Emergence of nonlinear damping in nanomechanical systems from thermal interactions

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Abstract. Atomically thin structures exhibit nonlinear damping that is amplitude-dependent. Different sources for this nonlinearity have been hypothesized, but consensus has not been reached. By performing molecular dynamics simulations, we show that nonlinear damping can emerge from coupling to a thermal bath. We perform ring-down with two different configurations. While an isolated crystalline membrane did not show signatures of nonlinear damping, we find that by linking the same system to a heat bath, ring-down measurements show two thermalization time constants. To confirm our observation, we use nonlinear membrane theory, couple it to a Nose-Hoover thermostat, and find that nonlinear damping is mediated through a quadratic coupling to the heat bath. Our simulations highlight the microscopic origins of damping in nanostructures, demonstrating the influence of heat baths in nonlinear dissipation processes experimentally probed in nanomechanical systems.

Introduction

Unlike typical macroscale structures that exhibit linear damping under external harmonic loadings, atomically thin structures tend to display amplitude-dependent nonlinear behaviour. Different physical sources for this behaviour have been enumerated, including coupling between flexural modes and in-plane phonons [1] and internal resonance [2]. Several studies have proposed that energy transfer between a structure and a thermal bath could also result in nonlinear damping [3]. However, it is hypothesized that these secondary resonators (thermal baths) mostly operate at particular resonances. In order to combine statistical thermodynamics and Newtonian mechanics for particles, molecular dynamics simulations have utilized thermostats to simulate thermal bath energy interactions. These thermostats are designed so that the entire system containing the nanostructure and heat bath satisfies the ergodicity criterion. Here we couple continuum mechanics with a Nose-Hoover thermostat to investigate the mechanical damping that can arise from such thermo-elastic interaction.

Results and Discussion

Simulations utilizing the NVE ensemble (a configuration with constant number of atoms, volume, and energy) conserve the entire atom system's energy. However, it has been demonstrated that if a membrane is not properly pre-tensioned or its effective temperature is low, the energy of the first mode will pass to higher modes and cause damping in the resonator due to thermalization [4]. In order to rule out such a damping, we perform our NVE simulation for a sufficiently pre-tensioned membrane at low temperatures and observe that the resonance is not dampened in a ring-down simulation. With the addition of interactions with a heat bath (NVT ensemble), however, the resonances exhibit nonlinear damping. To understand the phenomenon better, we incorporate the Nose-Hoover formalism into a membrane model and observe the same behavior due to the emergence of a nonlinear coupling term. We observe that the nonlinear damping behavior is highly dependent on the bath-to-resonator mass ratio and their thermal energy difference.

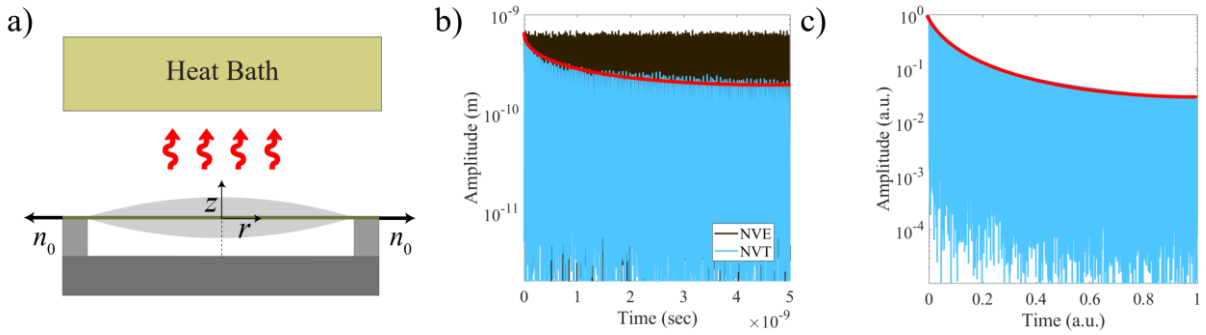

Figure 1: a) Circular membrane interacting thermodynamically with a thermal bath, b) ring-down simulation for a membrane using MD with NVE and NVT ensembles, and c) continuum model incorporating a Nose-Hoover thermostat showing nonlinear damping. Resonances with linear damping should decay linearly due to the logarithmic y-axis; however, the decay is clearly nonlinear.

References

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