# The Ballistic Heat Equation for a One-Dimensional Harmonic Crystal


**Anton Krivtsov**

**Abstract** The analytical model of unsteady ballistic heat transfer in a one-dimensional harmonic crystal is analyzed. A nonlocal temperature is introduced as a generalization of the kinetic temperature. A closed equation determining unsteady thermal processes in terms of the nonlocal temperature is derived. For an instantaneous heat perturbation a time-reversible equation for the kinetic temperature is derived and solved. This equation can be referred as the ballistic heat conduction equation, it is somewhat similar to the hyperbolic heat conduction equation, but it has important differences. The resulting constitutive law for the heat flux in the considered system is obtained. This law significantly differs from Fourier's law and it predicts a finite velocity of the heat front and independence of the heat flux on the crystal length. The analytical results are confirmed by computer simulations. Further developments of the presented approach are referred.

## 1 Introduction

An understanding of heat transfer at microlevel is essential to obtain link between microscopic and macroscopic description of solids [1–3]. As far as macroscopic scale level is concerned the Fourier law of heat conduction is widely and successfully used to describe heat transfer processes. At microscopic level, however, analytical and numerical investigations have shown substantial deviations from Fourier's law [4–6]. These inadequacies can be on principle addressed by using special laws of particles interactions [7–10] or complex enough structures [11, 12]. Recent experimental data however showed that Fourier's law is indeed violated in low-dimensional [13–15].

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The main reason is that at microlevel the ballistic heat transfer dominates, in contrast to macrolevel, where the diffusive (Fourier) heat conduction prevails. This motivates interest to the simplest lattice models, in particular harmonic one-dimensional crystals (chains), where the anomalies connected with the ballistic heat transfer are most prominent [1, 16, 17]. Problems of this kind previously have been mainly addressed in the context of the steady-state heat conduction [4–6, 17, 18]. The present work focuses on unsteady conduction regimes [12, 19–22].

Here we describe an approach that allows rigorous derivation of macroscopic heat conduction equations and corresponding anomalous heat conduction law for harmonic systems in a one-dimensional, non-quantum case. This approach for the simplest one-dimensional crystal was first presented in [23], below we show these results in more details. The obtained equations differ substantially from the earlier suggested heat transfer equations [24, 25], however they are in excellent agreement with molecular dynamics simulations and previous analytical estimations [20].

## 2 The System

We consider a one-dimensional crystal, described by the following equation of motion:

$$\ddot{u}_i = \omega_e^2(u_{i-1} - 2u_i + u_{i+1}) \tag{1}$$

where $u_i$ is the displacement, $i$ is the number of the particle, $\omega_e \stackrel{\text{def}}{=} \sqrt{C/m}$ is the elementary frequency, $m$ is the particle mass, $C$ is the stiffness of the interparticle bond, dot is the time derivative. The crystal is infinite: the index $i$ is an arbitrary integer. The initial conditions are

$$u_i|_{t=0} = 0\,, \qquad \dot{u}_i|_{t=0} = \sigma(x)\rho_i\,, \tag{2}$$

where $\rho_i$ are independent random values with zero expectation and unit variance; $\sigma^2(x)$ is variance of the initial velocities, which is a slowly varying function of the spatial coordinate $x = ia$, where $a$ is the lattice constant. These initial conditions correspond to an instantaneous temperature perturbation, which can be induced in crystals, for example, by an ultrashort laser pulse [26, 27]. The displacements as functions of time $u_i = u_i(t)$ can be found as a solution of the Cauchy problem (1)–(2). These functions are random—they depend linearly on the integration constants, which are linear functions of the random values $\rho_i$ (2).

