

Study of nuclear magnetic quadrupole moments at triatomic molecules

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C,P,T-invariance and its violations

These transformations were supposed not to change laws of nature:

$$P : \vec{r} \rightarrow -\vec{r}$$

$$T : t \rightarrow -t$$

$$C : q \rightarrow -q$$

Some interactions have Hamiltonians which are noninvariant with respect to these transformations.

Example with electron and its EDM

According to Wigner–Eckart theorem:

$$\vec{d}_e = \alpha \vec{s}$$

Under the mentioned transformations:

$$P : \quad -\vec{d}_e = \alpha \vec{s}$$

$$T : \quad \vec{d}_e = \alpha(-\vec{s})$$

So, existence of nonzero electric dipole moment of the electron (or any other particle) would indicate simultaneous P,T-violation.

Nuclear magnetic quadrupole moment arising

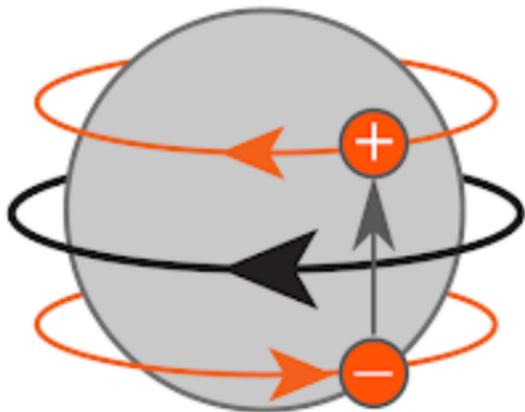


Figure: Rotation of the nucleon with EDM as a source of nuclear MQM
(figure from <http://www.hutzlerlab.com/research/nuclear-mqm>)

Nuclear MQM can also have collective nature, but even in this case it is also violating fundamental symmetries.

Efforts to detect NMQM

Most of experiments searching for nuclear MQMs are studying interaction of NMQM with the electrons at the molecules with heavy atoms.

Interaction of the NMQM with the electron is described by the Hamiltonian:

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

Here: M is the value of NMQM,

I is the nuclear spin,

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

$\vec{\alpha}$ are Dirac α -matrices

and \vec{r} is the electron displacement.

CP-odd energy shift

The aforementioned interaction leads to CP-odd energy shift of the molecular electronic levels:

$$\delta E \sim W_M \cdot M,$$

which is proportional to molecular constant

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

Calculation of this constant for some triatomic molecules is the main goal of the present study.

Historical background

Results of search for NMQM with several molecules

Molecule	$ W_M , 10^{33} \frac{\text{Hz}}{\text{e}\cdot\text{cm}^2}$	$ \delta E \leq \dots \text{ mHz}$	$ M \lesssim \dots, \text{ e}\cdot\text{cm}^2$
YbF (2011) ^a	1.3	6	$5.0 \cdot 10^{-35}$
HfF ⁺ (2017) ^b	0.5	0.6	$1.0 \cdot 10^{-35}$
ThO (2018) ^c	1.6	0.24	$1.5 \cdot 10^{-36}$
YbOH (soon)	1.1
LuOH ⁺ (soon)	1.3

^aJ.J. Hudson *et.al.*, Nature;

^bW.B. Cairncross *et.al.*, Physical Review Letters;

^cThe ACME Collaboration, Science;

Chosen molecules

The present study is devoted to calculation of W_M constant for YbOH molecule and LuOH^+ molecular cation.

Their advantages:

- ▶ heavy atom (effect is scaled as Z^2);
- ▶ open electronic shell;
- ▶ high nuclear spin $I(\text{Yb}) = 5/2$ and $I(\text{Lu}) = 7/2$;
- ▶ may be cooled by laser technique and polarized.

Many-electron system study

Electronic shells are described in terms of Dirac-Fock orbitals:

$$(\hat{h} + \hat{J} - \hat{K})\psi_i = \varepsilon_i\psi_i$$

\hat{h} is one-electron Hamiltonian;

\hat{J} is electron-electron Coulomb interaction;

\hat{K} is electron *exchange* operator;

ε_i is electron orbital energy of i -th electron;

ψ_i is its wavefunction in one-electron approximation.

