Chirality of a molecule and its anapole moment: theory

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Ref.: T. Fukuyama, T. Momose & DN, arXiv:1505.03888 [hep-ph], to appear in Eur. Phys. J. **D**

Anapole Moment: Definition

Suppose that there is a point particle f at rest in an external magnetic field. If the interaction Hamiltonian H_{ana} between f and the magnetic field $\vec{B}$ is given by

$$H_{\text{ana}} = -\vec{a} \cdot (\nabla \times \vec{B}) ,$$

then the vector $\vec{a}$ is called the **anapole moment** of f.

(I. B. Zel'dovich, JETP **33** (1957) 1531)

- If f has a non-zero spin, then $\vec{a} \propto \overrightarrow{\text{spin}}$
- H_{ana} is P-odd and T-even
  cf:
  EDM $\vec{d}$: $H_{\text{EDM}} = -\vec{d} \cdot \vec{E}$ (P-odd, T-odd)
  MDM $\vec{\mu}$: $H_{\text{MDM}} = -\vec{\mu} \cdot \vec{B}$ (P-even, T-even)

Anapole moment of a spin-1/2 particle

For a spin-1/2 particle f, in the language of field theory,

$$\langle f(p')|J_\mu^{\text{em}}|f(p)\rangle = \bar{u}_f(p')\Gamma_\mu u_f(p) \ ,$$

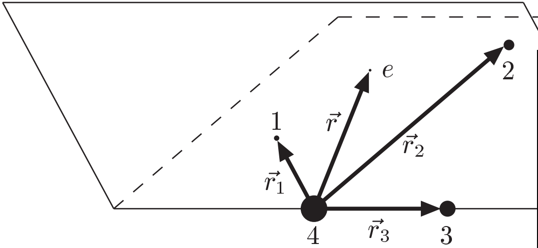
$$\Gamma_\mu = F_1(q^2)\gamma_\mu + \frac{i}{2m_f}F_2(q^2)\sigma_{\mu\nu}q^\nu - F_3(q^2)\sigma_{\mu\nu}q^\nu\gamma_5 - F_4(q^2)(\gamma_\mu q^2 - 2m_f q_\mu)\gamma_5$$

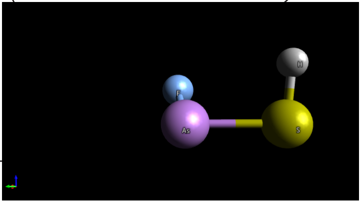
It is known that there are no other independent form factors of a spin-1/2 particle other than $F_1(q^2), \ldots, F_4(q^2)$ (See e.g., Nowakowski, Paschos, & Rodriguez, physics/0402058)

$F_1(0) = -eQ_f$	(electric charge)
$F_2(0) = -eQ_f a_f$	(a_f : anomalous magnetic moment)
$F_3(0) = d_f$	(EDM)
$F_4(0) = \tilde{a}_f$	(anapole moment)

If f is a Majorana particle, then $F_1(q^2) = F_2(q^2) = F_3(q^2) = 0$.

We have computed **the contribution from the chirality to the anapole moment of the chiral 4-atom molecule**,





which is the simplest molecule which has non-trivial chirality.
Here, parity is violated by the configuration of the atoms.

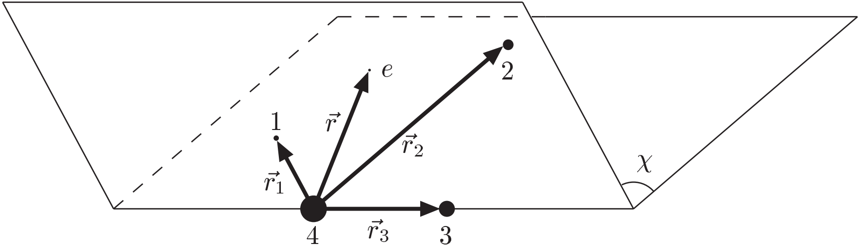
Our Setup:

- There is an unpaired electron e localized around the atom 4.
- Atom 4: the heaviest. Atom 3: the second heaviest

(the same setup as in Khriplovich & Pospelov, Z. Phys. **D17** (1990) 81).