## 3 Nonlocal Temperature

The first analytical solution of a steady heat conduction problem for a harmonic chain was obtained in [18] using a covariance matrix for coordinates and momenta. Then this approach was extended and applied to various harmonic systems [4, 11, 16, 17]. Study of the covariance matrix allowed obtaining analytical expressions for steady [28] and unsteady [29, 30] temperature profiles. Here a somewhat similar approach based on analysis of covariances for velocities [23, 31, 32] is used. Following [33] the *nonlocal temperature* $\theta_{ij}$ is defined as

$$k_B\theta_{ij} \stackrel{\text{def}}{=} m\langle \dot{u}_i \dot{u}_j \rangle, \tag{3}$$

where $k_B$ is the Boltzmann constant, angle brackets stand for mathematical expectation, $\langle \dot{u}_i \dot{u}_j \rangle$ is the velocity covariance (note that $\langle \dot{u}_i \rangle \equiv \langle \dot{u}_j \rangle \equiv 0$). Then differentiation of (3) with the use of the dynamics equation (1) allows to obtain the following closed differential-difference equation of the fourth order [31]

$$\ddddot{\theta}_{ij} - 2(\mathscr{L}_i + \mathscr{L}_j)\ddot{\theta}_{ij} + (\mathscr{L}_i - \mathscr{L}_j)^2\theta_{ij} = 0, \tag{4}$$

where $\mathscr{L}_i$ is the linear difference operator: $\mathscr{L}_i u_i \stackrel{\text{def}}{=} \omega_e^2(u_{i-1} - 2u_i + u_{i+1})$. Equation (4) is an exact one, it describes processes of two types: fast transition to the local equilibrium [32] and slow heat transfer process [23]. For continuum description of the heat transfer the nonlocal temperature is redefined as

$$(-1)^n\,\theta_n(x) \stackrel{\text{def}}{=} \theta_{ij}\,, \qquad n \stackrel{\text{def}}{=} j - i\,, \qquad x = \frac{i+j}{2}a, \tag{5}$$

where $n$ is the covariance index, $x$ is the macroscopic spatial coordinate. If $n = 0$ then $i = j$ and quantity $\theta_n$ coincides with the kinetic temperature $T$:

$$k_B\theta_0(x) = k_B T(x) = m\langle \dot{u}_i^2 \rangle, \tag{6}$$

where $i = x/a$. According to its definition, the nonlocal temperature reflects a nonlocal nature of thermal processes in harmonic crystals and can be considered as a generalization of the kinetic temperature.

To obtain the simplified equation for description of the heat transfer only, the following two approximations are used.

1. **Continualization**. The nonlocal temperature $\theta_n(x)$ is a slowly varying function of the spatial coordinate $x$ (on the distances of order of the lattice constant $a$). This allows replacing the finite differences by the spatial derivatives [34]. The approximation is adequate for processes that are sufficiently smooth in space, e.g. for spatial temperature profiles in a form of waves that are much longer then the lattice constant $a$.

2. **Slow process approximation**. This approximation allows to neglect the term with the fourth time-derivative in Eq. (4) resulting in the second order differential equation with respect to time. Alternatively the second order equation can be obtained [23] using the virial approximation [2]: time or spatial derivatives of mathematical expectations are small with respect to quantities that have non-zero values in thermodynamic equilibrium. This approximation is adequate for processes that are not too far from thermodynamic equilibrium. In particular, the virial approximation allows to express covariances of the bond strains in terms of the nonlocal temperature.

Then the following second order differential-difference equation can be obtained from Eq. (4):

$$\ddot{\theta}_n + \tfrac{1}{4}c^2(\theta_{n-1} - 2\theta_n + \theta_{n+1})'' = 0, \tag{7}$$

where $c = \omega_e a$ is the speed of sound. This is a closed equation describing unsteady thermal processes in the crystal in terms of the nonlocal temperature. The processes under consideration should be such that the nonlocal temperature is sufficiently smooth in time and space. Apart from this limitation any unsteady thermal processes in the considered system satisfy equation (7). This equation in its current form appeared for the first time in [33], its derivation can be found in [23] (in different designations) or in [35] (for more complex problem). After solution (analytical or numerical) of Eq. (7) the kinetic temperature can be obtained as $T(t, x) = \theta_n(t, x)|_{n=0}$.

