I. INTRODUCTION

Heat conductivity in one-dimensional (1D) lattices is a well-known classical problem related to 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 stated that if the potential of interaction is bounded (allows dissociation of the neighboring particles), then the heat conductivity converges [5, 6]. In the same time, it is still not clear whether this condition is mandatory and what are necessary and sufficient requirements for the convergence in systems of different dimensionality.

In this paper we address significant system properties, which directly effect the heat transport – a homogeneity and an ordering in the lattice. As for the nonhomogeneous systems, main attention has been attributed to chains with staggering 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. [7]). So, the staggering masses lead to 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 that the heat conduction coefficient $\kappa$ in this system diverges in the thermodynamical limit as $\kappa \sim N^\alpha$ for certain $\alpha > 0$ [8-11]. More detailed recent exploration of this system [12] 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. Due to numeric difficulties, it is hard to draw more clear-cut conclusion. In our paper we revisit these simulations and reveal, that close to the integrable limit the heat transport remains superdiffusive, as one would intuitively expect. This observation supports the claim that the observed "saturation" of the heat conduction coefficient is in fact a crossover regime, and the heat conductivity remains abnormal.

As extension of these studies, we explore also effect of the disorder on the heat transport. Two characteristics of the disorder are addressed – internal correlations in the disordered structure, and concentration of the "impurities" with different mass. These aspects of the disorder are studied for the system of rigid rods with abnormal heat conductivity, and also for two different models with convergent heat conductivity – Lennard-Jones (LJ) chain and chain of rotators. It is demonstrated that in any of these systems the disorder does not modify the convergence properties of the heat conduction coefficient in the thermodynamical limit. In the same time, the disorder strongly effects the heat transport. This effect is ambiguous and strongly depends on particular model and chosen set of parameters. It is demonstrated that the effect of the disorder is closely related to a particular mechanism of scattering for the heat flux in each specific model.

II. DIATOMIC GAS OF RIGID PARTICLES WITH RANDOM MASS DISTRIBUTION

We first consider a one-dimensional chain of rigid rods with size $d > 0$, with masses which can take only two values $M_1 = 1$ and $M_2 = m \geq 1$ (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:

\[
H = \sum_{n} \left[ \frac{p_{n}^{2}}{2m_{n}} x_{n}^{2} + V(x_{n+1} - x_{n}) \right].
\]  

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:

\[
V(r) = \infty \text{ if } r \leq d, \quad V(r) = 0 \text{ if } r > d.
\]  

Potential function (2) in fact corresponds to instant-
taneous elastic collisions of the rods. In this one-
dimensional chain, only neighboring rods can collide.
Namely, collision of the rod number \( n \) with the rod num-
ber \( n + 1 \) 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:

\[
\begin{align*}
\dot{v}_{n}' &= \frac{[2m_{n+1}v_{n+1} + (m_{n} - m_{n+1})v_{n}]}{(m_{n} + m_{n+1})}, \\
\dot{v}_{n+1}' &= \frac{[2m_{n}v_{n} + (m_{n+1} - m_{n})v_{n+1}]}{(m_{n} + m_{n+1})}.
\end{align*}
\]

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 probability.
To describe the correlation between the masses of neigh-
boring rods, we define additional parameter \( 0 \leq p_{m} < 1 \),
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 \( p_{m} = 0.5 \) corre-
sponds 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 equal masses are expected in the chain. Aver-
age length of such homogeneous clusters is estimated as
\( N_{p} = 1/(1 - p_{m}) \). Quite obviously, in the limit \( p_{m} \rightarrow 1 \) the
chain becomes almost homogeneous, in other terms, it
contains the homogeneous clusters of diverging length
\( N_{p} \rightarrow \infty \).

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-assigned to
\( v_{1} > 0 \); the latter is random with Maxwell distribution

\[
P(v) = (|v|m/T) \exp(-v^{2}m^{2}/2T),
\]

with mass \( m = m_{1} \) and temperature \( T = T_{+} \). Similarly,
the rod \( N \) interacts with Maxwell thermostat according to
values of 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 bound-
aries. In the moment of collision \( t = t_{j} \) the ther-
mostat changes the energy of the terminal rod by value
\( \Delta E_{n}(t_{j}) = m_{n}(v_{n}^{2}(t_{j} + 0) - v_{n}^{2}(t_{j} - 0))/2 \), 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 \( t_{j} \) \( j = 1 \) \( \in \) \( [0, t] \), then the average work done by the ther-
mostat is expressed as

\[
j_{i}(t) = \frac{1}{t} \sum_{j=1}^{N_{t}} \Delta E_{i}(t_{j}).
\]

and its average power \( J_{i} = \lim_{t \rightarrow \infty} j_{i}(t) \).

