Unsteady heat transport in a semi-infinite free end Hooke chain caused by instantaneous heat pulse

Sergei D. Liazhkov

June 23, 2022

Abstract

We consider unsteady ballistic heat transport in a semi-infinite Hooke chain with free end and some initial temperature profile. An analytical description of the evolution of the kinetic temperature is proposed in the frameworks of the lattice dynamics approach in both discrete (though the eigenfunction expansion method) and continuum formulations. By comparison of discrete and continuum descriptions for kinetic temperature field, we reveal some restrictions to the latter. Specifically, the far-field kinetic temperature field is well described by the continuum solution, which is violated near and at the free end (boundary). We show that thermal wave has a property to reflect from the boundary, after that the discrete solution for the kinetic temperature undergoes a jump near the free end. Based on the comparison of continuum and discrete descriptions of heat propagation in the semi-infinite and infinite Hooke chains, we formulate the principles of symmetry of the corresponding solutions.

1 Introduction

Heat transfer at macroscale is known to be diffusive and obeys the Fourier law. Using of the law as constitutive relation, a wide class of problems in continuum mechanics can be solved (see e.g. [1]).

However, theoretical studies [2, 3, 4] and experiments [5, 6, 7, 8, 9, 10] show that at micro- and nanoscale heat propagation is nondiffusive, e.g. ballistic. In particular, deviation from the Fourier law is shown in nanotubes [5], silicon membranes [7], silicon nanowires [8], graphene [10]. Therefore, development of theory, describing thermal processes at micro- and nano-scale, is required and also relevant for the reason of development of micro- and nanoelectronics (see e.g. [11]).

As a general rule, two approaches are used for description of heat transfer at microscale (or nanoscale), namely the lattice dynamics (LD) approach and investigation of the Boltzmann transport equation (BTE). Using the second, one can solve problems, which are undecidable by the LD method (see e.g. [12, 13, 14]) and analyze quantities, continuously changing in space (for instance, the kinetic temperature). Hence a question arises: for what circumstances the LD approach to description of non-stationary heat transport problems is needed or is it needed at all?

In study [15], the kinetic theory of unsteady heat transport in the infinite one-dimensional harmonic chain is linked with the LD theory. It is shown that solution for the kinetic temperature, obtained by the LD approach, takes into account not only heat transport but the transient process, performing at short times: oscillations of the kinetic temperature caused by equilibration of kinetic and potential energies. In turn, the solution of the collisionless BTE is related with heat transport only. In the present paper, we study heat transport in the semi-infinite
free end Hooke chain and show that only exact solution by LD approach has information about influences of free end boundary condition on this unsteady process.

Based on the LD approach, one can distinguish discrete and continuum descriptions of the ballistic heat transport. In the pioneering work of Klein and Prigogine [16] the evolution law of the discrete field (changing in dependence of number of particle) of the kinetic temperature, obtained using exact Schroedinger solution [17] of the dynamics equations for the Hooke chain. In the pioneering work by Krivtsov [20], the PDE for the continuum kinetic temperature (changing in dependence of continuous spatial coordinate) is derived. In the papers [18, 19], the discrete and continuum kinetic temperature fields are under comparisons. It is shown that evolution over time of the temperature fields caused by arbitrary initial perturbation (except point) leads to coincidence of these. However, aforesaid results are about energy propagation in infinite chains only.

The question of influences of spatial inhomogeneity on heat transport remains open. In particular, answer to this question, related to free boundaries, is necessary for development of theoretical models of the experiments associated with reflection of phonons [21, 22]. In the study [23], asymptotic expressions for heat flux and local temperature in the semi-infinite chain with absorbing boundary are obtained. However, the results give no clear information on the boundary effects.

In this paper, we qualitatively describe the process of heat propagation in the semi-infinite free end Hooke chain and, analogously to [18], compare discrete (exact) and continuum descriptions on this process. We expect that results, obtained in this paper, may serve for generalization to the complex structural and high dimensional lattices and thus for more accurate description of experiments by Northrop and Wolfe.

The paper is organized as follows. In Sect.2, we formulate the problem and derive exact expression for particle velocities, which is further applied to derive the expression for the kinetic temperature. In Sect.3, we perform the continualization for the kinetic temperature to determine this in the continuum limit. In Sect.4 the fundamental solution for the kinetic temperature in continuum limit is found. In Sect.5, the discrete and continuum kinetic temperature fields are in comparison. Examples of the rectangular (Sect.5.2) and step (Sect.5.3) are considered. In Sect.6, we compare theory of ballistic heat transport in the semi-infinite Hooke chain with infinite Hooke chain. In Sect.7, the results of the paper are discussed. The principles of symmetry of continuum and discrete solutions for the kinetic temperature are formulated based on results of Sect.4 and Sect.6 respectively.

2 Discrete solution for the kinetic temperature

The following exact expression for the kinetic temperature $T_n$ in the infinite Hooke chain has the form [16, 24]:

$$T_n = \sum_{j=-\infty}^{\infty} T_0^j J_2^j(n-j)(2\omega_e l), \quad \omega_e = \sqrt{\frac{c}{m}},$$

(1)

where $\omega_e$ is elementary atomic frequency; $c$ is stiffness of Hookean springs; $m$ is the particle mass; $T_0^n$ is initial temperature of particle $n$; $J$ is the Bessel function of the first kind. The formula (1) follows from exact solution for particle velocities, obtained by the Schroedinger approach [17] and condition implying uncorrelatedness of the initial velocities. In the similar way, the exact expression for the kinetic temperature of semi-infinite chain is further derived.
2.1 Mathematical formulation of the problem and derivation of expression for particle velocities

Initially, we consider the Hooke chain with two free ends, which consists of \( N \) particles\(^1\), interacting with the nearest neighbors. This system is governed by the dynamics equations

\[
\begin{align*}
\dot{u}_n &= v_n, \\
\dot{v}_n &= \omega_e^2 (u_{n+1} - 2u_n + u_{n-1}), \quad n = 1, \ldots, N - 2, \\
\dot{v}_0 &= \omega_e^2 (u_1 - u_0), \\
\dot{v}_{N-1} &= \omega_e^2 (u_{N-2} - u_{N-1})
\end{align*}
\]

where \( u_n \) and \( v_n \) are displacement and velocity for particle \( n \) respectively. The equations are supplemented by the following initial conditions:

\[
u_n = 0, \quad v_n = v_0^n.
\]

where \( v_0^n \) is the initial velocity field. Solution of Eqs. (2–3) can be sought in a form of Bessel function series, proposed in [24, 25]. However, the solution is rather cumbersome for further analysis. Therefore, using the eigenfunction expansion method (see e.g. chapter 31 in [26]) is optimal.

We seek \( u_n \) in the form, satisfying free boundary conditions:

\[
u_n = 0, \quad v_n = v_0^n.
\]

where \( v_0^n \) is the initial velocity field. Solution of Eqs. (2–3) can be sought in a form of Bessel function series, proposed in [24, 25]. However, the solution is rather cumbersome for further analysis. Therefore, using the eigenfunction expansion method (see e.g. chapter 31 in [26]) is optimal.

We seek \( u_n \) in the form, satisfying free boundary conditions:

\[
\begin{align*}
\hat{u}_k &= \sum_{n=0}^{N-1} u_n \cos \frac{(2n+1)\pi k}{N}, \\
\hat{v}_0 &= \sum_{n=0}^{N-1} v_0^n \cos \frac{(2n+1)\pi k}{N}
\end{align*}
\]

Applying (5) to (2) and (3) results in ODE with respect to \( \hat{u}_k \):

\[
\ddot{\hat{u}}_k + \omega_k^2 \hat{u}_k = 0, \quad \omega_k = 2\omega_e \sin \frac{\pi k}{N}, \quad \hat{u}_k|_{t=0} = 0, \quad \hat{v}_0^n |_{t=0} = \sum_{n=0}^{N-1} v_0^n \cos \frac{(2n+1)\pi k}{N},
\]

whence

\[
\hat{u}_k = \frac{\sin (\omega_k t)}{\omega_k} \sum_{n=0}^{N-1} v_0^n \cos \frac{(2n+1)\pi k}{N}.
\]

Here \( \omega_k \) is the \( k \)-th eigenfrequency of the chain. Substituting of (7) to (4) with subsequent differentiation with respect to time gives the following formula for the particle velocity:

\[
v_n = 2 \sum_{j,k=0}^{N-1} v_j^0 \cos \frac{(2j+1)\pi k}{N} \cos \frac{(2n+1)\pi k}{N} \cos (\omega_k t).
\]

Assume that the right end of the chain is located far away from the domain, wherein the perturbation could be concentrated. This assumption allows us to proceed to the thermodynamic limit (\( N \to \infty \)) and refer the chain to as the *semi-infinite free end chain*. We introduce a new

\(^1\)Number of particles \( N \) is constant in time.
variable $\theta = 2\pi k/N$ and replace the sum with respect to the number $k$ to the corresponding integral:

$$v_n = \frac{1}{\pi} \sum_{j=0}^{\infty} v_j^0 \int_{-\pi}^{\pi} \cos \left(\frac{2j+1}{2} \theta\right) \cos \left(\frac{2(n+1)}{2} \theta\right) \cos(\omega(\theta)t) d\theta,$$

$$\omega(\theta) = 2\omega_c \sin \frac{\theta}{2},$$  \hspace{1cm} (9)

where $\omega$ is the dispersion relation. Thus, we have the exact expression for velocity of each particle in the semi-infinite chain. In the next section, the formula (9) is employed to obtain the kinetic temperature.

