

$\mathcal{P}$, $\mathcal{T}$ -violating axion-mediated interactions in the RaOH moleculeAnna Zakharova^{*}*St. Petersburg State University, St. Petersburg, 7/9 Universitetskaya naberezhnaya, 199034, Russia
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If axions simultaneously have the scalar couplings to the nucleons and pseudoscalar couplings to the electrons, it may mediate a $\mathcal{P}$, $\mathcal{T}$ -violating interaction between the electronic shell and nuclei in the molecules. The polyatomic molecule RaOH, which is considered a promising platform for the $\mathcal{P}$, $\mathcal{T}$ -violation searches, is studied for its sensitivity to such interactions. Because of the long-range nature (on molecular scales) of the axion-mediated interaction, it is important whether the molecular parameter is sensitive to the vibration of the molecule. Our results imply that the impact of the vibrations on the axion-mediated electron-nucleon interaction in the molecule is similar to the impact on the short-range electron-nucleon scalar-pseudoscalar interaction studied earlier.

DOI: [10.1103/c3fg-p7w4](https://doi.org/10.1103/c3fg-p7w4)**I. INTRODUCTION**

An important question in fundamental physics is the origin of dark matter, the existence of which is predicted by observing the rotational curves of galaxies and data from gravitational lensing of galaxy objects, such as the Bullet Cluster. It also allows us to describe the formation of structures in the early Universe, and the observed inhomogeneities in cosmic microwave background radiation [1].

Pseudoscalar particles called axions are promising potential candidates for dark matter constituents [2–4]. Such particles with certain masses and coupling constant values may solve the strong $\mathcal{CP}$ problem [5], which remains an open problem of the Standard Model (SM) of particle physics [6,7]. QCD does not have other sources of $\mathcal{CP}$ violation except the axion-associated θ -term. In the SM, all known parity violations occur in the weak interaction, related to the mixing of the quark matrices (Cabibbo-Kobayashi-Maskawa) [8,9] and the neutrino matrices (Pontecorvo-Maki-Nakagawa-Sakata) [10,11]. Some physical effects, such as the electron electric dipole moment (eEDM) and scalar-pseudoscalar electron-nucleon interaction (NE-SPS), are strongly suppressed in the Standard Model [12–15]. However, some $\mathcal{CP}$ -violating scenarios, such as supersymmetry, predict much larger values for these

effects. The existence of new sources of $\mathcal{CP}$ violation may also be necessary to explain the problem of baryon asymmetry of the Universe and may lead to a value of the θ -term closer to the neutron electric dipole moment limit [16].

We can also consider axionlike particles that are light pseudoscalar particles, which may have a qualitatively similar behavior to the QCD axion but do not necessarily address the strong $\mathcal{CP}$ problem. Such particles may appear in diverse scenarios, resulting in a variety of their properties.

Molecular experiments allow us to study the effects related to $\mathcal{P}$ - and $\mathcal{T}$ -parity violation [13,17–20]. For example, an eEDM limit was obtained in an experiment with the diatomic molecule HfF⁺ [21]. Theoretical calculations are necessary to estimate the parameters of $\mathcal{P}$ - and $\mathcal{T}$ -parity violation for these effects [22]. The phenomena that may manifest itself in the molecular spectra include the interaction with cosmic fields of axions and dark photons, most straightforwardly in the chiral species such as the ground and vibrational states of the CHBrClF molecule [23]. Such interaction was also considered for a nonchiral molecule RaOCH₃ in nonequilibrium configurations [24].

Among the studies of the effects caused by new interactions with axions in molecules, one can highlight the papers about the effects of axion exchange between electrons and nuclei, as well as between electrons and electrons, studied for the diatomic molecules HfF⁺ [25], BaF [26], and the triatomic molecule YbOH [27,28]. Also, the interaction mediated by the axion produced by an electron-axion pseudoscalar vertex and a nucleon-axion or electron-axion scalar vertex were considered in [29,30]. In these works, the contribution of such interaction to the dipole moment of atoms and molecules was studied, and constraints on the corresponding interaction constants were obtained.