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 [12], we choose the temperature of the
left boundary as \( T_{+} = 6 \), and of the right boundary – as
\( T_{-} = 4 \) and simulate long time dynamics of the system.
It should be mentioned that this dynamics does not de-
pend on the absolute values of the temperatures, but only
on the ratio \( T_{+}/T_{-} \). After initial transient and formation of
stationary heat flux, we determine average powers of the
thermostats \( J_{1}, J_{N} \). The heat flux in the system
should satisfy obvious relationship \( J = J_{1} = -J_{N} \), which
can serve also as a test for validity of the numeric pro-
cedure. In our simulations these equations were obeyed
with very high accuracy. Distribution of the local tem-
perature in the chain is determined as \( T_{n} = \langle \dot{x}_{n}^{2}(t) \rangle_{t} \).

Simulation of the heat transport demonstrates that the
collisions of the rods with different mass bring about for-
mation of a linear thermal gradient in the chain, see Figure 1. We observe an effect of thermal resistance at the ends of the chain. As a result of this effect it turns out that the temperature of the leftmost rod $T_1 < T_+$, and of the rightmost rod $T_N > T_-$. This discrepancy decreased with an increase of the chain length. To avoid ambiguities related to this thermal resistance, we evaluated the value of the heat conduction coefficient in accordance with actual temperatures of the terminal rods rather than nominal temperature of the thermostats, and used the following relation:

$$\kappa(N) = JN/(T_1 - T_N).$$  \hspace{1cm} (3)

Dependence of the heat conduction coefficient $\kappa$ on the chain length $N$ for different values of the mass ratio $m$ and mass correlation parameter $p_m$ is presented in Figure 2. One can learn from this Figure, that for the case $p_m = 0$ (perfectly ordered diatomic chain) the dependence $\kappa(N)$ is similar to results presented previously in Ref. [12]. For large value of the mass ratio $m = 3$ the heat conduction coefficient increases approximately as $N^{0.3}$. However, for small mass ratio $m = 1.1$ for $N \sim 10^4$ the growth of the heat conduction coefficient slows down. It is extremely difficult to check the behavior of the coefficient for essentially longer chains.

Our simulations demonstrate that the randomness of the mass distribution in the chain does not cause any qualitative changes in the behavior of the heat conduction coefficient. Increase of the mass correlation parameter $p_m$ for fixed mass ratio and chain length leads to an increase of $\kappa$, as it is demonstrated in Figure 3. In the limit $p_m \rightarrow 1$ one obtains $\kappa(N) \rightarrow \infty$. The reason is that the modification (and scattering) of momenta of the individual rods is possible if the colliding particles have different masses. Average length of clusters of the rods with the same mass $N_p$ grows together with the mass correlation parameter $p_m$, so relative number of the scattering events (collisions of the rods with different mass) decreases. So, one can conjecture that the heat conduction coefficient will be proportional to the average length of the cluster with equal masses, which can be estimated as $N_p \sim 1/(1 - p_m)$. Curve 4 in Figure 3 confirms to some extent this conjecture.

Results presented in Figure 3 also point on different character of increase of the heat conduction coefficient with the system size for different values of the mass ratio. As one can observe, for relatively large mass ratio $m = 3$ and for all studied values of $p_m$ the heat conduction coefficient rapidly attains an asymptotic regime of divergence as approximately $N^{0.3}$. In the same time, for relatively small mass ratio $m = 1.1$ the heat conduction coefficient approaches extremely high values, as one would expect. However, it is possible to identify apparently convergent behavior at $N \sim 10^4$.

As it was mentioned before, our results for $p_m = 0$ reproduce simulations presented in [12]. There the authors have mentioned that on the basis of the simulation results it is not possible to reject possibility of convergence of the heat conduction coefficient for the case of small mass ratios. We demonstrate here that for other values of the mass correlation parameter the situation remains qualitatively the same. The authors of [12] also conjectured that the observed “convergence-like” behavior is
transient, and the heat conduction coefficient should attain the divergence regime for higher values of \( N \). This opinion seems very reasonable (it is completely counter-intuitive to expect that the system will switch to convergence while approaching the integrable limit of equal masses), but it is extremely difficult to perform such simulations for essentially longer chains. Therefore below we make an attempt to achieve numeric evidence on divergence of the heat conduction coefficient by exploration of an energy diffusion in the chain.

