Contribution ID: **1** Type: **Talk**

# Phase space probability distribution in force constants estimation

*Tuesday, 3 December 2019 15:00 (25 minutes)*

Recently developed methods [1–3] of computational investigation of anharmonic and temperature-dependent aspects of lattice dynamics are based on building of some form of model potential. Parameters of such a model are derived from the forces acting on atoms and requires replication of the conditions of thermal equilibrium – to obtain proper sampling of the phase space region occupied by the system. This requirement is very challenging when performing quantum mechanical calculations. Typically, it involves large number of atoms and long simulation times needed to approximate thermodynamical limit conditions. It is usually achieved by running a long molecular-dynamics calculation on the system, to thermalize all degrees of freedom, and selecting well-separated (independent) configurations from the obtained trajectory. While this approach provides good sampling of the phase space of the system, it is computationally very expensive and exceptionally wasteful. To obtain independent samples the selected times in the trajectory must be separated by multiple time steps – often tenths or hundreds. Thus, we are throwing away a large amount of computational time, often above 80%, to obtain good sampling of the probability distribution of the system. Furthermore, in the case of lattice-dynamical calculations, we are utilizing only the positions from the trajectory - since the velocity information is not used in the process. Together, this makes the described procedure limited to fairly small systems.
In this work we present an alternative scheme for creating a representation of the probability distribution in the configuration space, which aims to faithfully reproduce densities generated by the molecular dynamics, while being more effective in terms of computational time. This approach uses well-known techniques of probability distribution modelling, and apply knowledge of the behaviour of the system in thermodynamic equilibrium to obtain low sample rejection rate in the procedure. The proposed method, coupled with the effective-potential modelling provides a promising path to tackle problems of anharmonic and temperature-dependent lattice dynamics even in systems with large and complicated unit cells.

This work was partially supported by National Science Centre (NCN, Poland) under grant UMO-2014/13/B/ST3/04393.

Refs
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