^{129}Xe elektrinio dipolinio momento tyrimai atlikti daugiakonfigūracinio Dirako, Hartrio ir Foko artinyje

Multiconfiguration Dirac-Hartree-Fock calculations of atomic electric dipole moments for ^{129}Xe

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The existence of a non-zero permanent electric dipole moment (EDM) of an elementary particle or a composite system of particles would violate time reversal symmetry (T), as well as the combined charge conjugation and parity symmetry (CP), due to the CPT theorem [1]. One of the principal motivations behind the experimental searches of EDMs is to shed light on the observed matter-antimatter asymmetry in the Universe. The standard model cannot explain the matter-antimatter asymmetry in the Universe, as it predicts sources of CP violation (and of EDMs) several orders of magnitude weaker than those necessary to account for the observed baryon numbers. This leads to proliferation of the extensions to the Standard Model. Some of these extensions predict larger EDMs, sometimes within the reach of current experiments.

In the present work we computed the EDMs in the ground states of diamagnetic atom ^{129}Xe and compare our results with those of other authors. Our results were obtained within the multiconfiguration Dirac-Hartree-Fock (MCDHF) method, using the relativistic atomic structure package GRASP2K [2], which has been employed in the calculations of matrix elements of (P,T)-odd e-N tensor-pseudotensor (TPT) and pseudoscalar-scalar (PSS) interactions, nuclear Schiff moment (SM), and interaction of electron electric dipole (eEDM) moment with nuclear magnetic moments.

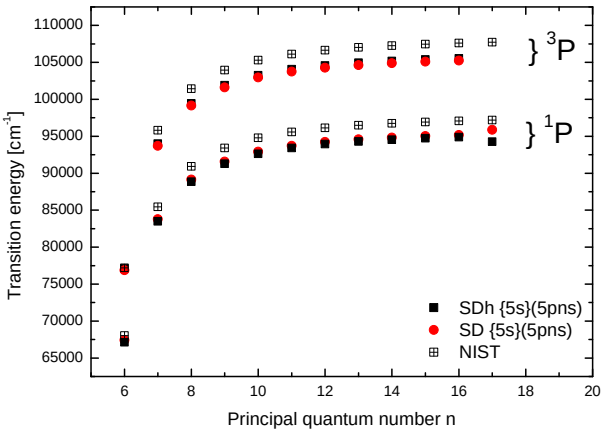

FIG. 1. Excitation energies of states $5p^5\ ns\ ^{1,3}P_1$ from strategies SD {5s}(5pns) and SDh {5s}(5pns) compared with NIST data base recommended values.

Calculations were performed for the ground state ($5p^6\ ^1S_0$) and for all excited states ($5p^5\ ns\ ^{1,3}P_1$) separately. Active space (AS_L, $L = 0-3$) of virtual orbitals for the ground and excited states was generated by single and double substitutions (SD) from $5s, 5p$ and ns shells, respectively. Sets of virtual orbitals (Layers L) included angular symmetries up to $l = s, p, d, f, g$ and listed below:
$L_0 = \{ns, np, nd, nf\}$;
$L_1 = \{(n+1)s, (n+1)p, (n+1)d, (n+1)f, (n+1)g\}$...
Active space (AS_L, $L = 0-3$) of virtual orbitals constructed in the following way:
$AS_0 = L_0$; $AS_1 = L_0 + L_1$...
At each stage only the outermost layer is optimized and the remaining orbitals (spectroscopic as well as other virtual layers) are kept frozen, this strategy was called SD {5s}(5pns). Later h symmetry was included in layers of orbitals (this strategy was called SDh {5s}(5pns)). Energies of levels $5p^5\ ns\ ^{1,3}P_1$ were computed up to $n = 16$, using these strategies. Computed energy levels are compared with NIST database in the Figure 1. The average energy difference is 0.021 ± 0.005, and 0.018 ± 0.006, for the first and the second strategy, respectively.

Using the wave functions obtained with these methods the contributions from four interactions were computed and are presented in the Table 1.

Table 1. TPT, PSS, SM, and eEDM contributions to atomic EDM of states $5p^5\ ns\ ^{1,3}P_1$ for Xe computed in strategies SD {5s}(5pns) and SDh {5s}(5pns).

Strategy	TPT	PSS	SM	eEDM
SD {5s}(5pns)	0.22	0.63	0.15	0.23
SDh {5s}(5pns)	0.23	0.66	0.16	0.24
[3](DHF)	0.45	1.3	0.29	0.85
[3](RPA)	0.57	1.6	0.38	1.0

More details about the computations and strategies will be provided during the conference.

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Keywords: tensor-pseudotensor interactions, pseudoscalar-scalar interactions, nuclear Schiff moment, electron electric dipole moment.

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