Nonstationary heat conduction in one-dimensional chains with conserved momentum

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This Rapid Communication addresses the relationship between hyperbolic equations of heat conduction and microscopic models of dielectrics. Effects of the nonstationary heat conduction are investigated in two one-dimensional models with conserved momentum: Fermi-Pasta-Ulam (FPU) chain and chain of rotators (CR). These models belong to different universality classes with respect to stationary heat conduction. Direct numeric simulations reveal in both models a crossover from oscillatory decay of short-wave perturbations of the temperature field to smooth diffusive decay of the long-wave perturbations. Such behavior is inconsistent with parabolic Fourier equation of the heat conduction. The crossover wavelength decreases with increase in average temperature in both models. For the FPU model the lowest-order hyperbolic Cattaneo-Vernotte equation for the nonstationary heat conduction is not applicable, since no unique relaxation time can be determined.

It is well known that parabolic Fourier equation of heat conduction implies infinite speed of the signal propagation and thus is inconsistent with causality [1–5]. Numerous modifications were suggested to recover the hyperbolic character of the heat transport equation [2]. Perhaps, the most known is the lowest-order approximation known as Cattaneo-Vernotte (CV) law [1,2]. In its one-dimensional (1D) version it is written as

$$\left(1 + \tau \frac{\partial}{\partial t}\right)\vec{q} = -\kappa\vec{\nabla}T, \qquad (1)$$

where κ is standard heat conduction coefficient and τ is characteristic relaxation time of the system. The latter can be of macroscopic order [5]. Importance of the hyperbolic heat conduction models for description of a nanoscale heat transfer has been recognized [6,7].

Only few papers dealt with numeric verification of such laws from the first principles [8]. As it is well known now from numerous numeric simulations and few analytic results, the relationship between the microscopic structure and applicability of the Fourier law for description of the stationary heat conduction is highly nontrivial and depends both on size and dimensionality of the model [9]. In particular, the heat conduction coefficient can diverge in the thermodynamic limit. Hyperbolic equations describing the nonstationary heat conduction inevitably include more empiric constants and therefore their relationship to the microscopic models can be even less trivial. To the best of our knowledge, no conclusive data exist in this respect.

This Rapid Communication deals with a study of spatial and temporal peculiarities of the nonstationary heat conduction in two simple one-dimensional models with conserved momentum—Fermi-Pasta-Ulam (FPU) chain and chain of rotators (CR). From the viewpoint of the stationary heat conduction, these two systems are known to belong to different universality classes. Namely, in the FPU chain the heat conduction coefficient diverges with the size of the system [10], whereas in the CR model it converges to a finite value

[11–13]. So, it is interesting to check whether other differences between these models will reveal themselves in the problem of nonstationary heat conduction.

In order to investigate this process, one should choose the parameters to measure. This question is not easy since the situation in this problem is different from the stationary heat conduction, where only one commonly accepted macroscopic equation exists and only one empiric parameter should be computed. The simplest CV law already has two independent coefficients, whereas more elaborate approximations can include even more parameters. Just because many different empiric equations exist, it is not desirable to pick one of them *ab initio* and to fit the data to find particular set of constants. Instead, it seems reasonable to look for some quantity which will characterize the process of the nonstationary conduction and can be measured from the simulations without relying on particular approximate equation. For this sake, we choose the characteristic *length* which characterizes the scale at which the nonstationarity effects are significant.

In order to explain the appearance of this scale, let us refer to 1D version of the CV equation for the temperature:

$$\tau\frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \alpha\frac{\partial^2 T}{\partial x^2}, \qquad (2)$$

where α is the temperature conduction coefficient.

Let us consider the problem of nonstationary heat conduction in a one-dimensional specimen with periodic boundary conditions $T(L,t)=T(0,t)$, where $T(x,t)$ is the temperature distribution, L is the length of the specimen, and $t \geq 0$. If it is the case, one can expand the temperature distribution to Fourier series, as a sum of spatial modes:

$$T(x,t) = \sum_{m=-\infty}^{\infty} a_m(t)\exp(2\pi inx/L), \qquad (3)$$

with $a_m(t)=a_{-m}^*(t)$, since $T(x,t)$ is real function.

