-1/2}\rangle, \tag{7}$$

where $\alpha_+ = \alpha_x + i\alpha_y$ is the Dirac matrix. Electronic matrix element of the h_A operator between $\Omega = +1$ and $\Omega = -1$ states (the present case) is zero. However, the vector PNC effect can contribute via the interference with the nonadiabatic effects due to the electron-rotation interaction through the intermediate $\Omega = 0$ states.

The PNC interaction induced by the scalar weak charge is given by the following Hamiltonian:

$$h_Z = -\frac{G_F}{2\sqrt{2}}\gamma_5[Zq_{w,p}\rho_{0p}(r) + Nq_{w,n}\rho_{0n}(r)]$$
$$\approx -Q^W\frac{G_F}{2\sqrt{2}}\gamma_5\rho_0(r), \tag{8}$$

where Q^W is the scalar weak charge of the ^{177}Hf nucleus. Hamiltonian (8) can couple electronic states only with $\Delta\Omega = 0$. However, due to the nonadiabatic interactions, the scalar weak charge can contribute to the considered PNC amplitude. Below, we consider contributions from the PNC effects induced by the tensor weak charge, vector anapole, and scalar weak charge.

III. ELECTRONIC STRUCTURE CALCULATION DETAILS

To calculate matrix elements of the PNC operators over electronic wave functions, we used the two-step approach [25–29]. This method allows one to avoid direct four-component relativistic treatment and use the highly accurate wave function inside the nucleus which is required for calculation of the matrix elements (5) and (7) containing integration over nucleus density. At 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 [30]. 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. An additional technical advantage is that one can also use very compact contracted basis sets [31,32]. At the second step, one uses the nonvariational procedure developed in Refs. [26–29] 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 and has been recently applied to study a number of diatomics [33–35].

To treat electron correlation effects we used the multireference linear-response coupled cluster method with single and double cluster amplitudes [36–38] for the calculation of the tensor PNC matrix element (5) and the multireference configuration interaction method to treat vector and scalar PNC matrix elements. In the correlation calculations, 20 electrons of Hf and F were included explicitly, whereas 60 ($1s..4f$) electrons of Hf were modeled by the GRECP operator. For the calculations, we have used the [12,16,16,10,8]/(6,5,5,3,1) basis set for Hf and [14,9,4,3]/(4,3,2,1) ANO-I basis set for F [39] used previously [40,41]. The uncertainty of the calculation for the considered off-diagonal electronic matrix element (5) (which has two-electron excitation as a leading contribution and therefore determined by pure correlation effects) can be estimated as 50% which is enough for the current purposes.

For the Hartree-Fock calculations and integral transformations we used the DIRAC15 code [42]. Relativistic correlation calculations were performed within the MRCC code [43].

IV. EVALUATION OF MOLECULAR PROPERTIES

The hafnium isotope ^{177}Hf has nuclear spin $I^1 = 7/2$, whereas the fluorine isotope ^{19}F has nuclear spin $I^2 = 1/2$. In this paper, we use coupling scheme,

$$\mathbf{F}_1 = \mathbf{J} + \mathbf{I}^1, \tag{9}$$

$$\mathbf{F} = \mathbf{F}_1 + \mathbf{I}^2, \tag{10}$$

where $\mathbf{J}$ is the total molecular angular momentum less the nuclear spins. The field-free energy levels of the ground rotational state with quantum number $J = 1$ splits by the hyperfine interaction with the hafnium nucleus into three groups which are characterized by $F_1 = 9/2$, $F_1 = 7/2$, $F_1 = 5/2$ quantum numbers. The hyperfine interaction with the fluorine nucleus further splits levels with total momentum $F = F_1 \pm 1/2$. Note that F_1 is not exact but a good quantum number since the hyperfine interaction with the fluorine nucleus is much weaker than the hyperfine interaction with the hafnium ones. Finally, each hyperfine level has two parity eigenstates known as the Ω doublet. These states are equal mixtures of $\Omega = \pm 1$ states.

Following Refs. [44,45], the energy levels and wave functions of the HfF$^+$ ion are obtained by the numerical diagonalization of the molecular Hamiltonian ($\hat{\mathbf{H}}_{\rm mol}$) on the basis set of the electronic-rotational wave functions,

$$\Psi_\Omega \theta^J_{M,\Omega}(\alpha,\beta) U^{\rm Hf}_{I^1M^1} U^{\rm F}_{I^2M^2}. \tag{11}$$

