Kapitza resistance in basic chain models with isolated defects

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Summary. Kapitza resistance due to isolated defect is explored numerically in benchmark chain models (linear, β-FPU, rotator and Frenkel-Kontorova). Kapitza resistance is found independent on chain length and temperature in linear model, but dependent on thermostat characteristics. In β-FPU model, the anomaly as in the heat conductivity continues, Kapitza resistance vanishes with the chain length and depend on temperature and thermostat. In Rotator and Frenkel-Kontorova models, which are characterized by normal heat conductivity, Kapitza resistance also shows convergence with chain length and independent on thermostat. Except for the linear model, the findings are similar to the heat conductivity characteristics in the respective models.

Kapitza resistance/Interfacial thermal resistance is defined as the ratio of discontinuity in the temperature gradient at the material interface to the heat flux flowing across the interface. It was first observed by Kapitza, in the junction between liquid helium II and a solid, during his experiments on superfluidity. Although numerous theoretical works have been devoted to explain Kapitza resistance, the two widely known models are Acoustic Mismatch Model (AMM) which is defined for very low temperatures and Diffuse Mismatch Model (DMM) which is defined for very high temperatures. Majority of the analytical, numerical works were based on AMM. The heat management problem, especially in nanoscale devices, involves the bulk conduction as well as the interfacial heat conduction. In this regard, Kapitza resistance and heat conductivity are two sides of a coin. We have well-known results for one-dimensional heat conduction problem and the studies divide models based on convergence and divergence of heat conductivity in the thermodynamic limit. But the behavior of Kapitza resistance in these models is less understood. More than just a theoretical concept, the divergence of heat conductivity is already established by experimental studies [1] for quasi-one-dimensional systems. Since interfacial thermal resistance is also a crucial factor that deciding the heat transport, the current study can shed light into thermal management problems in nano-scale devices. The present study conducted for Kapitza resistance behavior in basic benchmark models: linear, β-FPU, rotator and Frenkel-Kontorova. We choose isolated defect (isotopic defect/coupling defect) to create the interfacial boundary and to avoid the complications of the non-reciprocity.

We follow two numerical approaches: first, a semi-analytical method for linear model, which is based on the famous Rieder-Lebowitz-Lieb (RLL) method [2]; second, molecular dynamics simulations. In all cases, the non-equilibrium heat transport is established by connecting the chain to Langevin thermostats at both ends. In RLL method, the basic idea is to numerically solve the necessary and sufficient condition for the stationary state of a harmonic crystal from the generalized Liouville equation. In molecular dynamics simulations, we follow numerically the time evolution of the Hamiltonian with discrete time interval. We use Verlet algorithm to solve the equations of motion using homemade FORTRAN-95 codes. The results obtained for linear, β-FPU, rotator and Frenkel-Kontorova models are very-briefly discussed below.

It is well-known that in linear model, phonon does not exchange energy between modes and the phonon spectra is totally dependent on thermostat characteristics. We observed the heat flux and the temperature drop at the interface scales with the temperature and the Kapitza resistance is independent on chain length and temperature. We know heat conductivity was diverging with chain length in linear model. But we cannot say Kapitza resistance is normal for linear model because the Kapitza resistance is totally dependent on the thermostat since nothing in the chain can influence the phonons. Another observation for the linear model (more or less similar in other models also) is Kapitza resistance shows diverging behavior with the strength of the isolated defect when the strength goes to infinity.

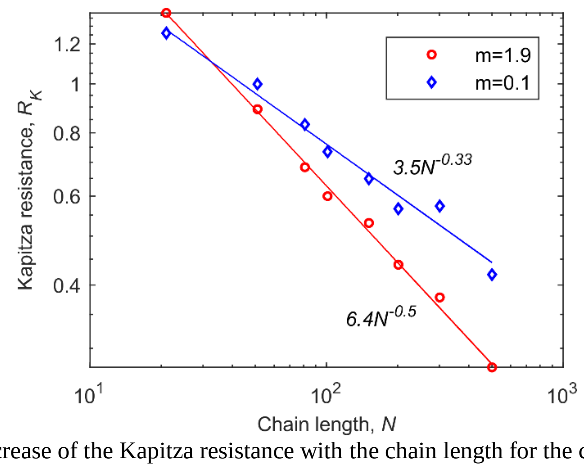

Figure 1: Power law decrease of the Kapitza resistance with the chain length for the chain with β-FPU interaction.

