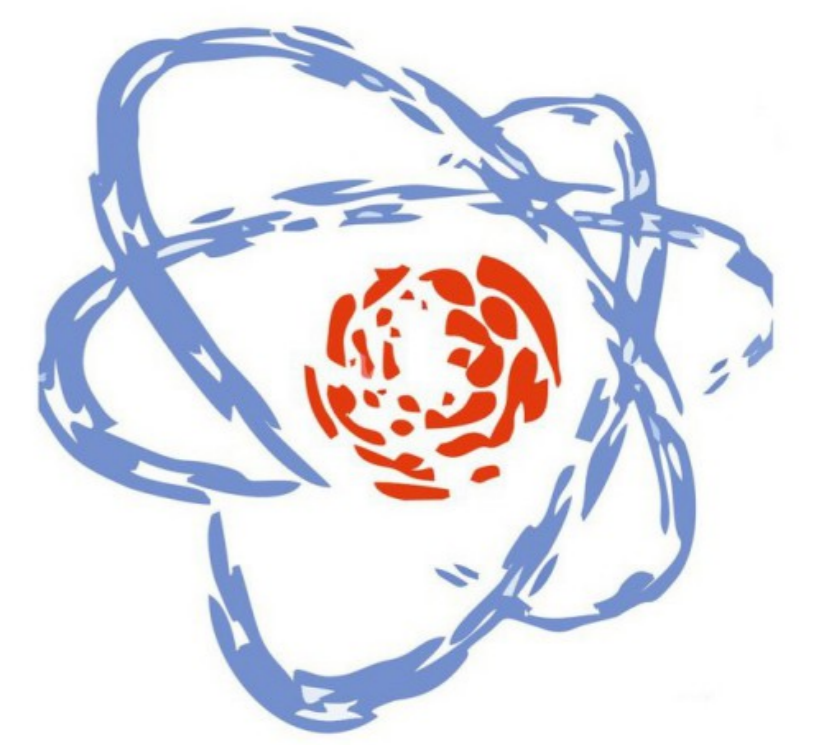


Coefficient of the anapole moment's enhancement in SiO^+ molecule



P. D. Turchenko*, L. V. Skripnikov

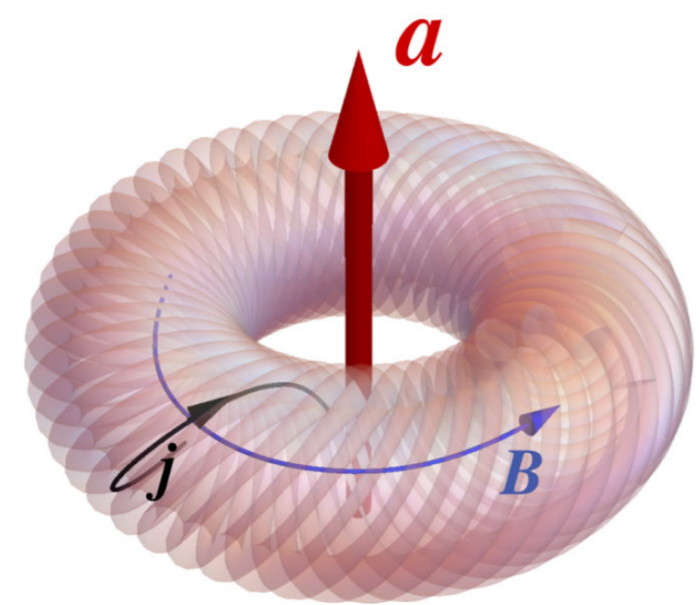
Petersburg Nuclear Physics Institute named by B.P. Konstantinov of National Research Centre "Kurchatov Institute" (NRC "Kurchatov Institute" - PNPI), 1 Orlova Roscha, Gatchina, Leningradskaya Oblast, Russia, 188300 and Saint Petersburg State University, 7-9 Universitetskaya Embankment, St Petersburg, Russia, 199034

*p.d.turchenko@vk.com

Abstract

Within the framework of fully relativistic approaches to describe multielectronic systems, the anapole moment gain in the cation was calculated $^{29}Si^{16}O^+$, equal to $W_a = 14.4$ Hz, the error does not exceed 3%. The obtained value can be used in interpreting the results of experiments by measurement of the anapole moment in the indicated cation. Some spectroscopic constants for the $X^2\Sigma_{1/2}^+$, $A^2\Pi_{1/2}$, $A^2\Pi_{3/2}$, $B^2\Sigma_{1/2}^+$ states have also been clarified at the level of quadruple excitations, necessary for setting up experiments on laser cooling of this molecule.