The initial conditions for Eq. (7) corresponding to the original initial conditions (2) are:

$$\theta_n|_{t=0} = T_0(x)\delta_n\,, \qquad \dot{\theta}_n|_{t=0} = 0, \tag{8}$$

where $T_0(x) = \frac{1}{2k_B}m\sigma^2(x)$ is the initial temperature distribution; $\delta_n = 1$ for $n = 0$, otherwise $\delta_n = 0$. The initial conditions (8) are taken after a fast transition process, which results, according to the virial theorem, in a double reduction of the initial kinetic temperature [32]. Note that in contrast with the random initial value problem (1)–(2), the initial value problem (7)–(8) is expressed in terms of mathematical expectations, and therefore it is a deterministic problem.

## 4 The Ballistic Heat Equation

Using an integral Fourier transform in the spatial coordinate $x$ the problem (7)–(8) can be solved analytically. For the Fourier image $\hat{\theta}_n(t, k)$ we obtain

$$\begin{aligned} \ddot{\hat{\theta}}_n &= \tfrac{1}{4}c^2k^2(\hat{\theta}_{n-1} - 2\hat{\theta}_n + \hat{\theta}_{n+1}), \\ \hat{\theta}_n|_{t=0} &= \hat{T}_0(k)\delta_n\,, \qquad \dot{\hat{\theta}}_n|_{t=0} = 0, \end{aligned} \tag{9}$$

where $k$ is the spatial frequency, $\hat{T}_0(k)$ is the Fourier image of the initial temperature distribution $T_0(x)$. Let us note the similarity between (1)–(2) and (9): initial value problem (9) can be interpreted as a motion of a harmonic chain having an initial shift of the central particle. This kind of problems can be effectively solved in terms of Bessel functions. In particular, Bessel functions were successfully applied to solution of shock-wave problems in harmonic chains [36, 37]. Similarly, the problem (9) has an analytical solution $\hat{\theta}_n(t,k) = \hat{T}_0(k) J_{2n}(ckt)$, where $J_{2n}$ are the Bessel functions of the 1st kind [38]. From the practical point of view the most interesting case is $n = 0$, which gives Fourier image $\hat{T}(t,k)$ of the kinetic temperature distribution:

$$\hat{T}(t,k) = \hat{T}_0(k) J_0(ckt). \tag{10}$$

From (10) it follows that the image $\hat{T}(t,k)$ satisfies the Bessel differential equation

$$\ddot{\hat{T}} + \frac{1}{t}\dot{\hat{T}} = -c^2 k^2 \hat{T}. \tag{11}$$

Fourier inversion of (11) gives a partial differential equation for the temperature field

$$\ddot{T} + \frac{1}{t}\dot{T} = c^2 T'', \tag{12}$$

which can be referred as the ballistic heat equation. The corresponding initial conditions follow from (8):

$$T|_{t=0} = T_0(x)\,, \qquad \dot{T}|_{t=0} = 0. \tag{13}$$

The obtained equation (12) is a particular case of the Darboux differential equation [39]. For description of the heat transfer in the harmonic one-dimensional crystal it was originally derived in [23]. Later it was proved that the same equation describes the ballistic heat transfer if the crystal is supported by an elastic foundation [40]. The ballistic heat equation describes the evolution of the temperature field after an instantaneous thermal perturbation happened at $t = 0$, that is why this equation can be used only with initial conditions (13). The condition $\dot{T}|_{t=0}$ means absence of the heat flux in the initial state. For more complex situation the general equation for nonlocal temperatures (7) should be used.