Heat transport in β-FPU model is always a puzzling problem since the observation of absence of thermalization by Fermi-Pasta-Ulam. Heat conductivity shows divergence with an exponent close to $1/3$ [3]. The anomaly continues in the case of Kapitza resistance which demands normalization of heat flux. Although the exponent dependent on the defect strength, still it is closer to $-1/3$ (Figure 1). The Kapitza resistance decreases with increase in temperature, which shows the temperature affects the phonon scattering process at the interface. As in the linear model, Kapitza resistance here also dependent on thermostat.

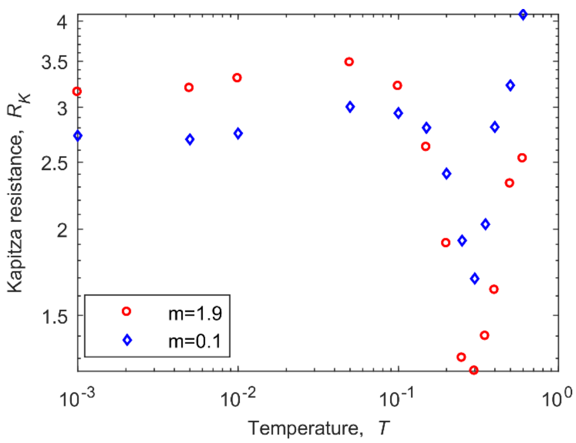

Figure 2: Temperature dependence of the Kapitza resistance in the chain of rotators.

Rotator model are well-known for momentum conserving models which obey convergence of thermal conductivity [4]. Kapitza resistance showed normal behavior here, that is, converges in the thermodynamic limit and independent thermostat characteristics at a temperature above the rotobreathers can get excited. The strong nonlinearity allows the system to forget about the thermostat characteristics and the phonon locking by the rotobreathers allows the normal diffusion. The activation of rotobreathers and its effect on the Kapitza resistance can be observed as a dip in the Kapitza resistance-temperature plot (Figure 2).

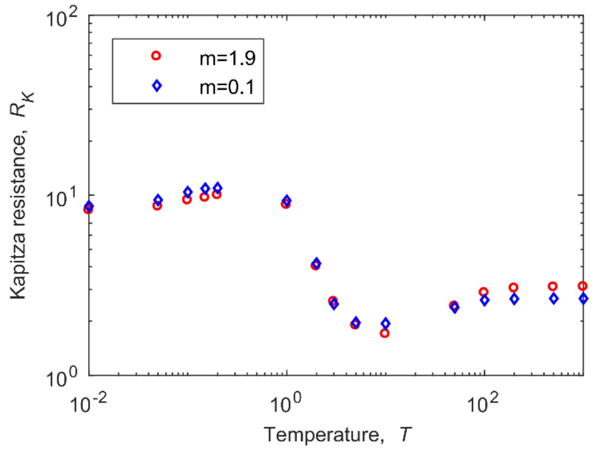

Figure 3: Dependence of the Kapitza resistance on the chain average temperature in the Frenkel-Kontorova model.

Coming to the Frenkel-Kontorova model, Kapitza resistance is normal and independent of thermostat characteristics at intermediate temperatures (Figure 3). We know the similar observation for heat conductivity since activation of topological kinks only happens at intermediate temperature range [5]. The linear characteristics at very low temperatures happens due to the weak nonlinearity and at high temperatures the chain detaches from the substrate.

In conclusion, linear model showed Kapitza resistance that is independent of chain size (contrary to heat conductivity) and temperature, but dependent on thermostat. The addition of cubic linearity makes the Kapitza resistance anomalous, that is, dependent on thermostat and chain length in the thermodynamic limit (need of normalized heat flux). Rotator and Frenkel-Kontorova models showed normal Kapitza resistance. In all the nonlinear models Kapitza resistance decreases, immediately after the very low temperature regime (linear regime) which needed to be investigated further.

References

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