Normal Heat Conductivity of the One-Dimensional Lattice with Periodic Potential of Nearest-Neighbor Interaction

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The process of heat conduction in a chain with a periodic potential of nearest-neighbor interaction is investigated by means of molecular dynamics simulation. It is demonstrated that the periodic potential of nearest-neighbor interaction allows one to obtain normal heat conductivity in an isolated one-dimensional chain with conserved momentum. The system exhibits a transition from infinite to normal heat conductivity with the growth of its temperature. The physical reason for normal heat conductivity is the excitation of high-frequency stationary localized rotational modes. These modes absorb the momentum and facilitate locking of the heat flux.

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The process of heat transport in one-dimensional lattices has become a challenging problem of nonlinear dynamics and statistical physics since the well-known work of Fermi, Pasta, and Ulam (FPU) [1]. They have revealed that weak anharmonicity of nearest-neighbor interaction is not sufficient to provide Fourier law of heat conductivity. This result questions the universal validity of the well-known Peierls model of the heat transport in dielectrics [2].

The general reason for the absence of the normal heat conductivity in the system of FPU is its closeness to the exactly integrable weakly nonlinear string described by the Korteveg–de Vries equation. Similarly, the exactly integrable Toda lattice reveals the absence of normal heat conductivity. Thus, the first necessary condition of the normal heat conductivity is stochastic behavior of the system. A widely studied system of this sort is the diatomic Toda lattice (the chain with the exponential potential of nearest-neighbor interaction and altering masses of the particles) [3]. It was demonstrated that this system has no normal heat conductivity at low temperatures even if the mass ratio is unfavorable for the integrability (1:2 [4]). However if the temperature is sufficiently high, the system becomes stochastic and demonstrates normal (linear) temperature distribution along the chain if the temperature gradient is applied. The reason for this effect is the closeness of the diatomic Toda lattice to the integrable Korteveg–de Vries string in the case of low temperatures and to the stochastic diatomic billiard in the case of high temperatures [5].

Recent large-scale numerical simulations had demonstrated that the stochastization of the system is necessary but not sufficient to provide Fourier law in the one-dimensional lattices. For a large variety of chains (FPU with quartic potential and others) exhibiting linear temperature distribution it was demonstrated that the coefficient of the heat conductivity diverges in the thermodynamic limit (as the number of particles N in the chain grows) as approximately $N^{0.37}$ [6]. Most recently the same situation was proved to be the case for the diatomic Toda lattice [7]. This paper also speculates that the heat conductivity in the linear chain with translationally invariant potentials (i.e., with conserved momentum) always diverges. It should be mentioned that for a few studied lattices with on-site potential (i.e., without conservation of momentum) normal heat conductivity is observed (ding-a-dong [8], ding-a-ling [9], and Frenkel-Kontorova models [10,11]). With the above situation in view, the chain with translationally invariant potentials and normal (saturating) heat conductivity may be of essential interest.

The present paper deals with the class of chains with the periodic potential of the nearest-neighbor interaction. Such a potential describes, for instance, the relative rotation of polymer fragments around the axis of the macromolecule [12]. This model is rather essential from the physical point of view since the interaction between macromolecules in a polymer crystal is much weaker than intermolecular interaction. Therefore in many situations the one-dimensional picture of processes in a polymer crystal is of real physical significance rather than of pure academic interest. To the best of our knowledge chains with a periodic potential have not been studied yet from the viewpoint of their heat conductivity. Moreover, the systems of this sort have essential peculiarity, namely, formation of nonlinear localized rotational modes [13].