2.2 Exact expression for the kinetic temperature

We consider an infinite set of realizations, which differ by the initial conditions (3). For the one-dimensional Hooke chain, we can characterize the thermal state via one parameter, which is referred to as the kinetic temperature:

$$m \langle v_n^2 \rangle \overset{\text{def}}{=} k_B T_n,$$

(10)

where $\langle \ldots \rangle$ stands for the mathematical expectation sign, namely averaging over realizations $^3$.

Substitution of the formula (8) to the definition of the kinetic temperature (10) yields

$$k_B T_n = \frac{1}{\pi^2} \int_{-\pi}^{\pi} \sum_{i,j=0}^{N-1} \langle v_i^0 v_j^0 \rangle \cos \left(\frac{2i+1}{2} \pi \theta_1 \right) \cos \left(\frac{2j+1}{2} \pi \theta_2 \right) \cos \left(\frac{2(n+1)+1}{2} \pi \theta_1 \right) \cos \left(\frac{2(n+1)+1}{2} \pi \theta_2 \right) \cos(\omega(\theta_1)t) \cos(\omega(\theta_2)t) d\theta_1 d\theta_2.$$  \hspace{1cm} (11)

From (10), the relation between initial velocity for particle $v_n^0$ and its initial kinetic temperature $T_n^0$ is

$$v_n^0 = \rho_n \sqrt{\frac{k_B T_n^0}{m}}, \quad \langle \rho_n \rangle = 0, \quad \langle \rho_j \rho_n \rangle = \delta_{jn},$$

(12)

where $k_B$ is the Boltzmann constant; $\delta_{jn}$ is the Kronecker delta; $\rho_n$ are uncorrelated random numbers with zero mean and unit variance. Thus, the initial conditions (3) imply an existence of a some initial temperature field in the chain and zero initial heat fluxes$^4$ [20, 30]. Uncorrelatedness of the initial velocities results in

$$T_n = \frac{1}{\pi^2} \sum_{j=0}^{\infty} T_j^0 \left( \int_{-\pi}^{\pi} \cos \left(\frac{2j+1}{2} \theta\right) \cos \left(\frac{2(n+1)+1}{2} \theta\right) \cos(\omega(\theta)t) d\theta \right)^2.$$  \hspace{1cm} (13)

The formula (13) is an exact solution for the discrete kinetic temperature of the semi-infinite chain with free end. If we decompose the product of cosines in (13) to sum of complex exponents, we obtain the representation of the kinetic temperature as superposition of waves with wavenumber $\theta$. We further refer (13) to as a discrete solution. From comparison of Eqs. (1) and (13) one can observe that the kinetic temperature can be represented as the discrete analogue of convolution of $T_n^0$ and squared velocity of particle $n$ in a chain, perturbed by instantaneous force with unit magnitude at the point $j$.

The expression (13) is further employed to obtain the kinetic temperature in the continuum limit.

$^2$In literature, this variable is systematically referred to as the continuous wave number (see [15, 28]).

$^3$Unambiguous determination of the temperature for systems far from equilibrium is unresolved fundamental problem [31]. In this paper, we calculate the kinetic temperature as average of kinetic energy over realizations, because it has simple physical meaning and can be measured in real experiments. Discussion of ergodic properties of the chain remains out of frameworks of this study.

$^4$The statement of problem corresponds to experimental heating the crystal by the ultrashort laser pulse.
3 Kinetic temperature in the continuum limit

In the section, we derive the kinetic temperature in continuum limit, namely is a function of continuum generalized coordinate. This representation suits for the general case when expression (13) becomes hard to use. We show that kinetic temperature in the continuum limit can be expressed as

$$T(x, t) = T_0^0(x) \frac{J_0(4\omega_e t)}{2} + \frac{1}{2\pi} \int_0^\pi T_0^0(|x + v_s t \cos \theta|) d\theta,$$

(14)

where

$\omega_e a$ is the sound speed; $a$ is the equilibrium distance (length of undeformed bond between particles); $T_0^0(x)$ is the field of continuum kinetic temperature, $T_0^0(an) = T_0^0$ (see derivation for details). Derivation of the formula (14) is given below.

We use an approach, proposed in study [15]. First of all, we separate the formula (13) into two terms, corresponding to the two physical processes:

$$T_n = T_n^F + T_n^S,$$

$$T_n^F = \sum_{j=0}^{\infty} T_0^0 F_{nj}, \quad T_n^S = \sum_{j=0}^{\infty} T_0^0 S_{nj},$$

$$F_{nj} = \frac{1}{2\pi^2} \int_{-\pi}^\pi \cos \frac{(2j+1)\theta_1}{2} \cos \frac{(2j+1)\theta_2}{2} \cos \frac{(2n+1)\theta_1}{2} \cos \frac{(2n+1)\theta_2}{2} \cos ((\omega(\theta_1) + \omega(\theta_2))t) d\theta_1 d\theta_2,$$

$$S_{nj} = \frac{1}{2\pi^2} \int_{-\pi}^\pi \cos \frac{(2j+1)\theta_1}{2} \cos \frac{(2j+1)\theta_2}{2} \cos \frac{(2n+1)\theta_1}{2} \cos \frac{(2n+1)\theta_2}{2} \cos ((\omega(\theta_1) - \omega(\theta_2))t) d\theta_1 d\theta_2,$$

(15)

We further show that the first term corresponds to high-frequency oscillations of the kinetic temperature, caused by equilibration of the kinetic and potential energies [29]. This is a fast process, occurring in time of order of several hundreds atomic periods. The second term corresponds to the slow process caused by ballistic heat transport. Characteristic time scale of this process is rather larger than of the thermal equilibration. Following [15], we perform a continualization for the «slow» and «fast» terms of the kinetic temperature, $T_n^S$ and $T_n^F$ respectively.

We introduce a mesoscale, which is larger than the distance between particles, $a$, but smaller than a some macroscale $^5$, $A$ and divide the chain into the equal intervals, indexed by $s$. Each interval $s$ has the length $2a\Delta N$, $\Delta N \gg 1$, $a\Delta N \ll A$ and is limited by the boundary-particles, $j_s$. We assume that the initial temperature profile, enclosed in the intervals $s$, changes slowly.

![Initial temperature profile](image)

$^5$A macroscale can be interpreted as a scale of the order of the length of chain.
Therefore, the length of the mesoscale is $2a\Delta N$. Then, the expressions for $T_n^S$ and $T_n^F$ in the formula (15) can be rewritten as

$$T_n^{(F,S)} = \sum_{s=0}^{\infty} \sum_{j_s = j_s - \Delta N + 1}^{j_s + \Delta N} T_j^0 (F, S)_{nj} \approx \sum_{s=0}^{\infty} \sum_{j_s = j_s - \Delta N + 1}^{j_s + \Delta N} (F, S)_{nj}$$

$$= 2a\Delta N \sum_{s=0}^{\infty} T_j^0 g_{n,j_s}^{(F,S)} (\Delta N), \quad g_{n,j_s}^{(F,S)} (\Delta N) = \frac{1}{2a\Delta N} \sum_{j=j_s-\Delta N+1}^{j_s+\Delta N} (F, S)_{nj}$$ \hspace{1cm} (16)

where $g_{n,j_s} (\Delta N)$ determines contribution of the point $j_s$ to the temperature at point $n$. It can also be interpreted as a discrete fundamental solution, obtained by averaging of the $T_n$ over the mesoscale. Further, we derive the continuum fundamental solution, corresponding to the slow term $g^S$ (see Sect.3.1) and to the fast term $g^F$ (see Sect.3.2).