Substituting Eq. (2) into Eq. (3), one obtains the equations for time evolution of the modal amplitudes:

$$\tau \ddot{a}_m + \dot{a}_m + 4\pi^2 m^2 \alpha a_m / L^2 = 0. \tag{4}$$

Solutions of Eq. (4) are written as

$$a_m(t) = C_{1m} \exp(\lambda_1 t) + C_{2m}(\lambda_2 t),$$

$$\lambda_{1,2} = (-1 \pm \sqrt{1 - 16\pi^2 m^2 \alpha \tau / L^2})/2, \tag{5}$$

where C_{1m} and C_m are constants determined by the initial distribution.

From Eq. (5) it immediately follows that for sufficiently short modes the temperature profile will relax in oscillatory manner:

$$m > L/4\pi\sqrt{\alpha\tau},$$

$$a_m(t) \sim \exp(-t/2\tau)\exp(i\omega_m t),$$

$$\omega_m = (\sqrt{16\pi^2 m^2 \alpha \tau / L^2 - 1})/2\tau. \tag{6}$$

If the specimen is rather long ($L \gg 4\pi\sqrt{\alpha\tau}$) then for small wave numbers (acoustic modes):

$$\lambda_1 \approx -1/\tau, \quad \lambda_2 \approx -4\pi^2 m^2 \alpha / L^2. \tag{7}$$

The first eigenvalue describes fast initial transient relaxation, and the second one corresponds to stationary slow diffusion and, quite naturally, does not depend on τ. So, we can conclude that there exists a critical length of the mode

$$l^* = 4\pi\sqrt{\alpha\tau}, \tag{8}$$

which separates between two different types of the relaxation: oscillatory and diffusive. The oscillatory behavior is naturally related to the hyperbolicity of the system. Existence of this critical scale characterizes the deviance of the system from parabolic Fourier law.

This critical wavelength scale l^* can be measured directly from the numeric simulation without relying on any particular empiric equation of the nonstationary heat conduction. The numeric experiment should be designed in order to simulate the relaxation of thermal profile to its equilibrium value for different spatial modes of the initial temperature distribution. We simulate the periodic chain of particles with conserved momentum with Hamiltonian

$$H = \sum_{n=1}^{N} \frac{1}{2} \dot{u}_n^2 + V(u_{n+1} - u_n), \tag{9}$$

where u_n is the displacement of nth particle and $V(u_{n+1} - u_n)$ is the potential of nearest-neighbor interaction. In order to obtain the initial nonequilibrium temperature distribution, all particles in the chain were embedded in the Langevin thermostat [9]. For this sake, the following system of equations was simulated:

$$\ddot{u}_n = V'(u_{n+1} - u_n) - V'(u_n - u_{n-1}) - \gamma_n \dot{u}_n + \xi_n,$$

$$n = 1, \ldots, N \tag{10}$$

where γ_n is the relaxation coefficient of the nth particle and the white noise ξ_n is normalized by the following conditions:

$$\langle \xi_n \rangle = 0, \quad \langle \xi_n(t_1)\xi_k(t_2) \rangle = 2\sqrt{\gamma_n \gamma_k} T_n \delta_{nk} \delta(t_1 - t_2), \tag{11}$$

where T_n is the prescribed temperature of the nth particle. The numeric integration has been performed for $\gamma_n = 0.1$ for every n and within time interval $t = 250$. After that, the Langevin thermostat was switched off [i.e., the dissipation and random force terms in Eq. (10) were set to zero] and relaxation of the system to a stationary temperature profile was studied for various initial distributions T_n for two particular choices of the nearest-neighbor interaction described above (FPU and chain of rotators):

$$V_1(x) = x^2/2 + x^4/4, \quad V_2(x) = 1 - \cos x.$$

The temperature of individual particle was defined as $T_n = \langle \dot{u}_n^2 \rangle$, where the averaging was performed over 20 successive time steps.