Let us consider a chain of molecules having a fixed distance l between the nearest neighbors. The molecules are allowed to rotate around the chain axis. Let the variable $\phi_n(t)$ denote the rotation of the nth molecule around the chain axis in an immovable system of coordinates. Thus a dimensionless Hamiltonian of the system will be

$$H = \sum_n \left\{ \frac{1}{2} \dot{\phi}_n^2 + U(\phi_{n+1} - \phi_n) \right\}, \tag{1}$$

where the dot denotes differentiation with respect to time t and $U(\phi)$—the potential of the nearest-neighbor interaction is a non-negative 2π-periodic function which satisfies the following conditions: $U(0) = 0$, $U'(0) = 0$, and $U''(0) = 1$. For the sake of the present simulation this potential is chosen in the simplest form

$$U(\phi) = 1 - \cos\phi \,. \tag{2}$$

While simulating the heat conductivity in atomic chains, the Nose-Hoover [14] model of a heat bath is commonly used. However, it was demonstrated that this model does not ensure correct energy distribution for the chain [15]. Therefore the classic Langevin model of the heat bath is used. A chain of N molecules is considered, N_0 molecules from each side being coupled to the Langevin heat baths with temperatures T_+ and T_-, respectively. Equations of motion for this system are written as

$$\begin{aligned}
&\ddot{\phi}_n = F(\phi_{n+1} - \phi_n) - F(\phi_n - \phi_{n-1}) - \gamma\dot{\phi}_n + \xi_n \,, \\
&\quad n = 1, \ldots, N_0 \,, \\
&\ddot{\phi}_n = F(\phi_{n+1} - \phi_n) - F(\phi_n - \phi_{n-1}) \,, \\
&\quad n = N_0 + 1, \ldots, N - N_0 \,, \\
&\ddot{\phi}_n = F(\phi_{n+1} - \phi_n) - F(\phi_n - \phi_{n-1}) - \gamma\dot{\phi}_n + \eta_n \,, \\
&\quad n = N - N_0 + 1, \ldots, N \,,
\end{aligned} \tag{3}$$

where function $F(\phi) = dU(\phi)/d\phi$, γ is a coefficient of linear relaxation, and ξ_n, η_n are white Gaussian noise governed by the following correlation relationships: $\langle \xi_n(t) \rangle = 0$, $\langle \eta_k(t) \rangle = 0$, $\langle \xi_n(t_1)\eta_k(t_2) \rangle = 0$, $\langle \xi_n(t_1)\xi_k(t_2) \rangle = 2\gamma T_+ \delta_{nk}\delta(t_2 - t_1)$, and $\langle \eta_n(t_1)\eta_k(t_2) \rangle = 2\gamma T_- \delta_{nk}\delta(t_2 - t_1)$.

The system of equations (3) has been integrated numerically. All values and processes were analyzed for time scales of 10^6–10^7, whereas the thermal equilibrium was approached at the scale 10^5. Then temperature profile

$$T_n = \langle \dot{\phi}_n^2(t) \rangle_t = \lim_{t\to\infty} \frac{1}{t} \int_0^t \dot{\phi}_n^2(\tau)\, d\tau \tag{4}$$

and local heat flux

$$J_n = \langle j_n(t) \rangle_t = \lim_{t\to\infty} \frac{1}{t} \int_0^t j_n(\tau)\, d\tau \tag{5}$$

of the chain were computed. Here $j_n = -[F(\phi_{n+1} - \phi_n) + F(\phi_n - \phi_{n-1})]\dot{\phi}_n/2$. The chain has been simulated for the following values of parameters: $\gamma = 0.1$, $N_0 = 50$, $N = 150$, 200, 300, 500, 700, 900, 1300, 1700, 2100, 2400, and zero initial conditions $\{\phi_n = 0, \dot{\phi}_n = 0\}_{n=1}^{N}$. Thermal equilibrium was approached within the time scale $t = 10^5$. Time averages (4) and (5) were computed afterwards over the characteristic scale $t = 10^6$–10^7.

The linear temperature distribution formed due to the temperature gradient at the ends of the chain is presented in Fig. 1. The heat flux J_n in the chain outside the heat baths $N_0 < n \le N - N_0$ is constant $J_n = J$. The temperatures of the ends of the chain are well defined (although they are different from the prescribed temperatures of the heat baths), and thus reliable calculation of the heat conductivity of the chain is possible:

$$\kappa(N_1) = JN_1/(T_{N_0+1} - T_{N-N_0}) \,, \tag{6}$$

where $N_1 = N - 2N_0$ is a length of the chain fragment outside the heat baths. The limit value

$$\kappa = \lim_{N_1\to\infty} \kappa(N_1) \tag{7}$$

corresponds to the coefficient of heat conductivity of the chain under temperature $T = (T_+ + T_-)/2$.