### 3.1 Slow term

The following formula for $g_{n,j_s}^S (\Delta N)$ is calculated up to the order $O\left(\frac{1}{\Delta N}\right)$ (see Appendix A) and is represented below:

$$g_{n,j_s}^S (\Delta N) \approx \frac{1}{16\pi^2 a} \int_{-\pi}^{\pi} \left[ \cos (\Delta \theta \omega' (\theta_1) t) \cos((n + j_s)\Delta \theta) \text{sinc}(\Delta N\Delta \theta) \right] d\theta_1 d\theta_2 +$$

$$\frac{1}{16\pi^2 a} \int_{-\pi}^{\pi} \left[ \cos (\Delta \theta \omega' (\theta_1) t) \cos((n - j_s)\Delta \theta) \text{sinc}(\Delta N\Delta \theta) \right] d\theta_1 d\theta_2 +$$

$$\frac{1}{16\pi^2 a} \int_{-\pi}^{\pi} \left[ \cos (\Delta \theta \omega' (\theta_1) t) \cos(\theta_1 (2n + 1) - (n + j_s)\Delta \theta) \text{sinc}(\Delta N\Delta \theta) \right] d\theta_1 d\theta_2 +$$

$$\frac{1}{16\pi^2 a} \int_{-\pi}^{\pi} \left[ \cos (\Delta \theta \omega' (\theta_1) t) \cos(\theta_1 (2n + 1) - (n - j_s)\Delta \theta) \text{sinc}(\Delta N\Delta \theta) \right] d\theta_1 d\theta_2,$$ \hspace{1cm} (17)

where $\Delta \theta = \theta_1 - \theta_2$, $(\cdot)' = \frac{d}{d\theta_1}$, $\text{sinc}(x) = \frac{\sin x}{x}$. We change the variables $\theta = \theta_1, \varphi = \Delta \theta$ and rewrite the formula (17), using trigonometric identities and symmetry of the integrands with
The discrete fundamental solution:

\[ g_{n,j_s}(\Delta N) = \frac{1}{8\pi} \int_0^{\pi} \left[ \psi_1(n + j_s + \omega'(\theta)t) + \psi_1(n + j_s - \omega'(\theta)t) \right] d\theta \]

\[ + \frac{1}{8\pi} \int_0^{\pi} \left[ \psi_1(n - j_s + \omega'(\theta)t) + \psi_1(n - j_s - \omega'(\theta)t) \right] d\theta \]

where \( H \) has the following approximate form (see Appendix B):

\[ \psi_1(\Xi) = \frac{1}{2\pi a} \int_{-\pi}^{\pi} \cos (\Xi q) \text{sinc}(q\Delta N) dq, \]

\[ \psi_2(\Xi) = \frac{1}{2\pi a} \int_{-\pi}^{\pi} \sin (\Xi q) \text{sinc}(q\Delta N) dq, \]

where \( \psi_1 \) and \( \psi_2 \) are referred to as wave packets propagating with group velocity \( v_g = a\omega' \).

Averaging of the function \( g_{n,j_s} \) over mesoscale leads to a sum of the integrals of these wave packets. In the limit case \( \Delta N \gg 1 \) the wave packet \( \psi_2 \) is negligible and the expression for \( \psi_1 \) has the following approximate form (see Appendix B):

\[ \psi_1(\Xi) \approx \frac{1}{2a\Delta N} H \left( 1 - \frac{|\Xi|}{\Delta N} \right), \]

where \( H(x) \) is the Heaviside function. Using the limit case for \( \Delta N \), we obtain the final form of the discrete fundamental solution:

\[ g_{n,j_s}(\Delta N) \approx \frac{1}{4\pi} \int_0^{\pi} \left[ \psi(n - j_s + \omega'(\theta)t, \Delta N) + \psi(n + j_s + \omega'(\theta)t, \Delta N) \right] d\theta \]

\[ + \frac{1}{4\pi} \int_0^{\pi} \left[ \psi(n + j_s + \omega'(\theta)t, \Delta N) + \psi(n + j_s - \omega'(\theta)t, \Delta N) \right] d\theta, \]

\[ \psi(\Xi, \Delta N) = \frac{1}{2a\Delta N} \cos^2 \left( \frac{\theta(2n + 1)}{2} \right) H \left( 1 - \frac{|\Xi|}{\Delta N} \right). \]

We introduce continuous functions \( T^S(x) \), \( T^0(x) \), \( g^S_c(x,y) \) such that

\[ T^0(an) = T^0_n, \quad g^S_c(x,y) = \lim_{a\Delta N \to 0} g^S_{n,j_s}(\Delta N), \]

\[ T^S(x) = \lim_{a\Delta N \to 0} T^S_n = \int_0^\infty T^0(y) g^S_c(x,y) dy. \]

In the limit case \( a\Delta N/A \to 0 \), the function \( \psi \) can be replaced by the Dirac delta function. Using formulas (20) and (21), we obtain the fundamental solution for the slow term of the kinetic temperature:

\[ g^S_c(x,y) = g^S(x - y) + g^S(x + y), \quad g^S(x) = \frac{1}{2\pi} \int_0^{\pi} \delta(x + v_y(\theta)t) d\theta + \frac{1}{2\pi} \int_0^{\pi} \delta(x - v_y(\theta)t) d\theta. \]

(22)
where \( v_g(\theta) = v_s \cos \frac{\theta}{2} \) is the group velocity \(^6\).

The slow term \( T^S \) is further obtained as the integral convolution of this fundamental solution with field of the initial temperature:

\[
T^S = \frac{1}{4\pi} \int_0^\infty T^0(y) \int_0^\pi \delta(x - y + v_g(\theta)t) \, d\theta \, dy + \frac{1}{4\pi} \int_0^\infty T^0(y) \int_0^\pi \delta(x - y - v_g(\theta)t) \, d\theta \, dy + \frac{1}{4\pi} \int_0^\infty T^0(y) \int_0^\pi \delta(x + y - v_g(\theta)t) \, d\theta \, dy.
\]

(23)

It is shown from formula (23) that \( T^S \) is represented as sum of superpositions of independent localized wave packets. In contrast to the infinite chain, these wave packets can propagate both from the boundary (is described by first and third terms in (23)) and towards boundary (is described by second term in (23)). Fourth term is equal to zero, because \( T^0(-x) = 0 \). Using the property of convolutions and property of group velocity function, we simplify the formula (23):

\[
T^S = \frac{1}{2\pi} \int_0^\pi T^0(|x + v_st \cos \theta|) \, d\theta.
\]

(24)

**Remark** In the [15], the heat transport in the infinite Hooke chain is investigated in the frameworks of both the lattice dynamics approach and the Boltzmann kinetic theory. Following the second, solution for the continuum kinetic temperature is derived using the distribution function as solution of the collisionless Boltzmann transport equation. The result coincides with predictions from the lattice dynamics approach. As for the semi-infinite free end Hooke chain, the kinetic temperature can be obtained in the same way, if the solution of the collisionless Boltzmann transport equation with evenness condition at the boundary \( x = 0 \) is known. The result must coincide with (24).

### 3.2 Fast term

Analogously, using the assumption (16) with \( a\Delta N \ll A \) and \( \Delta N \gg 1 \) and (21), we obtain the expression for the fast term \( T^F \). Since the main contribution to the terms \( T^F \) comes from points \( \theta_1 \approx \theta_2 \), as it was shown is Sect.3.1, then \( \omega(\theta_1) + \omega(\theta_2) \approx 2\omega(\theta_1) \). According to Sect. 3.1, the fundamental solution, \( g^F \), can be written as

\[
g^F_e(x,y) = \frac{\delta(x-y) + \delta(x+y)}{2\pi} \int_0^\pi \cos(2\omega(\theta)t) \, d\theta = \frac{\delta(x-y) + \delta(x+y)}{2} J_0(4\omega_e t).
\]

(25)

Then, the formula for \( T^F \) has the form

\[
T^F = \frac{T^0(x)H(x) + T^0(-x)H(-x)}{2} J_0(4\omega_e t) = \frac{T^0(x)}{2} J_0(4\omega_e t).
\]

(26)

Therefore, the expression for the fast term of the kinetic temperature, \( T^F \) coincides with the same formula for the infinite chain [29].

Thus, the final expression for the kinetic temperature in the continuum limit (14) is the sum of the contribution of fast processes caused by equilibration of kinetic and potential energies \( (T^F) \) and contribution of slow processes caused by ballistic heat transport \( (T^S) \). We further refer the formula (14) to as a continuum solution.

