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Improving the hyperfine structure theory in hydrogen molecular ions

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The hydrogen molecular ions H2+ and HD+ are promising systems for fundamental constants metrology. Their spectrum offer many ultra-narrow ro-vibrational transitions, the frequencies of which are sensitive to the proton-electron mass ratio, proton charge radius, and Rydberg constant [1]. Several projects aiming at high-accuracy measurements using Doppler-free spectroscopy schemes [2-4] are in progress.
The interpretation of experimental data requires improved theoretical description of the hyperfine structure [4]. The leading terms of the hyperfine Hamiltonian, i.e. the spin-spin Fermi contact interactions, have been calculated with high precision [5], but the theoretical accuracy is limited by the spin-orbit and spin-spin tensor interactions, which have been so far evaluated in the framework of the Breit-Pauli Hamiltonian [6,7]. The calculation of higher-order relativistic corrections to these interaction terms, following the NRQED approach, will be presented.
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