Are there really phase transitions in 1-d heat conduction models?

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Recently, it has been claimed (O. V. Gendelman and A. V. Savin, Phys. Rev. Lett. 84, 2381 (2000); A.V. Savin and O.V. Gendelman, arXiv: cond-mat/0204631 (2002)) that two nonlinear classical 1-d lattice models show transitions, at finite temperatures, where the heat conduction changes from being finite to being infinite. These are the well known Frenkel-Kontorova (FK) model and a model for coupled rotators. For the FK model we give strong theoretical arguments why such a phase transition is not to be expected. For both models we show numerically that the effects observed by Gendelman et al. are not true phase transitions but are rather the expected cross-overs associated to the conductivity divergence as $T \to 0$ and (for the FK model) $T \to \infty$.

Heat conduction in classical one-dimensional lattices has recently been investigated by many authors (see [1] for a recent review). A large class of 1-d systems can be described by the general Hamiltonian

$$H = \sum_{i=1}^{N} \left( \frac{p_i^2}{2m} + U(q_{i+1} - q_i) + V(q_i) \right) \quad (1)$$

where $N$ is the system size, $p_i$ is the momentum of the $i$th particle, $q_i$ is its displacement from the equilibrium position, $U$ is the internal potential, and $V$ is an external potential. In the following we shall always use $m = 1$, without loss of generality. Real isolated systems must have $V = 0$, since any external potential would itself involve a “scaffolding” which is not rigid and would thus also contribute to heat conduction. Thus, for real systems the support of the external potential must be included in the description of the system, and $V$ has to be replaced by a contribution to the internal potential $U$. Nevertheless, we shall in the following keep the ansatz (1), understanding that we are calculating only part of the complete heat conduction when $V \neq 0$. In the following we shall also assume that the system has no frozen disorder.

It is well known that heat conduction is infinite, if all potentials are harmonic [2] or if the system is integrable. In this case phonons resp. solitons are not scattered. Thus they propagate ballistically, given a constant heat flux $J$ (independent of $N$) when a finite constant temperature difference $\Delta T$ is applied to the two ends of a chain of length $N$. Thus formally, the conductivity $\kappa = JN/\Delta T$ is proportional to $N$. For non-integrable models with an acoustic phonon branch, i.e. without an external potential, one expects ballistics transport in the infinite wave length limit (since phonon scattering in general decreases with energy), which leads to a power behavior $\kappa \sim N^\alpha$ with $0 < \alpha < 1$ [3]. This is the case, e.g., for the Fermi-Pasta-Ulam (FPU) model [6] and for the diatomic Toda lattice [7].

An exception to this seems to happen for coupled rotators [8, 10].

$$U(q_{i+1} - q_i) = -\cos(q_{i+1} - q_i) \quad , \quad V(q_i) = 0 \quad , \quad (2)$$

which seem to have finite $\kappa$ [8]. This is explained [10] by the fact that single highly excited rotators essentially decouple from neighboring rotators, acting thus as barriers for the propagation of any phonons, even soft ones.

Soft acoustic phonons are essentially Goldstone modes due to Galilei invariance. Finite heat conduction (in $d = 1$) is therefore expected when $V \neq 0$, since then translation invariance is broken and an acoustic branch does not exist in the phonon spectrum. This is e.g. the case for the Frenkel-Kontorova (FK) model

$$U(q_{i+1} - q_i) = \frac{1}{2}(q_{i+1} - q_i)^2 \quad , \quad V(q_i) = -\varepsilon \cos q_i \quad . \quad (3)$$

(notice that this is the commensurate FK model, where the harmonic part of the potential leads to the same particle distance in the ground state as the cosine potential; we shall only discuss this case in the following). In this model, all phonons have a finite mean free path, bounded from above by a finite constant which is independent of the wave number $k$, but which diverges for $T \to 0$ and for $T \to \infty$. The latter follows from the fact that $V$ given by Eq.(3) effectively becomes negligible when $T \to \infty$, and effectively becomes a sum of harmonic potentials when $T \to 0$. Thus there is no ballistic transport, and no obvious mechanism which could lead to an infinite conductivity for any finite $T$, while one expects $\kappa$ to diverge when $T \to 0$ or $T \to \infty$ [11].

It was thus very surprising when Savin and Gendelman [12] claimed to have clear evidence for phase transitions in the FK model, at which the conductivity changed from finite to infinite. They claimed that $\kappa$ is finite only in an interval $T_{c1} < T < T_{c2}$, with $T_{c1}$ and $T_{c2}$ dependent on $\varepsilon$, while $\kappa = \infty$ outside this interval.