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The polyatomic molecules such as the triatomic molecules RaOH and YbOH are a promising platform for future parity-violation searches. It is important to stress that the measurement of the $\mathcal{P}$, $\mathcal{T}$ on the triatomic molecules involves their excited rovibrational states. In addition to the doublets associated with the rotation of the electron shell, triatomic linear molecules have l doublets [31–34]. In hexatomic molecules of the “symmetric top” type, additional doublets appear associated with the rotation of the CH_3 ligand in two opposite directions [24,35,36]. Measurement of the relative shifts within different parity doublets allows one to significantly suppress many systematic effects. The possibility of laser cooling of the polyatomic molecules also presents a huge advantage for the experiment [37–42]. The laser cooling of the triatomic molecule SrOH was demonstrated in [43]. For the molecule RaOH, only limited spectroscopic data exist, such as in [44] where the band origins, rotational constant, and spin-rotation constant were obtained.

The axion-mediated interaction can manifest itself in the molecular spectra the same way as such $\mathcal{P}$, $\mathcal{T}$ -violating effects as the eEDM and the scalar-pseudoscalar electron-nucleon interaction. It is important to compute the sensitivities to the different effects to be able to distinguish them from each other using multiple measurements on different molecular species.

If we suppose the existence of the axion exchange interaction of the electrons with nuclei characterized by the product of coupling constants $g_{e,P} \cdot g_{N,S}$, this $\mathcal{P}$, $\mathcal{T}$ -odd effect can be estimated from the splitting between levels with opposite values of M (projection of total angular momentum on space-fixed frame) given by

$$\Delta E_{\mathcal{P},\mathcal{T}} \simeq P g_{e,P} g_{N,S} \Omega W_{\text{ax}}, \quad (1)$$

where Ω is the projection of the electron spin on the molecular axis. The parameter W_{ax} is determined from the molecular electronic structure calculation. $P \leq 1$ is the degree of polarization of the molecule [34]. Because the states of interest are excited rovibrational states, it is important to study the impact of the molecule geometry on the molecular parameters. Previously, we have studied such impact on the enhancement of the eEDM and NE-SPS for the triatomic molecules RaOH [31] and YbOH [32], as well as the hexatomic molecules RaOCH_3 [35] and YbOCH_3 [36]. While the impact is noticeable, it is not particularly large for these properties. The axion-mediated interaction differs from these interactions because of its long-range nature; therefore, one may find it interesting to check whether the impact of the molecular vibrations may become significant in this case. In this paper, we study the molecular parameter for the electron-nucleon axion-mediated interaction for the triatomic molecule RaOH.

II. AXION-MEDIATED INTERACTION OF ELECTRONS AND NUCLEI

The interaction terms between the axion and the fermions of the Standard Model may be written as

$$\mathcal{S}_{\text{int}} = \sum_{f \in \text{SM}} (g_{f,S} \bar{\Psi}_f a \Psi_f + i g_{f,P} \bar{\Psi}_f a \gamma_5 \Psi_f). \quad (2)$$

If both scalar interaction with nucleons $g_{N,S}$ (with $N = p, n$) and pseudoscalar interaction with electrons $g_{e,P}$ are present, the process of axion exchange, represented by the Feynman diagram in Fig. 1, induces the following one-electron operator of electron interaction with the nucleus A , written in the atomic units as

$$\hat{H}_{eN} = i \frac{g_{e,P}}{4\pi} \sum_{i=1}^{N_e} \sum_{k=1}^A \int d^3 \mathbf{R}_k g_{N_k,S} \rho_k(\mathbf{R}_k) \frac{e^{-m_a c |\mathbf{r}_i - \mathbf{R}_k|}}{|\mathbf{r}_i - \mathbf{R}_k|} \gamma_0^{(i)} \gamma_5^{(i)}, \quad (3)$$

where N_e is the number of electrons, A is the atomic weight of the nucleus (i.e., number of nucleons), $\mathbf{r}_i$ is the coordinate of the i th electron, $\mathbf{R}_k$ is the coordinate of the k th nucleon, $N_k = p, n$ is the type of nucleon, ρ_k is the nucleon density function normalized by 1, and m_a is the axion mass. The gamma matrices $\gamma_0^{(i)}$ and $\gamma_5^{(i)}$ are acting on the spinor of the i th electron. In atomic units the speed of light is $c \simeq 137$.

A number of approximations can be employed in this operator.