The all-electron wavefunction is constructed as the corresponding determinant:

$$\Phi = \det\{\psi_1(x_1), \dots, \psi_N(x_N)\}$$

Electron correlation consideration

In order to obtain molecular wavefunction beyond the one-electron approximation, the *coupled cluster approach* was used. It is based on exponential form of the wavefunction:

$$\Psi = \exp(\hat{T})\Phi$$

Excitation operator includes excitations of different orders:

$$\hat{T} = \hat{T}_1 + \hat{T}_2 + \hat{T}_3 + \dots,$$

and \hat{T}_i may be written as, i.e.

$$\hat{T}_1 = \sum_{\substack{i \in \text{occupied} \\ a \in \text{virtual}}} \hat{T}_i^a = \sum_{\substack{i \in \text{occupied} \\ a \in \text{virtual}}} t_i^a \hat{a}^+ \hat{i}$$

with unknown amplitudes t_i^a .

Example

$$\hat{T}_i^a \begin{vmatrix} \psi_1(x_1) & \dots & \psi_1(x_N) \\ \vdots & & \vdots \\ \psi_i(x_1) & \dots & \psi_i(x_N) \\ \vdots & & \vdots \\ \psi_N(x_1) & \dots & \psi_N(x_N) \end{vmatrix} = t_i^a \begin{vmatrix} \psi_1(x_1) & \dots & \psi_1(x_N) \\ \vdots & & \vdots \\ \psi_a(x_1) & \dots & \psi_a(x_N) \\ \vdots & & \vdots \\ \psi_N(x_1) & \dots & \psi_N(x_N) \end{vmatrix}$$

Coupled cluster equations

The substitution $\Psi = \exp(\hat{T})\Phi$ modifies the Schrödinger equation:

$$\exp(-\hat{T})\hat{H}\exp(\hat{T})\Phi = E\Phi.$$

Now it is system of nonlinear scalar equations with unknown excitation amplitudes t_{ij} and total energy E .

(Φ is Dirac-Fock wavefunction, it is determined on the previous step)

Calculation of mean values

Hellmann-Feynman theorem states, that for the eigenvalue E_λ and the eigenfunction ψ_λ of the Hamiltonian $\hat{H}(\lambda)$ with the free parameter λ the following equation takes place:

$$\frac{dE_\lambda}{d\lambda} = \langle \psi_\lambda | \frac{d\hat{H}(\lambda)}{d\lambda} | \psi_\lambda \rangle.$$

If one defines $\hat{H}(\lambda) = \hat{H}_0 + \lambda\hat{A}$, the HFT gives the way to calculate mean value of an arbitrary operator \hat{A} :

$$\bar{A} = \left. \frac{dE_\lambda}{d\lambda} \right|_{\lambda=0}$$

Results for YbOH

The final results for YbOH molecule are:

$$W_M = -1.07(6) \cdot 10^{33} \frac{\text{Hz}}{e \cdot \text{cm}^2}$$

$$M = 1.0 \cdot 10^{-27} \bar{\theta} e \cdot \text{cm}^2 + 0.6 \cdot 10^{-10} (\tilde{d}_u - \tilde{d}_d) e \cdot \text{cm}$$

Current limitations for $\bar{\theta}$ and $|\tilde{d}_u - \tilde{d}_d|$ (are obtained from neutron EDM measurement) would lead to energy shift $\delta E \simeq 60 \mu\text{Hz}$, and the experiment is expected to be highly more sensitive.

Results for LuOH⁺

The final results for YbOH molecule are:

$$W_M = -1.25(10) \cdot 10^{33} \frac{\text{Hz}}{e \cdot \text{cm}^2}$$

$$M = 1.6 \cdot 10^{-27} \bar{\theta} e \cdot \text{cm}^2 + 0.7 \cdot 10^{-10} (\tilde{d}_u - \tilde{d}_d) e \cdot \text{cm}$$

The corresponding energy shift is expected to be ~ 2 times higher than the one for YbOH. So, obtainment of new restrictions for fundamental parameters of Standard Model is possible with both of these molecules.

Thank you for your attention!