Indeed, the same authors had also claimed that there is a phase transition in the rotator model [8, 10]. There, the density of highly excited rotators should of course go to zero for $T \to 0$. Thus one expects that soft phonons exist in this limit, and $\kappa \to \infty$ for $T \to 0$. Instead of this, it was claimed in [8, 10] that $\kappa = \infty$ in an entire interval $0 \leq T \leq T_c$.

In the present paper we want to test these claims by performing simulations on larger lattices and with higher
and with \( T_{\text{N}} \leq 9, 10, 12 \). The temperature difference \( \Delta T \) of the chains are 64, 128, 256, 512, 1024, and 2048. While the gradients in the central region are roughly constant, most of the temperature variation happens for short chains in the thermostated boundaries.

In order to mimic the simulations of [9, 10, 12] as close as possible, we also used Langevin thermostats (we do not agree with these authors that Nosé-Hoover thermostats would be unsuitable, but we just don’t want any discussion about this point). More precisely, we simulated a chain of \( N_0 + N + N_0 \) oscillators. The central \( N \) oscillators follow their Hamiltonian equations of motion, while the outer \( 2N_0 \) ones satisfy \( \dot{q}_n = -\frac{\partial \phi}{\partial q_n} - \gamma \dot{q}_n + \xi_n \) and with \( \phi = U + V \) being the total potential, \( \xi_n \) being white Gaussian noises, \( \langle \xi_n(t)\xi_k(t') \rangle = 2\gamma T_0 \delta_{nk} \delta(t - t') \) and with \( T_n = T_{\text{high}} \) for \(-N_0 \leq n \leq 0\) and \( T_n = T_{\text{low}} \) for \( N < n < N + N_0 \). We used \( N_0 = 40 \) and \( \gamma = 0.1 \), as in [9, 10, 12]. The temperature difference \( \Delta T \equiv T_{\text{high}} - T_{\text{low}} \) was chosen between 10% and 20%.

For the integration we used a simple leap frog [13]. On the one hand this is symplectic and thus more suited for the central region than, say, a Runge-Kutta integrator. On the other hand it should be more robust than higher order symplectic integrators in the boundary regions which are not Hamiltonian. Step size was 0.05, and total integration times were typically \( 10^7 - 10^9 \) units (i.e. \( 10^8 - 10^9 \) steps), with some runs going up to \( 5 \times 10^8 \) units. We checked that this was sufficient to reach a steady state and that the time-averaged heat flux \( J \) was independent of the site.

We verified also that the temperature profiles were roughly linear in the central region \( 0 \leq n \leq N \), but we could not verify the absence of temperature jumps at its boundaries claimed in [9, 10, 12]. More precisely, such jumps were absent only for very large lattices and small conductivities, i.e. if the heat flux was small. Otherwise, for small lattices and/or large conductivities, there were very large jumps, mostly located in the boundary regions \(-40 < n < 0\) and \( N < n < N + 40\) (see Fig. 1). Thus while the profile in the central region was essentially linear (in contrast to simulations with Nose-Hoover thermostats coupled to single particles, as e.g. in [9, 10], it would be very wrong to estimate the conductivity simply by dividing the flux by the nominal imposed \( \Delta T \)). It seems that this was done in several cases in [9, 10, 12], which explains some – but not all – of the differences between their results and those of the present paper. In other cases the authors of [9, 10, 12] must have taken into account boundary jumps, otherwise their results would disagree much more with ours than they actually do. Unless otherwise said, we will estimate \( \kappa \) by dividing the flux by the temperature drop over the inner half of the central region.

Notice that a similar behavior was found also for the rotator model and for the discrete \( \phi^4 \) model. The latter is given by the Hamiltonian [14]

\[
H = \frac{1}{2} \sum_i \left( \dot{\phi}_i^2 + (q_{i+1} - q_i)^2 + \alpha q_i^2 + \frac{1}{2} \beta q_i^4 \right). \tag{4}
\]

Conductivities for the \( \phi^4 \) model with \( T = 2 \) and \( \beta = 1 - \alpha \) are shown in Fig. 2 for various values of \( \beta \in [0, 1] \). The \( \phi^4 \) model is a prototype model with finite conductivities. Indeed we see that all measured values of \( \kappa \) are not only finite but are independent of \( N \). This would not have been the case if we had not taken the temperature jumps into account and would have used the nominal value of \( \Delta T \) when estimating \( \kappa \) from \( J/\Delta T \). The values of \( \kappa \) shown in Fig. 2 are in very good agreement with those of [14].

