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Analytic approach to anharmonic modes of lattice vibrations.

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The classical theory of lattice dynamics deals with harmonic crystals. While this theory is very effective with describing large number of physical phenomena connected with lattice vibrations, it leaves out an important aspect of the lattice dynamics: anharmonic effects. Without this component many important physical phenomena cannot be properly described: thermal expansion, phase transitions, thermal equilibrium, thermal conductivity, multi-phonon processes - to name just a few. Over the years a number of effective methods have been developed to deal with cases where the anharmonicity could be treated as a small perturbation in the harmonic model. In many situations this approach is useful and effective (e.g. Quasi Harmonic Approximation for dealing with thermal expansion). Unfortunately, in cases where forces in the crystal are strongly anharmonic (e.g. phase transitions, phonon modes with strongly anharmonic potentials) this approach is much less effective.

In crystals the anharmonic component may take various forms. In many materials (e.g. PbTe, TiO2) one or more of vibrational modes is characterized by a strongly anharmonic potential of the general form of the fourth order polynomial.
The equation of motion in such a potential can be solved analytically and the result can be further analysed to obtain experimentally verifiable properties: mode frequency as a function of temperature, thermal displacements, line profile etc. Even in cases where the potential does not allow for analytical solution, the procedure can still be carried out, however with higher computational cost, using numerical integration of the equation of motion.

This work presents a computational scheme for this type of calculation and demonstrates the derivation of temperature dependence of phonon frequency in the case of anharmonic mode in rutile titanium dioxide. The calculation is based on the DFT-derived potential for the mode.

Author: Dr JOCHYM, Pawel T. (Dept. of Computational Material Science, Institute of Nuclear Physics PAN, Cracow, Poland)

Co-author: Dr WEHINGER, Bjoern (Department of Quantum Matter Physics, University of Geneva; Laboratory for Neutron Scattering and Imaging, PSI, Switzerland)

Presenter: Dr JOCHYM, Pawel T. (Dept. of Computational Material Science, Institute of Nuclear Physics PAN, Cracow, Poland)

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