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Correction for Vibrational Frequencies to the Molecular Parameter Characterizing Nuclear Spin-Dependent Parity-Violating Effects in the $^{29}Si^{16}O^+$ Cation

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In an earlier work [1], the calculation of the molecular parameter W_a, which characterizes nuclear spin-dependent effects parity violating (NSD-PV) in the $^{29}Si^{16}O^+$ cation for the ground state, was discussed. One of these effects is the nuclear anapole moment [2], which dominates in NSD-PV [3]. The work [1] lists various sources of contributions and their uncertainties, to which the vibrational correction of the molecule can also be added.

When taking the vibrational correction into account in the first approximation, it becomes clear that to describe it correctly, non-adiabatic effects must be considered. In the adiabatic approximation, the terms of the ground $\Sigma\frac{1}{2}$ state and the excited $\Pi\frac{1}{2}$ state "repel" each other due to spin-orbit interaction. As a result, the function $W_a(R)$ (where R is the internuclear distance) has a discontinuity at the "pseudo-crossing" point of these terms, which prevents proper averaging over the vibrational frequencies of the ground state. Therefore, to solve the non-adiabatic vibrational problem using scalar-relativistic calculations, it is necessary to include the non-diagonal matrix element of the spin-orbit interaction between these terms.

In this work, using the coupled-channel method [4], a solution to the non-adiabatic vibrational problem is discussed, and a Python program was written to calculate non-adiabatic vibrational wave functions. The obtained result is essential for the interpretation of an experiment being prepared by a group from MIT [5], which aims to refine the Standard Model in the sector of weak interactions.

References

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