

# ORIGINAL ARTICLE

S. N. Gavrilov · A. M. Krivtsov · D. V. Tsvetkov

# Heat transfer in a one-dimensional harmonic crystal in a viscous environment subjected to an external heat supply

Received: 29 November 2017 / Accepted: 8 May 2018

© Springer-Verlag GmbH Germany, part of Springer Nature 2018

Abstract We consider unsteady heat transfer in a one-dimensional harmonic crystal surrounded by a viscous environment and subjected to an external heat supply. The basic equations for the crystal particles are stated in the form of a system of stochastic differential equations. We perform a continualization procedure and derive an infinite set of linear partial differential equations for covariance variables. An exact analytic solution describing unsteady ballistic heat transfer in the crystal is obtained. It is shown that the stationary spatial profile of the kinetic temperature caused by a point source of heat supply of constant intensity is described by the Macdonald function of zero order. A comparison with the results obtained in the framework of the classical heat equation is presented. We expect that the results obtained in the paper can be verified by experiments with laser excitation of low-dimensional nanostructures.

**Keywords** Ballistic heat transfer · Harmonic crystal · Kinetic temperature

## 1 Introduction

An understanding of heat transfer at the microlevel is essential to obtain a link between the microscopic and the macroscopic descriptions of solids. As far as the macroscopic level is concerned, Fourier's law of heat conduction is widely and successfully used to describe heat transfer processes. However, it is well known that for one-dimensional crystals substantial deviations from Fourier's law are observed [1–5]. Extensive investigations over the last decades were devoted to resolving these anomalies, and many of the recent developments in this area are reviewed in book [6]. One of the possible solutions is to use special laws of particle interactions

Communicated by Andreas Öchsner.

This work is supported by Russian Science Foundation (Grant No. 18-11-00201).

S. N. Gavrilov (⋈) · A. M. Krivtsov

Institute for Problems in Mechanical Engineering RAS, V.O., Bolshoy pr. 61, St. Petersburg, Russia 199178

S. N. Gavrilov

E-mail: serge@pdmi.ras.ru

A. M. Krivtsov

E-mail: akrivtsov@bk.ru

S. N. Gavrilov · A. M. Krivtsov · D. V. Tsvetkov Peter the Great St. Petersburg Polytechnic University, Polytechnicheskaya str. 29, St. Petersburg, Russia 195251

D. V. Tsvetkov

E-mail: DVTsvetkov@ya.ru

Published online: 21 May 2018

[7–11], in particular, systems on a nonlinear elastic support with no momentum conservation [8], or systems possessing the possibility of bond break [9–11]. Such systems under certain conditions demonstrate normal heat conductivity even in one dimension. As it is shown in [12], one-dimensional case is still very specific; therefore, another way to avoid anomalies is to use sufficiently complex structures and increase the system dimensionality [13,14]. However, recent experimental observations demonstrate that Fourier's law is indeed violated in low-dimensional nanostructures [15–20], where the ballistic heat transfer is realized. This fact is in agreement with the phonon theory [21,22], which relates the heat conductivity with the phonon mean free path. At the macroscale, the phonon mean free path is a small quantity in comparison with the characteristic size of the system, but this is not true for microscale and nanoscale systems [23]. This motivates the interest in the simplest lattice models, in particular, in harmonic one-dimensional crystals (chains), where these anomalies are most prominent [24,25]. Problems of this type were previously addressed mainly in the context of steady-state heat conduction [1–5,26–35], and unsteady conduction regimes came into the focus in [14,36–44].

Simple lattice models can be used for the analytical investigation of the thermomechanical processes in solids at the microscale [40,45–48], and, in particular, in the carbon nanostructures [49,50]. One-dimensional systems due to their simplicity can be used to obtain analytical solutions in a closed form without loss of generality [5,41,46,51], or to get the asymptotic description of non-stationary processes in media with complex structure [51–56]. In previous studies [43,44,57], a new approach was suggested which allows one to solve analytically non-stationary thermal problems for a one-dimensional harmonic crystal—an infinite ordered chain of identical material particles, interacting via linear (harmonic) forces. In particular, a heat transfer equation was obtained that differ from the extended heat transfer equations suggested earlier [58–61]; however, it is in an excellent agreement with molecular dynamics simulations and previous analytical estimates [36]. Later, this approach was generalized to a number of systems, namely to a one-dimensional crystal on an elastic substrate [42], and to two- and three-dimensional harmonic crystals [62,63]. In most of above-mentioned papers [42– 44,62,63], only isolated systems were considered. The motivation for this paper is to consider a system that can exchange energy with its surroundings. Therefore, now we assume that the crystal is surrounded by a viscous environment (a gas or a liquid) which causes an additional dissipative term in the equations of stochastic dynamics for the particles. Additionally, we take into account sources of heat supply. This is a more realistic model, and thus, we expect that the theoretical results obtained in the paper can be verified by experiments with laser excitation of low-dimensional nanostructures [18–20,64].

The paper is organized as follows. In Sect. 2, we consider the formulation of the problem. In Sect. 2.1, some general notation is introduced. In Sect. 2.2, we state the basic equations for the crystal particles in the form of a system of stochastic differential equations. In Sect. 2.3, we introduce and deal with infinite set of covariance variables. These are the mutual covariances of the particle velocities and the displacements for all pairs of particles. We use the Itô lemma to derive (see "Appendix A") an infinite deterministic system of ordinary differential equations which follows from the equations of stochastic dynamics. This system can be transformed into an infinite system of differential-difference equations involving only the covariances for the particle velocities. In Sect. 3, we introduce a continuous spatial variable and write the finite difference operators involved in the equation for covariances as compositions of finite difference operators and operators of differentiation. To do this, we use some identities of the calculus of finite differences (see "Appendix B"). In Sect. 4, we perform an asymptotic uncoupling of the equation for covariances. Provided that the introduced continuous spatial variable can characterize the behavior of the crystal, one can distinguish between slow motions, which are related to the heat propagation, and vanishing fast motions [42,44], which are not considered in the paper. Slow motions can be described by a coupled infinite system of second-order hyperbolic partial differential equations for quantities which we call the non-local temperatures. The zero-order non-local temperature, which is proportional to the statistical dispersion of the particle velocities, is the classical kinetic temperature. In Sect. 5, we obtain an expression for the fundamental solution for the kinetic temperature and solve the non-stationary problem of the heat propagation from a suddenly applied point source of constant intensity. In contrast to the case of a crystal without viscous environment (Sect. 5.1), in the case of a crystal surrounded by a viscous environment (Sect. 5.2) there exists a steady-state solution describing the kinetic temperature distribution caused by a constant point source. In Sect. 6, we present the results of the numerical solution of the initial value problem for the system of stochastic differential equations and compare them with the obtained analytical solution. In Sect. 7, we compare our results with the classical results obtained in the framework of the heat equation based on Fourier's law. In the conclusion (Sect. 8), we discuss the basic results of the paper.

#### 2 Mathematical formulation

#### 2.1 Notation

In the paper, we use the following general notation:

t the time:

 $H(\cdot)$  the Heaviside function;

 $\delta(\cdot)$  the Dirac delta function;

 $\langle \cdot \rangle$  the expected value for a random quantity;

 $\delta_{pq}$  the Kronecker delta ( $\delta_{pq}=1$  if p=q, and  $\delta_{pq}=0$  otherwise);  $\delta_n$   $\delta_n=1$  if n=0 and  $\delta_n=0$  otherwise;

 $J_0(\cdot)$  the Bessel function of the first kind of zero order [65];

 $I_0(\cdot)$  the modified Bessel function of the first kind of zero order [65];

 $K_0(\cdot)$  the Macdonald function (the modified Bessel function of the second kind) of zero order [65];

 $erfc(\cdot)$  the complementary error function [65].

## 2.2 Stochastic crystal dynamics

Consider the following system of stochastic ordinary differential equations [66,67]:

$$dv_i = F_i dt + b_i dW_i, \qquad du_i = v_i dt, \tag{2.1}$$

where

$$F_i = \omega_0^2 \mathcal{L}_i u_i - \eta v_i, \tag{2.2}$$

$$dW_i = \rho_i \sqrt{dt}, \tag{2.3}$$

$$\omega_0 \stackrel{\text{def}}{=} \sqrt{C/m}.\tag{2.4}$$

Here i is an arbitrary integer which describes the position of a particle in the chain; the stochastic processes  $u_i(t)$  and  $v_i(t)$  are the displacement and the particle velocity, respectively;  $F_i$  is the force on the particle;  $W_i$ are Wiener processes;  $b_i(t)$  is the intensity of the random external excitation;  $\eta$  is the specific viscosity for the environment; C is the bond stiffness; m is the mass of a particle;  $\mathcal{L}_i$  is the linear finite difference operator:

$$\mathcal{L}_i u_i = u_{i+1} - 2u_i + u_{i-1}. \tag{2.5}$$

Note that the results of the paper can be generalized for more complex finite difference operators and related physical systems (e.g., a crystal on an elastic support, next neighbor interactions).

