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Heat conduction in 1D harmonic crystal: Discrete and continuum approaches

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ABSTRACT

In this work the energy transfer in a one-dimensional harmonic crystal is investigated. In particular, a comparison between the discrete approach presented by Klein, Prigogine, and Hemmer with the continuum approach presented by Krivtsov is made. In the pioneering work of Klein and Prigogine the transfer of thermal energy is considered. In particular, an expression is obtained, which allows to calculate the thermal energy of each particle as a function of time. Later, Hemmer derived and used similar expressions to solve several particular problems in context of heat conduction. In the work of Krivtsov—in contrast to the discrete approach—a partial differential continuum equation is derived from the lattice dynamics of a 1D harmonic crystal. This so-called ballistic heat equation describes the propagation of heat at a finite speed in a continuous one-dimensional medium. The current work compares analyses based on the discrete equation of Klein, Prigogine, and Hemmer with those from the continuum-PDE-based one by Krivtsov. There is an important difference between the approaches. The continuum approach is derived from the dynamics of the crystal lattice, in which only kinetic degrees of freedom were excited and then thermal equilibration occurred. In contrast to that we consider in the discrete approach explicitly given equal kinetic and potential initial energies. Several exactly solvable initial problems are studied by using both methods. The problem of point perturbation shows a discrepancy in the results obtained in the framework of the continuous and discrete approaches. It is caused by the fact that the smoothness conditions of the initial perturbation is violated for the continuum approach. For other problems it is shown that at large spatial scales, where the one-dimensional crystal can be considered as a continuous medium, the discrete and the continuum relations converge. The asymptotic behavior of the difference between two aforementioned approaches is analyzed.

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1. Introduction

The one-dimensional chain is a very instructive object for investigating properties of crystals on the micro- and nanoscale. It allows to derive all statistical quantities analytically from the dynamics of the lattice. One of the first pioneering papers where the one-dimensional chain was examined goes back to Schrödinger in 1914, [1]. An exact solution for the displacements of particles for an arbitrary initial configuration in terms of Bessel functions was obtained. It was observed that unlike to the case of signals in an elastic string the perturbations in the one-dimensional harmonic chain propagate at an infinite speed.

Later these results were used by Klein and Prigogine [2] for the description of stochastic non-equilibrium transient processes in a 1D chain. A formula, which determines the evolution of initial distribution of individual particles' energies, was obtained. Afterwards, in 1959, Hemmer obtained a similar expression [3] and illustrated some important aspects of this process based on the example of several initial value problems. Hemmer pointed out that the process described by this formula is not consistent with the classical law of Fourier. However, no continuum based alternatives were proposed at that time. In several later works including [4,5] it was shown that, indeed, the heat flow in a one-dimensional harmonic crystal cannot be described by Fourier's law in the stationary non-equilibrium case. Since then, discrete systems were considered by many authors as an attractive model for the investigation of heat conduction [6–12]. However, a number of questions regarding continuum description remain to be addressed.

Recently, a continuum based approach was proposed by Krivtsov in [13,14]. This approach is aimed at building continuum models of heat conduction based on lattice dynamics. In the

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last years this approach was extensively developed for more complex systems [15–22]. It was shown by Krivtsov that in the one-dimensional chain two different types of processes occur, namely (a) fast motions [13], when the kinetic and potential energies equilibrate, and (b) slow motions [14], when the temperature propagates along the spatial coordinate. By using covariance analysis an equation for the generalized nonlocal temperatures was obtained from the lattice dynamics, and after spatial continualization a continuum equation for the temperature was obtained in [14]. This equation describes the propagation of heat in a one-dimensional chain at a finite speed (this is a "slow" process (b)). The finite signal speed in this model does not contradict the results showing infinite speed of mechanical signals in discrete systems [1,3,7] since in the derivation of Krivtsov [14] coarse graining of the initial discrete model is performed. The model introduced in [14] is a relevant model for the description of the ballistic heat process on a continuum scale. However, it lacks the ability to describe several phenomena observed on the discrete level.

The aim of the presenting work is to consider the process of heat conduction in a 1D crystal from the viewpoints of two approaches: the continuum and the discrete one. In order to illustrate the differences and the similarities of the approaches, several initial problems are considered.

2. One-dimensional harmonic chain

The harmonic chain allows us to investigate anomalous heat conduction phenomena in a simple and powerful manner. Following on to the work [14] we consider an infinite harmonic chain. Each particle with mass m is connected to its neighbors by Hookean springs with stiffnesses C. The equation for the particle motion reads in nearest neighbor approximation:

$$\ddot{u}_n = \omega_0^2(u_{n-1} - 2u_n + u_{n+1}), \quad \omega_0 = \sqrt{\frac{C}{m}}, \tag{1}$$

where u_n is the displacements of the particle with index n, dot $\dot{(\ldots)}$ denotes a derivative with respect to time t. Let us consider the chain described by (1) with the following stochastic initial conditions:

$$u_n|_{t=0} = 0, \qquad \dot{u}_n|_{t=0} = \sigma(x)\rho_n, \tag{2}$$

where ρ_n are independent random variables with zero mathematical expectation $\langle\rho_n\rangle = 0$ and unit variance $\langle\rho_n^2\rangle = 1$ (see for details Ref. [14]); $\sigma(x)$ is the smooth function of a spatial coordinate $x = an$; σ^2 is the variance of the initial particle velocity; a is a distance between neighboring particles at the equilibrium. Such initial conditions can be implemented by an ultrafast laser heating [23].

For a spatially homogeneous problem $\sigma(x) = \text{const}$, after the beginning of the process described by Eq. (1) and the initial conditions (2), the kinetic and potential energies of each particle oscillate, until they eventually tend to an equal value. These oscillations decay according to a power law (for an analytical explanation see [13,22] and Section 5 in this work). At large times, $t \gg 2\pi/\omega_0$ the energies can be assumed equal. We will now explain this process in more detail.

Following [13,14,24] we introduce the kinetic, potential, and total specific (per particle) energies, K_n, P_n, E_n of a particle, respectively:

$$K_n = \frac{1}{2}m\langle\dot{u}_n^2\rangle, \quad P_n = \frac{1}{2}C\langle\epsilon_n^2\rangle, \quad E_n = K_n + P_n, \tag{3}$$

where $\epsilon_n = u_n - u_{n+1}$ (this definition is after works [1,3]), and $\langle\ldots\rangle$ is the mathematical expectation value. At the initial moment, $t = 0$, the displacements and deformations are zero, and the velocities are assigned randomly to the particles, according to Eq. (2). Therefore the initial kinetic energy $K_n^0 = K_n|_{t=0}$ will be equal to the total energy, and the potential initial energy $P_n^0 = P_n|_{t=0}$ is zero:

$$K_n^0 = E_n, \quad P_n^0 = 0. \tag{4}$$

The kinetic and potential energies will equilibrate at large times: $K_n|_{t\gg 2\pi/\omega_0} \simeq P_n|_{t\gg 2\pi/\omega_0}$. New equilibrated energies can be introduced $K_n^{\text{eq}} = K_n|_{t\gg 2\pi/\omega_0}$, $P_n^{\text{eq}} = P_n|_{t\gg 2\pi/\omega_0}$. Thus, the following equality holds:

$$K_n^{\text{eq}} = P_n^{\text{eq}} = \frac{E_n}{2}. \tag{5}$$

After this transition process the kinetic temperature can be defined proportional to the kinetic energy:

$$\frac{1}{2}k_B T_n \overset{\text{def}}{=} K_n^{\text{eq}} = \frac{E_n}{2}, \tag{6}$$

where k_B is the Boltzmann constant. Note that the definition of temperature in non-equilibrium is a classical challenge that has received considerable attention in the community [25–28]. The equality $k_B T = E$, which follows from (6), corresponds to the description of a classical harmonic oscillator in contact with a heat bath of temperature T (see Appendix B). Alternatively to the definition (6) one can assume each particle to be at local quasi-equilibrium with its surroundings and, following the considerations from Appendix B, define the temperature as proportional to the total energy $k_B T = E$. This case, however, is beyond the scope of this work.

