From High-Resolution Spectroscopy to Light-Dressed Molecules

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We report new developments in the general quantum-dynamical code GENIUSH [1,2], originally invented to variationally solve the time-independent rovibrational Schrödinger equation for N-atomic molecules using a general and exact kinetic energy operator, arbitrarily-chosen vibrational coordinates and body-fixed frame embeddings. The up-to-date version of GENIUSH includes time-dependent quantum-dynamical features and is able to solve the time-dependent Schrödinger equation for molecules coupled to time-dependent external electric fields. The power of the theoretical framework developed is demonstrated by new time-dependent rovibrational results for the coherent inhibition and enhancement of tunneling in ammonia isotopomers, both achieved by nonresonant laser fields [3]. These time-dependent quantum-dynamical computations rely on the concept of light-dressed states, treat all rotational and vibrational degrees of freedom in a numerically exact way and assume neither the alignment nor the orientation of the molecule under investigation. If time permits, we will also present novel results for the spectroscopy of light-dressed polyatomic molecules with an emphasis on the signature of light-induced conical intersections [4] on light-dressed spectra [5].

References

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