III. DIFFUSION OF ENERGY PULSES IN THE CHAIN WITH RANDOM MASS DISTRIBUTION

For simulation of the energy diffusion we consider the chain comprising \( N = 20000 \) particles. The thermostats are removed and the terminal rods elastically interact with the walls. Initially all the rods are randomly placed in the interval \((d, N - d)\) and 60 rods at the left end of the system are thermalized with average temperature \( T = 10 \). Then, we simulate the diffusion of energy (temperature) along the chain. To improve the accuracy, all results of such simulations are averaged over \( 10^4 \) independent realizations of the initial temperature distribution. Thus, for every time instance one obtains average temperature distribution in the chain \( T_n(t) = \langle \dot{x}_n^2(t) \rangle \). Results of these simulations are presented in Figures 4 and 5. As one could expect, the character of the thermal diffusion depends on the value of mass ratio \( m \). For \( m = 1 \) one observes a ballistic flow – all energy leaves the left end of the chain, and the heat pulse becomes wider and lower, since the initial pulse contains particles with different velocities. For \( m > 1 \) the flow includes both ballistic and diffusive components, and some residual energy remains at the left end of the system.

It is convenient to describe evolution of the temperature distribution in the chain with the help of the fol-
The mean quadratic deflection from the initial state (concentration at the left end of the chain):

$$\sigma^2 = \sum_{n=1}^{N} (n - 1/2)^2 c_n.$$  \hspace{1cm} (4)

Here \(\{c_n = T_n/2E\}_{n=1}^{N}\) characterizes the temperature distribution in given time instant, \(E = \sum_{n=1}^{N} T_n/2\) is a total constant energy of the chain.

Numeric simulation demonstrates that the mean quadratic deflection at large times asymptotically obeys power law : \(\langle \sigma^2 \rangle \sim t^{\beta}\) when \(t \rightarrow \infty\). These results are illustrated in Figure 6. Li and Wang suggested [13] that the exponent \(\beta\) describing the mean square displacement of diffusion particles \(\langle x^2(t) \rangle \sim t^{\beta}\) should be related with \(\alpha\) through equation

$$\alpha = 2 - 2/\beta.$$  \hspace{1cm} (5)

This equation implies that normal diffusion (\(\beta = 1\)) leads to the normal (non-divergent) heat conductivity (\(\alpha = 0\)). In the same time, superdiffusion (\(\beta > 1\)) correspond to divergent (\(\alpha > 0\)) heat conductivity.

Numeric results in Figure 6 for homogeneous chain with \(m = 1\) yield value \(\beta = 2\), which corresponds to purely ballistic energy transport. For mass ratio \(m = 2\) one obtains \(\beta = 1.32\), and for \(m = 1.05\) or \(m = 1.1\) with \(p_m = 0, 0.5, 0.75\) this exponent is approximately \(\beta = 1.345\). So, for all these values of parameters we obtain somewhat different exponents, but the same qualitative result – the system exhibits superdiffusion, and, consequently, the heat conductivity diverges in the thermodynamic limit.

For mass ratio close to unity one can observe a crossover between different short-time and long-time types of behavior. Namely, the mean quadratic deflection \(\sigma^2\) at small times \(t \sim 10^3\) grows with exponent \(\beta\) close to unity (cf. curves 2, 3, 4, 5 and line 9 in Figure 6). However, for larger times \(t \sim 10^4\) the system achieves the superdiffusion regime with \(1 < \beta < 2\), as it is demonstrated in Figure 6. Therefore, one should expect that the heat conduction coefficient in all considered cases should diverge in thermodynamic limit if the system size is large enough. The diffusion “test” presented here demonstrates no signs of convergent heat conductivity for all studied values of parameters, but instead supports the conjecture of [12] on transient character of the apparent “convergence”.