---

\(^6\)Here evenness properties of the Dirac delta function and \( v_g \) are used.
4 Point heat perturbation. Principle of continuum solution symmetry

We consider the point instantaneous thermal perturbation in the point, located at a some distance from the boundary, namely $ha$, $h \in \mathbb{N} \cup \{0\}$. We determine the initial temperature, corresponding to the considered case:

$$T^0(x) = A\delta(x - ha), \quad (27)$$

where $A$ is a constant with dimension $K \cdot m$. Since thermal equilibration occurs instantly, we neglect them. Therefore,

$$T \approx T^S = \frac{A}{2\pi} \int_0^{\pi} \delta(|x + v_s \cos \theta t| - ha) d\theta. \quad (28)$$

Calculation of integrals (28) is carried out using the following formula [32]:

$$\int_D \delta(f(\Xi)) d\Xi = \sum_i \frac{1}{|f'(\Xi_i)|}, \quad f(\Xi) = 0, \quad (29)$$

where $\Xi_i$ are zeros of function $f$, lying inside the domain $D$. Therefore, we have the following formula for the continuum kinetic temperature

$$T = \frac{A}{2\pi} \left( \frac{H(v_s t - |x - ha|)}{\sqrt{v_s^2 t^2 - (x - ha)^2}} + \frac{H(v_s t - |x + ha|)}{\sqrt{v_s^2 t^2 - (x + ha)^2}} \right). \quad (30)$$

We have obtained the continuum temperature in the semi-infinite chain in the case of a heat pulse. However, if we consider the infinite chain with thermal sources located at the points $ha$ and $-ha$, the obtained continuum solution is the same [27], [Sokolov2021]. Therefore, the continuum kinetic temperature in the semi-infinite Hooke chain with free end and some source coincides with the continuum kinetic temperature in the infinite Hooke chain with the same and mirrored sources. The aforesaid rule will be further referred to as a principle of continuum solution symmetry.

We consider point heat perturbation, located at some point from the boundary $(h = 10)$. Behavior of thermal waves, propagation of which obeys the formula (30) is represented in figure 2.

Figure 2: Thermal waves. $\omega_e t = 5$ (solid line), $\omega_e t = 10$ (dashed line), $\omega_e t = 18$ (dash-dotted line).
Figure 2 shows travelling to both directions waves in the semi-infinite chain. Wave, emanated from the point \( x = ha \), travels to the left end, *instantly* reflects from the boundary at the moment \( t = ha/v_s \) and travels backwards. Specifically, it is shown that, the temperature profile is *not symmetric* with respect to the heat source after the reflection.

Thus, we have analytically described a property of the ballistically propagating thermal waves to reflect from boundaries. In the next section, we compare continuum and discrete descriptions of the kinetic temperature field in cases of perturbation on the finite domain.

5 Examples

In this section, evolution of the kinetic temperature fields in the cases of rectangular and step thermal perturbations are under investigation. We compare discrete and continuum temperature fields and show that continuum descriptions of heat transport have some restrictions.

5.1 Simulation details

For further analyzing of derived formulas for the kinetic temperatures, we make these dimensionless. First of all, we introduce the following dimensionless variables \( \tilde{x}, \tilde{u}, \tilde{v}, \tilde{t}, \tilde{T} \) such as:

\[
\begin{align*}
\tilde{x} &= x/a, \quad \tilde{u} = u/a, \\
\tilde{v} &= v/v_s, \quad \tilde{t} = \omega_s t, \quad \tilde{T} = T k_B/(mv_s^2).
\end{align*}
\]

(31)

In the points of particle locations \( \tilde{x} \equiv n \). We denote further the continuum kinetic temperature as \( \tilde{T}(\tilde{x}) \) and the discrete kinetic temperature as \( \tilde{T}_n \).

We rewrite the dynamics equations (2) as

\[
\begin{align*}
\dot{\tilde{u}}_n &= v_n \dot{\tilde{t}}, \\
\dot{\tilde{v}}_n &= \left( \tilde{u}_{n+1} - 2 \tilde{u}_n + \tilde{u}_{n-1} \right) \dot{\tilde{t}}, \quad n = 1, 2, ..., N - 2, \\
\dot{\tilde{v}}_{N-1} &= \left( \tilde{u}_{N-2} - \tilde{u}_{N-1} \right) \dot{\tilde{t}}, \\
\dot{\tilde{v}}_0 &= \left( \tilde{u}_1 - \tilde{u}_0 \right) \dot{\tilde{t}},
\end{align*}
\]

(32)

with initial conditions

\[
\begin{align*}
\tilde{u}_n &= 0, \quad \tilde{v}_n = \rho_n \sqrt{\tilde{T}_n^0}, \quad \langle \rho_n \rangle = 0, \quad \langle \rho_m \rho_n \rangle = \delta_{mn}.
\end{align*}
\]

(33)

In numerical simulations, the kinetic temperatures are calculated numerically as follows:

\[
\tilde{T}_n = \frac{1}{R} \sum_{i=1}^{R} \tilde{v}_{n,i}^2,
\]

(34)

where \( R \) is number of realizations, which differs by random initial conditions (33), \( R = 10^5 \). Particle velocity, \( \tilde{v}_{n,i} \), is obtained for each realization \( i \) via solving of dynamics equations (32) with initial conditions (33) using the fourth-order symplectic Candy and Rozmus integrator [34] with optimizing parameters proposed in [35] and time-step \( \Delta \tilde{t} = 0.01 \).

Analytical discrete and continuum solutions for the kinetic temperature are respectively rewritten as

---

7The chain with \( N = 500 \) particles is used. For that, \( \tilde{t} \) is taken to be less than the time of thermal wave propagation to the right end.

8Random numbers \( \rho_n \) are uniformly distributed in the segment \([-\sqrt{3}; \sqrt{3}]\).
\[ \tilde{T}_n = \frac{1}{\pi^2} \sum_{j=0}^{\infty} \tilde{T}_j^0 \left( \int_{-\pi}^{\pi} \cos \left( \frac{(2j+1)\theta}{2} \right) \cos \left( \frac{(2n+1)\theta}{2} \right) \cos \left( 2\tilde{t} \sin \frac{\theta}{2} \right) d\theta \right)^2, \]  

(35)

\[ \tilde{T}(\tilde{x}, \tilde{t}) = \frac{\tilde{T}_0^0(\tilde{x})}{2} J_0(4\tilde{t}) + \frac{1}{2\pi} \int_0^{\pi} \tilde{T}_0^0(|\tilde{x} + \tilde{t} \cos \theta|) d\theta. \]  

(36)

5.2 Rectangular initial perturbation

Consider a rectangular heat perturbation, which is defined by following formula:

\[ \tilde{T}_0^0(\tilde{x}) = H(\tilde{x} - \tilde{L}_1) - H(\tilde{x} - \tilde{L}_1 - \tilde{L}_2), \quad \tilde{L}_1 > 0, \quad \tilde{L}_2 > 0, \]  

(37)

where \( \tilde{L}_1 a \) is a distance from the boundary to the perturbation, \( \tilde{L}_2 a \) is a width of perturbation. We take \( \tilde{L}_1 = 25 \) and \( \tilde{L}_2 = 50 \) and investigate temperature profiles in two cases: before reflection of thermal wave and after reflection. Discrete and continuum kinetic temperatures, corresponding to the case before reflection, are represented in figure 3.

Figure 3: Discrete and continuum solutions for kinetic temperature in the semi-infinite Hooke chain, in the case of rectangular initial perturbation. \( \tilde{t} = 20 \) (left) and \( \tilde{t} = 100 \) (right).

It is seen in figure 3 (left) that the continuum and discrete solutions practically coincide before thermal wave reaches the boundary, except regions near wavefront and on the boundaries of initial perturbation. Aforesaid mismatches are caused by finiteness of the perturbation length and fast process, which takes place at relatively short times. The mismatches, mentioned above become infinitesimal at \( \tilde{t} = 100 \) (see right Fig. 3), when energy of the fast process is much less than energy transferred along the chain. However, the discrete kinetic temperature undergoes a jump near the boundary (see inlet of right Fig. 3). Therefore, the discrete and continuum solutions disagree after reflection of thermal wave from the boundary. In order to investigate this jump in detail, we consider behavior of the temperatures at the boundary.