Fourier inversion of the representation (10) gives an analytical solution of the initial value problem (12)–(13):

$$T(t,x) = \frac{1}{\pi}\int_{-1}^{1} \frac{T_0(x - cts)}{\sqrt{1 - s^2}}\, ds. \tag{14}$$

Similar integral representation without obtaining equation (12) was derived in [41] using heat energy density correlation functions. Substitution $s = \cos\varphi$ gives an alternative integral form

$$T(t,x) = \frac{1}{\pi}\int_0^{\pi} T_0(x + ct\cos\varphi)\,\mathrm{d}\varphi. \tag{15}$$

The physical meaning of this representation is that $ct\cos\varphi$ is the group velocity of Eq. (1), where $\varphi$ is a half of the wave number. Representation (15) can be interpreted as superposition of the classical wave equation solutions for all wave numbers. Further investigations have shown that the similar rule is fulfilled for much more general harmonic systems [42, 43].

Thus, an evolution of the temperature field in a one-dimensional crystal after an instantaneous thermal perturbation is described by partial differential equation (12) with initial conditions (13) or by integral formulas (14)–(15). According to (14) the thermal front propagates with the sound speed $c$ (in contrast to the thermal conductivity based on Fourier's law where an unphysical instantaneous signal propagation is realized). The obtained wave behavior of the heat front is similar to predictions of the wave theories of heat conduction [24, 25]. However, the obtained solution has important differences, which will be shown in the text to follow.

## 5 Heat Flux

For the considered system the heat flux can be represented [5, 6, 44] as

$$q = \tfrac{1}{2}C\langle(u_i - u_{i+1})(\dot{u}_i + \dot{u}_{i+1})\rangle. \tag{16}$$

The heat flux $q$ satisfies the energy balance equation

$$\rho k_B \dot{T} = -q', \tag{17}$$

where $\rho = 1/a$ is the density (number of particles per unit volume), $k_B\dot{T}$ stands for the heat energy for the considered system. Joint consideration of Eqs. (12) and (17) gives the constitutive law for the heat flux

$$\dot{q} + \frac{1}{t}q = -k_B c^2 \rho T', \tag{18}$$

which replaces Fourier's law in the considered system. Alternatively, the law (18) can be derived directly, in the same way as the ballistic heat conduction Eq. (12) is derived. Integral representations for the heat flux follows from (14) and (18):

$$q(t,x) = \frac{k_B c\rho}{\pi}\int_{-1}^{1} \frac{T_0(x - cts)}{\sqrt{1-s^2}}\,sds. \tag{19}$$

The alternative representation corresponding to (15) is

$$q(t,x) = \frac{k_B c\rho}{\pi} \int_0^\pi T_0(x + ct\cos\varphi)\cos\varphi \, \mathrm{d}\varphi. \tag{20}$$

## 6 Comparison of Different Equations Describing the Heat Conduction

Let us consider three models of heat conduction: the classic heat equation based on Fourier's law of heat conduction; the hyperbolic heat equation (thermal wave equation) based on the Maxwell-Cattaneo-Vernotte law [24, 25]; the obtained above ballistic heat equation (12). Brief comparison of these models is given in Table 1. The hyperbolic heat equation and Eq. (12) have similar form and somewhat similar behavior (e.g. a finite velocity of the heat front propagation). However, there are significant differences:

1. The main difference is that $\tau$, a material constant, is replaced in (12) by the physical time $t$. Consequently, these equations are close for intermediate tomes $t \approx \tau$, however they are substantially different for small and large times. Moreover, for $t \to 0$, from the first glance, the ballistic equation (12) has singularity. However, same as for the hyperbolic equation, the solution of this equation does not have any time singularity, which can be easily seen from formula (15). For $t \to \infty$ the asymptotics of the hyperbolic and ballistic equations are different: exponential and power decay respectively—see Table 1(b).
2. The ballistic heat equation, as opposite to the hyperbolic and Fourier equations, is not time-invariant—it changes with substitution $t$ by $t + t_0$. This is because it describes reaction of the system on the instantaneous thermal perturbation at