Finally, it is instructive to check the accuracy of semi-empiric estimation (5) with respect to results of the independent numeric simulations of the heat diffusion and heat conduction. The conclusion is that this formula provides correct qualitative relationship between exponents \(\alpha\) and \(\beta\), but is not completely accurate. For instance, for mass ratio \(m = 3\) we obtained \(\beta = 1.32\), and according to (5) it yields \(\alpha = 0.48\). However, direct simulation of the heat conduction in this case brings \(\alpha = 0.3\). So, the conclusion on divergence of the heat conduction coefficient in all cases is based on the fact that exponent \(\beta\) attains almost the same values for all parameter values, rather than on exact value of this exponent.

In previous sections we explored the effect of disorder on heat transport in systems with divergent heat conductivity. In order to get closer to realistic physical situation, we continue with consideration of one-dimensional chains, in which the heat conduction coefficient converges in the thermodynamical limit.

**IV. HEAT TRANSPORT IN RANDOM DIATOMIC LENNARD-JONES CHAIN**

As an example of more realistic model with convergent heat conductivity, we consider a chain with common Lennard-Jones (LJ) interatomic potential:

$$V(r) = 4\epsilon[(\sigma/r)^6 - 1/2]^2.$$  \hspace{1cm} (6)

We set the following values of parameters: \(\epsilon = 1/72, \sigma = 2^{-1/6}\). For this choice of the parameters, the potential has a minimum for the distance between particles \(r_0 = 1\) and stiffness in the minimum \(k = V''(r_0) = 1\). Consequently, a sound velocity in the homogeneous \((m = 1)\) chain \(v_0 = r_0\sqrt{k/m} = 1\).

Recently it was established that the homogeneous Lennard-Jones chain has convergent heat conductivity [5, 6]. Efficient phonon scattering exists due to thermally
activated large elongations of the interparticle bonds; possibility of such large elongations stems from bound-
edness of the LJ potential [6]. One expects that inho-

Figure 7: Dependence of the thermal conductivity \( \kappa \) on the
length \( N \) of the diatomic LJ chain for temperature \( T = 0.0005 \)
and mass ratio \( m = 2 \). The curves represent the results for
three values of the mass correlation parameter \( p_m = 0, 0.5 \)
and 0.75 (curves 1, 2 and 3 respectively). Horizontal lines
correspond to the values of the heat conduction coefficient
obtained with the help of Green-Kubo relation.

Therefore for \( m > 1 \) the heat conductivity of the LJ chain
should be convergent and lower than in the homogeneous
case.

To verify this conjecture, we simulate the heat trans-
port in random LJ chain with end regions attached to
Langevin thermostats. The method of simulation is de-
scribed in details in paper [5]. For this sake, we consider
the chain with \( N = 80 + 10 \times 2^l, l = 1, 2, ..., 10 \) particles
and fixed boundary conditions, attach the leftmost 40
particles to the Langevin thermostat with temperature
\( T_+ \) and 40 rightmost particles – to the Langevin ther-
omestat with temperature \( T_- \), where \( T_{\pm} = (1 \pm 0.1)T \). Here \( T \)
is the average temperature of the chain. Local tempera-
ture distribution in the chain is defined as \( T_n = \langle \delta x_n^2 \rangle \),
the heat flux – as \( J = \langle J_n \rangle \), where \( J_n = -\dot{x}_n V''(x_{n+1} - x_n) \)
is a local instantaneous flux of energy through site number
\( n \). In internal fragment of the chain \( 40 < n \leq N - 40 \) one
observes constant heat flux and approximately linear
thermal profile. Thus, it is possible to define the heat
conduction coefficient as \( \kappa(N_i) = J N_i / (T_{41} - T_{N-40}) \),
\( N_i = N - 81 \) is the length of the chain fragment between
the thermostats.

Thermal conductivity can also be found with the help
of Green-Kubo relation [14]

\[
\kappa = \lim_{t \to \infty} \lim_{N \to \infty} \frac{1}{N T^2} \int_0^t c(\tau) d\tau, \tag{7}
\]

where \( c(t) = \langle J_n(\tau) J_n(\tau - t) \rangle_\tau \) autocorrelation function
of the heat flux; the latter is defined as \( J_n(t) = \sum_{\tau} J_n(\tau) \).

To find the autocorrelation function \( c(t) \), we simulate a
cyclic chain with \( N = 10^4 \) units, initially completely
immersed in the Langevin thermostat with temperature
\( T \). After thermal equilibration with the thermostat, it is
removed and Hamiltonian dynamics of the chain is sim-
ulated. To increase the accuracy of the autocorrelation
function measurement, we average its value over \( 10^4 \)
independent realizations of the initial chain thermalization.

