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Characterizing Equilibration Times in Suspended Atomic Chains CHRISTOPHER WATENPOOL, DONALD PRIOUR, Youngstown State University — Carbyne, chains of carbon atoms with alternating single and triple bonds, represents a covalently bonded one dimensional atomic chain, and has been of recent technological interest. Some realizations involve a carbyne chain suspended (e.g., between two graphene flakes). While locally stiff, such a geometry would nevertheless be subject to thermally induced transverse perturbations; we also account for anharmonic effects in the interactions among neighboring carbon atoms. This circumstance, with a weakly anharmonic linear chain experiencing fluctuations in a 3D environment, is fundamentally distinct from the case of a similar chain with motion solely in the longitudinal direction. This contrast presents an opportunity to examine whether equilibration is facilitated by transverse motions or slowed by the presence of long time oscillations as seen in the case of anharmonic chains with only 1D motion allowed. With molecular dynamics simulations, we consider on the one hand an isolated chain with transverse motions allowed and determine if the 3D environment hastens equilibration; we also couple the chains to a heat bath (which would obviate long time oscillations), and we calculate exponents for the asymptotic scaling of equilibration times with respect to the size of the system.

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