First, we approximate the nucleon density with a single function ρ , which can be identified as the charge density,

$$\hat{H}_{eN} \simeq iA \frac{g_{e,P} \bar{g}_{N,S}}{4\pi} \sum_{i=1}^{N_e} \int d^3 \mathbf{R} \frac{\rho(\mathbf{R}) e^{-m_a c |\mathbf{r}_i - \mathbf{R}|}}{|\mathbf{r}_i - \mathbf{R}|} \gamma_0^{(i)} \gamma_5^{(i)}, \quad (4)$$

where $\bar{g}_{N,S}$ is introduced for the nucleus with the atomic weight A and charge Z ,

$$\bar{g}_{N,S} = \frac{(A - Z)g_{n,S} + Zg_{p,S}}{A}. \quad (5)$$

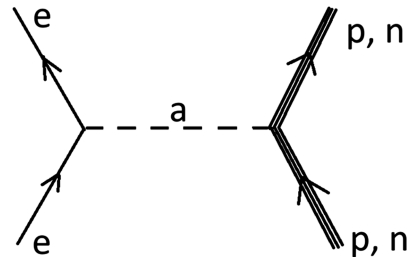


FIG. 1. Feynman diagram for the axion-mediated electron-nucleon interaction.

In fact, the results of [26] imply that the non-point-like description of the atomic nuclei becomes important only for $m_a \gtrsim 10$ MeV. This is consistent with our own computation.

The molecular parameter is then introduced as

$$W_{\text{ax}} = \frac{1}{g_{e,P} \bar{g}_{N,S} \Omega} \langle \Psi | \hat{H}_{eN} | \Psi \rangle, \quad (6)$$

where the γ_5 present in the operator damps this interaction unless the electrons have the relativistic momenta. Combined with A scaling, this means that, despite its long-range nature, only the contribution of the interaction of electrons with heavy nuclei and their neighborhood (though significant in size) will matter. Consequently, for the RaOH molecule considered in this paper, we take into account only the contribution of the interaction of electrons with the heavy ($A = 226$) radium atom. Equation (5) gives the expectation value of the axion-mediated $\mathcal{P}$ - and $\mathcal{T}$ -violating part of the Hamiltonian. This value can be used to obtain the product of constants $g_{e,P} \cdot g_{N,S}$ from energy shifts of molecular levels that could, in principle, be detected experimentally.

Second, the typical molecular length scale corresponds to the Compton length of masses in the ~ 1 keV range. This is much larger than the astrophysically acceptable masses of the axion. Therefore, we can approximate the exponent in the numerator as $e^{-m_a c |\mathbf{r}_i - \mathbf{R}_k|} \simeq 1$. However, it is still interesting to consider the opposite limit of $m_a c \gtrsim 10$ GeV in which this interaction becomes an effective NE-SPS interaction,

$$\hat{H}_s = i g_s \frac{G_F}{\sqrt{2}} Z \rho(\vec{r}) \gamma_0 \gamma_5 \quad (7)$$

with the parameter describing the sensitivity to this interaction,

$$W_s = \frac{1}{g_s \Omega} \langle \Psi | \hat{H}_s | \Psi \rangle, \quad (8)$$

where the Fermi constant is $G_F = 2.2225 \times 10^{-14}$ in atomic units. In the high-mass limit, when $m_a c$ is comparable or less than the radius of the nucleus, these parameters are related to each other as

$$W_{\text{ax}} \simeq \frac{\sqrt{2} A}{Z G_F} \frac{W_s}{m_a^2 c^2}. \quad (9)$$

As we have previously computed the value of W_s in [31], we will use this relation to check the validity of our computation.

III. ONE-CENTER RESTORATION METHOD

The computational complexity for the RaOH molecule is high due to the large number of electrons and the necessity

to introduce a large number of the basis functions to account for the states with large momenta. To overcome that, we use generalized effective core potential (GRECP) to describe the core electrons [45–47]. However, only the two-component solutions can be obtained this way, and they have incorrect smoothed behavior in the core region. To overcome that problem, the one-center restoration method was developed in [48]. Let us elucidate the main idea of this method.