**Frenkel-Kontorova model:** In all simulations, \( N \) ranged from 32 to 2048. We made simulations for \( \varepsilon = 1, 0, 3.0 \) and 10.0. According to [12], \( T_{c1} \) is only weakly dependent on \( \varepsilon \): \( T_{c1} = 2.6, 2.3, \) and \( 2.0 \) for \( \varepsilon = 1, 0, 3.0, 10.0 \). On the other hand, \( T_{c2} \) should strongly increase with \( \varepsilon \), \( T_{c2} = 3.3, 15, \) and 150 for the above three values.

Conductivities for \( \varepsilon = 1.0 \) are shown in Fig. 3. Obviously, they are finite for \( T = 2 \) and \( T = 8 \), showing...
that the temperature range with finite conductivities is underestimated in [12]. For $T = 0.5$ and $T = 32$ we see a slow increase of $\kappa$ with $N$, over a wide range of the latter, but it seems to stop for the very largest lattices ($N > 1000$). Finally, for $T = 0.125$ and $T = 128$ there is a slow increase for all $N > 300$. The latter could be taken as an indication that $\kappa$ diverges for these temperatures, but we think that this would be wrong. On the one hand, the increase with $N$ is very slow, much slower than in Fig. 4 of [12]. We would get a similarly fast increase as in [12] if we would use the nominal temperature difference, i.e. if we would disregard the jumps seen in Fig. 1. On the other hand, the data for $0.5 \leq T \leq 32$ show us that the saturation of $\kappa$ happens at larger and larger lattice sizes as we go away from the central energy region, just as we have expected. Thus we must expect in any case an increase of $\kappa$ for all reachable lattice sizes, and observing it does not give any relevant information.

Analogous results for $\varepsilon = 3.0$ are given in Fig. 4. There we show data for the temperature range $[0.75, 75]$. This is again much larger than the range where convergent conductivities were found in [12]. This time all curves become horizontal for large $N$, i.e. the conductivity is finite in the entire range. It of course depends strongly on $T$, see Fig. 5. It diverges both for $T \to 0$ and for $T \to \infty$, since the problem effectively becomes harmonic in both limits.

Finally, our last simulations for the FK model, for $\varepsilon = 10$, are summarized in Fig. 6. There we only show results for low temperatures, $0.5 \leq T \leq 2.75$. Except for the last temperature, they are all in the regime where the authors of [12] have found divergent $\kappa$. In contrast, all our curves are either horizontal for all $N$ or become horizontal for large $N$, suggesting that $\kappa$ is finite for all finite $T$.

**Rotator model:** For the rotator model, we simulated larger systems, with $N$ ranging from 32 to 8192. Conductivities are plotted in Fig. 7 against $N$ for $T = 0.6, 0.45, 0.3,$ and $0.2$ (from bottom to top). According to [9], the phase transition from a high-$T$ phase with finite conduction to a low-$T$ phase with infinite conduc-
FIG. 7: Heat conductivity versus system size for the rotator model. Again, statistical and integration errors are less than the symbols.

...tion occurs at some $T_c$ between 0.2 and 0.3. According to that, the lowest three curves in Fig. 7 should become flat for $N \to \infty$, while the uppermost should continue to grow. This is not what is found, although our values for $T = 0.2$ and 0.3 agree numerically quite well with those of [9]. But while the curve for $T = 0.2$ increases with the same average slope as in Fig. 2 of [9], it is definitely S-shaped and stops to rise for the largest values of $N$.

**Conclusion:** In this paper we studied the size dependence of the effective finite size conductivity of nonlinear 1D lattices, as a function of temperature. We used straightforward but high statistics simulations to show that there are no indications of the phase transitions suggested in [9, 10, 12] on the basis of similar simulations. For the FK model, this is in agreement with expectations, since phonons should have a finite free path in this model for all finite temperatures. For the rotator model it is less obvious. It suggests that the blocking of the propagation of soft phonons by localized excitations [9] is effective at all finite temperatures. It becomes of course less and less important as $T \to 0$, since the density of such excitation decreases exponentially with $1/T$. But it is present at all finite $T$, and it becomes dominant for $N \to \infty$.

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