2.1. The continuum approach of Krivtsov [14]

Recall the equation of motion (1) and the initial conditions (2). In case of a spatially nonhomogeneous problem, $\sigma(x) \neq \text{const}$ and when $\sigma(x)$ is a smooth function, the following equation, which describes the dynamics of the kinetic temperature field $T(x,t)$ can be derived based on the analysis of equations of motions (1) (see for details [29]):

$$\ddot{T} + \frac{1}{t}\dot{T} = c^2 T'', \qquad c = \omega_0 a. \tag{7}$$

Here c is the speed of sound in the one-dimensional crystal, prime $(\ldots)'$ denotes derivative with respect to spatial coordinate x. In the framework of the continuum model we assume that

- the spatial coordinate x is continuous, $x \in \mathbb{R}$;
- the relation following from (6),

$$k_B T(x) = E(x) \tag{8}$$

is considered to hold for all values of the spatial coordinate x.

The initial conditions which follow from the stochastic initial conditions (2) are used with Eq. (7):

$$T|_{t=0} = T^0(x), \qquad \dot{T}|_{t=0} = 0, \tag{9}$$

where $T^0(x)$ is the initial temperature profile. The initial conditions (9) for the PDE (7) are the consequence of the initial conditions (2) for the Eq. (1) of lattice dynamics. A solution for this initial value problem (7), (9) can be found in the following form [24]:

$$T(x,t) = \frac{1}{\pi}\int_{-1}^{1}\frac{T^0(x-cts)}{\sqrt{1-s^2}}\,\mathrm{d}s = \frac{1}{2\pi}\int_0^{2\pi} T^0\Big(x + ct\cos\frac{p}{2}\Big)\mathrm{d}p. \tag{10}$$

The second relation for the kinetic temperature in (10) shows that there is no singularity, which by premature judgment of the form of Eq. (7) seems to occur at $t = 0$.

In the case when $\sigma(x)$ is a slowly varying function of coordinate, first, at each point in space, thermal equilibration occurs locally, similar to the one described above for the spatially homogeneous problem. The initial kinetic temperature T^0 is defined as

proportional to the kinetic energy (5) that is reached after equilibration:

$$T^0 = \frac{2K^{\mathrm{eq}}}{k_B} = \frac{m\sigma^2}{2k_B}. \tag{11}$$

Let us comment on the term "initial" used in Eq. (11). Strictly speaking, the relation (8) holds only for large times. However, in Eq. (11) we assume Eq. (5) valid from the very beginning of the process. This assumption is an approximation.

To summarize, there are limitations to (7). The continuous approach implicitly assumes that

- the process of thermal equilibration in the case of slowly varying $\sigma(x)$ is close to the one observed in the case of constant $\sigma(x)$;
- the ballistic heat Eq. (7) becomes valid only for large times after equilibration, i.e., when (8) holds.

2.2. The discrete approach

Following on to the works [2,3] the infinite system of equations of motion (1) is considered. The following quantities [1] are introduced (they are called *Schrödinger coordinates* in [3]):

$$\xi_{2n} \overset{\mathrm{def}}{=} m^{\frac{1}{2}}\dot{u}_n, \quad \xi_{2n+1} \overset{\mathrm{def}}{=} C^{\frac{1}{2}}(u_n - u_{n+1}). \tag{12}$$

It is seen (for more details see [1,2]) that the system of Eq. (1) can be solved in terms of (12), giving the solution

$$\xi_n = \sum_{k=-\infty}^{\infty} \xi_n^0 J_{n-k}(2\omega_0 t), \tag{13}$$

where J_n is the Bessel function of the first kind, ξ_n^0 are the values of ξ_n at the initial moment of time. Eq. (13) describes the evolution of coordinates ξ_n based on the deterministic initial values ξ_n^0.

Following [2] let us now assume that the initial conditions ξ_n^0 are random and obey $\langle \xi_n^0 \rangle = 0$, $\langle \xi_k^0 \xi_n^0 \rangle = \delta_{k,n}$, where $\delta_{k,n}$ is the Kronecker delta, since we are interested in the macroparameters of the system, e.g., the temperature. Following [2] we introduce the values

$$\mathcal{E}_n = \frac{1}{2}\langle {\xi_n}^2 \rangle. \tag{14}$$

It was shown in [2,3] that the evolution of (14) can be described by the relation

$$\mathcal{E}_n(t) = \sum_{k=-\infty}^{\infty} \mathcal{E}_k^0 J_{n-k}^2(2\omega_0 t), \tag{15}$$

where $\mathcal{E}_n^0 = \frac{1}{2}\langle {\xi_n^0}^2 \rangle$ are the values of (14) at the initial moment of time. From (14), (12), (3) follows that introduced values (14) are connected with kinetic and potential respectively

$$\mathcal{E}_{2n} = K_n, \quad \mathcal{E}_{2n+1} = P_n. \tag{16}$$

Therefore, it is seen from Eq. (6) and the first equality from (16) that the kinetic temperature T_n of a particle with index n can be calculated by use of (15),

$$k_B T_n = 2\mathcal{E}_{2n} = 2\sum_{k=-\infty}^{\infty} \mathcal{E}_k^0 J_{2n-k}^2(2\omega_0 t). \tag{17}$$

To summarize this section, two expressions describing the evolution of initial temperature field are considered. One is a function of time and spatial coordinate (10), the other is a function of time and the particle index (17). We will further compare the temperature fields described by both equations using the examples of several initial value problems.

Within the framework of the discrete approach, there are initial values $\mathcal{E}_{2n}^0$ and $\mathcal{E}_{2n+1}^0$, they correspond to kinetic and potential energies respectively of a particle with index n at the position $x = an$. As discussed above, the continuum approach implies local thermal equilibrium. Thus these initial values are assigned with an equal value corresponding to the kinetic temperature in the continuum model $T^0(x)$ at the coordinate $x = an$, i.e.,

$$\mathcal{E}_{2n}^0 = \mathcal{E}_{2n+1}^0 = k_B T^0(an)/2. \tag{18}$$

3. Comparison of the approaches

In the next sections, we will consider several initial value problems (see Tab. 1) for the two aforementioned approaches.

The approaches are compared in dimensionless form. Equation (7) depends on the continuous coordinate x while (15) depends on the dimensionless index n. A dimensionless coordinate is chosen as $\tilde{x} = x/a$. In this case x matches the position of the particle with index n, namely $x = an$, then $\tilde{x} = n$. We choose $\tau = \omega_0 t$ as the dimensionless time. For the temperature we choose $\tilde{T} = T/T_{\mathrm{ref}}$, where T_{ref} is the background temperature.

3.1. The problem of point thermal perturbation

Continuum approach. Let us consider an initial localized infinitely narrow perturbation. For the continuum Eq. (7) the initial conditions are modeled by the Dirac delta function $\delta(x)$,

$$T^0(x) = a\Delta T\delta(x). \tag{19}$$

Substitution of the initial conditions (19) into the first relation from (10) gives the solution of Eq. (7):

$$T(x,t) = \frac{a\Delta T\,\mathcal{H}(ct - |x|)}{\pi\sqrt{c^2t^2 - x^2}}, \tag{20}$$

where $\mathcal{H}(x)$ is the Heaviside function. Eq. (20) in dimensionless form reads:

$$\tilde{T}(\tilde{x},\tau) = \frac{\mathcal{H}(\tau - |\tilde{x}|)}{\pi\sqrt{\tau^2 - \tilde{x}^2}}. \tag{21}$$

The total energy assigned to the system E^{tot} at time $t = 0$, according to initial conditions Eqs. (20) and (8) is:

$$E^{\mathrm{tot}} = \int_{-\infty}^{\infty} \rho\, E(x)\,\mathrm{d}x = \int_{-\infty}^{\infty} \rho k_B \Delta T a\delta(x)\mathrm{d}x = k_B\Delta T, \tag{22}$$

where $\rho = 1/a$ is the number of particles per unit length.