The formula for the continuum temperature at the boundary, \( \tilde{T}(0, \tilde{t}) \), has the following form, which can be obtain by substitution of (37) to (36) with \( \tilde{x} = 0 \) and subsequent integration from 0 to \( \pi \):

\[ \tilde{T}(0, \tilde{t}) = \frac{1}{\pi} \left[ \arccos \left( \frac{\tilde{L}_1}{\tilde{t}} \right) H \left( \tilde{t} - \tilde{L}_1 \right) - \arccos \left( \frac{\tilde{L}_1 + \tilde{L}_2}{\tilde{t}} \right) H \left( \tilde{t} - \tilde{L}_1 - \tilde{L}_2 \right) \right]. \]  

(38)

From the formula (38), one can conclude that evolution of the kinetic temperature at the boundary, caused by rectangular perturbation in the chain, has three stages. The first stage is
related with fast processes and propagation of thermal waves before reflection ($t < \tilde{L}_1a/v_s$). The second stage, related to reflection of thermal wave, begins at $t = \tilde{L}_1a/v_s$ and has duration $t = \tilde{L}_2a/v_s$. Finally, the third stage begins after reflection of the wave from boundary at $t = (\tilde{L}_1 + \tilde{L}_2)a/v_s$ and is related to relaxation of the temperature on the boundary. Evolution of this is presented in figure 4.

![Figure 4: Evolution of the kinetic temperature at the boundary.](image)

One can see from the figure 4 that the discrete solution for the kinetic temperature at the boundary significantly differs from the continuum after reaching of thermal wave of the end. Growth of the discrete solution at the boundary, caused by reflection of thermal wave and decrease of this, caused by propagation of wavefront backwards are faster than the same stages of evolution of the continuum solution.

Thus, process of heat propagation in the semi-infinite Hooke chain caused by rectangular perturbation can be generally described by the continuum model, if we deal with propagation of the wavefront. However, continuum description the field of kinetic temperature at and near the boundary has inaccuracies.

### 5.3 Step initial perturbation

We consider step heat perturbation:

$$\tilde{T}^0(\tilde{x}) = H(\tilde{L} - \tilde{x}), \quad \tilde{L} > 0,$$

(39)

where $\tilde{L}a$ is a width of perturbation. Id est, the initial heat pulse affects the boundary. The discrete and continuum kinetic temperatures, corresponding to the case, are presented in figure 5, for $\tilde{L} = 50$. 

12
Figure 5: Discrete and continuum kinetic temperatures in the semi-infinite chain corresponding to the cases before ($\tilde{t} = 20$, left) and after reflection ($\tilde{t} = 80$ (blue line) and $\tilde{t} = 100$ (black line), right).

It is shown in Fig. 5 that discrete and continuum solutions are significantly different near the boundary after reflection of thermal wave by virtue of the jump (see inlet in right Fig. 5). However, some mismatches between discrete and continuum solutions are observed both before ($t < \tilde{L}/v_s$) and after ($t > \tilde{L}/v_s$) reflection of thermal wave from the boundary. Before the reflection, these mismatches are caused by influences of the fast process, occurring at the same time of wavefront propagation. The fast process strongly affects on the oscillations of discrete kinetic temperature near the boundary, which cannot be described via the continuum solution. Although propagation of the wavefront obeys the continuum description, unexpectedly, the mismatches between discrete and continuum kinetic temperature field remain. Namely the discrete solution diverges from the (see Fig. 5). An explanation of these divergences from physical point of view is beyond the scope of present paper.

Analogously to 5.2 formula for the continuum kinetic temperature at the boundary is expressed as:

$$\tilde{T}(0, \tilde{t}) = \frac{H(\tilde{L} - \tilde{t}) + J_0(4\tilde{t})}{\pi} \arcsin \left( \frac{\tilde{L}}{\tilde{L}} \right) H(\tilde{t} - \tilde{L}).$$

Evolution of the kinetic temperature occurs in two stages: equilibration of the kinetic temperature (at times $\tilde{t} < \tilde{L}$). At times ($\tilde{t} > \tilde{L}$) the wavefront propagates after reflection of this from boundary. Then the kinetic temperature at the boundary decays. Evolution of functions of the temperatures at the boundary are presented in Fig. 6.
Figure 6 shows significantly different behavior of the discrete and continuum kinetic temperatures not only at \( \tilde{t} > \tilde{L} \) (when discrete solution also asymptotically deviates from the continuum) but also at \( \tilde{t} < \tilde{L} \).

**Remark** According to the preliminary calculations, both discrete and continuum solutions for the kinetic temperature at the boundary are scale invariant with respect to \( \tilde{L} \), i.e.

\[
\tilde{T}(\tilde{t}) \bigg|_{\tilde{t} = 0, \tilde{T}_0|_{\tilde{L} + \Delta \tilde{L}}} = \tilde{T}(\tilde{L} + \Delta \tilde{L} \tilde{t}) \bigg|_{\tilde{t} = 0, \tilde{T}_0|_{\tilde{L}}}.
\]

Thus, the discrete kinetic temperature significantly differs from the continuum kinetic temperature by virtue of jump near the boundary. The discrete solution at the boundary decays substantially faster than continuum solution. This observation requires detailed asymptotic analysis based on the stationary phase method [36, 37] and therefore needs a separate investigation, which remains beyond the scope of present paper.

In the next section, we compare discrete and continuum description of heat transport in the semi-infinite and infinite chains.

### 6 Principle of discrete solution symmetry

In the section, we investigate heat transport in the infinite Hooke chain in the case of initial perturbation determined as

\[
\tilde{T}^0(\tilde{x}) = H(\tilde{x} - \tilde{L}_1) - H\left( \tilde{x} - (\tilde{L}_1 + \tilde{L}_2) \right) + H\left( \tilde{x} + (\tilde{L}_1 + \tilde{L}_2) \right) - H(\tilde{x} + \tilde{L}_1),
\]

where the parameters \( \tilde{L}_1 \) and \( \tilde{L}_2 \) are defined in Sect. 5.2. The initial temperature profile (41) assumes two mirrored with respect to zero heat sources.

Further, we consider two cases. The first case is with symmetry of heat sources but the different corresponding initial velocities. Therefore, the governing dynamics equations are

\[
\frac{d^2\tilde{u}_n}{dt^2} = \tilde{u}_{n+1} - 2\tilde{u}_n + \tilde{u}_{n-1}, \quad n = -N, \ldots, -2, -1, 0, 1, 2, \ldots, N.
\]

with initial conditions

\[
\tilde{u}_n = 0, \quad \tilde{v}_n = \frac{d\tilde{u}_n}{dt} = \rho_n \sqrt{\tilde{T}_n^0}, \quad \langle \rho_n \rangle = 0, \quad \langle \rho_m \rho_n \rangle = \delta_{mn},
\]

where \( \tilde{T}_n^0 \) is determined by the formula (37). Equations (42–43) are solved numerically with periodic boundary conditions in the same way as discussed in Sect. 5.1. In the thermodynamic
limit \((N \to \infty)\), analytical solution of the problem is also presented both in the discrete
and continuum formulations. The discrete solution for the kinetic temperature is proposed in
pioneering work by Klein and Prigogine \[16\] based on the Schroedinger approach \[17\] to solving
the dynamics equations (42):

\[
\tilde{T}_n = \sum_{j=-\infty}^{\infty} \tilde{T}_j^0 r^2_{2(n-j)}(2\tilde{t}).
\]  

(44)

The continuum solution is proposed by Krivtsov \[29, 20\]:

\[
\tilde{T}(\tilde{x}, \tilde{t}) = \tilde{T}_0(\tilde{x}) \frac{\tilde{T}_0(\tilde{x})}{2} J_0(4\tilde{t}) + \frac{1}{2\pi} \int_0^{\pi} \tilde{T}_0(\tilde{x} + \tilde{t} \cos \theta)d\theta.
\]  

(45)

The discrete and continuum kinetic temperatures for different moments of time and at
\(\tilde{L}_1 = 25, \tilde{L}_2 = 50\) are presented in Fig. 7.

Figure 7: Discrete and continuum solutions for kinetic temperature in the infinite Hooke chain,
in the case of rectangular initial perturbation (formula (41)). \(\tilde{t} = 20\) (left) and \(\tilde{t} = 100\) (right).

It is seen from Fig.7 that the continuum and discrete kinetic temperatures are in good
agreement. Moreover, in the domain \(\tilde{x} \geq 0\) the continuum kinetic temperature field coincides
with the same field in the semi-infinite chain\[9\]. As expected, the principle of continuum solu-
tion principle, formulated in Sect.5 is fulfilled. However, the corresponding discrete solutions
disagree. The reason of the mismatch is the random initial velocities are uncorrelated. If so,
then the discrete solutions are not symmetric with respect to zero even in case of mirrored heat
sources.

Let us consider another case, which is governed by the dynamics equations (32) with initial
conditions (33). However, firstly, we enumerate particles as follows:

\[
n = -N, ..., -2, -1, 1, 2, ..., N.
\]  

(46)

Secondly, we require the following condition for the initial velocities

\[
\rho_{-n} = \rho_n,
\]  

(47)

which assumes a symmetry with respect to zero of both initial temperature profile and field of
initial velocities simultaneously.