The normal random variables  $\rho_i$  are such that

$$\langle \rho_i \rangle = 0, \quad \langle \rho_i \rho_i \rangle = \delta_{ii},$$
 (2.6)

and they are assumed to be independent of  $u_i$  and  $v_i$ . The initial conditions are zero: for all i,

$$u_i(0) = 0, v_i(0) = 0.$$
 (2.7)

In the case  $b_i \equiv b$ , Eq. (2.1) are the Langevin equations [68,69] for a one-dimensional harmonic crystal (an ordered chain of identical interacting material particles, see Fig. 1) surrounded by a viscous environment (e.g., a gas or a liquid). Assuming that  $b_i$  may depend on i, we introduce a natural generalization of the Langevin equation which allows one to describe the possibility of an external heat excitation (e.g., laser excitation). This external excitation is assumed to be localized in space (in the paper we mostly consider the case of a point heat source) and much more intensive than the stochastic influence caused by a nonzero temperature of the environment. Therefore, we neglect in (2.1) the constant stochastic term that does not depend on i. Note that since  $b_i$  does not depend on  $u_i$  and  $v_i$  for all i, j, it is not necessary to distinguish between the Stratonovich and Itô formalism [66] in the case of Eq. (2.1).



Fig. 1 A one-dimensional harmonic crystal

## 2.3 The dynamics of covariances

According to (2.2),  $F_i$  are linear functions of  $u_i$ ,  $v_i$ . Taking this fact into account together with (2.6) and (2.7), we see that for all t

$$\langle u_i \rangle = 0, \quad \langle v_i \rangle = 0.$$
 (2.8)

Following [70], consider the infinite sets of covariance variables

$$\xi_{p,q} \stackrel{\text{def}}{=} \langle u_p u_q \rangle, \quad v_{p,q} \stackrel{\text{def}}{=} \langle u_p v_q \rangle, \quad \kappa_{p,q} \stackrel{\text{def}}{=} \langle v_p v_q \rangle,$$
 (2.9)

and the quantities

$$\beta_{p,q} \stackrel{\text{def}}{=} \delta_{pq} \, b_p b_q. \tag{2.10}$$

In the last equation, we take into account the second equation of (2.6). Thus, the variables  $\xi_{p,q}$ ,  $v_{p,q}$ ,  $\kappa_{p,q}$  and  $\beta_{p,q}$  are defined for any pair of crystal particles. For simplicity, in what follows we drop the subscripts p and q, i.e.,  $\xi \stackrel{\text{def}}{=} \xi_{p,q}$ . By definition, we also put  $\xi^{\top} \stackrel{\text{def}}{=} \xi_{q,p}$ , etc. Now we differentiate the variables (2.9) with respect to time taking into account the equations of motion (2.1). This yields the following closed system of differential equations for the covariances (see "Appendix A"):

$$\partial_t \xi = \nu + \nu^\top,$$

$$\partial_t \nu + \eta \nu = \omega_0^2 \mathcal{L}_q \xi + \kappa,$$

$$\partial_t \kappa + 2\eta \kappa = \omega_0^2 \mathcal{L}_p \nu + \omega_0^2 \mathcal{L}_q \nu^\top + \beta,$$
(2.11)

where  $\partial_t$  is the operator of differentiation with respect to time;  $\mathcal{L}_p$  and  $\mathcal{L}_q$  are the linear difference operators defined by (2.5) that act on  $\xi_{p,q}$ ,  $\nu_{p,q}$ ,  $\kappa_{p,q}$ ,  $\beta_{p,q}$  with respect to the first index subscript p and the second one q, respectively. Now we introduce the symmetric and antisymmetric difference operators

$$2\mathcal{L}^{S} \stackrel{\text{def}}{=} \mathcal{L}_{p} + \mathcal{L}_{q}, \qquad 2\mathcal{L}^{A} \stackrel{\text{def}}{=} \mathcal{L}_{p} - \mathcal{L}_{q}, \tag{2.12}$$

and the symmetric and antisymmetric parts of the variable  $\nu$ :

$$2\nu^{S} \stackrel{\text{def}}{=} \nu + \nu^{\top}, \qquad 2\nu^{A} \stackrel{\text{def}}{=} \nu - \nu^{\top}.$$
 (2.13)

Note that  $\xi$  and  $\kappa$  are symmetric variables. Now equations (2.11) can be rewritten as follows:

$$\partial_t \xi = 2\nu^{\mathrm{S}}, \quad (\partial_t + 2\eta)\kappa = 2\omega_0^2 \mathcal{L}^{\mathrm{S}} \nu^{\mathrm{S}} + 2\omega_0^2 \mathcal{L}^{\mathrm{A}} \nu^{\mathrm{A}} + \beta,$$
 (2.14)

$$(\partial_t + \eta)\nu^{A} = -\omega_0^2 \mathcal{L}^{A} \xi, \qquad (\partial_t + \eta)\nu^{S} = \omega_0^2 \mathcal{L}^{S} \xi + \kappa. \tag{2.15}$$

Applying the operator  $\partial_t + \eta$  to Eq. (2.14) and substituting expressions (2.15) yield a closed system of two equations of second order in time:

$$\partial_t(\partial_t + \eta)\xi = 2(\omega_0^2 \mathcal{L}^{S} \xi + \kappa), \tag{2.16}$$

$$(\partial_t + \eta)(\partial_t + 2\eta)\kappa = 2((\omega_0^2 \mathcal{L}^S)^2 - (\omega_0^2 \mathcal{L}^A)^2)\xi + 2\omega_0^2 \mathcal{L}^S \kappa + (\partial_t + \eta)\beta.$$
 (2.17)

We can express  $\kappa$  in terms of  $\xi$  using Eq. (2.16):

$$\kappa = \frac{1}{2} (\partial_t^2 + \eta \partial_t - 2\omega_0^2 \mathcal{L}^S) \xi, \tag{2.18}$$

and substitute the result into Eq. (2.17). This yields

$$\frac{1}{2} \Big( \Big( (\partial_t + \eta)(\partial_t + 2\eta) - 2\omega_0^2 \mathcal{L}^{\mathbf{S}} \Big) (\partial_t^2 + \eta \partial_t - 2\omega_0^2 \mathcal{L}^{\mathbf{S}}) - 4 \Big( (\omega_0^2 \mathcal{L}^{\mathbf{S}})^2 - (\omega_0^2 \mathcal{L}^{\mathbf{A}})^2 \Big) \xi$$

$$= (\partial_t + \eta)\beta. \tag{2.19}$$

Simplifying the left-hand side of Eq. (2.19) results in an equation of fourth order in time for  $\xi$ :

$$\left( (\partial_t + \eta)^2 (\partial_t^2 + 2\eta \partial_t - 4\omega_0^2 \mathcal{L}^{S}) + 4(\omega_0^2 \mathcal{L}^{A})^2 \right) \xi = 2(\partial_t + \eta)\beta. \tag{2.20}$$

Now we apply the operator  $\frac{1}{2}(\partial_t^2 + \eta \partial_t - 2\omega_0^2 \mathcal{L}^S)$  to Eq. (2.20). Taking into account (2.18), this yields a fourth-order equation for the covariances of the particle velocities  $\kappa$ :

$$((\partial_t + \eta)^2(\partial_t^2 + 2\eta\partial_t - 4\omega_0^2 \mathcal{L}^S) + 4(\omega_0^2 \mathcal{L}^A)^2)\kappa = (\partial_t + \eta)(\partial_t^2 + \eta\partial_t - 2\omega_0^2 \mathcal{L}^S)\beta.$$
 (2.21)

In what follows, we deal with Eq. (2.21). According to Eqs. (2.7), (2.9), we supplement Eq. (2.21) with zero initial conditions. We state these conditions in the following form, which is conventional for distributions (or generalized functions) [71]:

$$\kappa \big|_{t<0} \equiv 0. \tag{2.22}$$

To take into account nonzero classical initial conditions, one needs to add the corresponding singular terms (in the form of a linear combination of  $\delta(t)$  and its derivatives) to the right-hand sides of the corresponding equations [71].

Let us note that Eq. (2.21) is a deterministic equation. What is also important is that (2.21) is a closed equation. Thus, the thermal processes do not depend on any property of the cumulative distribution functions for the displacements and the particle velocities other than the covariance variables used above.