In the case of small temperatures \( T \ll \epsilon \) the heat
transport occurs due to propagation of weakly interacting
linear waves (as it is commonly accepted, we call them
phonons despite purely classical character of our model).
If the temperatures are large, \( T \gg \epsilon \) only hard cores of

Figure 8: Dependence of the thermal conductivity \( \kappa \) on the
length \( N \) of the diatomic LJ chain for temperature (a)
\( T = 0.0005 \) and (b) \( T = 0.2 \). The mass ratio \( m = 2.1 \). The curves represent the results for three values of the mass cor-
relation parameter \( p_m = 0, 0.5 \) and 0.75 (curves 1, 2 and 3
respectively). Horizontal lines correspond to the values of the
heat conduction coefficient obtained with the help of Green-
Kubo relation.
the interatomic potentials have significant effect on the heat transport. So, the LJ chain can be considered as a set of almost completely rigid particles, and the heat transport occurs due to the collisions between these particles. Since the heat transport mechanisms for high and low temperatures are rather different, it is natural to expect different effect of the random mass distribution in these two cases.

First, let us consider the heat transport in the LJ chain for relatively low temperature \( T = 0.0005 \). In this limit the system becomes very close to a chain with parabolic interatomic potential. Therefore, the diatomic LJ chain with staggering masses (mass correlation parameter \( p_m = 0 \)) becomes close to well-known homogeneous diatomic chain with its typical acoustical and optical phonon branches. In the same time, for random chain with mass correlation parameter \( 0 < p_m < 1 \) it is well-known that some vibration modes become localized (Anderson localization). So, one can expect that as \( p_m \) grows above zero and the homogeneous diatomic chain becomes randomized, the heat conductivity of the chain should decrease. In the same time, as \( p_m \) approaches unity, the chain becomes closer to the monoatomic case, and the heat conductivity should increase. Therefore, one can qualitatively predict non-monotonous dependence of the heat conduction coefficient on the mass correlation parameter \( p_m \) for fixed temperature and mass ratio. Moreover, it is anticipated that this effect will be more pronounced for higher mass ratio.

Dependence of the heat conduction coefficient \( \kappa \) on the chain length \( N \) for different values of \( p_m \) is presented in Figures 7 and 8. For the case \( m = 2 \), \( T = 0.0005 \) the increase of \( p_m \) brings about significant (up to order of magnitude) decrease of the heat conductivity for all considered values of the chain length (see Fig. 7). For the mass ratio close to unity \( m = 1.1 \) the picture is less clear. The increase of \( p_m \) leads to relatively mild decrease of the heat conductivity only for short chains with \( N < 10^3 \), as it is illustrated in Figure 8 (a). Possible explanation is that the chain is rather close to the homogeneity, thus the Anderson localization is less pronounced and other effects (such as grow of expected length of the homogeneous clusters) can come into a competitor and blur the effect of localization. For longer chains, the heat transport is governed by phonons with large wavelength, which are less sensitive to small inhomogeneities of the mass distribution.

For high temperature \( T = 0.2 \) the chain dynamics is primarily governed by collisions between hard repulsive cores of the particles. It is possible to say that in this case the LJ chain is close 1D diatomic gas model, but not completely equivalent to it. The crucial difference is that for any finite values of the temperature the time of collisions is finite. Therefore, contrary to the 1D gas considered above, triple collisions of the particles have a nonzero probability. In recent paper [6] it is demonstrated that such triple collisions provide efficient scattering mechanism for energy transport in the system and ensure convergence of the heat conduction coefficient. Consequently, one should expect a monotonous growth of the heat conductivity with increasing \( p_m \) similarly to the diatomic gas. Numeric simulation presented in Figure 8 (b) confirms this similarity (cf. Figure 3). Important difference is that in the LJ chain the heat conductivity for \( p_m \rightarrow 1 \) remains finite and convergent in the thermodynamical limit.

Due to this convergence, it is reasonable to consider a dependence of the limit value of the heat conduction coefficient on the mass correlation parameter \( p_m \). For this sake, we simulated the chain with \( N = 20000 \) particles and evaluated the limit value of \( \kappa \) for different temperatures and mass ratios with the help of Green-Kubo relation (7). Methodology of this simulation has been described above, and the results are presented in Figure 9.