The alternative way to compute the heat conductivity of the chain is based on the Green-Kubo formula [16]

$$\kappa_s = \lim_{t\to\infty} \lim_{N\to\infty} \frac{1}{NT^2} \int_0^t c(\tau)\, d\tau \,, \tag{8}$$

where the correlation function $c(t) = \langle J_s(\tau)J_s(\tau - t) \rangle_\tau$, and $J_s(t) = \sum_n j_n(t)$ is the average heat flux in the chain.

While computing this correlation function the cyclic chains of $N = 4000$ molecules completely connected with the Langevin heat bath have been considered. When the thermal equilibrium has been approached, the bath has been removed and the heat flux in the free chain has been analyzed. In order to improve the accuracy the results were averaged over 500 different realizations of the Langevin bath.

Numerical simulation of the chain has demonstrated that there exists a certain critical value of the temperature T_0 in the interval $[0.2 \;\; 0.3]$. If $T < T_0$ then the heat conductivity of the chain diverges in the limit of $N_1 \to \infty$ and for $T > T_0$ the heat conductivity converges to finite value. The dependence of κ on N_1 at the temperature $T = 0.2$ is presented in Fig. 2. As is demonstrated there, the heat conductivity κ diverges approximately as $N_1^{0.26}$. This law of divergence remarkably coincides with those discovered for other systems earlier [6,7], although the power is slightly less than reported there. However, for the temperatures

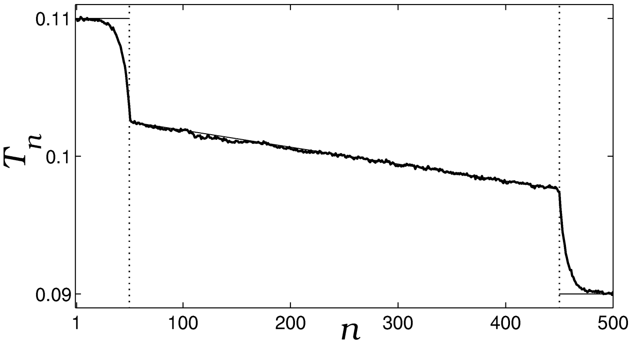

FIG. 1. Distribution of local temperature T_n in the chain with a periodic potential of nearest-neighbor interaction ($N = 500$, $N_0 = 50$, $T_+ = 0.11$, $T_- = 0.09$; time of averaging is $t = 5 \times 10^6$).

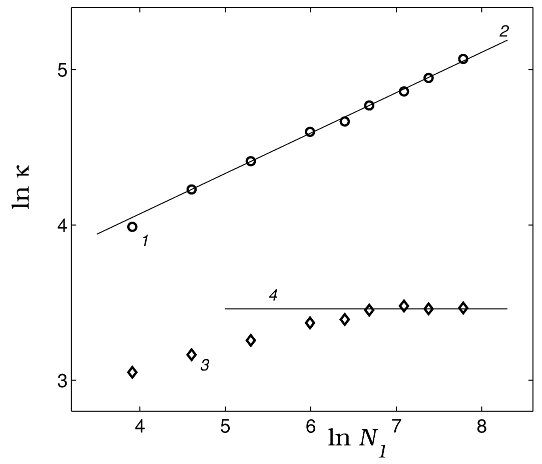

FIG. 2. Dependence of $\ln\kappa$ on $\ln N_1$. Markers 1 (circles) represent numerical data at the temperature $T = 0.2$ ($T_+ = 0.21$, $T_- = 0.19$). The line 2 approximating these data has slope $\delta = 0.26$. Markers 3 (diamonds) represent the numerical data at $T = 0.3$ ($T_+ = 0.33$, $T_- = 0.27$). Corresponding line 4 has zero slope ($\kappa = 31.8$).