Separate analysis of individual spatial modes will provide insight into the global behavior of the system only if these modes are, at least approximately, not interacting. For CV Eq. (2) this is the case since it is linear. However, we do not rely on it *a priori* and the absence of interaction between different spatial relaxation modes [defined by Eq. (3)] should be checked numerically. We simulate the relaxation of the initial thermal profile comprising five different modes:

$$T_n = T_0 + \sum_{i=4}^{8} A_i \cos[2\pi(n-1)/2^i] \tag{12}$$

in cyclic chain of $N = 2^{10}$ particles, with average temperature $T_0 = 1$ and modal amplitudes $A_4 = \cdots = A_8 = 0.02$ for the CR potential, and with $T_0 = 20$, $A_4 = \cdots = A_8 = 0.4$ for the FPU potential. Both simulations demonstrated almost complete lack of interaction between the modes. No other modes were excited with visible amplitudes. Each mode in the collective excitation relaxed similarly to the profile obtained when it was excited individually. So, it is possible to conclude that for given values of the parameters the equation of the nonstationary heat conduction should be approximately linear and separate analysis of spatial relaxation modes is justified.

In order to study the relaxation of different spatial modes of the initial temperature distribution, its profile has been prescribed as

$$T_n = T_0 + A \cos[2\pi(n-1)/Z], \tag{13}$$

where T_0 is the average temperature, A is the amplitude of the perturbation, and Z is the length of the mode (number of particles). The overall length of the chain L has to be multiple of Z in order to ensure the periodic boundary conditions. The results were averaged over 10^6 realizations of the initial profile in order to reduce the effect of fluctuations.

Typical result of the simulation is presented at Fig. 1. The chain of rotators of the same length $N = 1024$ and the same modal wavelength $Z = 64$ demonstrates qualitatively different relaxation behavior for different temperatures—the oscillatory one for lower temperature and the smooth decay—for higher temperature. This observation suggests that the critical wavelength mentioned above, if it exists, should decrease
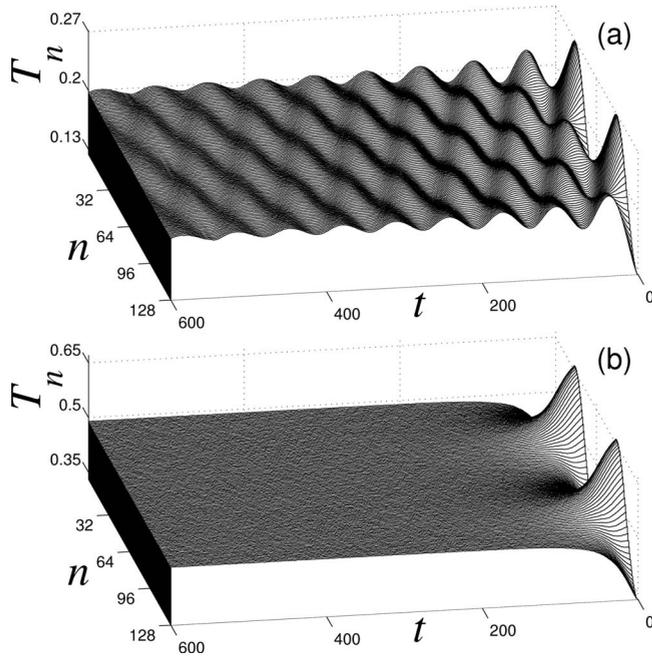
FIG. 1. Relaxation of initial periodic thermal profile in the chain of rotators, $Z=64$, $L=1024$, (a) $T_0=0.2$, $A=0.05$ (oscillatory decay) and (b) $T_0=0.5$, $A=0.15$ (smooth decay of the initial thermal profile).

with the temperature increase. However, its existence should be checked for constant temperature and varying wavelength.

