Physics Letters A ••• (••••) •••–•••

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Heat conduction in diatomic chains with correlated disorder

Alexander V. Savin [a,*], Vadim Zolotarevskiy [b], Oleg V. Gendelman [b]

[a] Semenov Institute of Chemical Physics, Russian Academy of Sciences, 4 Kosygin str., 119991 Moscow, Russia
[b] Faculty of Mechanical Engineering, Technion – Israel Institute of Technology, Haifa 32000, Israel

ARTICLE INFO

Article history:
Received 14 September 2016
Accepted 25 October 2016
Available online xxxx
Communicated by V.A. Markel

Keywords:
Heat transport
Diatomic chain
Correlated disorder
Billiard model
Lennard–Jones chain
Transport of energy

ABSTRACT

The paper considers heat transport in diatomic one-dimensional lattices, containing equal amounts of particles with different masses. Ordering of the particles in the chain is governed by single correlation parameter – the probability for two neighboring particles to have the same mass. As this parameter grows from zero to unity, the structure of the chain varies from regular staggering chain to completely random configuration, and then – to very long clusters of particles with equal masses. Therefore, this correlation parameter allows a control of typical cluster size in the chain. In order to explore different regimes of the heat transport, two interatomic potentials are considered. The first one is an infinite potential wall, corresponding to instantaneous elastic collisions between the neighboring particles. In homogeneous chains such interaction leads to an anomalous heat transport. The other one is classical Lennard–Jones interatomic potential, which leads to a normal heat transport. The simulations demonstrate that the correlated disorder of the particle arrangement does not change the convergence properties of the heat conduction coefficient, but essentially modifies its value. For the collision potential, one observes essential growth of the coefficient for fixed chain length as the limit of large homogeneous clusters is approached. The thermal transport in these models remains superdiffusive. In the Lennard–Jones chain the effect of correlation appears to be not monotonous in the limit of low temperatures. This behavior stems from the competition between formation of long clusters mentioned above, and Anderson localization close to the staggering ordered state.

1. Introduction

Heat conductivity in one-dimensional (1D) lattices is a well-known classical problem related to the microscopic foundation of Fourier's law. The problem started from the famous work of Fermi, Pasta, and Ulam (FPU) [1], where an abnormal process of heat transfer was initially revealed. Numerous aspects of the problem were widely addressed over last two decades [2–4]. It was established that mere nonlinearity of the interparticle interactions in one-dimensional models is insufficient for convergence of the heat conduction coefficient in the thermodynamical limit. Recently it was demonstrated that the heat conductivity converges in broad variety of models with bounded potential of the interatomic interaction [5,6]. Such models are characterized by possibility of dissociation between the neighboring particles. This conclusion on convergence, however, does not apply to "billiard" models, where interaction between the particles is reduced to instantaneous elastic impacts. It seems that the reason for this crucial difference is the nonzero time of interaction between the neighboring particles, when the potential is not ideally "impact". Thus, triple particle collisions are possible; the latter provide additional efficient scattering mechanism, as outlined in [6].

In this paper we address other system properties, which directly effect the heat transport – a homogeneity and an ordering in the lattice. Modifications of the heat transport caused by inhomogeneities in the mass or potential distribution were explored starting from the pioneering work on harmonic system with different masses [7]. Later works considered isotopic disorder [8], harmonic [9] and anharmonic random chains [10,11]. However, main attention of the studies on the nonhomogeneous systems has been attributed to chains with staggering [12,13] or randomly distributed masses. In particular, numerous papers simulated the heat transport in one-dimensional diatomic hard-point gas. This system is especially interesting, since the case of equal masses corresponds to completely integrable linear homogeneous billiard (even its version with external on-site potential is integrable, see, e.g. [14]). So, the staggering masses constitute a perturbation of the integrable case, and the question is whether this perturbation will lead to normal heat transport. Numerous numeric works on the diatomic billiard with staggering particles led to a conclusion

* Corresponding author.
E-mail address: asavin@center.chph.ras.ru (A.V. Savin).

http://dx.doi.org/10.1016/j.physleta.2016.10.046
0375-9601/

that the heat conduction coefficient κ in this system diverges in the thermodynamical limit as $\kappa \sim N^{\alpha}$ for certain $\alpha > 0$ [15–18]. More detailed recent exploration of this system [19] demonstrated, that when the mass ratio is slightly different from one, it is not possible to exclude normal heat conduction over longer and longer sizes as the integrable limit is approached. In the same time, it was conjectured [19] that also in this case the heat conductivity diverges, but for longer chains than are available for simulation.

An interesting idea for simulating the finite conductivity was to introduce scatterers in quasi-1D billiard gas channels. The first work in this field was carried out by Alonzo et al. [20], where a quasi-1D billiard in Lorentz gas channel was analyzed. The ends of the channel constituted the heat baths, and the movement of the particles inside the channel was interrupted by semicircular scatterers. The conductivity of this chaotic system obeyed Fourier's law. In order to investigate the role of chaos on the problem of heat conduction, the subsequent works implemented changes in geometry and order of the scatterers [21]. Some of the "modified" configurations showed normal heat conductivity. In some others, the heat conduction coefficient diverged [21]. Thus the assumption that chaos may be sufficient condition for a system to possess the finite heat conductivity has been disproved. Such billiard gas models might shed some light on the heat transport. In the same time, they lack certain basic features of the realistic systems, such as particle interactions, phonon transport, and local thermal equilibrium [21].