$T > T_0$ this divergence disappears and the limit is finite. As is also demonstrated in Fig. 2, for $T = 0.3$ the heat conductivity $\kappa(N_1)$ approaches its limit value $\kappa = 31.8$ with a growth of N_1.

As the last result is very different from the results for other chains with conserved momentum, the behavior of the heat conductivity was checked independently with the help of the Green-Kubo formula (8). The investigation of the correlation function $c(t)$ has confirmed the conclusion concerning the finite heat conductivity of the chain. The reason is that for the temperature region $T > T_0$ the correlation function decreases exponentially with time and therefore the integral in formula (8) converges. Hence the heat conductivity κ_c is finite. For $T_0 < T < 2$ the correlation function decreases monotonically and for $T > 2$ the decrease is exponential with oscillations. It should be mentioned that the two ways of numerical calculation of the heat conductivity provide almost equal results (the difference never exceeded a few percent).

Then the dependence of the heat conductivity on the temperature of the chain has been computed by means of the Green-Kubo formula (8). It was demonstrated that for $T \to \infty$ the coefficient of heat conductivity decreases exponentially and diverges for $T \to T_0$ (see Fig. 3).

In order to investigate the mechanism of heat conduction the dependence of the global heat flux J on the temperature gradient imposed on the chain was computed. The temperature T_- was set equal to zero. As is demonstrated in Fig. 4, the value of the heat flux grows monotonically for temperatures $T < T_r = 1.3$. At $T = T_r$ the heat flux approaches its maximum value and decreases with further growth of the temperature gradient. Such unexpected behavior is related to excitation of nonlinear localized rotational modes of the chain.

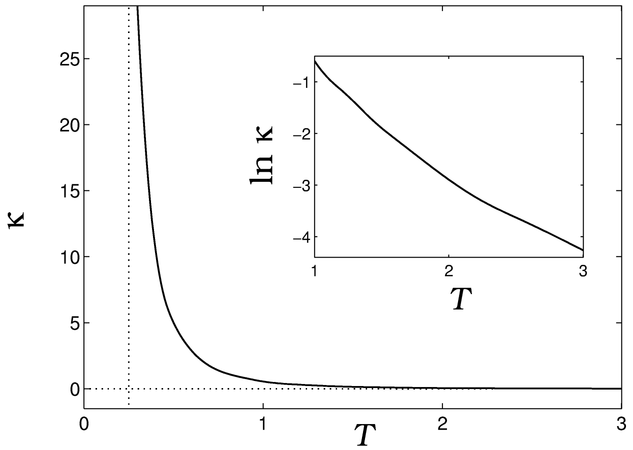

FIG. 3. Dependence of the heat conductivity κ on the temperature T. The inset demonstrates the same dependence in semilogarithmic coordinates. The heat conductivity decreases exponentially at sufficiently high temperatures.

Physically these modes correspond to fast rotation of one molecule, whereas the rotation angles of its neighbors remain small. Such modes are possible due to the periodic and finite potential of the nearest-neighbor interaction. A necessary condition of localization is that the average frequency of rotation has to be inside the attenuation zone of the linear spectrum of the chain. More exact measurements with numerical technique have demonstrated that for the chain considered the localized rotational modes exist for frequency region $\omega > 2.175\,62$ (and the phonon propagation zone is $0 \le \omega \le 2$). Numerical simulations demonstrate that these localized excitations prevent free propagation of phonons. Rotational localized excitation in the chain with finite temperature has a finite lifetime and is gradually destroyed due to interaction with phonons.

In order to elucidate the role of rotational localized excitations in the heat transfer and relaxation, another numerical experiment has been performed. The chain of $N = 300$ particles was heated in the Langevin thermal bath which was removed after the thermal equilibrium was approached. In order to provide a channel for energy

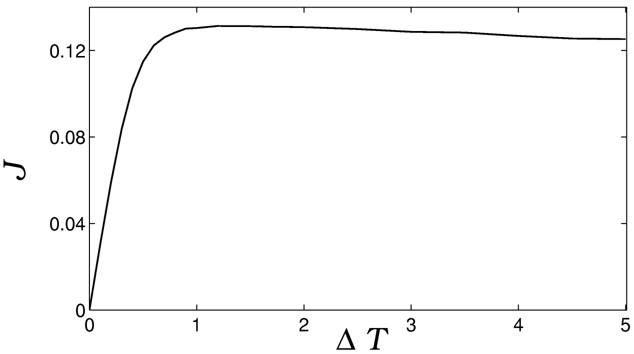

FIG. 4. Dependence of the heat flux J on the temperature gradient ΔT in the chain with $N = 300$, $N_0 = 50$, $T_+ = \Delta T$, $T_- = 0$.