*Discrete approach.*A similar problem at the discrete level is modeled by the perturbation of the one kinetic and one potential degree of freedom. Local equilibration is assumed. In this case, the initial conditions are written

$$\mathcal{E}_n^0 = \frac{k_B\Delta T}{2}[\delta_{n,0} + \delta_{n,1}]. \tag{23}$$

Note that the energy of the system is

$$E^{\mathrm{tot}} = \sum_{n=-\infty}^{\infty} \mathcal{E}_n^0 = k_B\Delta T, \tag{24}$$

which agrees with (22). By substituting the initial conditions (23) into Eq. (15) the solution reads [3]:

$$\mathcal{E}_n = \frac{k_B\Delta T}{2}\left[J_n^2(2\tau) + J_{n-1}^2(2\tau)\right]. \tag{25}$$

The relation for the temperature is obtained by using Eq. (25) together with (17):

$$T_n = \Delta T\left[J_{2n}^2(2\tau) + J_{2n-1}^2(2\tau)\right]. \tag{26}$$

By taking into account $T_{\mathrm{ref}} = \Delta T$, the dimensionless form of (26) reads:

$$\tilde{T}_n(\tau) = J_{2n}^2(2\tau) + J_{2n-1}^2(2\tau). \tag{27}$$

It is seen in Fig. 1 that the solution (27) has discrepancies with continuum solution (21), especially near the wavefront $\tilde{x} = \tau$. The

Table 1
Initial conditions for considered problems: point, step and rectangular initial profiles T^0.

	Point	Step	Rectangular
Plot			
Continuum, T^0	$\Delta T a\delta(x)$	$\begin{cases}\Delta T, & x \geq 0\\ 0, & x < 0\end{cases}$	$\begin{cases}\Delta T, & -l \leq x \leq l\\ 0, & x < -l,\ x > l\end{cases}$
Discrete, $\mathcal{E}_n^0$	$\frac{k_B}{2}\Delta T[\delta_{n,0} + \delta_{n,1}]$	$\begin{cases}\frac{k_B}{2}\Delta T, & n \geq 0\\ 0, & n < 0\end{cases}$	$\begin{cases}\frac{k_B}{2}\Delta T, & -2N \leq n \leq 2N+1\\ 0, & n < -2N,\ n > 2N+1\end{cases}$

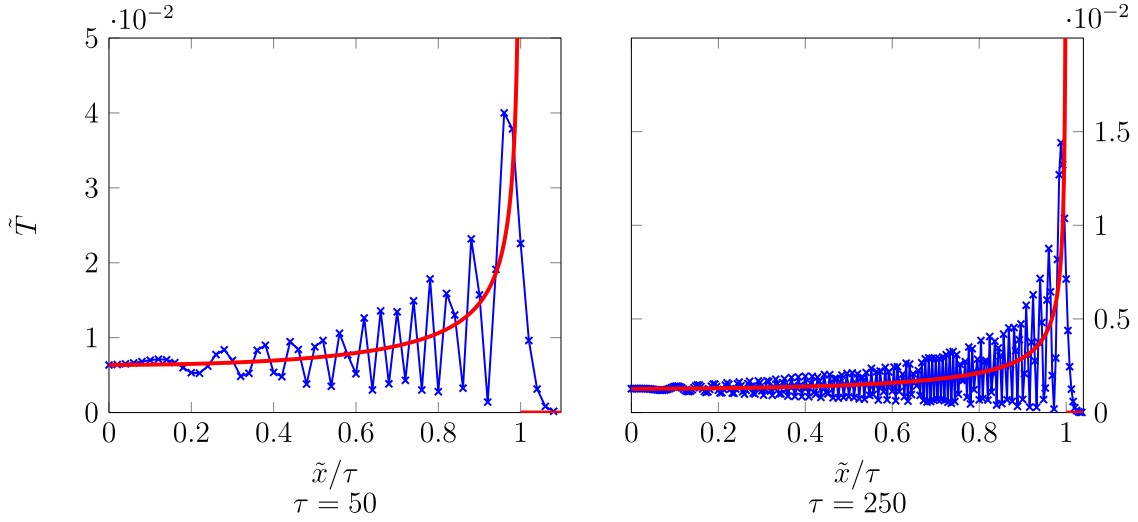

Fig. 1. Comparison of continuum (21) (red line) and discrete (27) (blue connected crosses) solutions for an initial point thermal perturbation at different values of dimensionless time τ.

continuum solution is an average curve for the discrete points. This mismatch between the obtained solutions is due to the fact that on the discrete level the function describing initial perturbation (23) is not smooth in space. A rigorous comparison of point perturbations deserves a separate consideration and is beyond the scope of this work.

3.2. The heat step problem

Continuum approach The contact between a hot and a cold half-space is investigated. For Eq. (7) this problem was first considered in [14]. The problem is described by the following initial conditions:

$$T^0 = \begin{cases}\Delta T, & x \geq 0,\\ 0, & x < 0.\end{cases} \tag{28}$$

In [14] the solution of Eq. (7) with the initial conditions (28) was obtained,

$$T(x,t) = \begin{cases}\frac{\Delta T}{\pi}\arccos\left(-\frac{x}{ct}\right), & |x| \leq ct,\\ \Delta T, & x > ct,\\ 0, & x < -ct.\end{cases} \tag{29}$$

Eq. (29) can be represented in dimensionless form as follows:

$$\tilde{T}(\tilde{x},\tau) = \begin{cases}\frac{1}{\pi}\arccos\left(-\frac{\tilde{x}}{\tau}\right), & |\tilde{x}| \leq \tau,\\ 1, & \tilde{x} > \tau,\\ 0, & \tilde{x} < -\tau,\end{cases} \tag{30}$$

where the temperature is normalized by ΔT.

Discrete approach. Following the work [3], the initial problem, corresponding to (28) is considered. According to (18),

$$\begin{aligned}&\mathcal{E}_n^0 = \tfrac{1}{2}k_B\Delta T, && n \geq 0,\\ &\mathcal{E}_n^0 = 0, && n < 0.\end{aligned} \tag{31}$$

By substituting the initial conditions (31) into Eq. (15) the solution is:

$$\mathcal{E}_n = \frac{1}{2}k_B\Delta T\sum_{k=-n}^{+\infty} J_k^2(2\omega_0 t). \tag{32}$$

By applying Eqs. (17) to (32), the corresponding kinetic temperatures are obtained:

$$T_n = \Delta T\sum_{k=-2n}^{+\infty} J_k^2(2\omega_0 t). \tag{33}$$

In dimensionless form Eq. (33) reads:

$$\tilde{T}_n = \sum_{k=-2n}^{+\infty} J_k^2(2\tau). \tag{34}$$

Relation (34) can be transformed by using the relation $1 = J_0^2(2\tau) + 2\sum_{k=1}^{+\infty} J_k^2(2\tau)$ (see [30] pg. 363 for details) to avoid infinite summation:

$$\tilde{T}_n = \begin{cases}\frac{1}{2}\left(1 + J_0^2(2\tau) + 2\sum_{k=1}^{2n} J_k^2(2\tau)\right), & n \geq 0,\\ \frac{1}{2}\left(1 - J_0^2(2\tau) - 2\sum_{k=1}^{-2n-1} J_k^2(2\tau)\right), & n < 0.\end{cases} \tag{35}$$

The solutions (30) and (34) are plotted in Fig. 2 for comparison. The continuum equation (7) describes the propagation of heat with finite speed. In the region $\tilde{x} > \tau$ and $\tilde{x} < -\tau$ the original temperature distribution remains. It can be seen in Fig. 2 that the continuum solution (30) has a pronounced wavefront which has vertical tangent, a jump in the spatial derivative, and propagates at finite speed. The discrete solution tends to converge to the continuum one except for a region near the wavefront, where it detaches from continuum curve and smoothly reaches the horizontal line (see inlet Fig. 2).