Here, Ψ_Ω is the electronic wave function, $\theta^J_{M,\Omega}(\alpha,\beta) = \sqrt{(2J+1)/4\pi} D^J_{M,\Omega}(\alpha,\beta,\gamma=0)$ is the rotational wave function, α, β, γ are the Euler angles, $U^{\rm Hf}_{I^1M^1}$ and $U^{\rm F}_{I^2M^2}$ are the Hf and F nuclear spin wave functions, and M (Ω) is the projection of the molecule angular momentum $\mathbf{J}$ on the laboratory $\hat{z}$ (internuclear $\hat{n}$) axis, $M^{1,2}$ are the projections of the nuclear angular momenta on the same axis. We write the molecular Hamiltonian for the ^{177}Hf ^{19}F$^+$ molecule in the form

$$\hat{\mathbf{H}}_{\rm mol} = \hat{\mathbf{H}}_{\rm el} + \hat{\mathbf{H}}_{\rm rot} + \hat{\mathbf{H}}_{\rm hfs} + \hat{\mathbf{H}}_{\rm PNC}. \tag{12}$$

Here $\hat{\mathbf{H}}_{\rm el}$, $\hat{\mathbf{H}}_{\rm rot}$, $\hat{\mathbf{H}}_{\rm hfs}$, and $\hat{\mathbf{H}}_{\rm PNC}$ are the electronic, the rotation of the molecule, hyperfine, and PNC interactions ($\hat{\mathbf{H}}_{\rm PNC} = h_Z + h_A + h_Q$), respectively,

$$\hat{\mathbf{H}}_{\rm rot} = B_{\rm rot}\mathbf{J}^2 - 2B_{\rm rot}(\mathbf{J}\cdot\vec{\mathbf{J}}^e) \tag{13}$$

is the rotational Hamiltonian. Explicit forms of other Hamiltonians can be found in Refs. [18,41].

V. RESULTS AND DISCUSSIONS

Calculated value of the molecular constant which characterizes the tensor weak PNC interaction in the molecule [given by Eq. (5)] is $W_q = i \times 6.0 \times 10^{-12}$ a.u. Taking $Q_p = 3365$ mb for ^{177}Hf and assuming $Q_n \approx (N/Z)Q_p$ [4] one obtains $Q^{TW} \approx -4.91$ b which is close to a more accurate calculation, -5.44 b, given in Ref. [46]. Thus, finally we have $W_q Q^{TW} \approx 8 \times 10^{-3}$ Hz.

Table I gives calculated transition matrix elements of the quadrupole weak interaction h_Q in terms of $W_Q Q^{TW}$ as well as the dipole moment between components of the Ω doublet and splitting for hyperfine sublevels of the ground rotational level of the $^3\Delta_1$ electronic state of ^{177}HfF$^+$.

TABLE I. Transition dipole moment (in atomic units for $m_F = 1$[a]), off-diagonal matrix elements of h_Q (in units of $W_q Q^{TW}$), h_Z (in units of $10^{-8} W_z Q^W$) between components of Ω doublets and Ω-doublet splittings, Δ (in megahertz), for the ground rotational $J = 1$ hyperfine levels of the $^3\Delta_1$ electronic state of ^{177}Hf ^{19}F$^+$. Individual contributions from the Coriolis interaction with $^3\Pi_{0^+}$ (in units of $10^{-3} W_a^{(1)} \kappa$) and $^3\Pi_{0^-}$ (in units of $10^{-3} W_a^{(2)} \kappa$) are given for h_a.

F_1	F	d	h_Q	$h_a(^3\Pi_{0^+})$	$h_a(^3\Pi_{0^-})$	h_Z	Δ
9/2	5	−0.1660	−0.0960	0.1280	−0.1506	−0.8405	3.6
	4	−0.2030	−0.0961	0.1282	−0.1508	−0.8407	3.6
7/2	4	0.0618	0.3335	−0.0613	0.0721	−0.8427	−15.7
	3	0.0803	0.3337	−0.0611	0.0719	−0.8430	−15.7
5/2	2	0.2310	−0.2843	−0.2009	0.2364	−0.8509	12.0
	3	0.1656	−0.2847	−0.2010	0.2366	−0.8506	12.1

[a] Values for the transition dipole moment for other m_F's can be obtained by multiplying on m_F, matrix elements of h_Q, h_A, and h_Z between components of Ω doublets and Ω-doublet splittings are independent of the m_F quantum number.

As was noted above, the vector PNC interaction induced by the nuclear anapole moment can also contribute to the considered effects via the interference with the nonadiabatic (Coriolis) interaction described by the second term of rotational Hamiltonian given by Eq. (13). The latter electron-rotation interaction can couple states with $\Delta\Omega = \pm 1$. We have estimated the effect by numerical diagonalization of the corresponding spin-rotational Hamiltonian $\hat{\mathbf{H}}_{\rm mol}$ [see Eq. (12)]. For this, the interaction through the $^3\Pi_{0^+}$ and $^3\Pi_{0^-}$ intermediate states has been considered, i.e., we have considered the basis of electronic-rotational wave functions (11) with $^3\Delta_1$, $^3\Delta_{-1}$, $^3\Pi_{0^+}$, and $^3\Pi_{0^-}$ electronic parts. Corresponding contributions are given in Table I in terms of the following molecular electronic constants:

$$W_a^{(1)} = \frac{G_F}{\sqrt{2}} \langle ^3\Delta_1 | \rho_0(r)\alpha_+ | ^3\Pi_{0^+} \rangle \approx i \times 21 \text{ Hz},$$

$$W_a^{(2)} = \frac{G_F}{\sqrt{2}} \langle ^3\Delta_1 | \rho_0(r)\alpha_+ | ^3\Pi_{0^-} \rangle \approx i \times 17 \text{ Hz}.$$