In this paper we also consider the thermal transport in the chain models, which include the particles with two different masses, but do that in more general setting. Key difference from the previous studies is that the ordering of these particles in the chains is neither perfectly periodic (homogeneous or staggering) nor completely random. Instead, the mass distribution in the chain is characterized by the correlated disorder. More exactly, the masses of neighboring particles are equal with probability p_m, and $0 \le p_m \le 1$. Increase of this parameter favors clustering in the chain. All previously studied cases (complete order and uncorrelated disorder) correspond to special values of p_m. The effect of the correlated disorder is studied for the system of rigid particles with abnormal heat conductivity, and also for a model with convergent heat conductivity – Lennard–Jones (LJ) chain. It is demonstrated that in any of these systems the correlated disorder does not modify the convergence properties of the heat conduction coefficient in the thermodynamical limit, but strongly effected the quantitative characteristics of the heat transport.

2. Diatomic gas of rigid particles with random mass distribution

Let us consider the one-dimensional chain of rigid rods with size $d > 0$, with masses which can take only two values $M_1 = 1$ and $M_2 = m \ge 1$ (dimensionless parameter m is interpreted as the mass ratio). To be specific, we choose the length of the rods as $d = 0.1$ and average distance between their centers $a = 1$. In other terms, numeric density of the rods is adopted to be unit. The rods are numbered in ascending order of coordinates of their centers. Hamiltonian of the system is expressed in the following form:

$$H = \sum_n \left[\frac{p_n^2}{2m_n} + V(x_{n+1} - x_n) \right]. \quad (1)$$

Here m_n is a mass of the n-th rod, x_n – coordinate of its center, $p_n = m_n \dot{x}_n$. The interaction of absolutely rigid particles is described by the following hard-core potential:

$$V(r) = \infty \text{ if } r \le d, \quad V(r) = 0 \text{ if } r > d. \quad (2)$$

Potential function (2) describes instantaneous elastic collisions of the rods. In this one-dimensional chain, only neighboring rods can collide, and collision of the rod number n with the rod number $n+1$ occurs if the distance between their centers $x_{n+1} - x_n = d$. As it is well-known, if before the collision velocities of the rods are $v_n = \dot{x}_n$ and $v_{n+1} = \dot{x}_{n+1}$, then after the collision the velocities will take the following values:

$$v'_n = [2m_{n+1}v_{n+1} + (m_n - m_{n+1})v_n]/(m_n + m_{n+1})$$
$$v'_{n+1} = [2m_n v_n + (m_{n+1} - m_n)v_{n+1}]/(m_n + m_{n+1}).$$

Between the collisions, the rods move as free particles.

In considered model, each rod can have the mass $m_n = 1$ or the mass $m_n = m$ with equal concentration. To describe the correlation between the masses of neighboring rods, we define additional parameter $0 \le p_m \le 1$, which denotes a probability for the neighboring rod to have the same mass. The case $p_m = 0$ corresponds to the chain with alternating masses, the case $p_m = 0.5$ corresponds to completely random distribution of the masses in the chain (lack of correlation between the neighbors). The higher value of p_m, the longer clusters of particles with equal masses are expected in the chain. Average length of such homogeneous clusters is estimated as $N_p \sim 1/(1 - p_m)$. In the limit $p_m \longrightarrow 1$ the chain becomes almost homogeneous, in other terms, it contains the homogeneous clusters of diverging length $N_p \longrightarrow \infty$.

For simulation of the heat transport in this model with N rods, we include the interaction of terminal rods with boundary thermostats. The rod with $n = 1$ interacts with thermostat of temperature T_+, the rod number N – with thermostat of temperature T_-. Interaction of the first rod with the thermostat occurs when $x_1 = d/2$. In this moment, the velocity of this rod is re-ascribed to $v_1 > 0$; the latter is random with Maxwell distribution

$$P(v) = (|v|m/T)\exp(-v^2 m/2T)$$

with mass $m = m_1$ and temperature $T = T_+$. Similarly, the rod N interacts with Maxwell thermostat when $x_N = N - d/2$. In this moment, the velocity of this is re-ascribed to random value $v_N < 0$ with Maxwell distribution with mass $m = m_N$ and temperature $T = T_-$.

As it was mentioned above, the rods interact with the thermostats only when they collide with the boundaries. In the moment of collision $t = t_j$ the thermostat changes the energy of the terminal rod by value $\Delta E_i(t_j) = m_i[v_i^2(t_j + 0) - v_i^2(t_j - 0)]/2$, where $i = 1, N$. If over time interval $[0, t]$ there were N_t collisions of the terminal rod with the boundary in time instances $(\{t_j\}_{j=1}^{N_t} \in [0, t])$, then the average work done by the thermostat is expressed as

$$j_i(t) = \frac{1}{t}\sum_{j=1}^{N_t} \Delta E_i(t_j),$$

and its average power $J_i = \lim_{t\to\infty} j_i(t)$.

For simulation of the heat transport in the system we choose the following initial conditions:

$$x_n(0) = n - 1/2, \quad \dot{x}_n(0) = v_n, \quad n = 1, 2, ..., N.$$

Here v_n is a random value with Maxwell distribution $P(v) = \sqrt{m_n/2\pi T}\exp[-m_n v^2/2T]$, where $T = (T_+ + T_-)/2$.

Following paper [19], the temperature of the left boundary is set to $T_+ = 6$, and of the right boundary – to $T_- = 4$. Then, long time dynamics of the system is simulated. It should be mentioned that this dynamics does not depend on the absolute values of the temperatures, but only on the ratio T_+/T_-. After initial transient and formation of stationary heat flux, average powers of the thermostats J_1, J_N are computed. The heat flux in the system should

Please cite this article in press as: A.V. Savin et al., Heat conduction in diatomic chains with correlated disorder, Phys. Lett. A (2016), http://dx.doi.org/10.1016/j.physleta.2016.10.046