It can be seen from Fig. 3 that on the large times, i.e., if the distance traveled by a thermal wave greatly exceeds the interatomic

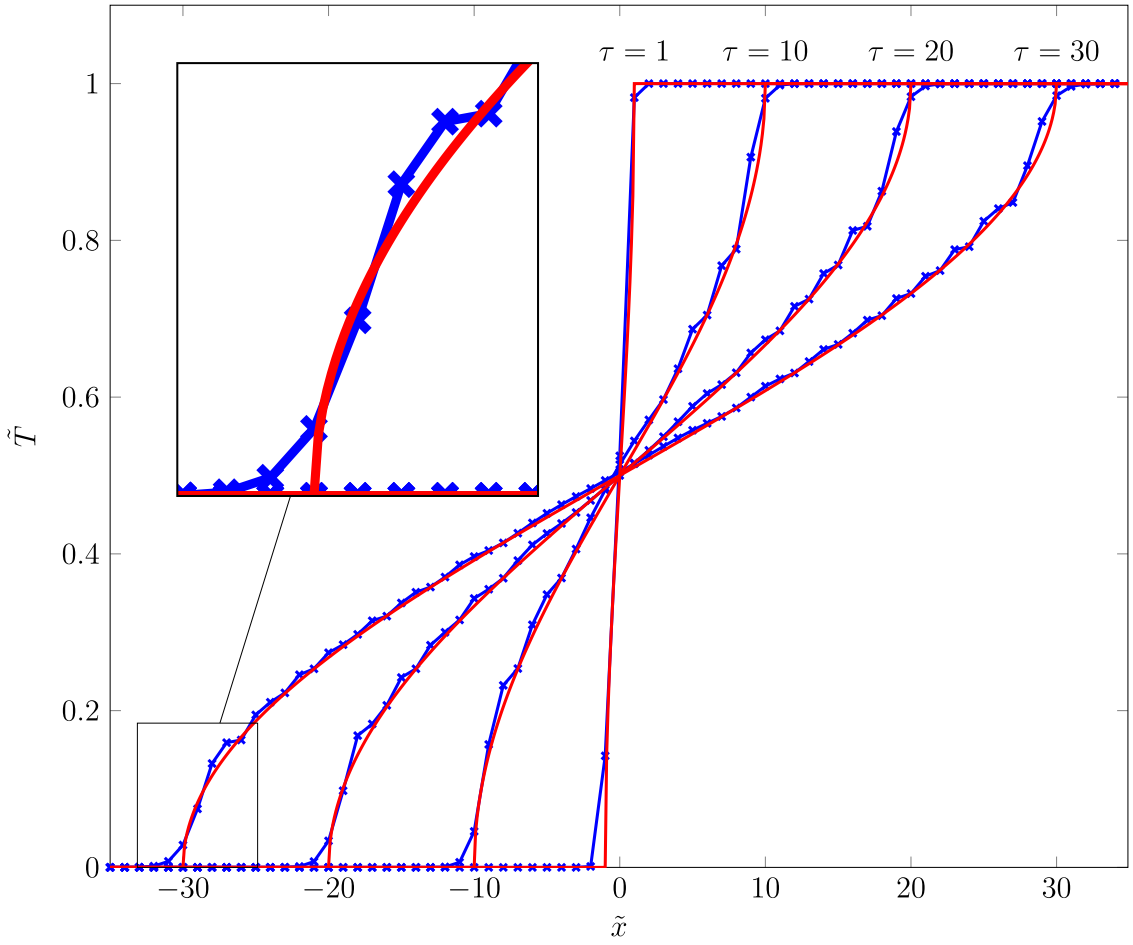

Fig. 2. Propagation of the heat front for the problem of a heat step for the continuum (30) (red solid line) and the discrete (34) (blue connected crosses) solutions at different values of dimensionless time τ.

distance, the solutions converge and the discrete and the continuum solution become indistinguishable for an observer on that scale.

3.3. Rectangular initial perturbation. Comparison on a large scale

Continuum approach. Let us consider a rectangular initial temperature perturbation. It was considered in [31] in context with the ballistic heat equation. The initial conditions are written as $T^0(x) = \Delta T$ for $|x| \le l$, otherwise $T^0 = 0$, where l is the width of the initial impulse. We are interested in the behavior at large times. The solution for $t > l/c$, $x \ge 0$ is the following one [31]:

$$T(x,t) = \begin{cases} 0, & ct + l \le x, \\ \frac{\Delta T}{\pi} \arccos \frac{x-l}{ct}, & ct - l \le x \le ct + l, \\ \frac{\Delta T}{\pi}\left(-\arccos \frac{x+l}{ct} + \arccos \frac{x-l}{ct}\right), & 0 \le x \le ct - l; \end{cases} \tag{36}$$

for $x < 0$ the solution is symmetric. Eq. (36) in dimensionless form reads:

$$\tilde{T}(\tilde{x},\tau) = \begin{cases} 0, & \tau + l/a \le \tilde{x}, \\ \frac{1}{\pi} \arccos \frac{\tilde{x}-l/a}{\tau}, & \tau - l/a \le \tilde{x} \le \tau + l/a, \\ \frac{1}{\pi}\left(-\arccos \frac{\tilde{x}+l/a}{\tau} + \arccos \frac{\tilde{x}-l/a}{\tau}\right), & 0 \le \tilde{x} \le \tau - l/a. \end{cases} \tag{37}$$

Discrete approach. On the discrete level the initial conditions for the rectangular impulse are modeled as follows. The particles with indices from $-N$ to N are thermally excited, $aN = l$. Thus thermal energies $\mathcal{E}_n^0$ with indices from $-2N$ to $2N+1$ are excited. The degree of freedom with index $2N+1$ is also excited, since we want that the kinetic and the potential degrees of freedom are both equally excited. The amplitude of perturbation $\frac{1}{2}k_B\Delta T$ is chosen to correspond to the initial conditions on to continuum level, as it was done in the problem of step perturbation. In analogy to (31) the initial conditions for the discrete problem are written as follows:

$$\begin{array}{ll} \mathcal{E}_k^0 = \frac{1}{2}k_B\Delta T, & -2N \le k \le 2N+1, \\ \mathcal{E}_k^0 = 0, & k < -2N, \quad k > 2N+1. \end{array} \tag{38}$$

The solution for the initial conditions (38) is:

$$\mathcal{E}_n = \frac{1}{2}k_B\Delta T \sum_{k=-2N}^{2N+1} J_{n-k}^2(2\omega_0 t). \tag{39}$$

