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Covariant measurements of chaos in chemical reaction dynamics[1]

JASON R. GREEN, University of Cambridge, R. STEPHEN BERRY, University of Chicago, DAVID J. WALES, University of Cambridge — Accurate characterization and measurement of classical chaos are needed to place limits on predictions of atomic motion in few-body and many-body systems. Quantifying chaos requires determination of the many local phase-space directions that indicate the sensitivity of motion to initial conditions. Here we show that coordinate-independent (covariant) directions have the qualitative and quantitative properties needed to provide a detailed understanding of the degree of randomness in reaction dynamics. Furthermore, we show that these directions allow accurate determination of time-scale separation in the exploration of phase space. In particular, they reveal separate time scales in the emerging local ergodicity of a model triatomic Lennard-Jones cluster. Over a range of total energies, there is a phase space region of highly chaotic behavior, characterizing motion in each local potential well, and a region with more regular dynamics, characterized by a longer time scale, corresponding to motion across the saddles. Exploiting covariant directions as a computational tool provides new insight into the dynamics of clusters and floppy molecules, and into quantitative theories of nonequilibrium statistical mechanics.

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