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Classical Simulation *versus* Perturbation Theory of Anharmonicity in 2D Lennard-Jones Triangular Lattice XIAO SHEN, TAO SUN, JULIE STERN, PHILIP B. ALLEN, SUNY at Stony Brook — Classical molecular dynamics simulation and perturbation theory are two methods that can treat the anharmonicity in solids. Classical molecular dynamics simulation can treat anharmonic effects to high order. Perturbation theory beyond lowest order is difficult, and has convergence issues. However, perturbation theory easily treats the thermodynamic limit, while simulation is necessarily done on a finite system. This raises interesting questions such as whether molecular dynamic simulation will give the correct decay rate when the phonon mean free path is larger than the simulation cell. We try to answer such questions, and explore the limits of both methods, by comparing their results. The system we studied is a two dimensional triangular lattice model with a Lennard-Jones potential.

Xiao Shen
SUNY at Stony Brook

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