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Relativstic corrections to the hyperfine structure of hydrogen molecular ions

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Recent advances of Doppler-free rovibrational spectroscopy of HD+ ions [1,2] underline the high potential of these systems for accurate tests of molecular theory and determination of fundamental constants. However, analysis of experimental data is made more complex by the hyperfine structure. Measurement of a sufficient number of hyperfine components is required in order to extract a spin-averaged rovibrational transition frequency [3], which can then be accurately compared to the theory [4]. In practice, this may be difficult to achieve due to technical reasons [1,2], and one then has to use the theoretical determination of hyperfine shifts to extract the spin-averaged transition frequency. In Ref [1] the comparison between theory and experiment was limited by the HD+ hyperfine structure theory.

In this poster we will describe our calculations of relativistic corrections to the hyperfine structure of HD+ and H2+, especially to the spin-orbit and spin-spin tensor interactions. The complete effective Hamiltonian at orders m alphaˆ6 and m alphaˆ6 (m/M) is derived in the NRQED framework. Induced corrections are then calculated by applying the nonrelativstic perturbation theory, using three-body variational wavefunctions. Comparisons are made with experimental data whenever available.

[1] S. Alighanbari et al., Nature Phys. 14, 555 (2018).
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[4] V.I. Korobov, L. Hilico, J.-Ph. Karr, Phys. Rev. Lett. 118, 233001 (2017).

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