From Figure 9 one can learn that the character of dependence \( \kappa(p_m) \) substantially depends on the temperature and mass ratio. Common feature of all these dependencies is a rapid growth of the heat conductivity as \( p_m \rightarrow 1 \). For relatively low temperature \( T = 0.0005 \) and for both considered mass ratio \( m = 1.1 \) and \( m = 2 \) these dependencies are not monotonous. In particular, for \( m = 1.1 \) the heat conductivity achieves a minimum for \( p_m = 0.2 \) and for \( m = 2 \) the minimum is achieved for \( p_m = 0.75 \) (see Fig. 9, curves 1 and 3). As it was mentioned above, this non-monotonicity may be attributed to Anderson localization of oscillatory states in the chain with random structure – two terminal states with \( p_m = 0 \) and \( p_m = 1 \) are ordered. Naturally, this effect is much more pronounced for higher mass ratio \( m = 2 \).

For the case of relatively high temperatures this phenomenon of non-monotonicty disappears. Namely, for
mass ratio $m = 2$ and temperature $T = 0.01$ the heat conductivity is almost constant over the interval $0 \leq p_m < 0.9$ and rapidly grows for $p_m > 0.9$ (see Figure 9, curve 4). For mass ratio $m = 1.1$ and temperature $T = 0.2$ the heat conductivity exhibits a monotonous growth over the whole interval $0 < p_m < 1$ (see Figure 9, curve 2). This behavior is another illustration of primarily collisional dynamics of the LJ chain in the limit of high temperatures – it behaves similarly to the gas of rigid particles, cf. Figure 3. It is important to observe that in this regime there is no significant physical difference between the ordered staggered state with $p_m = 0$ and disordered states with small values of $p_m$. The reason is that the collision mechanism is local and not sensitive to the long-range order or disorder.

In this Section we have observed that the introduction of disorder into the diatomic LJ chain brings about significant modifications in its heat conductivity properties. This model is a simple illustration of binary mixture with equal concentration of components. As it was demonstrated above, it allows revealing a relationship between structural patterns typical for the binary mixtures (order vs. disorder, cluster formation) on the heat conductivity. Natural extension of such model is a relaxation of requirement of equal component concentration. This leads to a diatomic model with varying concentration of the components. This latter model is considered in the next Section.

V. EFFECT OF ISOTOPIC IMPURITIES ON THE HEAT CONDUCTIVITY IN LJ CHAIN

Let us consider the LJ chain, in which some particles have relative mass $m = 1.1$ (isotopic impurities). Parameter $0 \leq p_d \leq 0.5$ denotes a concentration of the isotopic impurities. In other terms, the mass of each particle is randomly set to $m$ with probability $p_d$ or to unity – with probability $1 - p_d$. Evaluation of the heat conduction coefficient here will be performed for system size $N = 20000$ with the help of Green-Kubo relation (7). The results are averaged over $10^4$ independent realizations of thermalization and distribution of the impurities. As it is demonstrated in Figure 10, the autocorrelation function of the heat flux decreases exponentially for all considered values of $p_d$.

We first explore the dependence of heat conductivity on the concentration of impurities for different temperatures, which determine different regimes of the heat transport. For this sake, we consider three different temperatures of the system: $T = 0.001 \ll \epsilon$, $T = 0.01 \sim \epsilon$ and $T = 0.1 \gg \epsilon$. Dependence of the heat conduction coefficient $\kappa$ on the concentration of impurities $p_d$ for these temperatures is presented in Figure 11. We observe that the increase of the concentration brings about monotonous decrease of the heat conduction coefficient for all temperatures; the minimal value is attained for $p_d = 0.5$.

![Figure 10: Exponential decrease of the autocorrelation function $c(t)$ for the LJ chains with concentration of impurities $p_d = 0, 0.05, 0.1, 0.2, 0.5$ (curves 1, 2, 3, 4, 5 respectively). Temperature of the system $T = 0.01$, mass of each impurity $m = 1.1$.](image1)

![Figure 11: Dependence of the thermal conductivity $\kappa$ on the concentration of impurities $p_d$ in the LJ chain with temperatures $T = 0.001$, $T = 0.01$ and $T = 0.1$ (curves 1, 2 and 3).](image2)