Anapole moment



Anapole moment \mathbf{a} of the system is defined as:

$$\mathbf{a} = -\pi \int r^2 \mathbf{j}(\mathbf{r}) d^3r,$$

where $\mathbf{j}(\mathbf{r})$ — is the bulk current density [1]. Among its properties we can emphasize the following:

1. the anapole contribution to the vector potential has the form $\mathbf{A}_a(\mathbf{R}) = \mathbf{a}\delta(\mathbf{R})$;
2. only nuclei with nonzero spin I can have the anapole moment \mathbf{I} , since $\mathbf{a} \sim \mathbf{I}$;
3. anapole arises as a result of intranuclear forces that violate \mathcal{P} -parity.

Figure 1: Classical analog of the anapole – toroidal winding with current

SiO^+ cation

In the present work, the $^{29}Si^{16}O^+$ molecule was studied. This choice is due to the fact that in two-atomic molecules there are rotational levels of opposite parity close in energy, which can be used to enhance the effects of \mathcal{P} parity violation. The properties of SiO^+ include the following:

1. the ^{16}O nucleus does not possess nuclear spin, while ^{29}Si – does, so the properties of the anapole moment will be localized on the latter;
2. SiO^+ molecule consists of light elements, which contributes to a simpler interpretation from the point of view of nuclear theory, since light nuclei require less laborious calculations.

Detection of the anapole moment using a molecule allows us to relate the experimental observations to the property of the nucleus.

Literature review

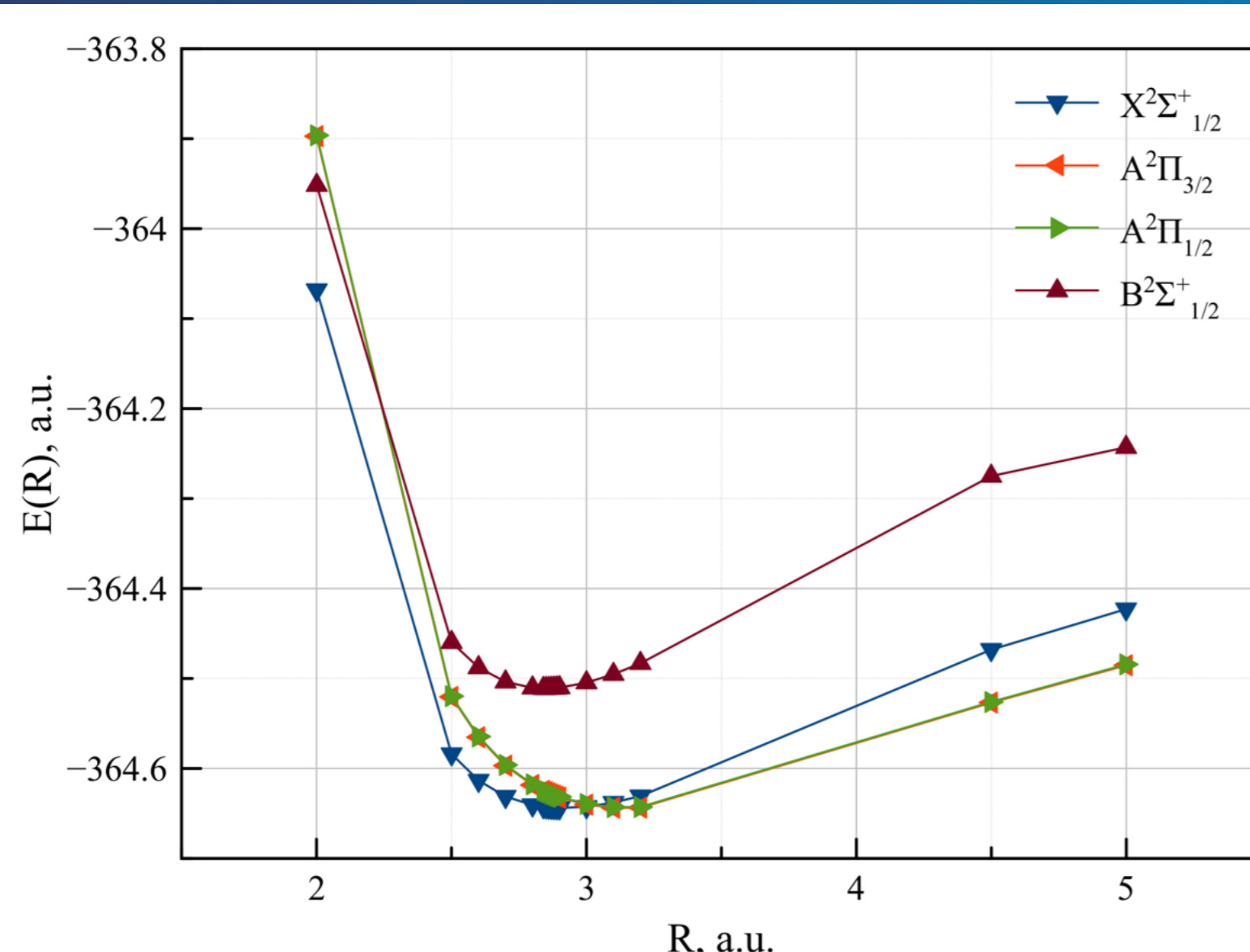
To date, the anapole moment of the nucleus was measured in 1997 in the ^{133}Cs atom, but the error of the experiment was impressive [2]. Also in 2018 an upper limit was placed on the value of the anapole moment in the $^{138}Ba^{19}F$ molecule [3]. More recently, a paper has appeared [4], which describes an experiment to determine the anapole moment in the $^{29}Si^{16}O^+$ cation. In the experiment, the authors plan to obtain the signal $S \sim k_a W_a$, where k_a — is a dimensionless constant related to the anapole moment (its determination is the ultimate goal of the joint work of theorists and experimenters on the way of searching for the anapole moment), W_a is the molecular parameter of the interaction between the anapole moment and electrons, the calculation of which is the goal of the present work.