First, we construct the equivalent bases. The atomic problem for the heavy atom is solved by using two approaches to get two sets of solutions. The first set of solutions is obtained by using the full-electron Hartree-Fock-Dirac method, resulting in

$$\Phi_{nljm}(\mathbf{r}) = \begin{pmatrix} f_{nlj}(r) \mathcal{Y}_{ljm}(\theta, \phi) \\ i g_{nlj}(r) \mathcal{Y}_{2j-l,jm}(\theta, \phi) \end{pmatrix}, \quad (10)$$

where $\mathcal{Y}_{ljm}$ are two-component spinor spherical harmonics. The second set of solutions is obtained by using GRECP resulting in two-component basis,

$$\tilde{\Phi}_{nljm}(\mathbf{r}) = \tilde{f}_{nlj}(r) \mathcal{Y}_{ljm}(\theta, \phi). \quad (11)$$

These two sets of solutions are mapped to each other based on an identification of the quantum numbers. This way the equivalent bases are constructed.

Second, the two-component molecular spinor $\tilde{\Psi}$ obtained in the GRECP approximation is represented in the vicinity of the nucleus as the superposition of the two-component basis,

$$\tilde{\Psi}(\mathbf{r}) = \sum_{njl} C_{njl} \tilde{\Phi}_{njl}(\mathbf{r}), \quad (12)$$

and then the four-component spinor is constructed using the same coefficients with four-component basis functions, which are equivalent to the two-component ones,

$$\Psi(\mathbf{r}) = \sum_{njl} C_{njl} \Phi_{njl}(\mathbf{r}). \quad (13)$$

The property is computed using the constructed four-component molecular spinors. Details of implementation are given in [49].

IV. COUPLED-CHANNELS TECHNIQUE

For the molecular wave function we assume the validity of the Born-Oppenheimer approximation,

$$\Psi_{\text{total}} \simeq \Psi_{\text{nuc}}(R, \hat{R}, \hat{r}) \psi_{\text{elec}}(R, \theta | q), \quad (14)$$

where q means coordinates of the electronic subsystem, $\hat{r}$ and $\hat{R}$ are directions of the OH axis and the Ra center of

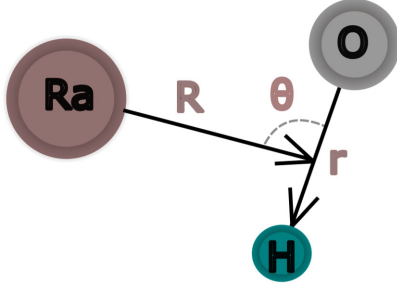


FIG. 2. Jacobi coordinates.

mass of the OH axis, respectively, θ is the angle between the above axes, and R is the distance between the radium atom and the ligand center of mass (Fig. 2). We consider the fixed ligand stretch since the Ra–OH bond stretching and bending frequencies are much smaller than the vibrations of the OH, using the equilibrium distance $r = 1.832$ a.u. [50]. The Dirac-Coulomb equation in the classical field of fixed nuclei has a solution $\psi(R, \theta|q)$. The corresponding Hamiltonian can be written in such form,

$$\hat{H}_{nuc} = -\frac{1}{2\mu} \frac{\partial^2}{\partial R^2} + \frac{\hat{L}^2}{2\mu R^2} + \frac{\hat{j}^2}{2\mu_{OH} r^2} + V(R, \theta), \quad (15)$$

where μ and μ_{OH} are the reduced masses of the Ra–OH and the OH ligand, respectively, $\hat{L}$ is the angular momentum of the rotation of the heavy radium atom and the ligand around their common center of mass, $\hat{j}$ is the angular momentum of the ligand rotation, and $V(R, \theta)$ is the effective adiabatic potential.

Thus, the solution of the Schrödinger equation is the nuclear wave function $\Psi_{nuc}(R, \hat{R}, \hat{r})$,

$$\hat{H}_{nuc} \Psi_{nuc}(R, \hat{R}, \hat{r}) = E \Psi_{nuc}(R, \hat{R}, \hat{r}). \quad (16)$$

We use the following series expansion to solve Eq. (16):

$$\Psi_{nuc}(R, \hat{R}, \hat{r}) = \sum_{L=0}^{L_{\max}} \sum_{j=0}^{j_{\max}} F_{JjL}(R) \Phi_{JjLM}(\hat{R}, \hat{r}), \quad (17)$$

where

$$\Phi_{JjLM}(\hat{R}, \hat{r}) = \sum_{m_L, m_j} C_{Lm_L, jm_j}^{JM} Y_{Lm_L}(\hat{R}) Y_{jm_j}(\hat{r}), \quad (18)$$

where Y_{Lm_L} is the spherical function, and C_{Lm_L, jm_j}^{JM} are the Clebsch-Fock-Gordan coefficients.