# 3 Continualization of the finite difference operators

In this section, we use some identities of the calculus of finite differences (see "Appendix B"). Following [43,70], we introduce the discrete spatial variable

$$k \stackrel{\text{def}}{=} p + q \tag{3.1}$$

and the discrete correlational variable

$$n \stackrel{\text{def}}{=} q - p \tag{3.2}$$

instead of discrete variables p and q. We can also formally introduce the continuous spatial variable

$$x \stackrel{\text{def}}{=} \frac{ak}{2},\tag{3.3}$$

where a is the lattice constant (the distance between neighboring particles). We have

$$q = \frac{x}{a} + \frac{n}{2}, \qquad p = \frac{x}{a} - \frac{n}{2}.$$
 (3.4)

To perform the continualization, we assume that the lattice constant is an infinitesimal quantity and introduce a dimensionless formal small parameter  $\epsilon$  in the following way:

$$a = \epsilon \hat{a},\tag{3.5}$$

where  $\hat{a} = O(1)$ . To preserve the speed of sound in the crystal  $c \stackrel{\text{def}}{=} a\omega_0$  as a quantity of order O(1), we additionally assume that

$$\omega_0 = \epsilon^{-1} \hat{\omega}_0, \tag{3.6}$$

where  $\hat{\omega}_0 = O(1)$ . Thus,  $c = \hat{a}\hat{\omega}_0 = O(1)$ . The basic assumption that allows one to perform the continualization is that any quantity  $\zeta_{p,q}$  defined by (2.9) or (2.10), where p and q are defined by (3.4), can be calculated as a value of a smooth function  $\zeta_n(x)$  of the continuous spatial slowly varying coordinate

$$x = \epsilon \hat{a}k \tag{3.7}$$

and the discrete correlational variable n:

$$\hat{\zeta}_n(x) \stackrel{\text{def}}{=} \zeta_{k+\frac{n}{2}, k-\frac{n}{2}} = \zeta_{p,q}. \tag{3.8}$$

In accordance with (3.8), one has

$$\mathcal{L}_{p}\zeta_{p,q} = \hat{\zeta}_{n-1}\left(x + \frac{a}{2}\right) - 2\hat{\zeta}_{n}(x) + \hat{\zeta}_{n+1}\left(x - \frac{a}{2}\right),$$

$$\mathcal{L}_{q}\zeta_{p,q} = \hat{\zeta}_{n+1}\left(x + \frac{a}{2}\right) - 2\hat{\zeta}_{n}(x) + \hat{\zeta}_{n-1}\left(x - \frac{a}{2}\right).$$
(3.9)

Applying the Taylor theorem to these formulas yields

$$\mathcal{L}_{p}\zeta_{p,q} = \mathcal{L}_{n}\hat{\zeta}_{n} + \frac{a}{2} \partial_{x}(\hat{\zeta}_{n-1} - \hat{\zeta}_{n+1}) + \frac{a^{2}}{8} \partial_{x}(\hat{\zeta}_{n-1} + \hat{\zeta}_{n+1}) + o(\epsilon^{2}), \mathcal{L}_{q}\zeta_{p,q} = \mathcal{L}_{n}\hat{\zeta}_{n} + \frac{a}{2} \partial_{x}(\hat{\zeta}_{n+1} - \hat{\zeta}_{n-1}) + \frac{a^{2}}{8} \partial_{x}(\hat{\zeta}_{n+1} + \hat{\zeta}_{n-1}) + o(\epsilon^{2}).$$
(3.10)

An alternative way of continualization can be realized by letting the number of particles diverge, rather than invoking an increasingly small separation [72]. Despite the algorithmic difference, these approaches lead to the same result.

Now we perform the continualization of the operators  $\mathcal{L}^{S}$ ,  $\mathcal{L}^{A}$ . Using (3.10), we obtain

$$\mathcal{L}^{S} = \mathcal{L}_{n} + O(\epsilon^{2}), \tag{3.11}$$

$$\mathcal{L}^{A} = -\frac{a}{2} \mathcal{D}_{n} \partial_{x} + O(\epsilon^{2}), \tag{3.12}$$

$$\mathcal{L}^{A} = -\frac{a}{2} \, \mathcal{D}_n \partial_x + O(\epsilon^2), \tag{3.12}$$

where

$$\mathcal{D}_n f_n = f_{n+1} - f_{n-1}. \tag{3.13}$$

Now we calculate  $(\mathcal{L}^{A})^{2}$  using (3.12), (B.6), (B.10). This yields

$$(\mathcal{L}^{\mathcal{A}})^2 = a^2 \mathcal{M} + o(\epsilon^2), \tag{3.14}$$

$$\mathcal{M} \stackrel{\text{def}}{=} -\frac{1}{4} \mathcal{L}_n (-1)^n \mathcal{L}_n (-1)^n \partial_x^2. \tag{3.15}$$

#### 4 Slow motions

Taking into account assumption (3.6), Eq. (2.21) can be rewritten in the following form:

$$\left( (\partial_t + \eta)^2 \left( \epsilon^2 (\partial_t^2 + \eta \partial_t) - 4 \hat{\omega}_0^2 \mathcal{L}^{\mathrm{S}} \right) + 4 \frac{\hat{\omega}_0^4}{\epsilon^2} (\mathcal{L}^{\mathrm{A}})^2 \right) \kappa 
= (\partial_t + \eta) \left( \epsilon^2 (\partial_t^2 + \eta \partial_t) - 2 \hat{\omega}_0^2 \mathcal{L}^{\mathrm{S}} \right) \beta.$$
(4.1)

Equation (4.1) is a differential equation whose highest derivative with respect to t is multiplied by a small parameter. Therefore, one can expect the existence of two types of solutions, namely solutions slowly varying in time and fast varying in time [73]. The presence of fast and slow motions is a standard property of statistical systems. Fast motions are oscillations of temperature caused by equilibration of kinetic and potential energies. Slow motions are related to macroscopic heat propagation.

Considering slow motions, we assume that

$$\epsilon^2 (\partial_t^2 + \eta \partial_t) \kappa \ll \hat{\omega}_0^2 \mathcal{L}^S \kappa, \qquad \epsilon^2 (\partial_t^2 + \eta \partial_t) \beta \ll \hat{\omega}_0^2 \mathcal{L}^S \beta.$$
(4.2)

Vanishing solutions that characterize fast motions, which do not satisfy (4.2), are not considered in this paper. In [44], the properties of fast motions are investigated in the case of the system under consideration without viscous environment ( $\eta = 0$ ) and external heating ( $\beta = 0$ ). In [42], fast motions in a one-dimensional harmonic crystal on an elastic substrate are considered (again under the zero external action condition).

Now, taking into account (3.14), we drop the higher-order terms and rewrite equation (4.1) in the form of an equation for slow motions:

$$2((\partial_t + \eta)^2 \mathcal{L}^S - c^2 \mathcal{M}) \kappa = (\partial_t + \eta) \mathcal{L}^S \beta.$$
(4.3)

Applying the operator  $(\mathcal{L}^{S})^{-1}$  to Eq. (4.3) results in

$$\ddot{\kappa} + 2\eta\dot{\kappa} + \left(\eta^2 - c^2(\mathcal{L}^{S})^{-1}\mathcal{M}\right)\kappa = \frac{1}{2}(\dot{\beta} + \eta\beta) + C,\tag{4.4}$$

where  $\mathcal{L}^S C \equiv 0$ . Here and in what follows we use more compact notation: the overdot means  $\partial_t$ , and the prime means  $\partial_x$ . Taking into account the initial conditions in the form of Eq. (2.22), one can show that C=0.

Now we perform the continualization of the equations. According to Eqs. (3.11), (3.14), (3.15), we have

$$(\mathcal{L}^{S})^{-1}\mathcal{M} = -\frac{1}{4}(-1)^{n}\mathcal{L}_{n}(-1)^{n}\partial_{x}^{2} + o(\epsilon^{2}).$$
(4.5)

Now we multiply (4.4) by  $(-1)^n m k_B^{-1}$  (here  $k_B$  is the Boltzmann constant) and rewrite Eq. (4.4) in the following form:

$$\ddot{\theta}_n + 2\eta\dot{\theta}_n + \eta^2\theta_n + \frac{c^2}{4}\mathcal{L}_n\theta_n'' = (\dot{\chi} + \eta\chi)\delta_n, \tag{4.6}$$

where, according to (3.8), we introduce the following quantities depending on the continual spatial variable x:

$$\theta_n(x,t) \stackrel{\text{def}}{=} (-1)^n m k_B^{-1} \hat{\kappa}_n(x,t), \tag{4.7}$$

$$\chi(x,t) \stackrel{\text{def}}{=} \frac{1}{2} m k_B^{-1} \hat{\beta}_0(x,t). \tag{4.8}$$

We call  $\theta_n$  the non-local temperatures and identify  $\chi$  as the heat supply intensity [note that  $\hat{\beta}_n \equiv 0$  for  $n \geq 1$  due to (2.10)]. Also, we identify  $T \stackrel{\text{def}}{=} \theta_n \big|_{n=0}$  as the kinetic temperature, since in the framework of the kinetic theory of gases expression (4.7) for  $\theta_0$  coincides with the expression for the temperature of an ideal gas consisting of particles with one degree of freedom. Now we recall the explicit form (2.5) for  $\mathcal{L}_n$  and rewrite Eq. (4.6) as the infinite system of partial differential equations

$$\ddot{\theta}_n + 2\eta \dot{\theta}_n + \eta^2 \theta_n + \frac{c^2}{4} (\theta_{n-1} - 2\theta_n + \theta_{n+1})'' = \phi(x, t) \delta_n, \tag{4.9}$$

$$\phi = \dot{\chi} + \eta \chi, \tag{4.10}$$

which describe the heat propagation in the crystal. The particular case of this equation for the case  $\eta = 0$ ,  $\chi \equiv 0$  was obtained previously in [74].

Note that Eq. (4.9) for slow motions involve only the product  $c = \omega_0 a$  and do not involve the quantities  $\omega_0$  and a separately, so they do not involve  $\epsilon$ . Provided that the initial conditions also do not involve  $\epsilon$ , the solution of the corresponding initial value problem and all its derivatives are quantities of order O(1). The rate of vanishing for fast motions depends on  $\epsilon$ : the smaller  $\epsilon$ , the higher the rate. Thus, for sufficiently small  $\epsilon$ , exact solutions of Eq. (2.21) quickly transform into slow motions.