Such simulations are presented at Fig. 2 (for the CR) and Fig. 3 (for the FPU chain). In both models one observes oscillatory decay for the short wavelengths and smooth exponential decay for relatively long waves. It means that for both models there exists some critical wavelength l^* which separates two types of the decay and thus the effect of the nonstationary heat conduction is revealed.
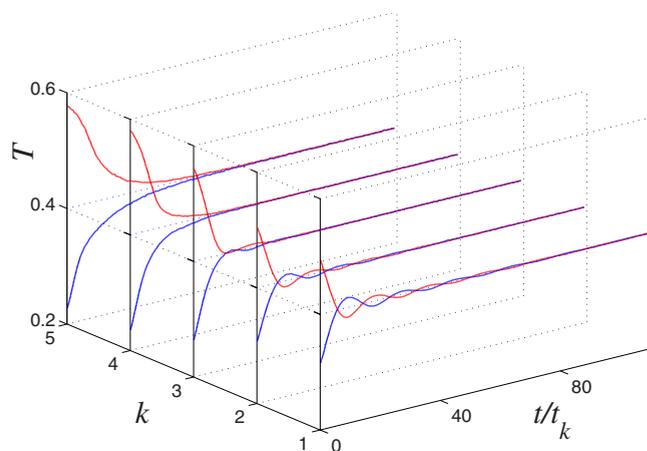
FIG. 2. (Color online) Evolution of the relaxation profile in the chain of rotators with change in the mode length Z. Time dependence of the mode maximum $T(1+Z/2)$ [red (gray) lines] and minimum $T(1)$ [blue (black) lines] are depicted with average temperature $T_0=0.4$ and $Z=16\times2^{k-1}$, $k=1,\ldots,5$, scaling time $t_k=2^{k-1}$. For all simulations length of chain $L=1024$.
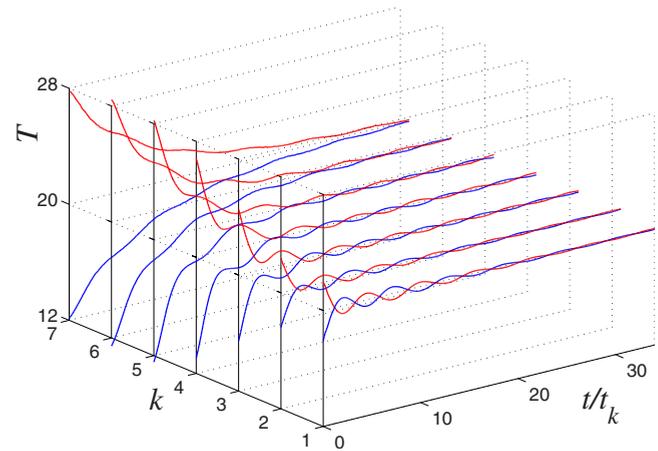
FIG. 3. (Color online) Evolution of the relaxation profile in the FPU chain with change in the mode length Z. Time dependence of the mode maximum $T(1+Z/2)$ [red (gray) lines] and minimum $T(1)$ [blue (black) lines] are depicted with average temperature $T_0=20$ and $Z=16\times2^{k-1}$, $k=1,\ldots,7$, scaling time $t_k=2^{k-1}$, length $L=1024$.

Results presented at Fig. 3 allow one to conclude that the critical wavelength for the FPU chain for given temperature may be estimated as $512<l^*<1024$. The interpretation of Fig. 2 is not that straightforward. It is clear that $32<l^*<128$, but for $Z=64$ the result is not clear. Within the accuracy of the simulation, it seems that only finite number of the oscillations is observed. It is possible to speculate that such behavior is not consistent with the lowest-order CV equation since expressions (6) and (7) suggest either infinite number of the oscillations or at most single crossing of the average temperature or no crossing at all. Possible interpretation may be that if the modal wavelength is close enough to the critical, the second-order CV model is not sufficient any more and the nonlocal effects of higher order should be taken into account. Still, these conclusions should be verified by more detailed simulations in the vicinity of the crossover wavelength.

The latter observation has motivated us to check whether the data of numeric simulations in these one-dimensional models offer a support for the CV macroscopic equation. For this sake, one can check another prediction of this equation—the independence of the amplitude decrement of the relaxation profile on the wavelength in the oscillatory regime [Eq. (6)]. The results of simulation are presented at Fig. 4 (CR) and Fig. 5 (FPU). One can see that for the chain of rotators the above prediction more or less corresponds to the simulation results. For the FPU chain the decrement is strongly dependent on the wavelength, at odds with the CV equation. In this latter case, no unique relaxation time exists.

