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First-Principles Computation of Graphene's Phonon Anharmonicity MORDECHAI KORNBLUTH, CHRIS A. MARIANETTI, Columbia University, Department of Applied Physics and Applied Mathematics — Here we use density-functional theory to compute an interatomic potential for graphene, including anharmonicities up to at least fourth order. We generate all group-theoretically allowed terms within a hexagon via the recently-developed slave mode expansion. This expands the potential in terms of the normal modes of overlapping hexagons, while obeying the space group symmetry and homogeneity of free space. We further introduce the notion of cooperative modes, which combine strain and $q = 0$ phonons to yield the same pure mode amplitude on each hexagon. Within the cooperative subspace, cooperative modes allow for arbitrarily-precise meshing to directly compute energies, or calculation of the anharmonic coefficients via finite-difference. We demonstrate the power of our approach in the context of strained graphene, which is known to have a novel strain-driven soft mode at the K-point. We identify the dominant anharmonic terms which drive the soft K mode, and study the role of finite temperatures using molecular dynamics and Monte-Carlo simulations.

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