## 5 Solution of the equations for slow motions

In what follows, we investigate the initial value problem for the system of partial differential equations (4.9) where the heat supply is given in the form of a point source

$$\chi = \bar{\chi}(t)\delta(x),\tag{5.1}$$

$$\bar{\chi}(t)\big|_{t<0} \equiv 0, \tag{5.2}$$

supplemented with zero initial conditions stated in the following form [see (2.22)]:

$$\theta_n(x,t)\big|_{t<0} \equiv 0. \tag{5.3}$$

## 5.1 The case $\eta = 0$

In this section, we consider a crystal without viscous environment and assume that  $\eta = 0$ . First, take  $\bar{\chi}(t) = \bar{\chi}_1 \delta(t)$ , where  $\bar{\chi}_1$  is a constant. This corresponds to the choice of heat supply in the form of a point pulse source. Thus, in accordance with Eq. (4.10),

$$\phi(x,t) = \bar{\chi}_1 \delta(x) \dot{\delta}(t). \tag{5.4}$$

Now we apply the discrete Fourier transform  $\mathcal{F}_n^y$  [75,76] with respect to the variable n to Eq. (4.9). This yields

$$\ddot{\theta}_{\mathcal{F}_n^y} - \mathcal{C}^2 \theta_{\mathcal{F}_n^y}'' = \bar{\chi}_1 \delta(x) \dot{\delta}(t), \tag{5.5}$$

where

$$\theta_{\mathcal{F}_n^y}(y, x, t) = \sum_n \theta_n \exp(-iny), \tag{5.6}$$

$$\mathcal{C} = c \left| \sin \frac{y}{2} \right|,\tag{5.7}$$

and y is the Fourier transform parameter. Here we have used the shift property [75,76] of the discrete Fourier transform:

$$\theta_{\mathcal{F}_{n+1}^{y}}(y,x,t) = \exp(\pm iy)\,\theta_{\mathcal{F}_{n}^{y}}(y,x,t). \tag{5.8}$$

Equation (5.5) is the inhomogeneous one-dimensional wave equation. Therefore, the solution can be written as the convolution of the right-hand side of (5.5) with the corresponding fundamental solution [71]:

$$\theta_{\mathcal{F}_n^y} = \bar{\chi}_1 \delta(x) \dot{\delta}(t) * \frac{1}{2\mathcal{C}} H(\mathcal{C}t - |x|) = \frac{\bar{\chi}_1}{2} \delta(\mathcal{C}t - |x|). \tag{5.9}$$

The inverse of  $\theta_{\mathcal{F}_0^y}$  (the kinetic temperature  $T = \theta_0$ ) can be expressed in the following form [75,76]:

$$\theta_0 = \frac{1}{2\pi} \int_{-\pi}^{\pi} \theta_{\mathcal{F}_n^y} \exp(iny) \, \mathrm{d}y \, \bigg|_{n=0} = \frac{\bar{\chi}_1}{4\pi} \int_{-\pi}^{\pi} \delta\left(ct \, \bigg| \sin\frac{y}{2} \, \bigg| - |x| \right) \mathrm{d}y. \tag{5.10}$$

To calculate the right-hand side of Eq. (5.10), one needs to use the formula (see [77])

$$\int_{I} \delta(f(y)) \, \mathrm{d}y = \sum_{i} \frac{1}{|f'(y_{i})|},\tag{5.11}$$

where  $y_i$  are the roots of f(y) lying inside the interval I. Taking

$$f(y) = ct \left| \sin \frac{y}{2} \right| - |x|, \tag{5.12}$$

one can find the corresponding roots

$$y_{1,2} = \pm 2 \arcsin \frac{|x|}{ct}, \quad ct \ge |x|.$$
 (5.13)

For ct < |x|, there are no roots. One has

$$f'(y_{1,2}) = \frac{ct}{2}\cos\frac{y_{1,2}}{2} = \frac{1}{2}\sqrt{c^2t^2 - x^2}.$$
 (5.14)

Applying (5.11), one gets

$$T = \bar{\chi}_1 \mathfrak{F}_1(x,t) \stackrel{\text{def}}{=} \frac{\bar{\chi}_1 H(ct - |x|)}{\pi \sqrt{c^2 t^2 - x^2}}.$$
 (5.15)

Formula (5.15) demonstrates that heat propagates at a finite speed c.

Now take  $\bar{\chi}(t) = \bar{\chi}_0 H(t)$ , where  $\bar{\chi}_0$  is a constant. This corresponds to the choice of heat supply in the form of a suddenly applied point source of constant intensity. Thus,

$$\phi(x,t) = \bar{\chi}_0 \delta(x) \delta(t), \tag{5.16}$$

in accordance with Eq. (4.10). In this case, an expression for the kinetic temperature can be obtained by integrating the right-hand side of Eq. (5.15) with respect to time:

$$T = \bar{\chi}_0 \mathfrak{F}_0 \stackrel{\text{def}}{=} \frac{\bar{\chi}_0}{\pi} \int_{|x|/c}^{t} \frac{d\tau}{\sqrt{c^2 \tau^2 - x^2}} = \frac{\bar{\chi}_0 H(ct - |x|)}{\pi c} \ln \frac{ct + \sqrt{c^2 t^2 - x^2}}{|x|}.$$
 (5.17)

The formula obtained agrees with previous results [57]. Note that for fixed  $x \neq 0$ , we have  $\mathfrak{F}_0 \propto \ln t$  ( $\mathfrak{F}_0$  is proportional to  $\ln t$ ) as  $t \to \infty$ . The solution  $\mathfrak{F}_0$  is self-similar. (It depends only on x/ct.)

The function  $\mathfrak{F}_0$  is the fundamental solution for the operator in the left-hand side of Eq. (4.9) (for n=0 and  $\eta=0$ ). The function  $\mathfrak{F}_1=\mathfrak{F}_0$  plays the role of the fundamental solution for the problem of the heat

propagation in a crystal without environment caused by a source of heat supply  $\chi(x, t)$ . The expressions for  $\mathfrak{F}_1$  were earlier obtained in [43,70,74] with a slightly different approach. Thus, in the case of an arbitrary function  $\chi(x,t)$ , the solution  $\theta_0$  of Eq. (4.10) that satisfies the zero initial condition in the form of Eq. (5.3) can be written as the convolution

$$\theta_0 = \chi * \mathfrak{F}_1 = \iint_{-\infty}^{\infty} \chi(\xi, \tau) \, \mathfrak{F}_1(x - \xi, t - \tau) \, \mathrm{d}\xi \, \mathrm{d}\tau$$

$$= \dot{\chi} * \mathfrak{F}_0 = \iint_{-\infty}^{\infty} \dot{\chi}(\xi, \tau) \, \mathfrak{F}_0(x - \xi, t - \tau) \, \mathrm{d}\xi \, \mathrm{d}\tau. \tag{5.18}$$

Here \* stands for the convolution of functions of two variables x and t. Using formulas (5.18) in practical applications, one should remember that the time derivative  $\dot{\chi}$  must be calculated in the sense of distributions (or generalized functions) [71]. Also note that the integration interval in (5.18) is in fact finite due to (5.2), (5.17).

#### 5.2 The case $\eta > 0$

In this section, we consider a crystal in a viscous environment and assume that  $\eta > 0$ . First, take  $\bar{\chi}(t) = \bar{\chi}_1 \delta(t)$ . This corresponds to the choice of heat supply in the form of a point pulse source. Thus,

$$\phi(x,t) = \phi_0 \stackrel{\text{def}}{=} \bar{\chi}_1 \delta(x) (\dot{\delta}(t) + \eta \delta(t)), \tag{5.19}$$

in accordance with Eq. (4.10). Applying the discrete Fourier transform  $\mathcal{F}_n^y$  with respect to the variable n to Eq. (4.9) and using the shift property (5.8) yield the following equation:

$$\ddot{\theta}_{\mathcal{F}_n^y} + 2\eta \dot{\theta}_{\mathcal{F}_n^y} - \mathcal{C}^2 \theta_{\mathcal{F}_n^y}'' + \eta^2 \theta_{\mathcal{F}_n^y} = \bar{\chi}_1 \delta(x) (\dot{\delta}(t) + \eta \delta(t)), \tag{5.20}$$

where the symbols  $\theta_{\mathcal{F}_n^y}(y, x, t)$  and  $\mathcal{C}$  are defined by Eqs. (5.6) and (5.7), respectively. The homogeneous equation that corresponds to Eq. (5.20) is a particular case of the telegraph equation

$$\ddot{W} + 2\eta \dot{W} - \mathcal{C}^2 W'' + \mathcal{B} W = 0. \tag{5.21}$$

The fundamental solution for the operator in the left-hand side of Eq. (5.21) is (see [78])

$$\Phi = \frac{e^{-\eta t} H(\mathcal{C}t - |x|) J_0(\sqrt{|\alpha|(t^2 - x^2/\mathcal{C}^2)})}{2\mathcal{C}}, \quad \alpha < 0,$$

$$\Phi = \frac{e^{-\eta t} H(\mathcal{C}t - |x|) I_0(\sqrt{|\alpha|(t^2 - x^2/\mathcal{C}^2)})}{2\mathcal{C}}, \quad \alpha > 0,$$
(5.22)

where  $\alpha \equiv \eta^2 - \mathcal{B}$ . The values of the coefficients in Eq. (5.20) correspond to the special limiting case of Eq. (5.21) where  $\alpha = 0$ , and the fundamental solution is given by the simple formula

$$\Phi = \frac{1}{2\mathcal{C}} \exp(-\eta t) H(\mathcal{C}t - |x|). \tag{5.23}$$

Calculating the convolution of the right-hand side of (5.19) with the fundamental solution (5.23) yields

$$\theta_{\mathcal{F}_n^y} = \bar{\chi}_1(\dot{\Phi} + \eta \Phi) = \frac{\bar{\chi}_1}{2} \exp(-\eta t) \delta(\mathcal{C}t - |x|); \tag{5.24}$$

therefore,

$$T = \theta_0 = \bar{\chi}_1 \mathfrak{F}_1^{\eta}(x, t) \stackrel{\text{def}}{=} \frac{\bar{\chi}_1 \exp(-\eta t)}{4\pi} \int_{-\pi}^{\pi} \delta\left(ct \left|\sin\frac{y}{2}\right| - |x|\right) dy$$
$$= \frac{\bar{\chi}_1 H(ct - |x|) \exp(-\eta t)}{\pi \sqrt{c^2 t^2 - x^2}}.$$
 (5.25)

The function  $\mathfrak{F}_1^{\eta}$  plays the role of the fundamental solution for the problem of the heat propagation in a crystal surrounded by a viscous environment caused by a source of heat supply  $\chi(x,t)$ .