From Eq. (39) the temperature of a particle is calculated by using formula (17):

$$T_n = \Delta T \sum_{k=-2N}^{2N+1} J_{2n-k}^2(2\omega_0 t). \tag{40}$$

The dimensionless form for the temperatures of particles with index n thus reads:

$$\tilde{T}_n(\tau) = \sum_{k=-2N}^{2N+1} J_{2n-k}^2(2\omega_0 t). \tag{41}$$

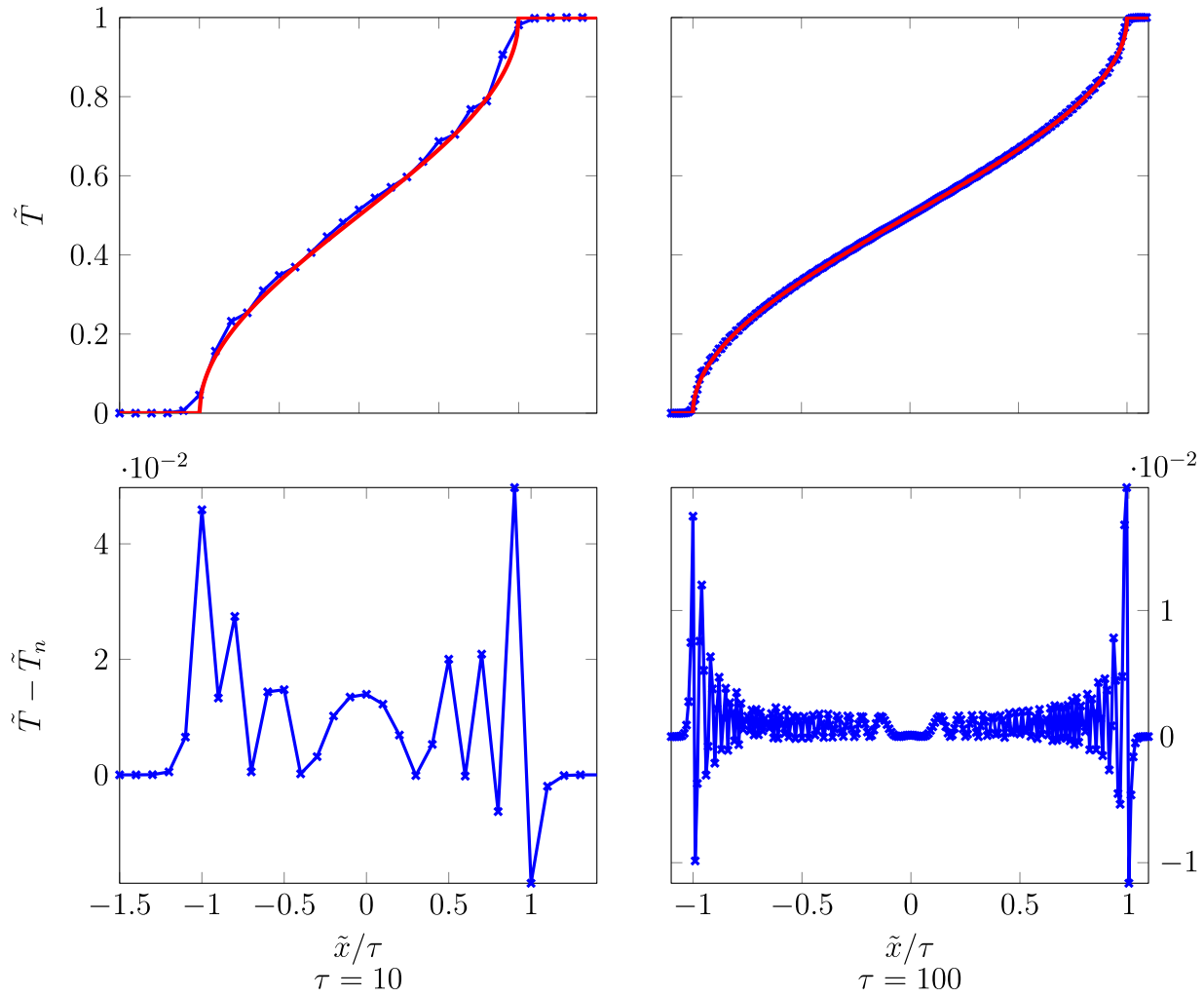

Fig. 3. Kinetic temperature profiles for the continuum (red solid line) and the discrete(blue connected crosses) solutions for the problem of heat step (upper row) and the difference between discrete and continuum solutions (lower row) at different values of dimensionless time τ.

On large spatial scales the width of the initial rectangular perturbation (38) tends to zero compared to the spatial scale of observation. In this context it is similar to the delta function (20). The amount of energy stored in the system is:

$$E^{\text{tot}} = \sum_{-2N}^{2N+1} \frac{1}{2} k_B \Delta T = \frac{4N+1}{2} k_B \Delta T. \tag{42}$$

In the following paragraph the solutions (41) and (37) are compared. In order to keep the same amount of energy in both problems, the solution (41) is normalized by the amount of stored energy (42) when plotted in Fig. 4. It is seen from Fig. 4 that for large times the discrete solution converges to the continuum one. The initial rectangular perturbation for the discrete equation is finite, unlike for the delta function. Therefore, the discrete solution has no singularity at the wavefront, unlike the continuum solution for the delta function.

The formula (39), describing the propagation of rectangular initial perturbation within the discrete approach, is obtained in this work by using the general solution from [3].

3.4. Rectangular initial perturbation. Comparison near the wavefront

Let us now compare the discrete solution (39) and the continuum one for an initial rectangular perturbation (36) near the wavefront (see Fig. 5). The behavior of the solution (36) was discussed in detail in [31]. It was shown in [31] that the width of the wavefront does not change in time and only depends on the width of the initial perturbation. The continuum solution has vertical tangents and jumps in the spatial derivative at points $\tilde{x} = \tau - N$, $\tilde{x} = \tau + N$.

Solutions for different initial width N at dimensionless time $\tau = 400$ are presented in Fig. 5. The spatial scale is normalized by the width of the initial impulse. Analogous to the case discussed in the section on the heat step perturbation, the discrete solution detaches from the continuum one in the points where the continuum solution has a vertical tangent and the spatial derivative has a jump (see Fig. 5 (a)). However, if the initial perturbation is wider, then the wavefront is observed on a bigger spatial scale, and this deviation becomes almost indistinguishable (see Fig. 5 (b)).

4. Asymptotics

Eq. (17) shows that the solution of a discrete problem (as a function of dimensionless time τ and particle index n) is represented as a superposition of terms of the form $J^2_{2n-k}(2\tau)$, where k is integer. We will consider the asymptotic behavior of the basic solution, $k = 0$,

$$T_n = J^2_{2n}(2\tau) \tag{43}$$

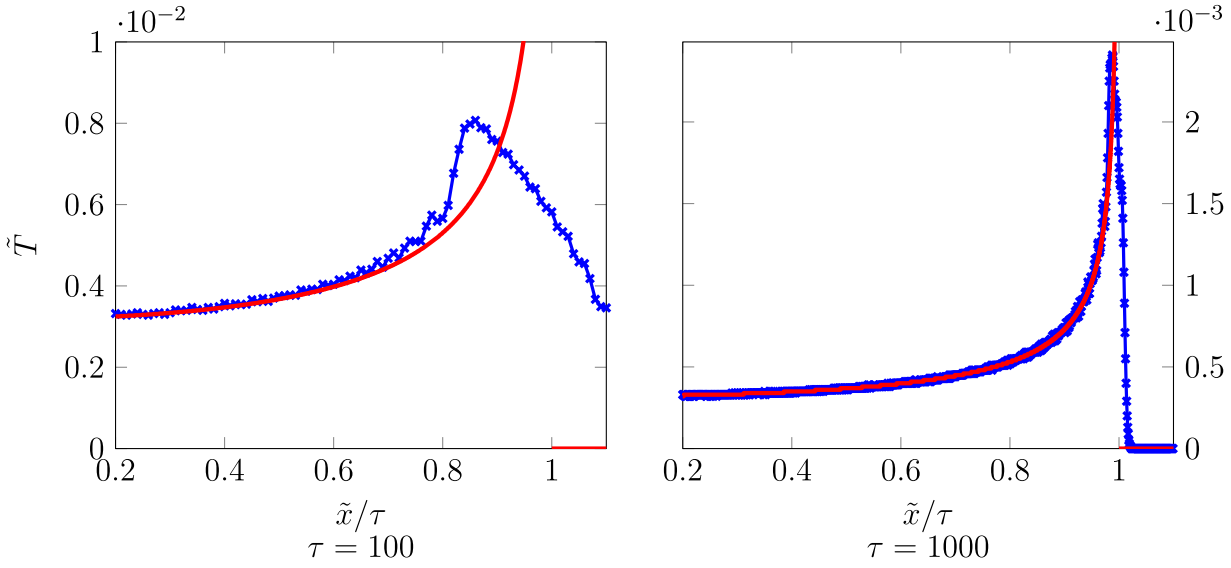

Fig. 4. Comparison of discrete (41) (blue connected crosses) and continuum (20) (red solid line) solutions at different values of dimensionless time τ.