Dependence of the heat conduction coefficient $\kappa$ on temperature $T$ for $p_d = 0$ and $p_d = 0.5$ is presented in Figure 12. Temperature dependence of the heat conductivity is not monotonous in both cases. Minimum of the heat conductivity corresponds to temperature $T_0 \approx \epsilon/2$. This pattern is related to weak phonon scattering for the low temperatures and collision-like dynamics for the high temperatures. Presence of the impurities in the chain does not change these patterns in qualitative manner, but quantitative changes are easily detected. In particular, the impurities most significantly attenuate the heat
conductivity in the limits of low and high temperatures (note logarithmic scale in Figure 10). To quantify this effect, is convenient to define a coefficient of maximal attenuation of the heat conductivity as $c_d = \kappa(0.5)/\kappa(0)$, where $\kappa(p_d)$ is the heat conduction coefficient in the LJ chain with concentration of impurities equal to $p_d$. Thus, for $T = 0.0005$ one obtains $c_d = 0.040$, for $T = 0.005$ – $c_d = 0.31$ and for $T = 0.1$ – $c_d = 0.037$. These findings may be easily explained, since the isotopic disorder strongly affects the phonons scattering at low temperatures – by modification of the spectrum and introducing new scatterers. For high temperatures the situation is even more profound – without disorder the system is close to integrable homogeneous billiard, and with disorder – to non-integrable random billiard considered above. However, for the crossover temperature $T \sim \epsilon/2$, there are no well-defined heat carriers and the chain exhibits strong chaos. This behavior is less sensitive to the disorder than the transport mechanisms, which work in the cases of high and low temperatures.

One can see that physical consequences of the isotopic disorder are determined by particular physical mechanism of the heat transport, rather than by mere fact of convergence or divergence of the heat conduction coefficient. To get additional evidence for this idea, we study the effect of isotopic disorder in other system, which has convergent heat conductivity, but completely different basic scattering mechanism – a chain of rotators.

VI. ISOTOPIC DISORDER IN THE CHAIN OF ROTATORS

The chain of rotators historically was the first to reveal the convergence of heat conductivity in 1D system in thermodynamic limit [15, 16]. This system is characterized by soft anharmonic periodic potential of the nearest-neighbor interactions:

$$V(r) = 1 - \cos(r).$$

The convergent heat conductivity in this system appears due to the scattering of phonons on rotobreathers, which appear due to thermal activation [15]. As in the previous Section, we introduce the isotopic disorder by including the particles with nonunit mass (one can interpret them as rotors with nonunit moment of inertia) in random manner with certain probability $p_d$. Then, the system is simulated and the heat conduction coefficient is evaluated by protocol based on the Green-Kubo relation, as it was described above.

Dependence of the heat conduction coefficient in the chain of rotators on its temperature is presented in Fig-
ure 13 for $p_d = 0$ and $p_d = 0.5$. One observes that for $p_d = 0$ the heat conduction coefficient $\kappa$ monotonously decreases with $T$ and for small temperatures is nicely described by the fitting $\kappa_0(T) = 0.0095 \exp(4.45/\sqrt{T})$. When one introduces the isotopic disorder (ratio of masses $m = 1.1$, concentration of impurities $p_d = 0.5$), one obtains very similar behavior with slightly different fitting $\kappa_{0.5}(T) = 0.0099 \exp(4.36/\sqrt{T})$ for the case $T \to 0$. So, the isotopic disorder leads to very slow decrease of the attenuation ratio $c_d = \kappa(0.5)/\kappa(0)$ as $T \downarrow 0$. For high temperatures, the isotopic disorder has almost no effect on the heat conduction. Slight reduction of $\kappa$ can be attributed to an increase of an average mass of the particles $\bar{m} = (1-p_d) + mp_d$; this effect leads to minor reduction of the heat conductivity $c_d = 1/\sqrt{\bar{m}}$ (for $m = 1.1$ and $p_d = 0.5$ one obtains $c_d = 0.976$).

From simple comparison between Figures 12 and 13, one can immediately conclude that the isotopic disorder has much stronger effect on the heat conductivity in the LJ chain than in the chain of rotators. In the latter case, the energy required for activation of the roto-breathers weakly depends on the isotopic disorder. The reason is the strongly localized profile of the roto-breather. In the same time, the fitting obtained in Figure 13 is quite surprising. If the roto-breathers are activated through a mechanism of thermal fluctuations, one would expect Arrenius behavior for the heat conduction coefficient (see, e.g. [6]). However, in this case we observe strongly non-Arrhenius behavior. One could conjecture that this result points on a fact that the roto-breathers appear (and disappear) as a result of interactions with small number of phonons, rather than by creation from the “thermal bath”. This issue seems rather challenging and calls for further exploration.

