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Oscillatory dynamics in simple systems at elevated temperatures – beyond a perturbational treatment of anharmonicity

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The importance of anharmonicity for describing fundamental materials properties, starting from finite heat conductivity due to phonon-phonon scattering, can hardly be overemphasized. For crystalline matter, the principal microscopic gauge is constituted by the broadening in energy of the phonon dispersions, corresponding to q-dependent phonon lifetimes, which is also the main unknown for microscopic computations of heat conductivity.

Here the case of elemental Al at temperatures up to the melting point will be considered. I will present experimental data obtained by inelastic neutron scattering with consideration to the necessary steps in data analysis for being able to extract the inherent linewidths. Further, I will present calculations of q-dependent line broadenings on the basis of density-functional theory, both in the standard approach of perturbation theory as well as via ab initio molecular dynamics, and I will discuss why perturbation theory fails at elevated temperatures.

A. Glensk et al., *Phys. Rev. Lett.* **123**, 235501 (2019)

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