Now take  $\bar{\chi}(t) = \bar{\chi}_0 H(t)$ . This corresponds to the choice of heat supply in the form of a suddenly applied point source of constant intensity. Thus,

$$\phi(x,t) = \phi_1 \stackrel{\text{def}}{=} \bar{\chi}_0 \delta(x) \left( \delta(t) + \eta H(t) \right), \tag{5.26}$$

in accordance with Eq. (4.10). Since  $\dot{\phi}_1 = \phi_0$ , the non-stationary solution can be obtained by integrating the right-hand side of Eq. (5.25) with respect to time:

$$T(x,t) = \frac{\bar{\chi}_0 H(ct - |x|)}{\pi} \int_{|x|/c}^t \frac{\exp(-\eta \tau)}{\sqrt{c^2 \tau^2 - x^2}} d\tau.$$
 (5.27)

In contrast to the case  $\eta = 0$ , for  $\eta > 0$  there exists a stationary solution which according to [79,80] can be expressed in a closed form:

$$T(x,\infty) = \frac{\bar{\chi}_0}{\pi} \int_{|x|/c}^{\infty} \frac{\exp(-\eta \tau)}{\sqrt{c^2 \tau^2 - x^2}} d\tau = \frac{\bar{\chi}_0}{\pi c} K_0 \left(\frac{\eta |x|}{c}\right). \tag{5.28}$$

Thus, the stationary spatial profile of the kinetic temperature caused by a point source of heat supply of constant intensity is described by the Macdonald function (the modified Bessel function of the second kind) of zero order.

It may be noted that, using the discrete Fourier transform, the steady-state solution (5.28) can be obtained as the solution  $\theta_0(x)$  of the problem for the static equations

$$\eta^{2}\theta_{n} + \frac{c^{2}}{4}(\theta_{n-1} - 2\theta_{n} + \theta_{n+1})'' = \eta \bar{\chi}_{0}\delta(x)\delta_{n}$$
(5.29)

that correspond to (4.9) with the boundary conditions at  $x \to \infty$ 

$$\theta_n(x) \to 0. \tag{5.30}$$

In the case of an arbitrary function  $\chi(x, t)$ , the solution  $\theta_0$  of Eq. (4.10) that satisfies the zero initial condition in the form of Eq. (5.3) can be written as the convolution of  $\chi$  with the fundamental solution  $\mathfrak{F}_1^{\eta}$  (5.25):

$$\theta_0 = \chi * \mathfrak{F}_1^{\eta} = \iint_{-\infty}^{\infty} \chi(\xi, \tau) \, \mathfrak{F}_1^{\eta}(x - \xi, t - \tau) \, \mathrm{d}\xi \, \mathrm{d}\tau. \tag{5.31}$$

Thus, we have obtained the analytical solution of the problem.

## 6 Numerics

In this section, we present the results of the numerical solution of the system of stochastic differential equations (2.1)–(2.3) with initial conditions (2.7). It is useful to rewrite Eqs. (2.1)–(2.3) in the dimensionless form

$$d\tilde{v}_i = (\mathcal{L}_i \tilde{u}_i - \eta \tilde{v}_i) d\tilde{t} + \tilde{b}_i \rho_i \sqrt{d\tilde{t}}, d\tilde{u}_i = \tilde{v}_i d\tilde{t},$$
(6.1)

where

$$\tilde{u} \stackrel{\text{def}}{=} \frac{u}{a}, \quad \tilde{v} \stackrel{\text{def}}{=} \frac{v}{c}, \quad \tilde{t} \stackrel{\text{def}}{=} \omega_0 t, \quad \tilde{b} \stackrel{\text{def}}{=} \frac{b}{c\sqrt{\omega_0}}, \quad \tilde{\eta} \stackrel{\text{def}}{=} \frac{\eta}{\omega_0}.$$
 (6.2)

We consider the chain of 2N + 1 particles and the periodic boundary conditions

$$u_{-N} = u_{N-1}, u_{-N+1} = u_N, v_{-N} = v_{N-1}, v_{-N+1} = v_N.$$
 (6.3)

To obtain a numerical solution in the case of the point source of the heat supply located at i=0, we assume that  $\tilde{b}_i \rho_i = \delta_{i0} \tilde{b} \rho_i$  and use the scheme

$$\Delta \tilde{v}_{i}^{j} = (\mathcal{L}_{i}\tilde{u}_{i}^{j} - \eta \tilde{v}_{i}^{j})\Delta \tilde{t} + \tilde{b}\delta_{i0}\rho^{j}\sqrt{\Delta \tilde{t}},$$

$$\Delta \tilde{u}_{i}^{j} = \tilde{v}_{i}^{j+1}\Delta \tilde{t},$$

$$\tilde{v}_{i}^{j+1} = \tilde{v}_{i}^{j} + \Delta \tilde{v}_{i}^{j},$$

$$\tilde{u}_{i}^{j+1} = \tilde{u}_{i}^{j} + \Delta \tilde{u}_{i}^{j},$$
(6.4)

where  $i = \overline{-N, N}$ . Here the symbols with superscript j denote the corresponding quantities at  $\tilde{t} = \tilde{t}^j \stackrel{\text{def}}{=} j \Delta \tilde{t}$ :  $\tilde{u}_i^j = \tilde{u}_i(\tilde{t}^j), \ \tilde{v}_i^j = \tilde{v}_i(\tilde{t}^j); \ \rho^j$  are normal random numbers that satisfy (2.6) generated for all  $\tilde{t}^j$ . Without loss of generality, we can take  $\tilde{b} = 1$ .

We perform a series of  $r = 1 \dots R$  realizations of these calculations (with various independent  $\rho_{(r)}^j$ ) and get the corresponding particle velocities  $v_{i(r)}^j$ . In accordance with (4.7), in order to obtain the dimensionless kinetic temperature

$$\tilde{T} = \frac{Tk_B}{mc^2},\tag{6.5}$$

we should average the doubled dimensionless kinetic energies:

$$\tilde{T}_i^j = \frac{1}{R} \sum_{r=1}^R (v_{i(r)}^j)^2. \tag{6.6}$$

Numerical results (6.6) for the kinetic temperature can be compared with the analytical unsteady solutions (5.27), (5.17) and steady-state solution (5.28) expressed in the dimensionless form:

$$\tilde{T}(\tilde{x}, \tilde{t}) = \frac{\tilde{b}^2 H(\tilde{t} - \tilde{x})}{2\pi} \int_{\tilde{x}}^{\tilde{t}} \frac{\exp(-\tilde{\eta}\tau)}{\sqrt{\tau^2 - \tilde{x}^2}} d\tau, \tag{6.7}$$

$$\tilde{T}(\tilde{x},\tilde{t})\big|_{\eta=0} = \frac{\tilde{b}^2 H(\tilde{t}-\tilde{x})}{2\pi} \ln \frac{\tilde{t}+\sqrt{\tilde{t}^2-\tilde{x}^2}}{|\tilde{x}|},\tag{6.8}$$

$$\tilde{T}(\tilde{x}, \infty) = \frac{\tilde{b}^2}{2\pi} K_0(\tilde{\eta}|\tilde{x}|), \tag{6.9}$$

where

$$\tilde{x} \stackrel{\text{def }}{=} \frac{x}{a} = i. \tag{6.10}$$

Note that the factor 1/2 in right-hand sides of Eqs. (6.7)–(6.9) appears according to Eq. (4.8).

A comparison between the analytical and numerical solutions is presented in Figs. 2, 3 and 4. Figure 2 corresponds to a crystal without viscous environment. Figure 3 corresponds to a crystal in a viscous environment in the case where  $\tilde{t}=70$  is small enough for the solution to be regarded as an unsteady one. Figure 4 corresponds to a crystal in a viscous environment in the case where  $\tilde{t}=500$  is large enough for the solution to be regarded as a steady-state one. All figures are presented for two numbers of realizations: (a) R=100 and (b) R=10,000. One can see that in all cases, for sufficiently large R=10,000 the analytical and numerical solutions are in a very good agreement.

