Abstract Submitted
for the OSF16 Meeting of
The American Physical Society

Circumventing Non Ergodic Dynamics in Anharmonic Atomic Chains CHRISTOPHER WATENPOOL, DONALD PRIOUR, Youngstown State University — Thermalization of chains in which atoms interact via a harmonic potential is precluded by the lack of interactions among normal modes, and is even hampered in anharmonic chains in the low temperature regime. Using molecular dynamics simulations (averaged over many runs to suppress noise), with Langevin Heat Baths applied at the ends, the energy exchange with the environment provides stochastic input, thereby facilitating equilibration while preserving the internal dynamics of the chain. We examine systems with a finite energy site stored in the lowest harmonic, as well as cold chains with zero energy per site. We use the ensemble averaged effective mode occupancy and effective temperature to calculate the time scale for equilibration. In the low temperature regime, we find the effective temperature (determined from the mean kinetic energy per site) to rise by a factor of two for chains with the fundamental excited before relaxing to the equilibrium value. Times for ensemble averaged mode occupancies to reach a threshold value are threshold independent and follow a smooth power law. For cold chains, relaxation times for the effective temperature are noisy with fluctuations among independent runs comparable to the mean value.

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Date submitted: 11 Sep 2016 Electronic form version 1.4