**Table 1** (a) Heat transfer equation, (b) equation connecting heat flux and temperature, (c) decay law for the sinusoidal heat perturbation. Notations: $t$ is time (variable), $\tau$ is the relaxation time (constant), $\beta$ is the thermal diffusivity, $\kappa$ is the thermal conductivity, $c$ is the sound speed, $\rho$ is the density, $k_B$ is the Boltzmann constant, $k$ is the spatial frequency. Approximation (c) for the hyperbolic heat equation is obtained for $c^2 = \beta/\tau$ and large $k$; approximation for $J_0$ is valid for relatively large $t$

| | Fourier heat equation | Hyperbolic heat equation | Ballistic heat equation |
|---|---|---|---|
| (a) | $\dot{T} = \beta T''$ | $\ddot{T} + \frac{1}{\tau}\dot{T} = \frac{\beta}{\tau}T''$ | $\ddot{T} + \frac{1}{t}\dot{T} = c^2 T''$ |
| (b) | $q = -\kappa T'$ | $\dot{q} + \frac{1}{\tau}q = -\frac{\kappa}{\tau}T'$ | $\dot{q} + \frac{1}{t}q = -k_B c^2 \rho T'$ |
| (c) | $e^{-\beta k^2 t}$ | $\approx e^{-\frac{t}{2\tau}}\cos(kct)$ | $J_0(kct) \approx \frac{\cos(kct - \frac{\pi}{4})}{\sqrt{\frac{\pi}{2}kct}}$ |

$t = 0$, the general situation is described by more general Eq. (7), which is time-invariant.

3. The ballistic heat equation is time-reversible: it does not change with substitution $t$ by $-t$. Same fulfils for the original dynamical equation (1) and the general equation for nonlocal temperatures (7). On contrary, the Fourier and hyperbolic heat equations are not time-reversible. The contradiction between time-reversibility of the classical microscopic equations and irreversibility of the corresponding macroscopic continuum equations is one of the opened questions of the modern physics [2, 45]. The obtained reversible macroscopic equation of the ballistic heat conduction may be a step towards solution of this problem. In particular, it will be shown below that this equation describes irreversible processes, such as decay of the sinusoidal heat perturbation—see Fig. 1. Thus reversible equations can produce irreversible solutions, even in a finite domain.

## 7 Sinusoidal Temperature Perturbation

We consider now a sinusoidal temperature perturbation

$$T_0(x) = A_0 \sin kx + B, \tag{21}$$

where $A_0$ and $B$ are temperature constants, $k = 2\pi/\lambda$ is the spatial frequency, $\lambda$ is the wavelength of the perturbation. These initial conditions provide simple and informative testing of thermal transfer in closed systems [12, 23, 46]. This is especially important for the ballistic heat transfer analysis, because in this case any external heat supply can substantially affect the thermal processes [47, 48]. Formulas (14) and (19) give an exact analytical solution for the temperature and heat flux

$$\begin{aligned} T(t,x) &= A_0 J_0(kct) \sin kx + B, \\ q(t,x) &= -k_B c \rho A_0 J_1(kct) \cos kx, \end{aligned} \tag{22}$$

where $J_0$ and $J_1$ are the Bessel functions of the 1st kind. This solution was obtained in [23]. Previously, without obtaining equation (12), an existence of a Bessel function solution for the sinusoidal temperature distribution in the one-dimensional harmonic crystal was mentioned in [20], and solution similar to (22) for the temperature field was obtained in Master-degree thesis [49].

To justify the assumptions in derivation of the analytical solution we compare it with results of molecular dynamics (MD) simulations. Equation (1) is solved by the central differences method, the time step is $0.01\tau_0$, where $\tau_0 = 2\pi/\omega_e$. The initial conditions (21) are set by a random number generator, the wavelength $\lambda$ is equal to the length of the chain containing $10^4$ particles. To provide correspondence with the analytical approach used above, $10^4$ realizations of such chain with an independent random initiation are computed. To optimize the computations all chains are joined at end-points to form a long chain ($10^8$ particles) with periodic boundary conditions.

