Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Relaxation-Excitation Mode Analysis of the Energy Landscape Statistics in Liquids ZHIKUN CAI, YANG ZHANG, University of Illinois at Urbana-Champaign — Despite theoretical and computational advances, a gap still exists between the energy landscape theory and the experimental observables. To bridge this gap, we formulated a relaxation-excitation mode analysis (REMA) framework by incorporating the energy landscape picture into the kinetic theory of liquids. We derived from the Boltzmann equation a coordinate-space relaxation-excitation equation by statistically treating many-body collisions in the locally thermalized "collision zone". The elementary relaxation-excitation mode defined by the Green's function of this equation follows a distribution governed by the intrinsic roughness of the energy landscape. Consequently, the experimentally measurable self intermediate scattering function, e.g. from quasi-elastic and inelastic scattering experiments, becomes a joint Laplace-Fourier transform of the relaxation-excitation mode distribution. Numerical inversion unveils the important statistics of activation barriers and basin excitations of the energy landscape. We examined the self-consistency of REMA on three ideal systems analytically and applied REMA to analyze the hydrogen dynamics of liquid water via ab initio molecular dynamics simulations.

Zhikun Cai
Univ of Illinois - Urbana

Date submitted: 11 Nov 2016 Electronic form version 1.4