Our calculation: Anapole moment of a chiral molecule

We have computed the contribution from the chirality to the anapole moment of the chiral 4-atom molecule,



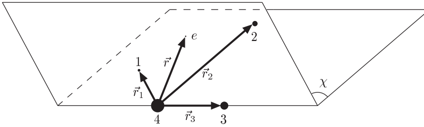
Our Assumptions:

- The Coulomb interactions between e and atoms 1 and 2 are treated as perturbation.
- The effect from atom 3 on e is taken into account as a slight shift of energy levels.

(the same assumptions as in Khriplovich & Pospelov, Z. Phys. **D17** (1990) 81).

Synopsis of our calculation (1)

We have computed **the contribution from the chirality to the anapole moment of the chiral 4-atom molecule**



If we choose $|p_{3/2}, 3/2\rangle$ to be the unperturbed state, then the states $|p_{1/2}\rangle$ and $|s_{1/2}\rangle$ mix into $|p_{3/2}, 3/2\rangle$ as a result of perturbation.
We sandwich the anapole operator $\vec{A} = \vec{a}\delta(\vec{r})$, where $\vec{a} = -\pi \int d^3\vec{r}\, r^2 \vec{j}(\vec{r})$, by these states: $\Longrightarrow$ Only those terms survive in which $\vec{a}$ is sandwiched by $|p_{1/2}\rangle$ and $|s_{1/2}\rangle$.

Synopsis of our calculation (2)

Our result:

$$\langle \vec{a} \rangle = \frac{\pi e}{m_e} \frac{4}{45} \left[r_1(s,p) - 4 r(s,p) \right] \frac{(\mathrm{Ry})^2}{E_s E_p} Z_1 Z_2$$
$$\times (\vec{J} \cdot \vec{n}_3)(\vec{n}_1 \cdot [\vec{n}_2 \times \vec{n}_3])$$
$$\times \left[C_1(r_1) C_2(r_2) \vec{n}_2 - C_1(r_2) C_2(r_1) \vec{n}_1 \right] ,$$

which is proportional to the P-odd geometric factor $(\vec{n}_1 \cdot [\vec{n}_2 \times \vec{n}_3])$, as expected. The red factors do not agree with Khriplovich-Pospelov.

$$r(s,p) \equiv \int_0^\infty dr \; r^3 R_s(r) R_p(r) \; ,$$

$$r_1(s,p) \equiv \int_0^\infty dr \; r^4 \left(R_s(r) \frac{dR_p(r)}{dr} - R_p(r) \frac{dR_s(r)}{dr} \right) \; ,$$

$$C_k(r_i) \equiv a_0 \int_0^\infty dr \; r^2 R_{1/2}(r) R_{3/2}(r) \left[\frac{r_i^k}{r^{k+1}} \theta(r - r_i) + \frac{r^k}{r_i^{k+1}} \theta(r_i - r) \right] ,$$

Synopsis of our calculation (3)

We have extended the analysis of ours (and Khriplovich and Pospelov's) to the cases where the initial (unperturbed) state is either $|s_{1/2}\rangle$ or $|p_{1/2}\rangle$.
When the initial state is $|s_{1/2}\rangle$,

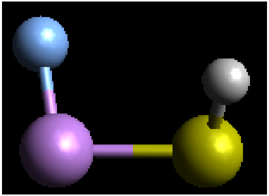
$$\begin{aligned}\langle\vec{a}\rangle = &\frac{2e\pi}{15m_e}\left(r_1(s,p) - 4r(s,p)\right)\left(\frac{1}{E(s_{1/2})-E(p_{3/2},3/2)} - \frac{1}{E(s_{1/2})-E(p_{3/2},-1/2)}\right)\frac{(\mathrm{Ry})^2}{E(s_{1/2})-E(p_{1/2})}Z_1 Z_2\left[\vec{n}_3\cdot\left(\vec{n}_1\times\vec{n}_2\right)\right] \\ &\times\left\{C_1(r_1)C_2(r_2)\vec{n}_2 - C_2(r_1)C_1(r_2)\vec{n}_1\right\} - \frac{4e\pi}{15m_e}\left(\tilde{r}_1(s,p)+2\tilde{r}(s,p)\right)\frac{1}{E(s_{1/2},1/2)-E(p_{1/2},-1/2)} \\ &\times\frac{(\mathrm{Ry})^2}{E(s_{1/2},1/2)-E(p_{3/2},1/2)}Z_1 Z_2\left[\vec{n}_3\cdot\left(\vec{n}_1\times\vec{n}_2\right)\right]\left\{\tilde{C}_1(r_1)C_2(r_2)\vec{n}_2 - C_2(r_1)\tilde{C}_1(r_2)\vec{n}_1\right\}\end{aligned}$$