To summarize, we reveal the hyperbolicity effects of the nonstationary heat conduction in one-dimensional models of dielectrics without relying on any particular empiric equation. There exists a critical modal wavelength l^* which separates between oscillating and diffusive relaxation of the temperature field; such crossover (actually, the oscillatory decay of the temperature field perturbations) is inconsistent with parabolic Fourier equation. So, if the size of the system is
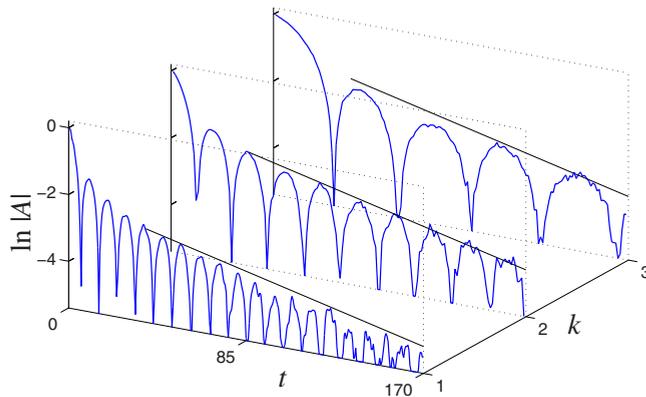
FIG. 4. (Color online) Exponential decay of the normalized oscillation amplitude in the chain of rotators $A(t)=[T(1+Z/2)(t)-T_0]/A)$ for the average temperature $T_0=0.3$, initial amplitude $A=0.05$ and different periods of the thermal profile $Z=16\times2^{k-1}$, $k=1,2,3$. The straight lines illustrate the decay of the maximum envelope according to $A=\exp(-\lambda t)$ with universal value $\lambda=0.015$ for all three simulations.

close to this critical scale, more exact macroscopic equations should be used for description of the nonstationary heat conduction. In both models studied the critical size decreases with the temperature increase. As for the CV equation itself, in the FPU chain this equation clearly contradicts the simulations for the short-wave perturbations of the temperature field. In the chain of rotators it seems to be inconsistent with the simulations in the vicinity of the critical wavelength, however is more or less justified for longer and shorter modes. One can speculate that this difference between two
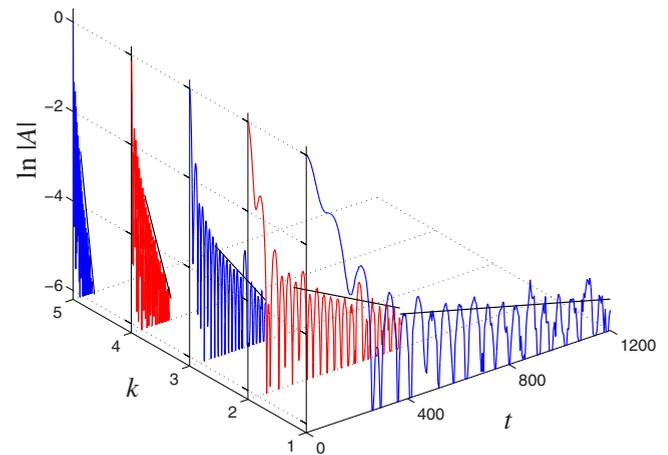
FIG. 5. (Color online) Exponential decay of the normalized oscillation amplitude in the FPU chain $a(t)=[T(1+Z/2)(t)-T_0]/A$ for the average temperature $T_0=10$, initial amplitude $A=0.05$ and different periods of the thermal profile $Z=16\times2^{k-1}$, $k=1,\ldots,5$. Blue (black) lines for $k=1$, 3, 5, and red (gray) lines for $k=2$, 4. The straight lines illustrate the decay of the maximum envelope according to $A=\exp(-\lambda t)$ with values $\lambda=0.0015$, 0.003, 0.008, 0.024, and 0.06 for $k=1$, 2, 3, 4, and 5.

models is related to their difference with respect to the stationary heat conduction—saturating versus size dependent behavior of the heat conduction coefficient [9–13].

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