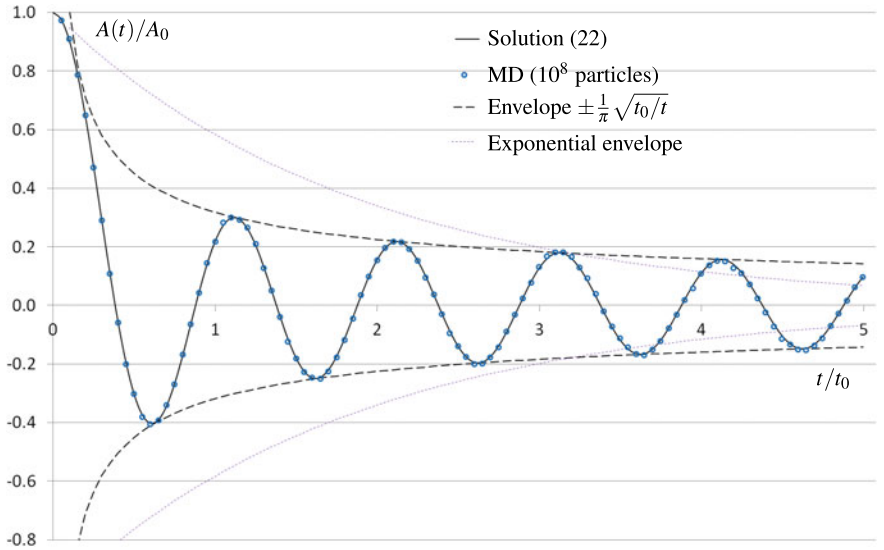


**Fig. 1** Oscillational decay of the thermal perturbation amplitude for 1D harmonic crystal. Comparison of the analytical solution (22) with the MD modeling results ($10^4$ joined chains containing $10^4$ particles each). Dashed lines show the envelope proportional to $1/\sqrt{t}$ and also an exponential envelope inherent to the hyperbolic heat equation

The results of the computations are compared with analytical solution (22) in Fig. 1. The horizontal axis in Fig. 1 represents the dimensionless time $t/t_0$, where $t_0 = \lambda/c$; the vertical axis stands for the oscillation amplitude $A(t)$, which is computed as the first coefficient of a spatial Fourier expansion of the temperature field. According to Fig. 1 there is an excellent agreement between the computational results and the analytical curve.

Due to the Bessel function properties [38], the temperature and heat flux (22) have an oscillational decay, where the oscillation amplitude is asymptotically proportional to $1/\sqrt{t}$. The same asymptotics has been obtained in [20] for one-dimensional harmonic crystals. In Fig. 1 the envelope proportional to $1/\sqrt{t}$ is shown by the dashed lines, perfectly bounding both analytical and computational graphs. The existing theories of heat conduction [24, 25], such as Fourier's, Maxwell-Cattaneo-Vernotte (MCV), dual-phase-lag [50], and spacetime-elasticity [21] yield linear differential equations with constant coefficients, and therefore all of them predict an exponential decay of the sinusoidal perturbation amplitude. In Table 1 a comparison of the analytically obtained decay law for $A(t)/A_0$ with the results based on some other theories is demonstrated, an exponential envelope inherent to the thermal wave model is also shown in Fig. 1. Thus, among the mentioned theories only the current one gives an analytical solution, which agrees with the MD simulations and asymptotic estimations of the oscillation decay for harmonic chains [20].