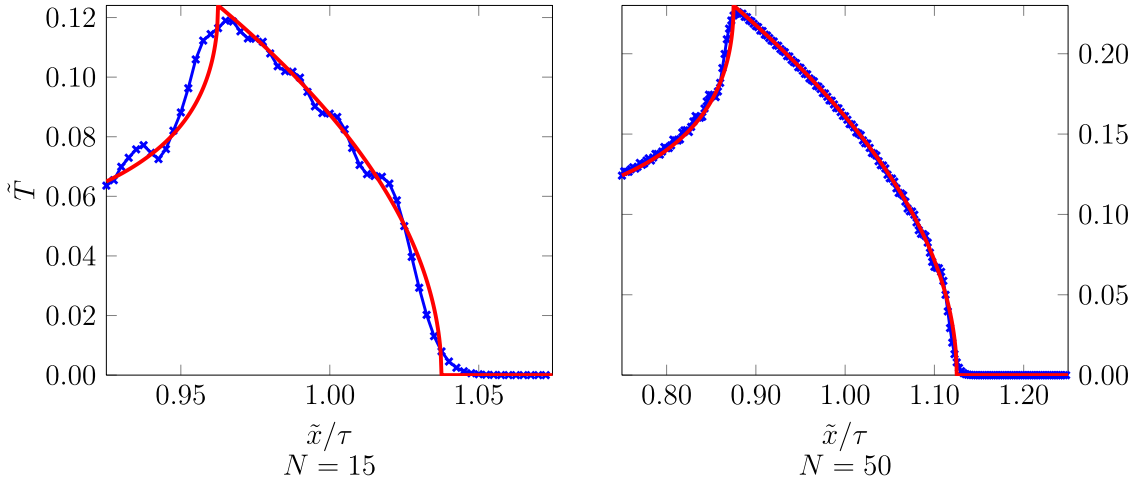

Fig. 5. Comparison of discrete (41) (blue connected crosses) and continuum (36) (red solid line) solutions for different initial impulse half-width $l = aN$.

for large distance $n \gg \tau$ and near the wavefront $n \sim \tau \gg 1$. The results obtained will also hold for solutions composed of a finite number of terms in (17).

Large distance asymptotics The asymptotic representation of the Bessel function of large index (see [32]) is given by

$$J_n(x) \sim e^n \left(\frac{x}{2}\right)^n n^{-2n-\frac{1}{2}} \left(c_0 + \frac{c_1}{n} + \frac{c_2}{n^2} + \ldots\right), \quad c_0 = 1/\sqrt{(2\pi)}, \tag{44}$$

where x is the argument and n is the index. We take only first term c_0 of the asymptotic expansion (44) into account. Applying the expansion (44) to (43) gives

$$T_n(\tau) = J_{2n}^2(2\tau) \sim \frac{1}{2\pi} e^{4n} \tau^{4n} (2n)^{-4n-1}. \tag{45}$$

The dominating decay behavior from formula (45) is:

$$T_n \sim (2n)^{-4n-1}. \tag{46}$$

From Eq. (46) it can be concluded that already at several interatomic distances from the wavefront the perturbation is of the order 10^{-10}.

Asymptotics near the wavefront We are interested in the asymptotics of (43) near the wavefront at large times. This corresponds to $n \sim \tau$. The asymptotics of Bessel functions for near-equal index and argument is given by Airy function Ai(x) (see [17] for details),

$$J_n(x) = \left(\frac{2}{n}\right)^{1/3} \mathrm{Ai}\left(\left(\frac{2}{n}\right)^{1/3} (n - x)\right) + O\left(n^{-1}\right). \tag{47}$$

Applying (47) to (43) gives the approximation of the wavefront

$$T_n(\tau) \sim \left(\frac{1}{n}\right)^{2/3} \mathrm{Ai}^2\left(\left(\frac{1}{n}\right)^{1/3} (2n - 2\tau)\right). \tag{48}$$

Eq. (48) allows further analysis. Airy function can be represented by an approximation

$$\mathrm{Ai}(x) = \frac{1}{2\sqrt{\pi}} x^{-1/4} e^{-\frac{2}{3}x^{3/2}}. \tag{49}$$

Substitution of (49) into (48) gives

$$T_n(\tau) = \frac{1}{4\sqrt{2}\pi n \sqrt{1 - \tau/n}} \exp\left[-\frac{8\sqrt{2}}{3} n \left(1 - \frac{\tau}{n}\right)^{3/2}\right]. \tag{50}$$

It is seen that for a fixed τ, for large n formula (50) gives

$$T_n(\tau) \sim \frac{A}{n} e^{-Bn}, \tag{51}$$

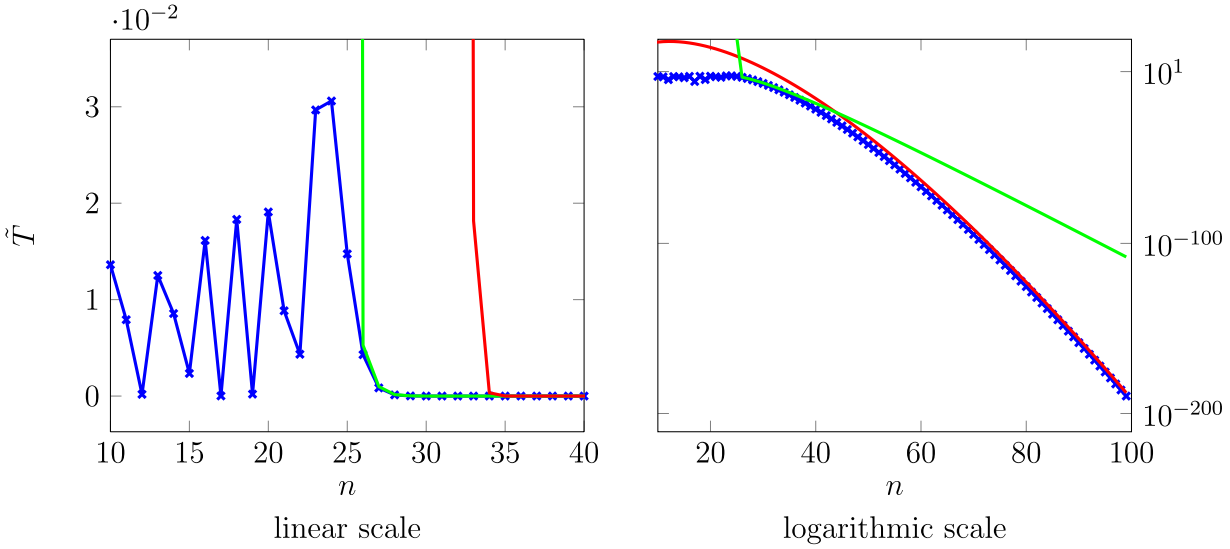

Fig. 6. Plot of basic solution (43) (blue connected crosses), large distance asymptotics (45) (red connected points), approximation (50) plotted for $n > \tau$ (green connected points).

where $A = (4\sqrt{2}\pi)^{-1}$, $B = 8\sqrt{2}/3$ are the constants. In Fig. 6, the basic solution (43), large distance asymptotics (45), and an approximation by Airy function (48) are presented.

