Abstract Submitted for the OSS15 Meeting of The American Physical Society

Departures from Standard Equipartition for Anharmonically Coupled Masses with a Quartic Term CHRISTOPHER WATENPOOL, DON-ALD PRIOUR, Youngstown State University — Using Monte Carlo simulations, we examine 1D chains of masses where a harmonic coupling is augmented by a quartic perturbation for which the strength may be weak, moderate, or strong. For the case of a single particle in a mixed harmonic/quartic well, thermodynamic observables may be calculated exactly with the thermally averaged potential energy ranging from $\frac{1}{2}k_{\rm B}T$ for the pristine harmonic well (i.e. consistent with standard equipartition) to $\frac{1}{4}k_{\rm B}T$ in the case of a dominant quartic term. We calculate and exhibit mean energies and RMS displacements for a variety of temperatures and perturbation strengths, and we extrapolate to the thermodynamic limit by considering large chains of masses. We comment on how the system auto-correlation time is impacted by the quartic perturbation.

> Christopher Watenpool Youngstown State Univ

Date submitted: 06 Mar 2015

Electronic form version 1.4