## 8 Stepwise Temperature Perturbation

Let us consider now a stepwise initial temperature distribution, modeling heat transfer between a hot and a cold body:

$$x < 0: \quad T(x) = T_2\,, \qquad x > 0: \quad T(x) = T_1, \tag{23}$$

where $T_2 > T_1$. In this case the integral representations (14), (19) yield for $|x| \le ct$ an exact analytical solution

$$\begin{aligned} T(t,x) &= T_1 + \tfrac{\Delta T}{\pi} \arccos \tfrac{x}{ct}, \\ q(t,x) &= \tfrac{k_B c \rho \Delta T}{\pi} \sqrt{1 - \left(\tfrac{x}{ct}\right)^2}, \end{aligned} \tag{24}$$

where $\Delta T = T_2 - T_1$; for $x > ct$ the original temperature distribution remains and the heat flux is zero. According to (24) the heat front propagates with the sound speed $c$ and the heat flux through cross-section $x = 0$ is constant and equal to $\frac{1}{\pi} k_B c \rho \Delta T$. In contrast, use of Fourier's law for the same problem gives the heat flux proportional to $t^{-1/2}$, which is infinite at $t = 0$ (an unphysical consequence of Fourier's law). Thus the heat flux $\frac{1}{\pi} k_B c \rho \Delta T$ is provided by the temperature difference that is realized on the spatial interval $x \in [-ct, ct]$ with increasing length of $2ct$. Consequently, the heat flux depends on the temperature difference rather than on the temperature gradient. This is in qualitative agreement with the known phenomenon of thermal superconductivity: the heat flux through a one-dimensional harmonic crystal placed between two thermal reservoirs does not depend on the length of the crystal [6, 18]. The same value $\frac{1}{\pi} k_B c \rho \Delta T$ was obtained in [51] as a steady-state limit of the heat flux for large $t$.

In Fig. 2 the analytical solution (24) is compared with computer simulations for $T_2 = 2T_1$. The above described computation procedure is used. Figure 2 shows the initial temperature distribution, the analytical solution, and the computation results obtained at $t = t_0/8$ using $10^6$ and $10^8$ particles ($t_0 = L/c$, where $L$ is the chain length; only half of the chain is shown in the figure). Convergence to the analytical solution with the increase of the system size is clearly seen.

Figure 3 shows a part of Fig. 2 corresponding to positive $x$. For symmetry reasons this case can be interpreted as a problem of a half-space heating: the initial temperature for $x > 0$ is $T_1$ and the boundary condition at $x = 0$ is $T = (T_2 + T_1)/2 > T_1$. The advantage of this formulation is that the constant boundary temperature is maintained without any thermostat. This is important since the heat transfer can substantially depend on the thermostat properties [47, 48]. Solutions of the considered problem using four different continuum equations are compared in Fig. 3 with the simulation results. Parameters are chosen in such a way that the total heat quantity transferred through the cross-section $x = 0$ (area under each curve) is equal for all models and the heat front (when it exists) propagates with the sound speed $c$. According to Fig. 3 the computation results almost coincide with the analytical solution of Eq. (12) and significantly differ from the solutions based on the other theories of

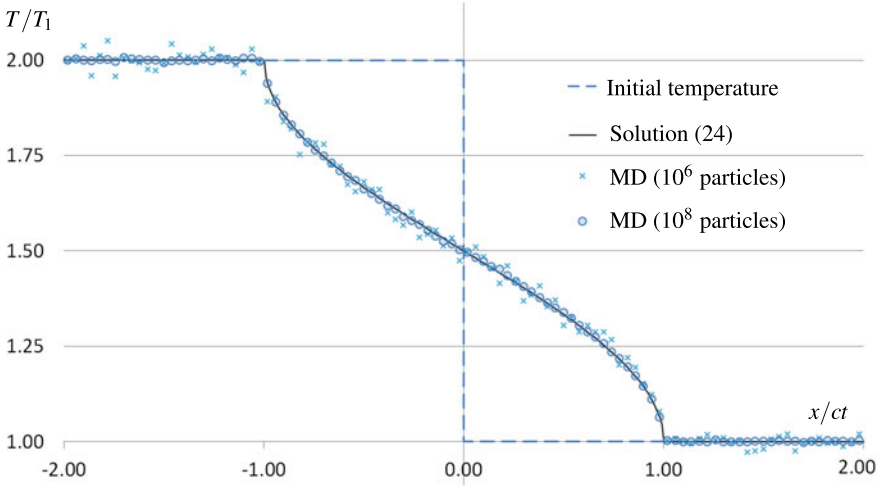


**Fig. 2** Heat transfer between hot (left) and cold (right) areas of 1D harmonic crystal. The analytical solution (24) is compared with the computer simulation (MD): $10^3$ chains containing $10^3$ particles each (cross is an average over 10 particles); $10^4$ chains containing $10^4$ particles (circle is an average over 100 particles)