## 7 Comparison with the Fourier thermal conductivity

Let us compare our results with the classical results obtained in the framework of the heat equation based on Fourier's law. Consider the case of the non-stationary temperature distribution caused by a suddenly applied point source of heat supply. For a crystal in an environment, the solution is given by formula (5.27). For large times, there exists a steady-state solution [see (5.28)], in contrast to the case  $\eta = 0$  of a crystal without environment, where the solution (5.17) of the same problem grows logarithmically. The dimensionless forms of solutions (5.27), (5.28), (5.17) are (6.7), (6.9), (6.8), respectively.

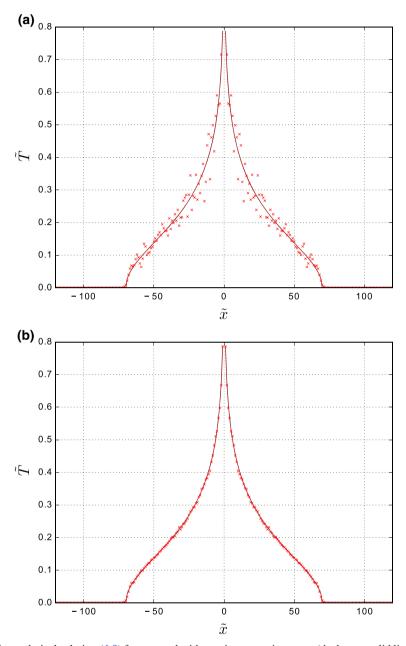
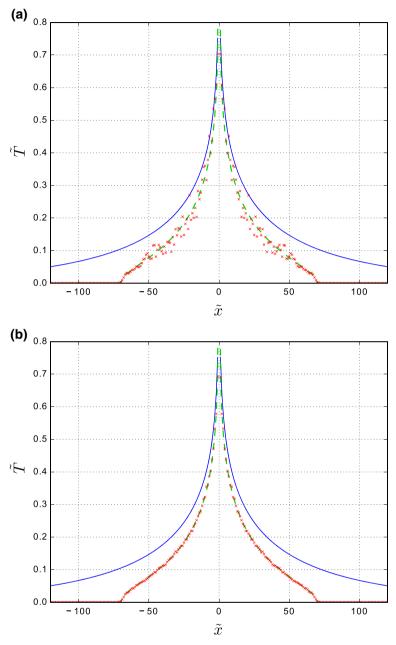


Fig. 2 Comparing the analytical solution (6.8) for a crystal without viscous environment (the brown solid line) and the numerical solution (the red crosses) in the case N=1000,  $\tilde{t}=70$ . **a** R=100, **b** R=1000

Introducing the dimensionless quantities  $\tilde{t}$ ,  $\tilde{T}$ ,  $\tilde{x}$  according to (6.2), (6.5), and (6.10), respectively, the classical heat equation in the case under consideration can be formulated in the following form

$$\frac{\partial \tilde{T}}{\partial \tilde{t}} - \kappa \frac{\partial^2 \tilde{T}}{\partial^2 \tilde{x}} = \lambda H(\tilde{t}) \delta(\tilde{x}), \tag{7.1}$$

where  $\kappa$ ,  $\lambda$  are positive dimensionless constants. The solution of (7.1) that equals zero for  $\tilde{t} < 0$  is (see [71])



**Fig. 3** Comparing the unsteady analytical solution (6.7) for a crystal in a viscous environment (the green dashed line), the corresponding steady-state analytical solution (6.9) in the form of the Macdonald function (the blue solid line) and the numerical solution (the red crosses) in the case  $\tilde{\eta}=0.01$ , N=1000,  $\tilde{t}=70$ . **a** R=100, **b** R=10,000

$$\tilde{T} = \frac{\lambda H(\tilde{t})}{2\sqrt{\varkappa\pi}} \int_{0}^{\tilde{t}} \frac{\exp\left(-\frac{|\tilde{x}|^{2}}{4\varkappa\tau}\right)}{\sqrt{\tau}} d\tau 
= \lambda H(\tilde{t}) \left(\sqrt{\frac{\tilde{t}}{\pi\varkappa}} \exp\left(-\frac{\tilde{x}^{2}}{4\varkappa\tilde{t}}\right) - \frac{|\tilde{x}|}{2\varkappa} \operatorname{erfc} \frac{|\tilde{x}|}{2\sqrt{\varkappa\tilde{t}}}\right).$$
(7.2)

For  $\tilde{t} \to \infty$  the right-hand side of (7.2) grows proportionally to  $\sqrt{\tilde{t}}$  being bounded at  $\tilde{x} = 0$ .

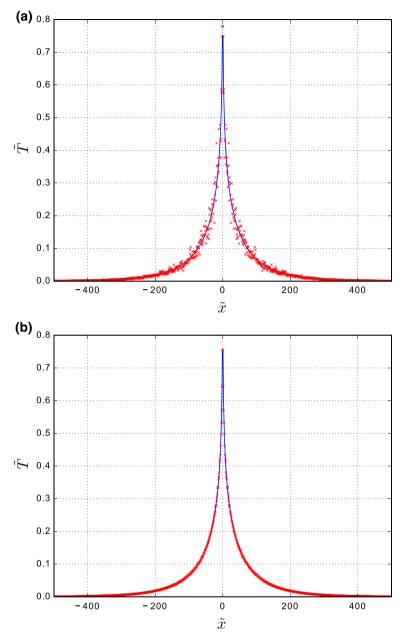


Fig. 4 Comparing the steady-state analytical solution (6.9) in the form of the Macdonald function (the blue solid line) and the numerical solution (the red crosses) in the case  $\tilde{\eta}=0.01$ , N=1000,  $\tilde{t}=500$ . **a** R=100, **b** R=10,000

Now we want to compare qualitatively the solutions (6.7) or (6.8) from the one hand, and (7.2) from the other hand. At first, we need to choose the reasonable values for material constants  $\varkappa$  and  $\lambda$  in (7.2). In order to make the solutions corresponding to different physical models more similar in some sense, for certain  $\tilde{t} = \tilde{t}_0$  we take constants  $\varkappa = \varkappa_0(\tilde{t}_0)$  and  $\lambda = \lambda_0(\tilde{t}_0)$  such that the following pairs of the quantities

$$\int_{-\infty}^{\infty} \tilde{T}(\tilde{x}, \tilde{t}_0) \, d\tilde{x} \quad \text{and} \quad \int_{-\infty}^{\infty} \tilde{x}^2 \tilde{T}(\tilde{x}, \tilde{t}_0) \, d\tilde{x}$$
 (7.3)

calculated by virtue of (6.8) and (7.2), respectively, are mutually equal. In such a way we get that  $\lambda_0 = 1/2$  and does not depend on  $\tilde{t}_0$ , while the quantity  $\varkappa_0$  depends on  $\tilde{t}_0$ .

The comparison between unsteady solutions for the crystal and the solution of the heat equation is given in Fig. 5. (All plots are calculated for  $\tilde{t}_0 = 30$ .) Certainly, the most important difference here is that according

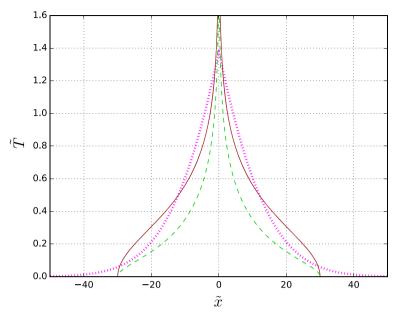


Fig. 5 A qualitative comparison between the non-stationary analytical solution (6.7) for a crystal in a viscous environment ( $\tilde{\eta} = 0.03$ , the green dashed line), the non-stationary analytical solution (6.8) for a crystal without viscous environment (the brown solid line) and the solution (7.2) of the heat equation ( $\kappa = 5.00$ , the magenta dotted line)

to (6.7) and (6.8) the heat propagates at a finite speed. Both solutions for the crystal are unbounded at x = 0, while the solution of the heat equation (7.2) remains to be finite.

#### 8 Conclusion

In the paper, we started with equations (2.1) for stochastic dynamics of a one-dimensional harmonic crystal in a viscous environment. We introduced in the standard way the kinetic temperature in the crystal as a quantity proportional to the statistical dispersion of the particle velocities. The most important results of the paper are the differential–difference equation (4.9) for the heat propagation in the crystal and the analytical formulas (5.17), (5.25) and (5.28) describing the ballistic heat propagation in the crystal from a point heat source. Formula (5.17) gives the non-stationary kinetic temperature distribution in a crystal without viscous environment caused by a point source of constant intensity. Formulas (5.25) and (5.28) correspond to the case of a crystal in a viscous environment. Formula (5.25) gives the non-stationary kinetic temperature distribution caused by a point pulse source (i.e., the fundamental solution). Formula (5.28) shows that the steady-state kinetic temperature distribution caused by a point source of constant intensity is described by the Macdonald function of zero order. The comparison between numerical solution of equations (2.1) and analytic solution of differential–difference equation (4.9) demonstrates a good agreement (see Figs. 2, 3, 4). In the case of the heat source of general structure, the formula for the kinetic temperature can be obtained as the convolution of the heat source function with the corresponding fundamental solution [see Eqs. (5.18), (5.31)].

A comparison of our results with the classical model based on the heat equation and Fourier's law demonstrates an essential difference in the kinetic temperature distribution near a point source of heat supply (see Sect. 7 and Fig. 5). In the framework of our model the heat propagates at the speed of sound for the crystal. We expect that the results obtained in the paper can be used to describe the heat transfer in low-dimensional nanostructures and ultra-pure materials [15,16,81]. On the other hand, we expect that the theoretical result expressed by formula (5.28) can be verified by experiments with laser excitation of nanostructures.