Using estimation $\kappa(^{177}\text{Hf}) \approx 0.1$ [47] and data from Table I one obtains that the tensor weak interaction is one to two orders of magnitude larger than the effect induced by the nuclear anapole moment.

The contribution of the PNC interaction induced by scalar weak charge has also been considered. As was noted above, this interaction can couple electronic molecular states with $\Delta\Omega = 0$. In our case, $^3\Pi_{0^+}$ and $^3\Pi_{0^-}$ electronic states can be mixed by this interaction. Therefore, this interaction can contribute to the mixing of $^3\Delta_1$ and $^3\Delta_{-1}$ states via the interference with nonadiabatic effects [in the second order of perturbation theory with respect to the interaction given by the second term of Eq. (13)]. Table I gives resulting contribution of the effect due to the scalar weak interaction in terms of the following molecular electronic constant:

$$W_z = \langle ^3\Pi_{0^+} | \frac{h_Z}{Q_W} | ^3\Pi_{0^-} \rangle \approx i \times 5 \text{ Hz}.$$

Taking $Q_W \approx -105$, one obtains that the resulting contribution is about two orders of magnitude smaller than the tensor weak interaction but on the same order as the nuclear anapole moment induced interaction.

Other molecules that are considered for the electron's EDM (eEDM) measurements, such as TaN, ThO, and ThF$^+$ can be considered to measure the weak quadrupole. In the experiments, one should use a heavy nucleus isotope with spin

$I > 1/2$, i.e., ^{181}Ta and ^{229}Th (the former one is stable). Note, however, that in the present case of the ^{177}HfF$^+$ cation, PNC effects induced by the anapole moment are not dominating. Contributions to this effect due to the nonadiabatic interaction of the Ω doublet with $^3\Pi_{0^+}$ and $^3\Pi_{0^-}$ states have opposite signs and partly cancel each other. Such a cancellation is not guaranteed for all $\Omega = 1$ molecules and should be checked for the corresponding system.

It follows from Table I that the PNC matrix element induced by the weak quadrupole is about several millihertz depending on the hyperfine sublevel. Therefore, for a reliable detection of the weak quadrupole moment, the sensitivity should be better than 1 mHz. Since the weak quadrupoles and the quadrupole moments of the neutron distribution have never been observed, a possibility of their detection is a sufficient motivation for the experiments. In Ref. [10] it was demonstrated for the BaF molecule that the present sensitivity to the PNC matrix element induced by the nucleus anapole moment achieves several hertz. At the same time, for the completely different electron EDM experiment on ^{180}HfF$^+$, the final value for the *e*EDM-sensitive frequency channel is less than 1 mHz (statistic) [11]. Thus, further development of the experimental methods as well as its adaptation to the molecules with $^3\Delta_1$ states is required.

In existing atomic experiments, the dominating contribution to PNC effects comes from the weak charge and anapole moment, therefore, the separation of a significantly smaller weak quadrupole contribution would be a very challenging task. In the considered case of the ^{177}HfF$^+$ cation, the weak quadrupole is the dominating contribution to PNC enhanced by a very small energy denominators between the $\Omega = 1$ doublet components (see Table I). Close levels of opposite parity with the difference of the electron angular momentum $\Delta J = 2$ (where the weak quadrupole induced PNC dominates) exist in rare-earth atoms [4]. However, such levels are unstable, and the weak quadrupole matrix elements between them are small (since they vanish in the absence of the configuration mixing). Therefore, the experiments with the $\Omega = 1$ molecules, such as ^{177}HfF$^+$, look more attractive than the atomic experiments aiming to measure the weak quadrupoles.

VI. CONCLUSION

In the present paper, the effect of the tensor weak interaction induced by the weak nuclear quadrupole moment has been calculated in the $^3\Delta_1$ electronic state of the ^{177}HfF$^+$ cation. The weak nuclear quadrupole moment is mainly determined by the neutrons' quadrupole distribution which is unknown and is of interest for the nuclear structure theory. It is shown that the tensor weak interaction gives the largest contribution with respect to other PNC effects induced by the nuclear anapole moment and nuclear weak charge. Thus, it is expected that in the corresponding experiment it will be possible to separate the tensor weak PNC effect from the other PNC effects.

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