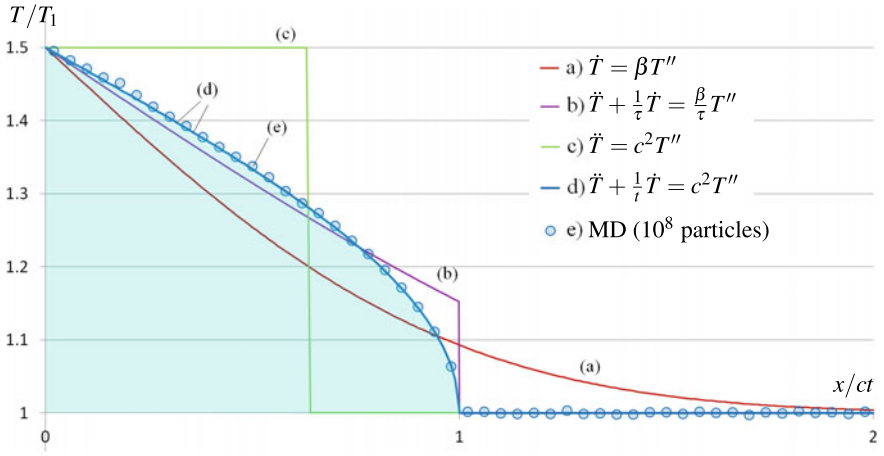


**Fig. 3** Heat propagation for different 1D models: **a** Fourier heat equation, **b** hyperbolic heat equation, **c** wave equation, **d** ballistic heat equation, **e** computer simulation for 1D harmonic crystal ($10^4$ chains containing $10^4$ particles each)

thermal conduction. Indeed, the Fourier heat equation predicts no heat front, the hyperbolic heat equation gives a stepwise front, while the real heat front is described by a smooth curve having a vertical tangent at $x = ct$. Note that the hyperbolic heat equation behaves as the wave equation at small times and as the Fourier heat equation at large times [52]. However, according to the analytical solution (24) and the

presented computer simulations, the heat transfer in a one-dimensional harmonic crystal is self-similar, i.e. $T = T(\frac{x}{ct})$, so it demonstrates same behavior for any times.

## 9 Conclusions and Further Research

An approach for description of the ballistic heat transfer in one-dimensional harmonic crystals is described. A notion of nonlocal temperature (a generalization of the kinetic temperature for two separate particles) is used for obtaining a closed system of equations for the thermal transfer description. For the case of an instantaneous heat perturbation this yields to a partial differential equation (12) for the kinetic temperature, which can be referred to as the ballistic heat equation. The resulting macroscopic constitutive law (18) (an alternative of Fourier's law for the considered system) predicts a finite velocity of the heat front and independence of the heat flux on the crystal length. The analytical findings are in excellent agreement with the molecular dynamics simulations and previous analytical estimations.

Further analysis of the ballistic heat equation (12) can be found in [53]. Application of the presented approach for more complex one-dimensional systems is given in [40], where a substrate potential is added, and in [35], where an external heat supply and a viscous environment are considered. Extension of this approach to systems of higher dimensions is presented in [42] for monoatomic and in [43] for polyatomic lattices. The presented approach in frames of the general approach for transition from discrete to continuum thermomechanics is outlined in [54]. The results of the referred investigations are relevant to aspects of nanotechnology that involve heat transfer processes in high purity nanostructures [13, 14, 55, 56].

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