Unveiling the highly nonlinear dynamics of KCN molecular system using Lagrangian descriptors

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In this work [1], we identify the phase-space structures which are responsible for the chaotic dynamics observed in KCN molecular system using the Lagrangian descriptors [3]. We show that the vibrational dynamics of this molecule is strongly determined by the invariant manifolds associated with a particular stretching periodic orbit previously described [2]. Likewise, the representation of these invariant manifolds on a Poincaré surface of section shown in Fig. 1 is also studied, concluding that the intricate depiction that is observed has its origin in the complex behavior of the manifolds, which is a consequence of the strong anharmonicities in the potential energy surface, as inferred from visual inspection of Fig. 2.

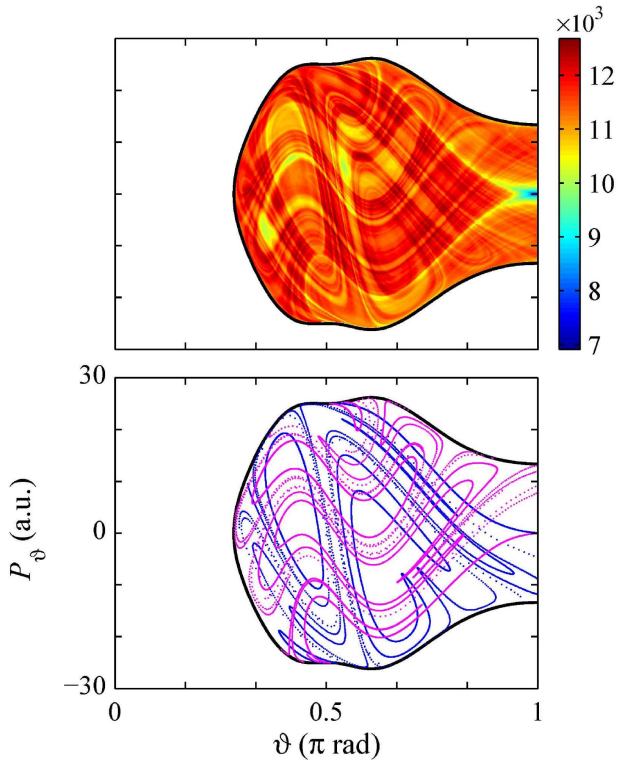

Fig. 1. Cuts of the phase space of the KCN molecular system along the Poincaré surface for a vibrational energy E=1300cm^{-1}. (Top) The Lagrangian descriptors integrated over 437.5 fs are able to unravel the homoclinic tangle (bottom) formed by the intersection of the stable (blue) and the unstable (pink) manifolds.

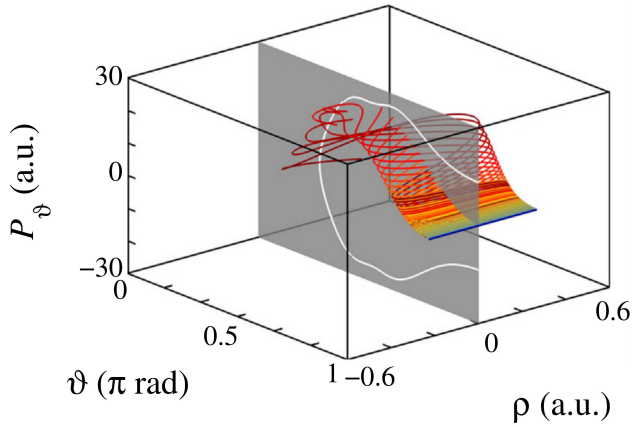

Fig. 2. The invariant manifolds of KCN molecular system are linear close to a stretching periodic orbit (blue line), but they get strongly distorted at larger distances due to the anharmonicities.

[1] F. Revuelta, F.J. Arranz, R.M. Benito, and F. Borondo, *Unraveling the highly nonlinear dynamics of KCN molecular system using Lagrangian descriptors*, Commun. Nonlinear Sci. Numer. Simul. **123**, 107265 (2023).

[2] H. Párraga, F. J. Arranz, R. M. Benito, and F. Borondo, *Above Saddle-Point Regions of Order in a Sea of Chaos in the Vibrational Dynamics of KCN*, J. Phys. Chem. A **122**, 343341 (2018).

[3] C. Lopesino, F. Balibrea-Iniesta S. Wiggins, and A. M. Mancho, *Lagrangian descriptors for two dimensional, area preserving, autonomous and nonautonomous maps*, Commun. Nonlinear Sci. Numer. Simul. **27**, 4051 (2015).