Kapitza thermal resistance in linear and nonlinear chain models.

The seminar will be given in English.

The interfacial thermal resistance, commonly known as Kapitza resistance, is defined as the ratio of discontinuity in the temperature gradient at the two different material interfaces to the heat flux flowing through the interface. In the present work, the Kapitza resistance is explored in various one-dimensional models for two cases: when an isolated defect is present in the chain and when an interface of two different material fragments exists. We present the exact analytic solutions for the Kapitza resistance for both cases in linear models, which has physical significance at very low/high temperature and/or short timescale in many realistic models. For the lightweight isotopic defect in the linear chain, one encounters a typical dip of the temperature profile, related to weak excitation of the localized mode in the attenuation zone. If the nonlinear interactions are included, this dip can still appear at a relatively short timescale, with subsequent elimination due to the nonlinear interactions.

We also show that the division of one-dimensional models into the universality classes established for the bulk one-dimensional heat conduction is valid in certain sense also for the boundary Kapitza resistance (except for linear models). In linear chains, the Kapitza resistance does not depend on the chain length in the thermodynamic limit, but substantially depends on the characteristics of thermostats used in the simulations. In the models with size-dependent heat conduction coefficient, the Kapitza resistance also is substantially size-dependent and thermostat dependent. Finally, in the models with normal heat conductivity the Kapitza resistance is also normal, i.e. size- and thermostat-independent in the thermodynamical limit.

ברכה,

מרץ 2021