Thus, we have a system of close-coupled equations for $F_{JjL}(R)$ [51],

$$\left[\frac{d^2}{dR^2} - \frac{L(L+1)}{R^2} - \frac{\mu j(j+1)}{\mu_{OH} r^2} + 2\mu E \right] F_{JjL}(R) = 2\mu \sum_{\tilde{j}, \tilde{l}} \mathcal{V}_{jL, \tilde{j}\tilde{L}}^J F_{J\tilde{j}\tilde{L}}(R), \quad (19)$$

where on the right side we have introduced a matrix potential

$$\mathcal{V}_{jL, \tilde{j}\tilde{L}}^J(R) = (-1)^{J+j+\tilde{j}} \sqrt{(2L+1)(2\tilde{L}+1)(2j+1)(2\tilde{j}+1)} \times \sum_{k=0}^{k_{\max}} V_k(R) \left\{ \begin{matrix} j & L & J \\ \tilde{L} & \tilde{j} & \lambda \end{matrix} \right\} \begin{pmatrix} L & \lambda & \tilde{L} \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} j & \lambda & \tilde{j} \\ 0 & 0 & 0 \end{pmatrix}, \quad (20)$$

where a matrix with curly brackets denotes a $6j$ symbol, matrices with round brackets denote $3j$ symbols, and $V_k(R)$ correspond to the decomposition of the potential in terms of the Legendre polynomials $P_k(x)$,

$$V(R, \theta) = \sum_{k=0}^{k_{\max}} V_k(R) P_k(\cos \theta). \quad (21)$$

To deal with the dependence on R we use the following approach. We choose a basis $f_n(R)$ of the eigenfunctions for longitudinal oscillations in the harmonic approximation,

$$\left[-\frac{1}{2\mu} \frac{d^2}{dR^2} + \frac{\mu \omega_{\parallel}^2}{2} (R - R_{eq})^2 \right] f_n(R) = \omega_{\parallel} \left(n + \frac{1}{2} \right) f_n(R). \quad (22)$$

Then we use the following decomposition:

$$F_{JjL}(R) = \sum_{n=0}^{n_{\max}} F_{JjLn} f_n(R). \quad (23)$$

The exact solution would correspond to the infinite sum, but for the numerical computations we use the finite basis approximation and cut our sum to $n_{\max}$. We considered different values of $n_{\max}$ to check numerical convergence. Here $n_{\max}$ is a maximal occupation number for the longitudinal vibrations. This means that higher value of $n_{\max}$ describes wider wave functions as well as more rapid oscillations in R . The electronic computations are performed on a discrete grid of R with minimal and maximal values defined by $R_{\min}$ and $R_{\max}$ correspondingly. We introduce matrix elements for the centrifugal term

$$C_{n\tilde{n}} = \int_{R_{\min}}^{R_{\max}} dR f_n(R) \frac{1}{R^2} f_{\tilde{n}}(R), \quad (24)$$

and the potential

$$\tilde{V}_{kn\tilde{n}} = \int_{R_{\min}}^{R_{\max}} dR f_n(R) \left(V_k(R) - \delta_{k,0} \frac{\mu \omega_{\parallel}^2}{2} (R - R_{eq})^2 \right) \times f_{\tilde{n}}(R). \quad (25)$$

The values for $R_{\min}$ and higher $R_{\max}$ are chosen in such a way that the obtained nuclear motion wave functions decrease rapidly beyond that range and do not impact the accuracy of the numerical computation.

