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Efficient Computation of Anharmonic Force Constants via q-space, with Application to Graphene MORDECHAI KORNBLUTH, CHRIS MARIANETTI, Columbia University — We present a new approach for extracting anharmonic force constants from a sparse sampling of the anharmonic dynamical tensor. We calculate the derivative of the energy with respect to q-space displacements (phonons) and strain, which guarantees the absence of supercell image errors. Central finite differences provide a well-converged quadratic error tail for each derivative, separating the contribution of each anharmonic order. These derivatives populate the anharmonic dynamical tensor in a sparse mesh that bounds the Brillouin Zone, which ensures comprehensive sampling of q-space while exploiting small-cell calculations for efficient, high-throughput computation. This produces a well-converged and precisely-defined dataset, suitable for big-data approaches. We transform this sparsely-sampled anharmonic dynamical tensor to real-space anharmonic force constants that obey full space-group symmetries by construction. Machine-learning techniques identify the range of real-space interactions. We show the entire process executed for graphene, up to and including the fifth-order anharmonic force constants. This method successfully calculates strain-based phonon renormalization in graphene, even under large strains, which solves a major shortcoming of previous potentials.

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