**Acknowledgements** The authors are grateful to D.A. Indeitsev, V.A. Kuzkin, E.V. Shishkina for useful and stimulating discussions.

# A The derivation of the dynamic equations for the covariances

Consider a system of stochastic differential equations

$$dx_i = a_i(\mathbf{x}, t) dt + \sum_{\alpha} b_{i\alpha}(\mathbf{x}, t) dW_j, \quad i = 1, ..., n,$$
 (A.1)

where  $\mathbf{x} = [x_1, \dots, x_n]^{\top}$  and  $W_j$  is a vector of uncorrelated Wiener variables. According to [67] [Chapter 6, formulas (6.4)–(6.17)], it follows from the Itô lemma that the following equation for the covariance variables holds:

$$\langle x_p x_q \rangle = \langle x_p a_q + x_q a_p + b_{q\alpha} b_{p\alpha} \rangle. \tag{A.2}$$

In the particular case (2.1), we have  $b_{i\alpha}(\mathbf{x}, t) = \delta_{\alpha i} b_i(\mathbf{x}, t)$ , whence

$$\langle x_p x_q \rangle^{\cdot} = \langle x_p a_q + x_q a_p \rangle + \delta_{pq} \langle b_p b_q \rangle. \tag{A.3}$$

Now we apply (A.3) to (2.1) and obtain

$$\langle u_{p}u_{q}\rangle^{\cdot} = \langle u_{p}v_{q}\rangle + \langle v_{p}u_{q}\rangle, 
\langle u_{p}v_{q}\rangle^{\cdot} = \langle u_{p}F_{q}\rangle + \langle v_{p}v_{q}\rangle, 
\langle v_{p}v_{q}\rangle^{\cdot} = \langle v_{p}F_{q}\rangle + \langle F_{p}v_{q}\rangle + \delta_{pq}\langle b_{p}b_{q}\rangle.$$
(A.4)

Applying these formulas to the particular case where  $F_i$  are given by Eq. (2.2) yields formula (2.11).

#### B Some identities of the calculus of finite differences

Consider an infinite sequence  $f_p$ , where p is an arbitrary integer. Introduce the left and right shift operators h and v, respectively:

$$hf_p \stackrel{\text{def}}{=} f_{p+1}, \quad \nu f_p \stackrel{\text{def}}{=} f_{p-1}.$$
 (B.1)

Clearly,

$$h\nu = 1 \iff \nu = h^{-1}.$$
 (B.2)

One has

$$\mathcal{L} = h + \nu - 2,\tag{B.3}$$

$$\mathcal{D} = h - \nu. \tag{B.4}$$

By definition, put

$$\Sigma \stackrel{\text{def}}{=} h + \nu + 2 = \mathcal{L} + 4. \tag{B.5}$$

One has

$$\mathcal{L}\Sigma f_p = f_{p+2} - 2f_p + f_{p-2} = \mathcal{D}^2 f_p.$$
(B.6)

Introduce the sign change operator  $(-1)^p$ . One has

$$h(-1)^p = (-1)^{p+1}h, (B.7)$$

$$\nu(-1)^p = (-1)^{p+1}\nu,\tag{B.8}$$

$$\mathcal{L}(-1)^p = (-1)^{p+1} \Sigma, \tag{B.9}$$

$$\Sigma = (-1)^{p+1} \mathcal{L}(-1)^p.$$
 (B.10)

### References

- Rieder, Z., Lebowitz, J., Lieb, E.: Properties of a harmonic crystal in a stationary nonequilibrium state. J. Math. Phys. 8(5), 1073–1078 (1967)
- 2. Bonetto, F., Lebowitz, J., Rey-Bellet, L.: Fourier's law: a challenge to theorists. In: Fokas, A., Grigoryan, A., Kibble, T., Zegarlinski, B. (eds.) Mathematical Physics 2000. World Scientific, Singapore (2000)
- 3. Lepri, S., Livi, R., Politi, A.: Thermal conduction in classical low-dimensional lattices. Phys. Rep. 377(1), 1–80 (2003)
- 4. Lepri, S., Livi, R., Politi, A.: On the anomalous thermal conductivity of one-dimensional lattices. Europhys. Lett. **43**(3), 271 (1998)

- 5. Dhar, A.: Heat transport in low-dimensional systems. Adv. Phys. 57(5), 457–537 (2008)
- 6. Lepri, S.: Thermal Transport in Low Dimensions: From Statistical Physics to Nanoscale Heat Transfer. Springer, Berlin (2016)
- Casati, G., Ford, J., Vivaldi, F., Visscher, W.: One-dimensional classical many-body system having a normal thermal conductivity. Phys. Rev. Lett. 52(21), 1861–1864 (1984)
- 8. Aoki, K., Kusnezov, D.: Bulk properties of anharmonic chains in strong thermal gradients: non-equilibrium  $\varphi^4$  theory. Phys. Lett. A **265**(4), 250–256 (2000)
- 9. Gendelman, O., Savin, A.: Normal heat conductivity in chains capable of dissociation. Europhys. Lett. 106(3), 34,004 (2014)
- 10. Savin, A., Kosevich, Y.: Thermal conductivity of molecular chains with asymmetric potentials of pair interactions. Phys. Rev. E 89(3), 032,102 (2014)
- 11. Gendelman, O., Savin, A.: Heat conduction in a chain of colliding particles with a stiff repulsive potential. Phys. Rev. E **94**(5), 052,137 (2016)
- 12. Spohn, H.: Fluctuating hydrodynamics approach to equilibrium time correlations for anharmonic chains. In: Lepri, S. (ed.) Thermal Transport in Low Dimensions: From Statistical Physics to Nanoscale Heat Transfer. Lecture Notes in Physics, pp. 107–158. Springer (2016)
- 13. Bonetto, F., Lebowitz, J., Lukkarinen, J.: Fourier's law for a harmonic crystal with self-consistent stochastic reservoirs. J. Stat. Phys. **116**(1), 783–813 (2004)
- 14. Le-Zakharov, A., Krivtsov, A.: Molecular dynamics investigation of heat conduction in crystals with defects. Dokl. Phys. 53(5), 261–264 (2008)
- 15. Chang, C., Okawa, D., Garcia, H., Majumdar, A., Zettl, A.: Breakdown of Fourier's law in nanotube thermal conductors. Phys. Rev. Lett. 101(7), 075,903 (2008)
- Xu, X., Pereira, L., Wang, Y., Wu, J., Zhang, K., Zhao, X., Bae, S., Bui, C., Xie, R., Thong, J., Hong, B., Loh, K., Donadio, D., Li, B., Özyilmaz, B.: Length-dependent thermal conductivity in suspended single-layer graphene. Nat. Commun. 5, 3689 (2014)
- 17. Hsiao, T., Huang, B., Chang, H., Liou, S., Chu, M., Lee, S., Chang, C.: Micron-scale ballistic thermal conduction and suppressed thermal conductivity in heterogeneously interfaced nanowires. Phys. Rev. B **91**(3), 035,406 (2015)
- 18. Cahill, D., Ford, W., Goodson, K., Mahan, G., Majumdar, A., Maris, H., Merlin, R., Phillpot, S.: Nanoscale thermal transport. J. Appl. Phys. 93(2), 793–818 (2003)
- 19. Liu, S., Xu, X., Xie, R., Zhang, G., Li, B.: Anomalous heat conduction and anomalous diffusion in low dimensional nanoscale systems. Eur. Phys. J. B 85, 337 (2012)
- 20. Chang, C.: Experimental probing of non-Fourier thermal conductors. In: Lepri, S. (ed.) Thermal Transport in Low Dimensions: From Statistical Physics to Nanoscale Heat Transfer. Lecture Notes in Physics, vol. 921, pp. 305–338. Springer (2016)
- 21. Peierls, R.: Quantum Theory of Solids. Oxford University Press, Oxford (1955)
- 22. Ziman, J.: Electrons and Phonons: The Theory of Transport Phenomena in Solids. Oxford University Press, Oxford (1960)
- 23. Hsiao, T., Chang, H., Liou, S., Chu, M., Lee, S., Chang, C.: Observation of room-temperature ballistic thermal conduction persisting over 8.3 μm in SiGe nanowires. Nat. Nanotechnol. **8**(7), 534–538 (2013)
- 24. Kannan, V., Dhar, A., Lebowitz, J.: Nonequilibrium stationary state of a harmonic crystal with alternating masses. Phys. Rev. E **85**(4), 041,118 (2012)
- 25. Dhar, A., Dandekar, R.: Heat transport and current fluctuations in harmonic crystals. Physica A 418, 49-64 (2015)
- 26. Allen, K., Ford, J.: Energy transport for a three-dimensional harmonic crystal. Phys. Rev. 187(3), 1132 (1969)
- 27. Nakazawa, H.: On the lattice thermal conduction. Prog. Theor. Phys. Suppl. 45, 231–262 (1970)
- 28. Lee, L., Dhar, A.: Heat conduction in a two-dimensional harmonic crystal with disorder. Phys. Rev. Lett. **95**(9), 094,302 (2005)
- Kundu, A., Chaudhuri, A., Roy, D., Dhar, A., Lebowitz, J., Spohn, H.: Heat conduction and phonon localization in disordered harmonic crystals. Europhys. Lett. 90(4), 40,001 (2010)
- 30. Dhar, A., Saito, K.: Heat transport in harmonic systems. In: Lepri, S. (ed.) Thermal Transport in Low Dimensions: From Statistical Physics to Nanoscale Heat Transfer. Lecture Notes in Physics, vol. 921, pp. 39–106. Springer (2016)
- 31. Bernardin, C., Kannan, V., Lebowitz, J., Lukkarinen, J.: Harmonic systems with bulk noises. J. Stat. Phys. **146**(4), 800–831 (2012)
- 32. Freitas, N., Paz, J.: Analytic solution for heat flow through a general harmonic network. Phys. Rev. E 90(4), 042,128 (2014)
- 33. Freitas, N., Paz, J.: Erratum: analytic solution for heat flow through a general harmonic network. Phys. Rev. E **90**(6), 069,903 (2014)
- 34. Hoover, W., Hoover, C.: Hamiltonian thermostats fail to promote heat flow. Commun. Nonlinear Sci. Numer. Simul. **18**(12), 3365–3372 (2013)
- Lukkarinen, J., Marcozzi, M., Nota, A.: Harmonic chain with velocity flips: thermalization and kinetic theory. J. Stat. Phys. 165(5), 809–844 (2016)
- 36. Gendelman, O., Shvartsman, R., Madar, B., Savin, A.: Nonstationary heat conduction in one-dimensional models with substrate potential. Phys. Rev. E **85**(1), 011,105 (2012)
- 37. Tsai, D., MacDonald, R.: Molecular-dynamical study of second sound in a solid excited by a strong heat pulse. Phys. Rev. E 14(10), 4714 (1976)
- 38. Ladd, A., Moran, B., Hoover, W.: Lattice thermal conductivity: a comparison of molecular dynamics and anharmonic lattice dynamics. Phys. Rev. E **34**(8), 5058 (1986)
- 39. Volz, S., Saulnier, J.B., Lallemand, M., Perrin, B., Depondt, P., Mareschal, M.: Transient Fourier-law deviation by molecular dynamics in solid argon. Phys. Rev. E **54**(1), 340 (1996)
- Daly, B., Maris, H., İmamura, K., Tamura, S.: Molecular dynamics calculation of the thermal conductivity of superlattices. Phys. Rev. E 66(2), 024,301 (2002)
- 41. Gendelman, O., Savin, A.: Nonstationary heat conduction in one-dimensional chains with conserved momentum. Phys. Rev. E 81(2), 020,103 (2010)