Then we get the finite linear system,

$$\begin{aligned} & \left[-2\mu\omega_{\parallel} \left(n + \frac{1}{2} \right) - \frac{\mu j(j+1)}{\mu_{OH} r^2} + 2\mu E \right] F_{JjLn} \\ & = 2 \sum_n L(L+1) C_{n\tilde{n}} F_{JjL\tilde{n}} + 2\mu \sum_{\tilde{j}, \tilde{l}, \tilde{n}} \tilde{V}_{jLn, \tilde{j} \tilde{L} \tilde{n}}^J F_{J\tilde{j} \tilde{L} \tilde{n}}, \end{aligned} \quad (26)$$

where we use

$$\begin{aligned} \tilde{V}_{jLn, \tilde{j} \tilde{L} \tilde{n}}^J & = (-1)^{J+j+\tilde{j}} \sqrt{(2L+1)(2\tilde{L}+1)(2j+1)(2\tilde{j}+1)} \\ & \times \sum_{k=0}^{k_{\max}} \tilde{V}_{kn\tilde{n}} \left\{ \begin{matrix} j & L & J \\ \tilde{L} & \tilde{j} & \lambda \end{matrix} \right\} \begin{pmatrix} L & \lambda & \tilde{L} \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} j & \lambda & \tilde{j} \\ 0 & 0 & 0 \end{pmatrix}. \end{aligned} \quad (27)$$

We use the following procedure to process the potential:

- (i) Adiabatic potential values are obtained in the electronic computations for a discrete grid of (R_i, θ_j) .
- (ii) We fit values for $\theta = 0^\circ$ using the Morse potential,

$$V(R, 0^\circ) = D_e \left(1 - \exp(-A(R - R_{eq}))^2 \right), \quad (28)$$

which gives R_{eq} and $\omega_{\parallel} = \sqrt{\frac{2D_e}{\mu}} A$.

- (iii) The dependence on θ is interpolated using Akima splines for each value of R_i .
- (iv) The Gauss-Legendre method is then used to obtain the coefficients of the Legendre polynomial expansion $V_k(R_i)$ on the grid of R_i values.
- (v) Then the dependence of the expansion coefficients V_k on R is also interpolated by Akima splines.
- (vi) The resulting interpolation is used to calculate the integrals $V_{kn\tilde{n}}$ [Eq. (25)].

Applying similar processing (except for the second step with Morse potential fit) and Eq. (27) to the property values, we also obtain the matrix elements of the properties $W_{jLn, \tilde{j} \tilde{L} \tilde{n}}$. The property average is obtained as

$$\langle W_{ax} \rangle = \sum_{j, l, n} \sum_{\tilde{j}, \tilde{l}, \tilde{n}} F_{JjLn}^* F_{J\tilde{j} \tilde{L} \tilde{n}} W_{jLn, \tilde{j} \tilde{L} \tilde{n}}. \quad (29)$$

V. RESULTS AND DISCUSSION

The molecular orbitals were obtained in the DIRAC19 software package using self-consistent field level. To describe the heavy radium atom, we used a ten-valence electron basis set adapted to GRECP developed by the quantum physics and chemistry department of PNPI [52]. We have used the equivalent bases adapted to this potential previously used in [31].

The functions f_{nlj} and g_{nlj} used to describe the equivalent bases functions are represented as a set of values on the uneven grid of r_i starting with $r_1 = 7.04 \times 10^{-6}$ to 150 a.u. Inside the nucleus region $r < r_1$, the following ansatz is used:

$$f_{nlj}(r) = r^{\gamma} \sum_{k=0}^5 a_k r^k. \quad (30)$$

These six terms correspond to a special ansatz to represent a wave function in the core region. This choice of ansatz was made before in the works about the one-center restoration

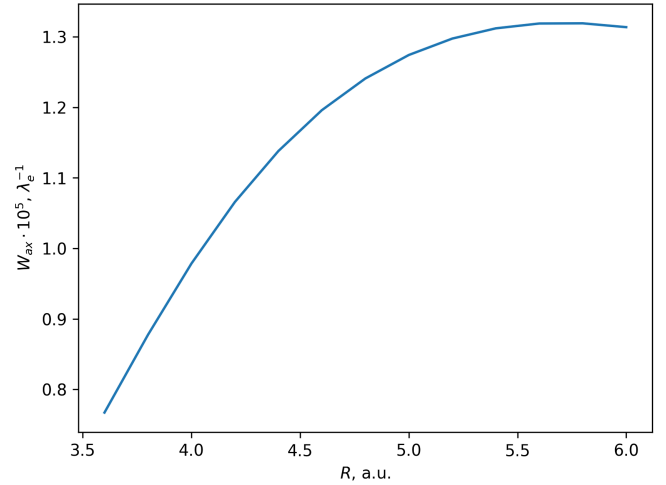


FIG. 3. The dependence of W_{ax} on R for $\theta = 0^\circ$.

