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Coherent inhibition and enhancement of tunneling in ammonia isotopomers

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BEFEKTETÉS A JÖVŐBE

Coherent inhibition and enhancement of tunneling in ammonia isotopomers

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Ammonia has been a prototype molecule for molecular spectroscopy and quantum tunneling dynamics for a long time (e.g., [1,2] and references cited therein). Recently, accurate full-dimensional potential energy and electric dipole moment hypersurfaces have become available for ammonia ([2, 3] and references cited therein). We have further developed and applied the general quantum-dynamical code GENIUSH [4,5] for the variational solution of the rovibrational Schrödinger equation. The numerical construction of the general and exact kinetic energy operator allows the application of arbitrarily chosen internal coordinates and body-fixed frame embeddings, including the Eckart frame. Our up-to-date version of GENIUSH is able to employ a contracted vibrational basis set consisting of products of reduced-dimensional vibrational eigenfunctions, facilitating the computation of highly-excited rovibrational eigenstates. Besides the computation of accurate rovibrational energy levels and wave functions GENIUSH has been extended to include dynamics under coherent infrared multiphoton excitation [6]. Our time-dependent quantum-dynamical computations treat all rotational and vibrational degrees of freedom in a numerically exact way and assume neither the alignment nor the orientation of the molecules under investigation. 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. The schemes proposed in this study achieve control of the time evolution of a quantum state initially localized in one of the potential wells by nonresonant laser fields and extend earlier vibrational studies [7-9].

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