First-principles calculation of anharmonic force constants\textsuperscript{1}

KEIVAN ESFARJANI, UC Santa Cruz, HAROLD STOKES, Brigham Young University — Calculation of anharmonic force constants in a crystal is a challenging task due to their large number, especially in a low symmetry crystal. Using the symmetry properties of the force constants coming from rotational, translational, as well as space group operation invariance, we formulate the exact constraints the latter have to satisfy. The other relations they have to satisfy come from total energy and forces for different atomic configurations. Using a singular value decomposition, we extract the force constants from the available linear relations and constraints. They will be used to calculate the phonon spectra and lifetimes, as well as scattering rates needed for the calculation of the thermal conductivity. This approach being systematic, can be extended to all crystals for which a first-principles-based interatomic potential up to fourth order can be obtained and used for molecular dynamics simulations.

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