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Nonlinear Dynamic Heat Capacity of a Simple Chain Polymer JONATHAN BROWN, JOHN MCCOY, New Mexico Tech — Molecular dynamics simulations were run on a simple bead-spring polymer system, known to be a glass former, with varying amplitude sinusoidal temperature oscillations. Small amplitude sinusoidal temperature produces a small amplitude sinusoidal energy, and dynamic heat capacity is the complex-valued transfer function between the two. For large amplitude temperature oscillations, the energy is no longer sinusoidal, and linear response theory breaks down. Instead, the resulting energy is can be written as a Fourier series. From the Fourier coefficients, we derived the entropy generated per cycle, which is related to the imaginary part of the dynamic heat capacity in the linear limit. Using this, we formulated a nonlinear extension of the dynamic heat capacity.

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