Thermal Conductivity in One Dimensional Systems?

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Fourier's law of heat conduction relates the nonequilibrium average of the heat flux per temperature gradient to the negative of the thermal conductivity. This linear relationship holds in the limit of small temperature gradients and large system sizes and is usually observed for solids, liquids and gases in three dimensions. The existence of the thermal conductivity in one-dimensional systems is still an open question and its divergence even more so in the large system size limit.

There are several important and still unanswered questions that we can address in this paper: what properties of the dynamical systems are responsible for the observed behavior in Equilibrium Molecular Dynamics (MD) simulations and Nonequilibrium Steady States generated by Nonequilibrium Molecular Dynamics (NEMD) simulations? A few key indicators that we will quantify include sample preparation, choice of thermostats in simulating a heat bath surrounding the one-dimensional chain, and several simulations approaches. These include the Green-Kubo Linear Response theory using equilibrium MD techniques; application of an external heat field to drive the system into a steady state, the Evans heat field method; and lastly, a nonequilibrium simulation of a lattice attached to hot and cold heat baths causing a flow of heat to take place along the lattice.