Nonadiabatic QED correction for hydrogen molecule

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The hydrogen molecule lies on the bleeding edge of both experimental and theoretical spectroscopy. Agreement between them at the 1 MHz level and below allows for verification of quantum electrodynamical (QED) and nonadiabatic effects description in bound systems, as well as serves as a cross-check for measurements. On the other hand, a discrepancy can be even more interesting and stimulating for research. For example, despite the constant progress in the theory [1] and the experiment [2], there still exist transitions in HD (e.g. 1–0 $R(0)$) with a noticeable ($\approx 2\sigma$) disagreement. The most likely cause on the theoretical side are the mixed nonadiabatic-QED effects, which have previously been included only for the ground rovibrational state of H_2 [3].

Derivation of formulas for these contributions is quite demanding in the perturbational (NAPT) framework. Instead, we approach the problem by solving the full Schrödinger equation in a "fully nonadiabatic" basis of explicitly correlated Gaussian (ECG) functions, which contain the electronic and the nuclear coordinates on an equal footing. This allows us to include the nuclear-mass-related effects even beyond the leading ones, as well as bypass difficulties present in the perturbational calculations, at the cost of doing it separately for each level considered. We hope our work can restore the consistency between the theory and the experiment for these problematic transitions, as well as help improve the quality of theoretical descripton overall. Furthermore, our precise results can have an added value of being reference points for NAPT calculations in the future.

During the talk, we will describe the methodology used and present the currently available preliminary results.

[1] M. Siłkowski, K. Pachucki, J. Komasa, M. Puchalski, Phys. Rev. A **107**, 032807 (2023)
[2] A. Fast, S. A. Meek, Phys. Rev. Lett. **125**, 023001 (2020)
[3] M. Puchalski, J. Komasa, P. Czachorowski, and K. Pachucki, Phys. Rev. Lett. **122**, 103003 (2019)