Computational methods

- The Dirac-Hartree-Fock (DHF) method was used for rough estimates and to obtain the Slater determinant
- The method of connected clusters (CC) was used to obtain high-precision results.
- W_a is calculated by the finite field method. The Hamiltonian of the system H is written through H_0 (Dirac-Coulomb Hamiltonian) and λ (numerical parameter) in the form $H = H_0 + \lambda W_a$, $\lambda \ll 1$. By the Gelman-Feynman theorem, knowing the eigenenergies E of the Hamiltonian H , we can find

$$\langle W_a \rangle = \left. \frac{\partial E(\lambda)}{\partial \lambda} \right|_{\lambda=0} \approx \frac{E(\lambda) - E(-\lambda)}{2\lambda}.$$

Potential energy curves at the CCSD level



Transition energies

The table presents the transition energies from some experiments in comparison with the energies obtained in the present work (the data are taken from [5]):

Transition energies to different excitation levels, values are in Hz

	$A^2\Pi_{1/2}$	$A^2\Pi_{3/2}$	$B^2\Sigma_{1/2}^+$
This work	1530	1680	25914
E.A. Colbourn et al., 1978		887	25740
S.N. Ghosh, et al., 2003			26017
R. Cameron et al., 1995		2242	26016

The values in this work were obtained by the CCSD(T) method. It can be seen that the energies of the $B^2\Sigma_{1/2}^+$ state are not far from each other, the energies of the $A^2\Pi_{3/2}$ are different. The challenge is to find out what causes this difference. A solution is currently being sought.

Coefficient W_a

At the CCSDT(Q) level, a W_a value was obtained at $R = 2.9$ a.u. (the equilibrium value was 2.87 a.u., equal to (14.4 ± 0.2) Hz Hz. The large error arises from the difference in the values obtained when taking different bases. At this point, a few steps remain to be taken to minimize that difference

Conclusions

In this work, the value of W_a at the CCSDT(Q) level was obtained and the energies of transitions to excited states at the CCSD(T) level were calculated. Currently, the value of W_a is refined at the CCSDTQ(P) level, averaged over vibrational frequencies, and its basis error is minimized. The energies of transitions to excited states are estimated at the CCSDT(Q) level.

Literature

1. I. B. K. V. V. Flambaum, *Journal of Experimental and Theoretical Physics* **79**, 1656 (1980).
2. C. S. W. et al., *Science* **275** (1997).
3. E. A. et al., *Physical Review Letters* **120** (2018).
4. J. K. et al., *arXiv* **2310.11192v1** (2023).
5. R. L. et al., *Chemical Physics* **525** (2019).