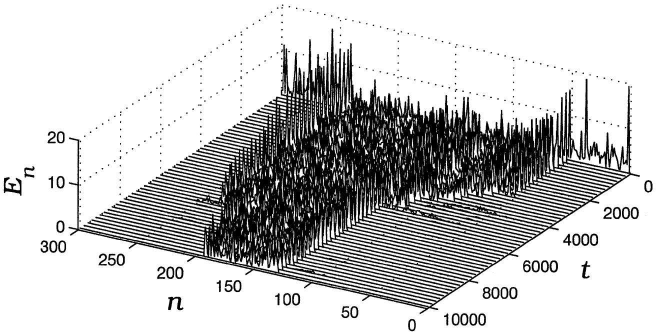

FIG. 5. Energy relaxation in the heated chain. Dependence of local energy E on the number of the molecule n and time t is represented. Initial temperature is $T = 3$, then the relaxation without energy supply and with friction within the heat baths is considered ($N = 300$, $N_0 = 50$, $T_+ = T_- = 0$).

absorption viscous damping at the ends of the chain has been introduced [it was sufficient to put $T_+ = T_- = 0$ in the system of equations (3)]. The numerical simulation has demonstrated an essential number of localized rotations in the chain. At $T = 1$ their number is rather small and they decay rapidly, thus they do not constitute any obstacle for the relaxation of energy. For $T = 2$ their effect on the relaxation is rather essential since the relaxation of energy in the middle of the chain becomes possible not before the localized rotations at the end parts of the chain are destroyed. Such stepwise character of relaxation dependent on the destroying of localized rotational modes for $T = 3$ is demonstrated in Fig. 5. The results of previous simulations demonstrate that at least at the qualitative level the process of the heat transfer in the chain with periodical potential of the nearest-neighbor interaction may be described as a sequence of "lockings" and "releases" of the heat flux. They occur due to the excitation and splitting of corresponding localized rotational modes, respectively. Thus, at high temperatures the diffusion of energy is governed mainly by the process described above rather than by interaction between long-wavelength Fourier modes being the reason for the divergence of the heat conductivity in the FPU-like chains [6].

Additional numerical simulation had demonstrated that the periodic waves in the chain of rotators become unstable as their energy approaches a certain critical value and localized rotational modes emerge as the result of this instability. The physical reason for this instability seems to be rather obvious—the periodic wave becomes unstable as the relative rotation of neighbor particles becomes close to 180°. So, with growth of the temperature the energy stored in the periodic waves is saturated, and the concentration and the lifetime of the rotational modes both increase. That in turn accounts for the saturation and decrease of the heat flux with the growth of the temperature at $T > T_r$ (Fig. 4).

Hence, the above results allow one to conclude that the transition from infinite to finite heat conductivity with the growth of temperature is observed in a one-dimensional chain with periodic potential of the nearest-neighbor interaction. The physical reason for normal heat conductivity is the excitation and splitting of nonlinear localized rotational modes. These modes prevent free propagation of the heat flux. Because of the finite lifetime of these rotational modes the process of the heat conduction constitutes successive lockings and releases of the heat flux.

Therefore the heat conductivity in the 1D chain may be normal despite the conservation of momentum. It is possible to speculate that it is not the case in previously studied chains with infinite nearest-neighbor potential (FPU, diatomic Toda lattice, and others) because localized vibrational modes known in such systems (discrete breathers [17]) do not reflect and lock the acoustic phonons like the localized rotational modes (rotobreathers) in the chain of rotators.

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