---

\[9\]One can see that, before reflection from the boundary, the discrete kinetic temperature can be described
by the solution (44).
The expression for particle displacement, $\tilde{u}_n$, can be represented as

$$
\tilde{u}_n = \frac{1}{N} \sum_{k=-N}^{-1} \tilde{u}_k e^{2\pi i n/N} + \frac{1}{N} \sum_{k=1}^{N} \tilde{u}_k^* e^{-2\pi i n/N},
$$

(48)

where $\tilde{u}_k(\tilde{t})$ and $\tilde{u}_k^*(\tilde{t})$ are unknown depending on time functions. From (48), the following representation for $\tilde{u}_{-n}$ follows

$$
\tilde{u}_{-n} = \frac{1}{N} \sum_{k=-N}^{-1} \tilde{u}_k e^{-2\pi i n/N} + \frac{1}{N} \sum_{k=1}^{N} \tilde{u}_k^* e^{2\pi i n/N}.
$$

(49)

The condition (47) must result in $\tilde{u}_k(\tilde{t}) = \tilde{u}_k^*(\tilde{t})$, whence $\tilde{u}_n = \tilde{u}_{-n}$. Therefore, the bond deformation between the particles $n = -1$ and $n = 1$ equals zero. Returning to the limit case ($N \to \infty$), we conclude that the Hooke chain with symmetric with respect to zero field of initial velocities is equivalent to the interacting two semi-infinite free end Hooke chains.

To the best of our knowledge, analytical solution for the kinetic temperature (both in the discrete and continuum formulations), corresponding to the problem (42), (43), (47) is unknown. We calculate numerically the kinetic temperature in the same way as discussed in Sect.5.1 and using periodic boundary conditions $^{10}$. Comparison between kinetic temperature field in the considered model at $\tilde{t} = 100$ with the corresponding solution for the semi-infinite chain (formulas (35) and (36)) is presented in Fig.8.

![Figure 8: The discrete kinetic temperature profile in the infinite Hooke chain in the case of rectangular initial perturbation (41) with condition (47) (black circles). The discrete kinetic temperature in the semi-infinite free end Hooke chain in the case of rectangular initial perturbation (37) (blue dashed line).](image)

From Fig.8 it is seen that the discrete solution for the semi-infinite chain in case of the rectangular perturbation is the same as solution for the infinite Hooke chain with absolutely mirrored heat sources (with symmetric initial velocity fields with respect to zero).

Thus, the discrete kinetic temperature in the semi-infinite Hooke chain with free end and some field of initial velocities *coincides* with the discrete kinetic temperature in the infinite Hooke chain with the same and mirrored velocity fields. The aforesaid rule will be further referred to as a *principle of discrete solution symmetry*.

$^{10}$In numerical calculations, we enumerate the particles in the sequence (see (42)).
7 Conclusions

Based on obtained in the paper results, we formulate the following principles, which the mechanism of ballistic heat transport in the semi-infinite free end Hooke chain is satisfied:

1. The continuum kinetic temperature field in the semi-infinite free end Hooke chain with some heat source (initial temperature field) coincides with the continuum kinetic temperature field in the infinite Hooke chain with the same and mirrored with respect to zero heat sources, corresponding to uncorrelated initial velocities. Herewith, the discrete solutions can mismatch by virtue of jump of the kinetic temperature near the boundary of the semi-infinite chain. This is the principle of continuum solution symmetry.

2. The discrete kinetic temperature field in the semi-infinite free end Hooke chain with some field of initial velocities coincides with the discrete kinetic temperature field in the infinite Hooke chain with the same and mirrored with respect to zero fields of initial velocities. This is the principle of discrete solution symmetry.

The principles, formulated above, may serve to solve the problem of unsteady heat transport problem in the semi-infinite (not only one-dimensional) lattices using known solutions for the infinite lattices.

It was analytically shown that process of ballistic heat propagation in the chain has at least two transient processes. The first is associated with reflection of thermal wave from the free boundary. The second transient process is related with propagation of thermal waves in the same direction. The discrete and continuum solutions for kinetic temperature at the boundary after reflection of thermal wave have significantly different behaviors.

It was shown by the examples of rectangular and step initial perturbations that the far field of the kinetic temperature obeys the continuum solution (14). However, the discrete and continuum kinetic temperature fields near the boundary mismatch. The continuum description of the ballistic heat transport has restrictions, attributable to the finiteness. Therefore, the Boltzmann kinetic theory needs taking into account the discreteness of structure. In order to use the continuum solution for kinetic temperature as the constitutive relation (in particular, for problems of thermoelasticity (see [38]) or thermoelectricity (see e.g. [39])), clarification of this with taking into account features of the discrete solution is needed. That can be done in two ways. The first is obtaining large-time asymptotics for the discrete kinetic temperature field in the similar way proposed in [19, 43]. The second way is to solve heat transport problem in the infinite chain with mirrored with respect to zero fields of initial velocities and then perform a continualization procedure, proposed either in [15] or in [27].

An explanation of jump of the kinetic temperature from the free end cannot be provided by the model of the semi-infinite chain. In order to understand this, heat transport through the boundary of the two chains with significantly different stiffnesses was numerically investigated analogously as discussed in 5.1. In this system, the jump of the kinetic temperature is the Kapitza jump, which was discovered experimentally long time ago [40]. From these observations, one can assume that the jump of the kinetic temperature near the free end is the limiting case of the Kapitza jump in the two interacting chains with stiffnesses, ratio of which is infinitesimal. However, verifying of this assumption requires a confirmation based on analytical treatments. The problem considered and solved in the present paper, can be auxiliary. In general, a problem of heat transport in the heterogeneous lattices is as yet hard to solve analytically but some progress in studying it is attained in both the steady-state [41, 42] and non-stationary [43] formulations.

We expect that results of the present paper may serve for development of full-fledged the-
or of heat transport in the semi-infinite lattices. However, real systems are generally anharmonic (nonlinear) and therefore investigation of heat propagation therein must take into account nonlinearity. On the other hand, heat transport regime remains quasi-ballistic in weakly anharmonic lattices at relatively short times and can be therefore qualitatively described in the harmonic approximation (see e.g. [38, 41, 42, 44, 45]).

8 Acknowledgements

The work is supported by the Russian Science Foundation (Grant No. 21-71-10129). The author is deeply grateful to V.A. Kuzkin, A.M. Krivtsov, S.N. Gavrilov, E.V. Shishkina, A.S. Sokolov and E.F. Grekova for useful and simulating discussions.

A Derivation of the discrete fundamental solution

Here, we derive the discrete fundamental solution, namely \( g_{n,j}(\Delta N) \).

Expanding a product of cosines in (15) yields

\[
S_{nj} = \frac{1}{16\pi^2} \int_{-\pi}^{\pi} \left[ \cos((n+j+1)(\theta_1 + \theta_2)) + \cos((n+j+1)(\theta_1 - \theta_2)) + \cos((n-j)(\theta_1 + \theta_2)) + \cos((n-j)(\theta_1 - \theta_2)) \right] \cos((\omega(\theta_1) - \omega(\theta_2))t) d\theta_1 d\theta_2.
\]

(50)

Therefore, the expression for \( g_{n,j}(\Delta N) \) can be rewritten as a sum of the following eight terms:

\[
g_{n,j}(\Delta N) = \frac{1}{16\pi^2 a} \int_{-\pi}^{\pi} \cos((\omega(\theta_1) - \omega(\theta_2))t) \sum_{i=1}^{8} \varphi_i(\theta_1, \theta_2) d\theta_1 d\theta_2, \\
\varphi_1(\theta_1, \theta_2) = \frac{1}{2\Delta N} \sum_{j=s+\Delta N+1}^{j_\ast} \cos((n+j+1)(\theta_1 + \theta_2)) = \frac{1}{2\Delta N} \cos\left(\frac{3(\theta_1 + \theta_2)}{2} + (\theta_1 + \theta_2)(n+j_s)\right) \frac{\sin((\theta_1 + \theta_2)\Delta N)}{\sin(\frac{\theta_1 + \theta_2}{2})}, \\
\varphi_2(\theta_1, \theta_2) = \frac{1}{2\Delta N} \sum_{j=s+\Delta N}^{j_\ast} \cos((n+j+1)\Delta\theta) = \frac{1}{2\Delta N} \cos\left(\left(n+j_s + \frac{3}{2}\right)\Delta\theta\right) \frac{\sin(\Delta N\Delta\theta)}{\sin(\frac{\Delta\theta}{2})}, \\
\varphi_3(\theta_1, \theta_2) = \frac{1}{2\Delta N} \sum_{j=s-\Delta N+1}^{j_\ast} \cos((n-j)(\theta_1 + \theta_2)) = \frac{1}{2\Delta N} \cos\left((\theta_1 + \theta_2)\left(\frac{1}{2} + j_s - n\right)\right) \frac{\sin((\theta_1 + \theta_2)\Delta N)}{\sin(\frac{\theta_1 + \theta_2}{2})}, \\
\varphi_4(\theta_1, \theta_2) = \frac{1}{2\Delta N} \sum_{j=s-\Delta N+1}^{j_\ast} \cos((n-j)\Delta\theta) = \frac{1}{2\Delta N} \cos\left(\Delta\theta\left(\frac{1}{2} + j_s - n\right)\right) \frac{\sin(\Delta N\Delta\theta)}{\sin(\frac{\Delta\theta}{2})},
\]