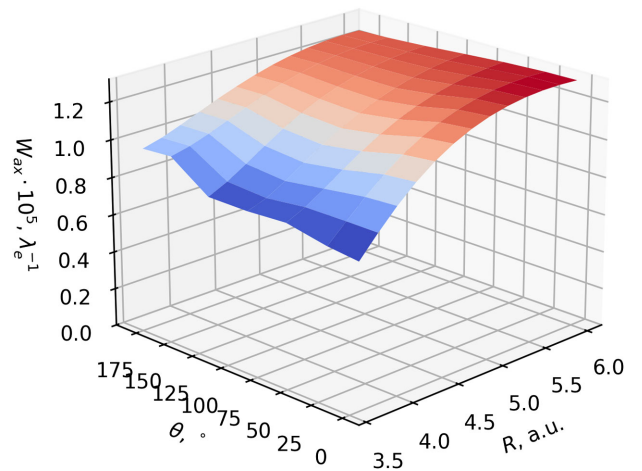


FIG. 4. The dependence of W_{ax} on R and θ .

technique [53] and used in the preceding work with the same equivalent basis sets for the radium atom [31]. This is important for an accurate description of the short-range electron-nucleon interactions. However, in our case, because of the significant long-range contribution, this region contribution is negligible when $m_a \ll 1$ MeV. This is in sharp contrast with the NE-SPS interaction.

The equilibrium geometry was determined in [31] to correspond to $R = 4.4$ a.u. The property was computed on a grid of values of R and θ . R was taken to span values from 3.6 to 6.0 a.u. with step 0.2 a.u., where θ was taken to be 0° , 25° , 57° , 90° , 122° , 155° , and 180° . The resulting value for the equilibrium geometry equals $1.1407 \times 10^{-5} \lambda_e^{-1}$, where $\lambda_e = \frac{\hbar}{m_e c}$ is the electron Compton length. Compare this with $3.36 \times 10^{-5} \lambda_e^{-1}$ for YbOH obtained in [27]. The dependence on the θ and R is depicted in Figs. 3 and 4. The values for several rovibrational states are given in Table I. To check the convergence and estimate numerical error, the computation was performed for $l_{\max}, j_{\max}, k_{\max} = 40, \dots, 43$, and $n_{\max} = 10, \dots, 13$.

Our results show that, despite the long-range nature of the property in question, its dependence on the geometry of the molecule is very similar to the short-range NE-SPS interaction. However, it should be stressed that previous studies of the axion-mediated interactions showed that electronic correlations can lead to significant corrections to the value of the molecular parameters. This may increase the sensitivity of W_{ax} to the vibrations of the molecule.

To test the validity of our computation, we have also computed the values for different masses m_a to compare the

TABLE I. Electron-nucleon axion-mediated interaction.

$v_{\parallel}$	$v_{\perp}$	l	$W_{\text{ax}}, 10^{-5} \lambda_e^{-1}$	Numerical relative error
Equilibrium configuration				
			1.1407	1.6791×10^{-5}
$J = 0$				
0	0	0	1.1347	1.6966×10^{-7}
1	0	0	1.1367	1.7668×10^{-7}
2	0	0	1.1379	5.3008×10^{-7}
0	2	0	1.1208	5.1133×10^{-7}
$J = 1$				
0	0	0	1.1347	1.6966×10^{-7}
0	1	1	1.1278	3.7887×10^{-7}

The YbOH equilibrium (fock space coupled cluster with singles and doubles, $m_a = 1..10$ eV) [27]

3.36

The BaF equilibrium (coupled cluster with singles and doubles, $m_a = 1..10^2$ eV) [26]

1.77

result with the prediction using the approximation (9) and the value for W_s taken from [31]. As both properties have shown very similar behavior, we have restricted ourselves to the equilibrium configurations. The dependence is depicted in Fig. 5. For $m_a > 5 \times 10^7$ eV, the deviation from predictions (9) is less than 10%. Note that, just as in [26], we see a change of the sign of the property near $m_a \sim 10^4$ eV which results in the blind spot for this mass range.