- 42. Babenkov, M., Krivtsov, A., Tsvetkov, D.: Energy oscillations in a one-dimensional harmonic crystal on an elastic substrate. Phys. Mesomech. **19**(3), 282–290 (2016)
- 43. Krivtsov, A.: Heat transfer in infinite harmonic one-dimensional crystals. Dokl. Phys. 60(9), 407–411 (2015)
- 44. Krivtsov, A.: Energy oscillations in a one-dimensional crystal. Dokl. Phys. 59(9), 427-430 (2014)
- 45. Hoover, W., Hoover, C.: Simulation and Control of Chaotic Nonequilibrium Systems. World Scientific, Singapore (2015)
- 46. Krivtsov, A.: From nonlinear oscillations to equation of state in simple discrete systems. Chaos Solitons Fractals 17(1), 79–87 (2003)
- 47. Berinskii, I.: Elastic networks to model auxetic properties of cellular materials. Int. J. Mech. Sci. 115, 481-488 (2016)
- 48. Kuzkin, V., Krivtsov, A., Podolskaya, E., Kachanov, M.: Lattice with vacancies: elastic fields and effective properties in frameworks of discrete and continuum models. Philos. Mag. **96**(15), 1538–1555 (2016)
- 49. Berinskii, I., Krivtsov, A.: Linear oscillations of suspended graphene. In: Shell and Membrane Theories in Mechanics and Biology, pp. 99–107. Springer, Cham (2015)
- 50. Berinskii, I., Krivtsov, A.: A hyperboloid structure as a mechanical model of the carbon bond. Int. J. Solids Struct. **96**, 145–152 (2016)
- 51. Shishkina, E., Gavrilov, S.: A strain-softening bar with rehardening revisited. Math. Mech. Solids 21(2), 137–151 (2016)
- 52. Gavrilov, S.: Dynamics of a free phase boundary in an infinite bar with variable cross-sectional area. ZAMM—J. Appl. Math. Mech. / Z. Angew. Math. Mech. 87(2), 117–127 (2007)
- 53. Gavrilov, S., Shishkina, E.: On stretching of a bar capable of undergoing phase transitions. Contin. Mech. Thermodyn. 22, 299–316 (2010)
- 54. Gavrilov, S., Shishkina, E.: A strain-softening bar revisited. ZAMM—J. Appl. Math. Mech. / Z. Angew. Math. Mech. 95(12), 1521–1529 (2015)
- 55. Shishkina, E., Gavrilov, S.: Stiff phase nucleation in a phase-transforming bar due to the collision of non-stationary waves. Arch. Appl. Mech. 87(6), 1019–1036 (2017)
- 56. Gavrilov, S., Herman, G.: Wave propagation in a semi-infinite heteromodular elastic bar subjected to a harmonic loading. J. Sound Vib. **331**(20), 4464–4480 (2012)
- 57. Krivtsov, A.: On heat transfer in a thermally perturbed harmonic chain. arXiv:1709.07924 (2017)
- 58. Chandrasekharalah, D.: Thermoelasticity with second sound: a review. Appl. Mech. Rev. 39(3), 355 (1986)
- 59. Tzou, D.: Macro-to Microscale Heat Transfer: The Lagging Behavior. Wiley, Hoboken (2014)
- 60. Cattaneo, C.: Sur une forme de l'équation de la chaleur éliminant le paradoxe d'une propagation instantanée. C. R. L'Acad. Sci. **247**(4), 431–433 (1958)
- 61. Vernotte, P.: Les paradoxes de la théorie continue de léquation de la chaleur. C. R. L'Acad. Sci. 246(22), 3154-3155 (1958)
- 62. Kuzkin, V., Krivtsov, A.: An analytical description of transient thermal processes in harmonic crystals. Phys. Solid State **59**(5), 1051–1062 (2017)
- Kuzkin, V., Krivtsov, A.: Fast and slow thermal processes in harmonic scalar lattices. J. Phys. Condens. Matter 29(50), 505,401 (2017)
- Indeitsev, D., Osipova, E.: A two-temperature model of optical excitation of acoustic waves in conductors. Dokl. Phys. 62(3), 136–140 (2017)
- 65. Andrews, L.: Special Functions of Mathematics for Engineers. SPIE Publications, Bellingham (1997)
- 66. Kloeden, P., Platen, E.: Numerical Solution of Stochastic Differential Equations. Springer, Berlin (1999)
- 67. Stepanov, S.: Stochastic World. Springer, Berlin (2013)
- 68. Langevin, P.: Sur la théorie du mouvement brownien. C. R. L'Acad. Sci. 146(530–533), 530 (1908)
- 69. Lemons, D., Gythiel, A.: Paul Langevin's 1908 paper on the theory of Brownian motion ["Sur la théorie du mouvement brownien"]. Am. J. Phys. **65**(11), 1079–1081 (1997)
- 70. Krivtsov, A.: Dynamics of heat processes in one-dimensional harmonic crystals. In: Problems of Mathematical Physics and Applied Mathematics: Proceedings of the Seminar in Honor of Prof. E.A. Tropp's 75th Anniversary, pp. 63–81. Ioffe Institute, St. Petersburg (2016) (in Russian)
- 71. Vladimirov, V.: Equations of Mathematical Physics. Marcel Dekker, New York (1971)
- Lepri, S., Mejía-Monasterio, C., Politi, A.: Nonequilibrium dynamics of a stochastic model of anomalous heat transport. J. Phys. A 43(6), 065,002 (2010)
- 73. Nayfeh, A.: Perturbation Methods. Wiley, Hoboken (2008)
- 74. Krivtsov, A.: On unsteady heat conduction in a harmonic crystal. arXiv:1509.02506 (2015)
- 75. Brigham, E.: The Fast Fourier Transform and Its Applications. Prentice Hall, Upper Saddle River (1974)
- 76. Slepyan, L., Yakovlev, Y.: Integral transform in non-stationary problems of mechanics. Sudostroenie (1980) (in Russian)
- 77. Gel fand, I., Shilov, G.: Generalized Functions. Properties and Operations, vol. 1. Academic Press, New York (1964)
- 78. Polyanin, A.: Handbook of Linear Partial Differential Equations for Engineers and Scientists. Chapman & Hall/CRC, Boca Raton (2002)
- 79. Prudnikov, A., Brychkov, Y., Marichev, O.: Integrals and Series. Elementary Functions, vol. 1. Gordon & Breach, New York (1986)
- 80. Aleixo, R., Oliveira, E.: Green's function for the lossy wave equation. Rev. Bras. Ensino Fis. 30(1), 1302 (2008)
- 81. Goldstein, R., Morozov, N.: Mechanics of deformation and fracture of nanomaterials and nanotechnology. Phys. Mesomech. **10**(5–6), 235–246 (2007)

**Publisher's Note** Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.