(51)
\[ \varphi_5(\theta_1, \theta_2) = \frac{1}{2\Delta N} \sum_{j=j_s-\Delta N+1}^{j_s+\Delta N} \cos \left( \frac{2j+1(\theta_1 + \theta_2)}{2} - \frac{2n+1(\theta_1 - \theta_2)}{2} \right) = \]

\[ = \frac{1}{2\Delta N} \cos \left( \frac{3}{2} j_s + n \right) + \varphi_2 \left( \frac{3}{2} j_s + n \right) \sin \left( \frac{(\theta_1 + \theta_2)\Delta N}{\sin \left( \frac{\theta_1 + \theta_2}{2} \right)} \right), \]

\[ \varphi_6(\theta_1, \theta_2) = \frac{1}{2\Delta N} \sum_{j=j_s-\Delta N+1}^{j_s+\Delta N} \cos \left[ \frac{2n+1(\theta_1 + \theta_2)}{2} - \frac{2j+1(\theta_1 - \theta_2)}{2} \right] = \]

\[ = \frac{1}{2\Delta N} \cos \left( \frac{3}{2} j_s + n \right) + \varphi_2 \left( \frac{3}{2} j_s + n \right) \sin \left( \frac{(\theta_1 + \theta_2)\Delta N}{\sin \left( \frac{\theta_1 + \theta_2}{2} \right)} \right), \]

\[ \varphi_7(\theta_1, \theta_2) = \frac{1}{2\Delta N} \sum_{j=j_s-\Delta N+1}^{j_s+\Delta N} \cos \left[ \frac{2n+1(\theta_1 + \theta_2)}{2} + \frac{2j+1(\theta_1 - \theta_2)}{2} \right] = \]

\[ = \frac{1}{2\Delta N} \cos \left( \frac{3}{2} j_s + n \right) + \varphi_2 \left( \frac{3}{2} j_s + n \right) \sin \left( \frac{(\theta_1 + \theta_2)\Delta N}{\sin \left( \frac{\theta_1 + \theta_2}{2} \right)} \right), \quad \Delta \theta = \theta_1 - \theta_2. \]

We rewrite the components \( \varphi_2, \varphi_4, \varphi_7, \varphi_8 \), containing the difference of wave numbers \( \Delta \theta \) as follows:

\[ \varphi_2 = \frac{\Delta \theta}{2} \left[ \frac{\cos \frac{3\Delta \theta}{2}}{\sin \frac{\Delta \theta}{2}} \left( \cos ((n + j_s)\Delta \theta) \right) - \frac{3\Delta \theta}{\sin \frac{\Delta \theta}{2}} \left( \sin ((n + j_s)\Delta \theta) \right) \right] \frac{\sin (\Delta N\Delta \theta)}{\sin \left( \frac{\Delta \theta}{2} \right)}, \]

\[ \sin(x) = \frac{\sin x}{x}, \]

\[ \varphi_4 = \frac{\Delta \theta}{2} \left[ \cot \frac{\Delta \theta}{2} \cos ((n - j_s)\Delta \theta) + \sin ((n - j_s)\Delta \theta) \right] \frac{\sin (\Delta N\Delta \theta)}{\sin \left( \frac{\Delta \theta}{2} \right)}, \]

\[ \varphi_7 = \frac{\Delta \theta}{2} \left[ \cos \frac{3\Delta \theta}{2} \cos (\Delta \theta(n + j_s) - \theta_1(2n + 1) - \frac{3\Delta \theta}{\sin \frac{\Delta \theta}{2}} \sin (\Delta \theta(n + j_s) - \theta_1(2n + 1)) \right] \frac{\sin (\Delta N\Delta \theta)}{\sin \left( \frac{\Delta \theta}{2} \right)}, \]

\[ \varphi_8 = \frac{\Delta \theta}{2} \left[ \cot \frac{\Delta \theta}{2} \cos (\theta_1(2n + 1) - \Delta \theta(n - j_s)) + \sin (\theta_1(2n + 1) - \Delta \theta(n - j_s)) \right] \frac{\sin (\Delta N\Delta \theta)}{\sin \left( \frac{\Delta \theta}{2} \right)}. \]

The formula (52) can be simplified due to our assumptions about continualization. At \( \Delta N \gg 1 \), the function \( \sin(x) \) is equal to 1 if \( \Delta \theta \) is zero and fast tends to zero if \( \Delta \theta \) is not equal to zero. Therefore, the main contribution, to the function \( g_{\theta_1}^{s}(\Delta N) \) comes from two close
wavenumbers $\theta_1, \theta_2$. Therefore, in the limit cases of $\Delta \theta \to 0$ and $\Delta N \gg 1$, we have

$$
\varphi_2 = \cos ((n + j_s) \Delta \theta) \operatorname{sinc}(\Delta N \Delta \theta) + O \left( \frac{1}{\Delta N} \right),
$$
$$
\varphi_4 = \cos ((n - j_s) \Delta \theta) \operatorname{sinc}(\Delta N \Delta \theta) + O \left( \frac{1}{\Delta N} \right),
$$
$$
\varphi_7 = \cos (\theta_1 (2n + 1) - (n + j_s) \Delta \theta) \operatorname{sinc}(\Delta N \Delta \theta) + O \left( \frac{1}{\Delta N} \right),
$$
$$
\varphi_8 = \cos (\theta_1 (2n + 1) - (n - j_s) \Delta \theta) \operatorname{sinc}(\Delta N \Delta \theta) + O \left( \frac{1}{\Delta N} \right),
$$
$$\varphi_1 = \varphi_3 = \varphi_5 = \varphi_6 = O \left( \frac{1}{\Delta N} \right). \tag{53}
$$

The difference $\omega(\theta_1) - \omega(\theta_2)$ can be decomposed into series:

$$
\omega(\theta_1) - \omega(\theta_2) \approx \omega'(\theta_1) \Delta \theta. \tag{54}
$$

Substitution of (53), (54) to (51) with dropping out of the terms of order $O \left( \frac{1}{\Delta N} \right)$ gives the formula (17).

B Derivation of formulas for wave-packets in the limit of mesoscale

We show that approximation of expressions for wave packets in (18) in the limit case ($\Delta N \gg 1$) approaches us to the Fourier transform of the $\operatorname{sinc}$ function.

Indeed,

$$
\frac{1}{2\pi a} \int_{-\pi}^{\pi+\pi} \cos (q\Xi) \operatorname{sinc}(q \Delta N) dq = \frac{1}{2\pi a \Delta N} \int_{(\pi-\pi)\Delta N}^{(\pi+\pi)\Delta N} \cos \left( \frac{q \Xi}{\Delta N} \right) \operatorname{sinc} q dq 
\approx \frac{1}{2\pi a \Delta N} \int_{-\infty}^{\infty} \cos \left( \frac{q \Xi}{\Delta N} \right) \operatorname{sinc} q dq = \operatorname{Re} \left( \frac{1}{2\pi a \Delta N} \int_{-\infty}^{\infty} e^{i \frac{q \Xi}{\Delta N}} \operatorname{sinc} q dq \right). \tag{55}
$$

Analogously,

$$
\frac{1}{2\pi a} \int_{-\pi}^{\pi} \sin (q\Xi) \operatorname{sinc}(q \Delta N) dq \approx \operatorname{Im} \left( \frac{1}{2\pi a \Delta N} \int_{-\infty}^{\infty} e^{\frac{i q \Xi}{\Delta N}} \operatorname{sinc} q dq \right). \tag{56}
$$

Since (see e.g. [46], chapter 1.)

$$
\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i \xi q} \operatorname{sinc} q dq = \frac{1}{2} H \left( 1 - |\xi| \right), \tag{57}
$$

then one gets

$$
\frac{1}{2\pi a \Delta N} \int_{-\infty}^{\infty} \cos \left( \frac{q \Xi}{\Delta N} \right) \operatorname{sinc} q dq = \frac{1}{2a \Delta N} H \left( 1 - \frac{|\Xi|}{\Delta N} \right), \tag{58}
$$
$$
\frac{1}{2\pi a \Delta N} \int_{-\infty}^{\infty} \sin \left( \frac{q \Xi}{\Delta N} \right) \operatorname{sinc} q dq = 0.
$$
References