and, similarly, in the case where $|p_{1/2}\rangle$ is the unperturbed state,

$$\begin{aligned}\langle\vec{a}\rangle = &+\frac{2e\pi}{15m_e}\left(r_1(s,p) - 4r(s,p)\right)\left(\frac{1}{E(p_{1/2})-E(p_{3/2},3/2)} - \frac{1}{E(p_{1/2})-E(p_{3/2},-1/2)}\right)\frac{(\mathrm{Ry})^2}{E(p_{1/2})-E(s_{1/2})}Z_1 Z_2\left[\vec{n}_3\cdot\left(\vec{n}_1\times\vec{n}_2\right)\right] \\ &\times\left\{C_1(r_1)C_2(r_2)\vec{n}_2 - C_2(r_1)C_1(r_2)\vec{n}_1\right\} + \frac{4e\pi}{15m_e}\left(\tilde{r}_1(s,p)+2\tilde{r}(s,p)\right)\frac{1}{E(p_{1/2},1/2)-E(s_{1/2},-1/2)} \\ &\times\frac{(\mathrm{Ry})^2}{E(p_{1/2},1/2)-E(p_{3/2},-1/2)}Z_1 Z_2\left[\vec{n}_3\cdot\left(\vec{n}_1\times\vec{n}_2\right)\right]\left\{\tilde{C}_1(r_1)C_2(r_2)\vec{n}_2 - C_2(r_1)\tilde{C}_1(r_2)\vec{n}_1\right\}\end{aligned}$$

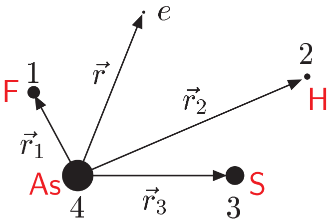
Concrete Example

Example of 4-atom chiral molecules: **FAsSH**



Molecular data:

$$\begin{aligned} &(Z_1, Z_2, Z_3, Z_4) = (9, 1, 16, 33), \\ &E(s_{1/2}) - E(p_{1/2}) = 29000\ [\mathrm{cm}^{-1}], \\ &E(p_{3/2}) - E(p_{1/2}) = 2500\ [\mathrm{cm}^{-1}], \\ &\vec{r}_1 = (0.83, -1.52, -0.29)\ [\text{Å}], \\ &\vec{r}_2 = (1.34, 0.00, 2.37)\ [\text{Å}], \\ &\vec{r}_3 = (0.00, 0.00, 2.23)\ [\text{Å}], \end{aligned}$$



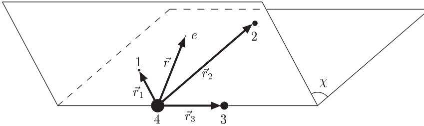
Result: $\langle \vec{a} \rangle \cdot \vec{n}_3 = 0.17\ \mu_B a_0$,

where μ_B is the Bohr magneton and a_0 the Bohr radius

Consistent with a very rough estimate by Khriplovich-Pospelov, $\langle \vec{a} \rangle \cdot \vec{n}_3 \simeq \mu_B a_0$

Summary and Discussions

We have computed the **anapole moment** of the 4-atom chiral molecule.



- Parity is violated by the configuration of the atoms, and a non-zero anapole moment is induced.
- We have corrected errors in a preceding study
- We have extended the framework to the cases where the initial (unperturbed) state is $|s_{1/2}\rangle$ or $|p_{1/2}\rangle$
- A similar method can be applied to the calculation of **the energy difference between enantiomers** due to Z-boson exchange (Khriplovich)
- See Momose-san's talk for experimetal aspects