The speed of signal propagation described by the discrete model is infinite, however, it is seen from (46) that on large distances the decay rate of the perturbation is very fast. In comparison, the classical Fourier model, which also predicts an infinite speed of signal propagation has an exponential decay rate, which is slower. In the discrete model the major amount of energy is transferred with the speed of sound in the medium, which coincides with the result of Krivtsov [14].

As seen from Fig. 6(a), an approximation Airy function (48) is good near the wave-front, but not so accurate for description of decay behavior ar large-distances. On the large distances the formula (45) gives a better approximation as seen from Fig. 6(b) on a logarithmic scale.

5. Equilibration of energies

Let us now follow the paper [13] and consider a situation, when the crystal is uniformly heated at time zero. Only the kinetic degrees of freedom are excited. For the discrete problem (15) the initial conditions are written:

$$\mathcal{E}_n^0 = \Delta\mathcal{E} \sum_{k=-\infty}^{\infty} \delta_{n,2k}. \tag{52}$$

By substituting (52) into (15) we obtain:

$$\mathcal{E}_n(t) = \Delta\mathcal{E} \sum_{k=-\infty}^{\infty} J_{n-2k}^2(2\omega_0 t). \tag{53}$$

Let us consider the solution (53) only for even or odd indices. It yields:

$$\mathcal{E}_n(t) = \begin{cases} \Delta\mathcal{E} \sum_{k=-\infty}^{\infty} J_{2k}^2(2\omega_0 t), & n \text{ is even}, \\ \Delta\mathcal{E} \sum_{k=-\infty}^{\infty} J_{2k+1}^2(2\omega_0 t), & n \text{ is odd}. \end{cases} \tag{54}$$

Let us consider the behavior of thermal energy associated with the kinetic part, namely when n is even. An algebraic transformation (see Appendix A) of the first relation from (54) yields,

$$\mathcal{E}_{2n}(t) = \Delta\mathcal{E} \sum_{k=-\infty}^{\infty} J_{2k}^2(2\omega_0 t) = \frac{\Delta\mathcal{E}}{2}[1 + J_0(4\omega_0 t)], \tag{55}$$

and in the dimensionless form,

$$\tilde{\mathcal{E}}_{2n}(t) = \frac{1}{2}[1 + J_0(4\tau)]. \tag{56}$$

Formula (56) was first derived from the discrete considerations in [2]. Formula (55) coincides with the formula derived in Ref. [13], where it has been obtained from covariance based approach.

We will finally compare the result (55) with a result obtained from computer simulations, a.k.a. Molecular Dynamics.

Numerical simulations Following [13,33] in the computer simulations we solve Eq. (1) numerically. In order to obtain the numerical solution we use the *leap frog* scheme:

$$\begin{aligned} \Delta v_{i,k} &= \omega_0^2 \big(u_{i+1,k} - 2u_{i,k} + u_{i-1,k}\big)\Delta t, \\ v_{i,k+1} &= v_{i,k} + \Delta v_{i,k}, \\ u_{i,k+1} &= u_{i,k} + v_{i,k+1}\Delta t, \end{aligned} \tag{57}$$

where in $\{\ldots\}_{i,k}$ the first lower index refers to i-th particle, second lower index refers to k-th timestep of simulation, Δt is the timestep. We consider a chain with N particles in total and with periodic boundary conditions,

$$u_1 = u_{N+1}, \quad u_0 = u_N. \tag{58}$$

In our simulation we use a timestep of $\Delta t = 0.01\frac{2\pi}{\omega_0}$, 401 particles and 10^4 realizations (samples). At timestep zero R realisations (samples) of the system are generated. All particles have zero displacements and random velocities corresponding to initial conditions (2). The average over realizations $\langle\ldots\rangle$ is used:

$$\langle y \rangle = \frac{\sum_{r=1}^{R} y^r}{R}, \tag{59}$$

where y is arbitrary quantity of interest, upper index $\{\ldots\}^r$ refer to value from r-th realization.

As seen explicitly from right hand side of Eq. (56) for a homogeneous problem behavior of kinetic energies does not depend on index n. Therefore, for certainty, in numerical calculation we consider the particle with index $\frac{N+1}{2}$ and find the average (59) of it's kinetic energy as a function of a discrete time $t_k = k\Delta t$:

$$\langle K_{\frac{N+1}{2}}(t_k) \rangle = \frac{\sum_{r=1}^{R} \frac{1}{2} m v^r_{\frac{N+1}{2},k}}{R}. \tag{60}$$

In Fig. 7 the average kinetic energy of a $(N+1)/2$-th particle (60) normalized to it's initial value at time zero $\langle K_{(N+1)/2}(0) \rangle$ and

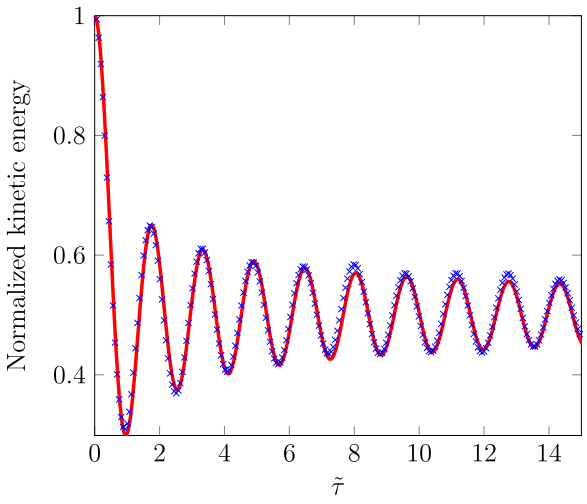

Fig. 7. Oscillations of kinetic energy. The red solid line refers to analytical expression (55), blue crosses are normalized kinetic energy (60) obtained from the simulation.

kinetic energy calculated by analytical expression (56) are plotted. As seen from Fig. 7 the potential and kinetic energies equilibrate, which corresponds to the virial theorem and was shown for a 1D crystal in [13]. In Ref. [18] this approach was extended to the description of such phenomena in 2D scalar lattices. However, it was shown in [18] that, in general, equilibrium temperatures, corresponding to different degrees of freedom of the unit cell, are not equal. This fact led to formulation of a *non-equipartition theorem* (see Ref. [18]).

To sum up this section, it has been demonstrated that three approaches: discrete (see Section 2.2 and Ref. [2,3]), continuum (see Section 2.1 and Ref. [13]), and numerical lead to the same result for the problem of a homogeneous initial perturbation. Potential and kinetic energies oscillate according to formula (55) and tend to equal value for large times. This result is consistent with the general concepts of statistical mechanics.

6. Conclusions

In this work, the heat conduction in the 1D chain is investigated. A comparison between the discrete approach from [2,3] and the continuum PDE derived in [14] was made.

The continuum approach is based on excitation of only kinetic lattice degrees of freedom, while initial potential degrees of freedom are zero. The function determining the amplitude of the initial perturbation is considered to be a smooth function of the spatial coordinate. Such initial conditions lead to fast equilibration between potential and kinetic energies locally in space. Strictly speaking, the obtained continuum PDE becomes valid after this initial equilibration. However, within the framework of the proposed continuum approach, the equilibration time is approximately assumed to be infinitely small and the proposed PDE is considered from the moment $t = 0$. On the other hand, the discrete approach has no limitiations on the ratio between initial kinetic and potential energies. However, in order to compare the discrete approach with the continuum one, we consider the initial kinetic and potential energies to be explicitly equal for each particle respectively within the framework of the discrete approach.