Finally, in Fig. 6, we contrast the expected sensitivity of the RaOH experiment with the existing laboratory limits on the product of the axion-nucleon scalar and axion-electron pseudoscalar coupling constants [54]. Current experiments with diatomic molecules setting a limit $d_e \leq 1.3 \times 10^{-30} e \cdot \text{cm}$ for $\mathcal{E} = 23$ GV/cm are able to sense energy differences $\Delta E = d_e \mathcal{E} \sim 0.7 \times 10^{-5}$ Hz [21], which gives us the conservative estimate for the RaOH experiment

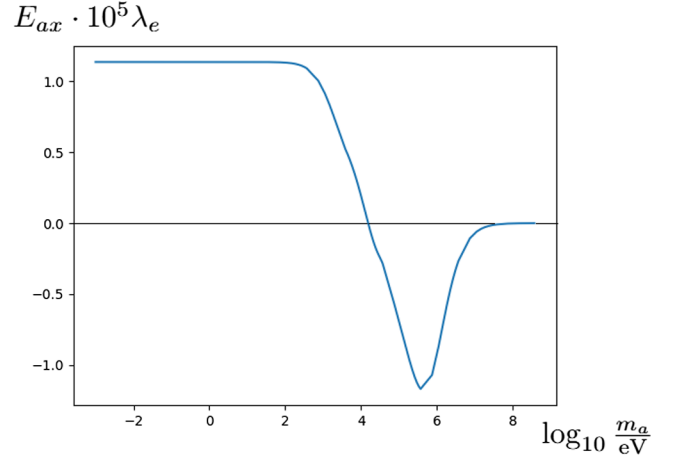


FIG. 5. The dependence of W_{ax} on m_a .

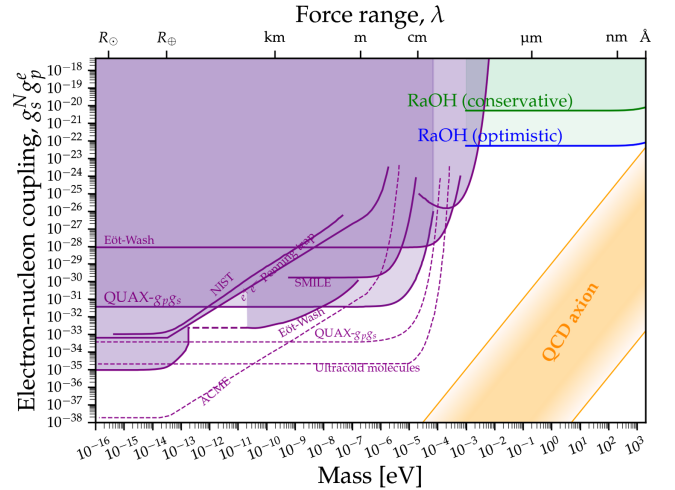


FIG. 6. The existing laboratory constraints on the $g_{e,p} g_{N,s}$ and the projected RaOH constraints. The conservative constraint corresponds to the present level of energy split measurement achieved on diatomics, whereas the optimistic ones are given by the expected increase of precision on the triatomic molecules.

constraint. It is expected [55] that for the triatomic molecules this sensitivity may be improved by about 2 orders of magnitude, which yields the optimistic constraint. This is still not enough to beat the astrophysical constraints coming from the red giants $g_{e,P}g_{N,S} < 10^{-26}$; however, this would make such molecular experiments best among laboratory experiments for the mass range $m_a > 1$ eV.

Radium is a heavier atom than ytterbium, which has resulted in higher values for sensitivities to such interactions as eEDM and NE-SPS for RaOH compared to YbOH molecules [31,35]. One could expect a higher value for the considered axion-mediated effect in the RaOH molecule, but this is not the case. Hence, while our result shows that the RaOH molecule is less sensitive to this particular interaction, this result nevertheless is interesting. On the other hand, it is important to know such parameters for future experiments. Considering a different ratio with YbOH value of this parameter compared to the eEDM and NE-SPS parameters, performing the measurement with

different molecules would allow one to distinguish different $\mathcal{P}$, $\mathcal{T}$ -odd effects from each other. Compared to YbOH, the eEDM and NE-SPS parameters for the RaOH are amplified by the same factor. In contrast, the axion-mediated interaction is significantly reduced. This could facilitate the distinguish of these effects.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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