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Time-series analysis of vibrational nuclear wave packet dynamics[1]

UWE THUMM, Kansas State University, THOMAS NIEDERHAUSEN, Kansas State University (now University of Madrid), BERNOLD FEUERSTEIN, Max-Planck Institut fuer Kernphysik, Heidelberg — We discuss the extent to which measured time-dependent fragment kinetic energy release (KER) spectra and calculated nuclear probability densities can reveal 1) the transition frequencies between stationary vibrational states, 2) the nodal structure of stationary vibrational states, 3) the ground-state adiabatic electronic potential curve of the molecular ion, and 4) the progression of decoherence induced by random interactions with the environment. We illustrate our discussion with numerical simulations for the time-dependent nuclear motion of vibrational wave packets in the D_2^+ molecular ion caused by the ionization of its neutral D_2 parent molecule with an intense pump laser pulse. Based on a harmonic time-series analysis, we suggest a general scheme for the full reconstruction, up to an overall phase factor, of the initial wave packets based on measured KER spectra, cf., Phys. Rev. A **77**, 063401 (2008).

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Uwe Thumm
Kansas State University

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