Examples of several initial profiles were considered. The problem of a point perturbation in a discrete system is of particular interest since, strictly speaking, it does not satisfy the condition of smoothness of the continuum model. As a result, discrepancies between kinetic temperature fields in the discrete and continuum models are observed. A rigorous description of point sources consistent with both approaches is beyond the scope of this paper.

For the rest of the considered problems, the discrepancy between the discrete and continuous approaches is also caused by the nonsmoothness of the initial conditions. However, in this case, the difference between approaches become indistinguishable when considering the process on scales much larger than the equilibrium distance between particles.

The discrete model [2,3] predicts infinite speed of signal propagation, in contrast to the continuum model [14]. Therefore, from the discrete viewpoint a localized initial perturbation causes an instant change in the field at large distances far away from the source. However, the asymptotical analysis of discrete model shows that this change rapidly decays as the observer moves away from the source and can be neglected on larger scales.

The obtained results help to understand the connection between the discrete and continuum description of heat conduction in low dimensional structures and allow to choose the type of description, depending on the considered scale level.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT authorship contribution statement

Aleksei A. Sokolov: Writing - original draft, Investigation. **Wolfgang H. Müller:** Writing - review & editing, Investigation, Conceptualization, Supervision. **Alexey V. Porubov:** Writing - review & editing. **Serge N. Gavrilov:** Writing - review & editing, Investigation.

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Appendix A. Representation of Bessel function of double argument

According to Ref. [30] the following relation holds:

$$J_0(2x) = J_0^2(x) + 2\sum_{k=1}^{\infty}(-1)^k J_k^2(x). \tag{A.1}$$

By adding and substituting $2\sum_{k=1}^{\infty} J_k^2(x)$ from the right part of Eq. (A.1) we obtain:

$$J_0(2x) = J_0^2(x) + 2\sum_{k=1}^{\infty}[(-1)^k + 1]J_k^2(x) - 2\sum_{k=1}^{\infty} J_k^2(x). \tag{A.2}$$

The factor $(-1)^k + 1$ in front of the Bessel function in the second term of (A.2) is equal to zero for odd values of k and to 2 for even values of k. Applying the relation (see Ref. [30])

$$1 = J_0^2(x) + 2\sum_{k=1}^{\infty} J_k^2(x) \tag{A.3}$$

to Eq. (A.2) yields

$$J_0(2x) = -1 + 2J_0^2(x) + 4\sum_{k=1}^{\infty} J_{2k}^2(x), \tag{A.4}$$

and by taking into account that $J_0^2(x) + 2\sum_{k=1}^{\infty} J_{2k}^2(x) = \sum_{k=-\infty}^{\infty} J_{2k}^2(x)$ it leads to:

$$\sum_{k=-\infty}^{\infty} J_{2k}^2(x) = \frac{1}{2}[1 + J_0(2x)]. \tag{A.5}$$

Appendix B. Mean energy of a harmonic oscillator

Let us consider the classical harmonic oscillator in 1D in a contact with a heat bath at temperature T. The oscillator's Hamiltonian is

$$H(q, p) = \frac{p^2}{2m} + \frac{1}{2} m\omega_0^2 q^2, \tag{B.1}$$

where $p = m\dot{q}$ is the momentum, q spatial coordinate of the oscillator. The partition function for this system is [34]

$$Z = \frac{1}{h} \int e^{-\beta H(q,p)} \mathrm{d}q\, \mathrm{d}p\,, \tag{B.2}$$

where $\beta = (k_B T)^{-1}$ is Boltzmann's factor, h is Planck's constant. The integration is done over all possible values of coordinate q and momentum p, and we denote here and further down $\int = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty}$. By substituting the Hamiltonian (B.1) into (B.2) one obtains:

$$\begin{aligned} Z &= \tfrac{1}{h} \textstyle\int e^{-\beta\left(\frac{p^2}{2m} + \frac{1}{2} m\omega_0^2 q^2\right)} \mathrm{d}q\, \mathrm{d}p = \\ &= \tfrac{1}{h} \textstyle\int_{-\infty}^{\infty} e^{-\beta \frac{p^2}{2m}}\, \mathrm{d}p \int_{-\infty}^{\infty} e^{-\frac{1}{2}\beta m\omega_0^2 q^2} \mathrm{d}q = \\ &= \tfrac{2}{\beta h\omega_0} \left(\textstyle\int_{-\infty}^{\infty} e^{-\xi^2} \mathrm{d}\xi\right)^2 = \tfrac{2\pi}{\beta h\omega_0} = \tfrac{k_B T}{\hbar\omega_0}, \end{aligned} \tag{B.3}$$

where $\hbar = h/(2\pi)$ is the reduced Planck constant. The mean value $\langle A \rangle$ of the value A is found by using the relation [34]:

$$\langle A \rangle = \int f(q, p) A(q, p) \mathrm{d}q\, \mathrm{d}p, \tag{B.4}$$

where $f(q, p)$ is the probability density function. The probability density function is calculated with the relation [34]

$$f(q, p) = \frac{1}{hZ} e^{-\beta H(q,p)}. \tag{B.5}$$

By substituting the probability density function (B.5) into the relation for the mean value (B.4) and by applying it to the energy (given by the Hamiltonian) one obtains:

$$\langle E \rangle = \frac{1}{hZ} \int e^{-\beta H} H\, \mathrm{d}q\, \mathrm{d}p = \frac{1}{hZ} \int \frac{\partial e^{-\beta H}}{\partial \beta} \mathrm{d}q\, \mathrm{d}p = \frac{1}{hZ} \frac{\mathrm{d}}{\mathrm{d}\beta} \int e^{-\beta H} \mathrm{d}q\, \mathrm{d}p = \frac{1}{Z} \frac{\mathrm{d}Z}{\mathrm{d}\beta}. \tag{B.6}$$

Then the mean energy of the system with partition function (B.2) is

$$\langle E \rangle = \frac{\mathrm{d} \ln Z}{\mathrm{d}\beta} = \frac{1}{\beta} = k_B T. \tag{B.7}$$

For the description of non-equilibrium process discussed in Section 2 we can consider each particle as an oscillator in quasi-equilibrium with the surroundings, if the temperature profile is a slowly changing function. Thus one can define the temperature by the relation (B.7). *Equipartition theorem* Let us consider the mean values of the kinetic and the potential energies, $K = p^2/(2m)$ and $P = \frac{1}{2} m\omega_0^2 q^2$, respectively, by using the relation (B.4). Substituting the kinetic energy K into (B.4) yields

$$\langle K \rangle = \frac{1}{hZ} \int \frac{p^2}{2m} e^{-\beta H} \mathrm{d}q\, \mathrm{d}p = \frac{2}{hZ\omega_0 \beta^2} \int_{-\infty}^{\infty} e^{-\xi^2} \mathrm{d}\xi \int_{-\infty}^{\infty} \zeta^2 e^{-\zeta^2} \mathrm{d}\zeta = \frac{1}{2\hbar\omega_0 \beta^2 Z} = \frac{1}{2} k_B T. \tag{B.8}$$

In a similar manner one obtains the mean potential energy

$$\langle P \rangle = \frac{1}{hZ} \int \frac{1}{2} m\omega_0^2 q^2 e^{-\beta H} \mathrm{d}q\, \mathrm{d}p = \frac{1}{2} k_B T, \tag{B.9}$$

which is equal to the mean kinetic energy. This result corresponds with the equipartition theorem. More generally it states, that each variable appearing quadratically in the Hamiltonian contributes $\frac{1}{2} k_B T$ to the total average energy.

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