[1] Rickert, W., Vilchevskaya, E.N., Müller, W.H. A note on Couette flow of micropolar fluids according to Eringen's theory Vol. 7, No. 1, 25–50 (2019)

[2] Rieder, Z., Lebowitz, J.L., Lieb, E. Properties of a harmonic crystal in a stationary nonequilibrium state. Journal of Mathematical Physics, Vol. 8, 1073 (1967)

[3] Lepri, S., Livi, R., Politi, A.: Thermal conduction in classical low-dimensional lattices. Phys. Rep. 377, 1 (2003)

[4] Dhar A., Heat transport in low-dimensional systems. Advances in Physics, pp. 457-537, (2008)

[5] Chang, C.W. Thermal transport in low dimensions. In: Lecture Notes in Physics, vol. 921, pp. 305–338 (2016)

[6] Huberman, S., Duncan, R.A., Chen, K., Song, B., Chiloyan, V., Ding, Z., Maznev, A.A., Chen, G., Nelson, K.A.: Observation of second sound in graphite at temperatures above 100 K. Science (2019)

[7] Johnson, J.A., Maznev, A.A., Cuffe, J., Eliason, J.K., Minnich, A.J., Kehoe, T., Sotomayor, Torres, C.M., Chen, G., Nelson, K.A.: Direct measurement of room-temperature nondiffusive thermal transport over micron distances in a silicon membrane. Phys. Rev. Lett. 110, 025901 (2013)

[8] Anufriev, R., Gluchko, S. Volz, S. Nomura, M. Quasi-ballistic heat conduction due to Levy phonon flights in silicon nanowires. Mesoscale and Nanoscale Physics (2018)

[9] Chang, C.W., Okawa, D., Garcia, H., Majumdar, A., Zettl, A.: Breakdown of Fouriers law in nanotube thermal conductors. Phys. Rev. Lett. 101, 075903 (2008)

[10] Xu, X., Wang Yu, Zhang, K et al. Length-dependent thermal conductivity in suspended single-layer graphene. Nature Communications (2014)

[11] Dwivedi, N., Ott, A.K., Sasikumar K., Dou, C., Yeo, R.J., Naranyanam, B., e t c. Graphene Overcoats for Ultra-High Storage Density Magnetic Media (2019)

[12] Majumdar, A. Microscale Heat Conduction in Dielectric Thin Films, J. Heat Transfer, 115(1): 7-16 (1993)

[13] Cahill, D.G., Ford, W.K., Goodson, K.E., Mahan, G.D., Majumdar, A., Maris, H.J., Merlin, R., Phillpot, S.R.: Nanoscale thermal transport. J. Appl. Phys. 93, 793 (2003)

[14] Spohn, H.: The phonon Boltzmann equation, properties and link to weakly anharmonic lattice dynamics. J. Stat. Phys. 124(2–4), 1041–1104 (2006)

[15] Kuzkin, V.A., Krivtsov, A.M. Unsteady ballistic heat transport: linking lattice dynamics and kinetic theory. ActaMechanica (2021)

[16] Klein, G., Prigogine, I. Sur la mecanique statistique des phenomenes irreversibles III. Physica, Vol. 19, 1053 (1953)

[17] Schrödinger, E. Zur dynamik elastisch gekoppelter punktsysteme. Annalen der Physik, Vol. 44, p. 916, (1914)
[18] Sokolov, A.A., Müller, W.H., Porubov, A.V., Gavrilov, S.N. Heat conduction in 1D harmonic crystal: Discrete and continuum approaches. International Journal of Heat and Mass Transfer, Vol. 176, 121442 (2021)

[19] Gavrilov, S.N. Discrete and continuum fundamental solutions describing heat conduction in a 1D harmonic crystal: Discrete-to-continuum limit and slow-and-fast motions decoupling, International Journal of Heat and Mass Transfer 194, 123019 (2022)

[20] Krivtsov, A.M. Heat transfer in infinite harmonic one dimensional crystals. Dokl. Phys. 60(9), 407 (2015)

[21] Northrop G.A. and Wolfe J.P. Phonon Imaging: Theory and Applications. Nonequilibrium Phonon Dynamics pp. 165-242 (1985)

[22] Wolfe, J.P. Imaging phonons. Acoustic wave propagation in solids. Cambridge University Press (1998)

[23] Gudimenko, A.I. Heat flow in a one-dimensional semi-infinite harmonic lattice with an absorbing boundary. Dal’nevost. Mat. Zh., 20, 1, pp.38–51 (2020) (in Russian)

[24] Hemmer, P.C. Dynamic and stochastic types of motion in the linear chain. Norges tekniske hoiskole, Trondheim, (1959)

[25] Takizawa, E, Kobayasi, K. On the Stochastic Types of Motion in a System of Linear Harmonic Oscillators. Chinese Journal of Physics, Vol. 6, No.1, 39-66 (1968)

[26] Mandel’shtam, L.I. Polnoe Sobranie Trudov (Complete Collected Works) (Ed. S M Rytov) Vol. 1 (Moscow: Izd. AN SSSR, 1948) (in Russian)

[27] Gavrilov, S.N., Krivtsov, A.M., Tsvetkov, D.V.: Heat transfer in a one-dimensional harmonic crystal in a viscous environment subjected to an external heat supply. Cont. Mech. Thermodyn. 31(1), 255–272 (2019)

[28] Kuzkin, V.A. Unsteady ballistic heat transport in harmonic crystals with polyatomic unit cell. Continuum Mechanics and Thermodynamics, 26 p. (2019)

[29] Krivtsov, A.,M. Energy Oscillations in a One-Dimensional Crystal. Doklady Physics. 2014, Vol. 59, No. 9, pp. 427–430

[30] Krivtsov, A.M. and Kuzkin, V.A. Encyclopedia of Continuum Mechanics, edited by H. Altenbach and A. Öchsner (Springer, Berlin, 2018)

[31] Casas-Vázquez, J., Jou, D. Temperature in nonequilibrium states: a review of open problems and current proposals, Rep. Prog. Phys. 66, pp. 1937–2023 (2003)

[32] Gelfand, I., Shilov, G.: Generalized Functions. Properties and Operations, vol. 1. Academic Press, New York (1964)

[33] Fedoryuk, M.V.: The stationary phase method and pseudodifferential operators. Russ.Math. Surv. 6(1), 65–115 (1971) (in Russian)

[34] Candy, J and Rozmus, W. A symplectic integration algorithm for separable Hamiltonian functions, J. Comput. Phys. 92, 230 (1991)

[35] McLachlan, R.I. and Atela, P. The accuracy of symplectic integrators, Nonlinearity 5, 541 (1992)
[36] Erdelyi, A. Asymptotic expansions. Courier Corporation, (1956)

[37] Fedoryuk, M. The Saddle-Point Method. Nauka, Moscow, (1977) (in Russian)

[38] Kuzkin, V.A., Krivtsov, A.M. Ballistic resonance and thermalization in Fermi-Pasta-Ulam-Tsingou chain at finite temperature, Phys. Rev. E, 101, 042209 (2020)

[39] Ivanova, E.A. Modeling of thermal and electrical conductivities by means of a viscoelastic Cosserat continuum, CMAT, 34, 555–586 (2022)

[40] Kapitza, P.L. The Study of Heat Transfer in Helium II, J. Phys. USSR 4, 181 (1941)

[41] Gendelman, O.V. and Paul, J. Kapitza thermal resistance in linear and nonlinear chain models: Isotopic Defect, Phys. Rev. E 103, 052113 (2021)

[42] Gendelman, O.V. and Paul, J. Kapitza resistance at a domain boundary in linear and nonlinear chains, Phys. Rev. E 104, 054119 (2021)

[43] Shishkina, E.V., Gavrilov, S.N. ArXiv 2206.08079

[44] Korznikova, E.A., Kuzkin, V.A., Krivtsov, A.M., Daxing Xiong, Vakhid A. Gani, Kudreyko, A.A., Dmitriev, S.V. Equilibration of sinusoidal modulation of temperature in linear and nonlinear chains, Phys. Rev. E 102, 062148 (2020)

[45] Liazhkov, S.D., Kuzkin, V.A. Unsteady two-temperature heat transport in mass-in-mass chains, Phys. Rev. E 105, 054145 (2022)

[46] Ango, A. Mathematics for Electro- and Radio Engineers. Nauka, Moscow (1965).