VII. CONCLUDING REMARKS

The results presented above address the effect of disorder on heat transport in one-dimensional models in two main aspects. The first one is internal correlation in the disordered structure. It is demonstrated that the effect of this internal correlation may be ambiguous and is governed by particular interatomic potential in the specific chain model. In the chain of rigid rods the growth of correlation leads to the growth of heat conductivity, since longer clusters leave less possibilities for the scattering of heat pulses. In the LJ chain the increase of the cluster length competes with a possibility of Anderson localization for the case of low temperatures, and therefore the heat conductivity depends on the correlation parameter in non-monotonous manner. From the other side, growing concentration of the impurities (particles with larger mass) always reduces the heat conductivity, but the extent of this reduction again strongly depends on the particular interatomic potential of interaction. In LJ chain a reduction by more than order of magnitude has been observed; in the chain of rotators the same concentration of the impurities led to reduction of the heat conductivity only by few percent. So, the effect of disorder is non-universal and cannot be explained without account of the structure of particular chain, and, even more important, of particular scattering mechanisms for the heat flux. In the same time, we have not observed any dependence of the convergence properties of the heat conduction coefficient on the amount of disorder in the system. It seems that this property is governed by more fundamental factors, such as topology of the potential.

VIII. ACKNOWLEDGMENTS

The authors are very grateful to Israel Science Foundation (grant 838/13) and to Lady Davis Fellowship Trust for financial support of their work. A.V.S. is grateful to the Joint Supercomputer Center of the Russian Academy of Sciences for the use of computer facilities.

[1] E. Fermi, J. Past,a and S. Ulam. Studies of nonlinear problems. Los Alamos Report No. LA.1940 (1955).
[2] S. Lepri, R. Livi, and A. Politi. Phys. Rep. 377, 1 (2003).
[3] S. Lepri, R. Livi, and A. Politi. Anomalous Transport: Foundations and Applications Weinheim:Wiley-VCH Verlag, Ch. 10, 2008).
[4] A. Dhar. Heat transport in low-dimensional systems. Advances in Physics 57, 5, 457-537 (2008).
[5] A. V. Savin and Yu. A. Kosevich. Thermal conductivity of molecular chains with asymmetric potentials of pair interactions. Phys. Rev. E 89, 032102 (2014).
[6] O. V. Gendelman and A. V. Savin. Normal heat conductivity in chains capable of dissociation. EPL, 106 34004 (2014).
[7] O.V.Gendelman and A.V.Savin. Heat Conduction in a One-Dimensional Chain of Hard Disks with Substrate Potential. Phys. Rev. Lett. 92 074301 (2004).
[8] A. Dhar. Heat Conduction in a One-Dimensional Gas of Elastically Colliding Particles of Unequal Masses. Phys. Rev. Lett. 86, 3554 (2001).
[9] A. V. Savin, G. P. Tsironis, and A. V. Zolotaryuk. Heat Conduction in One-Dimensional Systems with Hard-Point Interparticle Interactions. Phys. Rev. Lett. 88, 154301 (2002).
[10] P. Grassberger, W. Nadler, and L. Yang. Heat Conduction and Entropy Production in a One-Dimensional Hard-Particle Gas. Phys. Rev. Lett. 89, 180601 (2002).
[11] G. Casati and T. Prosen. Anomalous heat conduction in a one-dimensional ideal gas. Phys. Rev. E 67, 015203 (2003).
[12] S. Chen, J. Wang, G. Casati, and G. Benenti. Nonintegrability and the Fourier heat conduction law. Phys. Rev.
[13] B. Li and J. Wang. Anomalous Heat Conduction and Anomalous Diffusion in One-Dimensional Systems. Phys. Rev. Lett. 91, 044301 (2003).

[14] R. Kubo, M. Toda, and N. Hashitsume, in Statistical Physics II, edited by P. Fulde, Springer Series in Solid-State Sciences Vol. 31 (Springer, Berlin, 1991).

[15] O. V. Gendelman and A. V. Savin. Normal heat conductivity of the one-dimensional lattice with periodic potential of nearest-neighbor interaction. Phys. Rev. Lett., 84, 2381 (2000).

[16] C. Giardina, R. Livi, A. Politi, and M. Vassalli. Finite thermal conductivity in 1D lattices. Phys. Rev. Lett., 84, 2144 (2000).