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# Unsteady ballistic heat transport: linking lattice dynamics and kinetic theory

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**Abstract** The kinetic theory is widely used in the description of thermal transport at the micro- and nanoscale. In the theory, it is assumed that heat is carried by quasi-particles, obeying the Boltzmann transport equation. These quasi-particles are sometimes associated with phonons. However, since phonons are not localized in physical space, they cannot play the role of the quasi-particles used in the kinetic theory. In the present paper, we employ another interpretation of quasi-particles, namely wave packets. Our derivation is carried out for an infinite harmonic chain with a given initial temperature distribution. An exact formula describing the time evolution of the kinetic temperature of the chain is derived. A transition from the exact solution to a continuum limit is performed. It is shown that the resulting continuum solution coincides with the solution of the collisionless Boltzmann equation. The transition yields wave packets, localized in space and moving with group velocities. Therefore, the wave packets can be associated with quasi-particles. It is shown that the quasi-particle has finite lifetime and that its position is determined with some uncertainty.

## 1 Introduction

The derivation of the laws governing heat transport in solids is one of the key problems in modern mechanics and solid-state physics. In continuum mechanics, heat transport is modeled by the formulation of proper constitutive relations. In particular, at the macroscale, the Fourier law, assuming a linear relationship between heat flux and temperature gradient, is widely used. However, it has been shown in many theoretical [1–4] and experimental [5–8] works that the Fourier law may be violated at the micro- and nanoscale. Therefore, new constitutive relations, describing nanoscale heat transport, are required. A possible method for the derivation of these constitutive relations consists of using lower scale models. In the present paper, we consider two of these, specifically lattice dynamics and kinetic theory. Our main aim is a discussion of the link between these models.

In lattice dynamics, a material is represented by a set of interacting particles (atoms). Heat transport is associated with the propagation of thermal vibrations of these atoms<sup>1</sup> (see, e.g., [9]). The evolution of

<sup>1</sup> In the present paper, heat transport in dielectrics is considered, and therefore the contribution of electrons to heat transport is ignored.

<sup>2</sup> In harmonic crystals, the particles interact via linearized forces.

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the temperature profile is described via a solution of the lattice dynamics equations, with initial conditions corresponding to the initial temperature profile. For perfect (defect free) harmonic<sup>2</sup> crystals, this problem is solved analytically (see, e.g., papers [10–17]). This approach allows the definition of all the quantities of interest (kinetic temperature, heat flux, etc.) rigorously and the formulation of all assumptions explicitly.

In real crystals, nonlinearity, defects, and interfaces are usually present. Analytical solutions of the lattice dynamics equations are then generally not available. In this case, the kinetic theory of heat transport, originally formulated by Pierls [18], can be used. In kinetic theory, it is assumed that the heat is carried by a set of moving quasi-particles. The motion of the quasi-particles (evolution of their distribution function) is governed by the Boltzmann transport equation. Free motion of the quasi-particles corresponds to the ballistic heat transport regime, which is realized in harmonic crystals. The influence of lattice defects and nonlinearity of the interatomic interactions on heat transport are modeled by interactions (collisions) of the quasi-particles. Due to collisions, the quasi-particles may perform Brownian-type motion or the Levy walk. The former corresponds to the Fourier heat transport regime, while the latter corresponds to anomalous heat transport [19–21]. Kinetic theory is a valuable tool for the solution of many practical heat transport problems, which are beyond the range of applicability of the analytical solutions of the lattice dynamics equations (see, e.g., review [22]). However, proper links between lattice dynamics and kinetic descriptions of the heat transport are yet to be developed. In particular, the physical meaning of the quasi-particles, used in kinetic theory, is yet to be established.

In literature, quasi-particles are usually associated with phonons. The notion of the phonon is linked to the energy of harmonic plane waves in crystals. Since the harmonic waves are “infinite,” the phonons are not localized in physical space and cannot be regarded as quasi-particles. This fact was clearly demonstrated by Spohn [23]. In [23], it was shown that the distribution function for quasi-particles coincides with the Wigner function. An equation describing the evolution of the Wigner function for harmonic crystals was derived by Mielke [24], while a generalization for the weakly anharmonic case was carried out in [23, 25]. However, in these papers, no explicit expressions for the individual quasi-particles have been presented. We employ another approach. Instead of introducing an additional mathematical object (the Wigner function) and obtaining governing equations for this object, we derive all results directly from the exact expression for the kinetic temperature.

The difference between phonons and quasi-particles, used in kinetic theory, was first noted in the book by Frenkel [27], where the notion of the phonon was introduced.<sup>3</sup> It has been suggested that the role of the quasi-particle can be played by a wave packet, i.e. a group of harmonic waves with close wave numbers. Like quasi-particles, wave packets are localized in space and move with group velocities. However, to the best of our knowledge, a transition from the exact solution of the heat transport problem to an approximate solution in terms of wave packets has not yet been presented in the literature. Therefore, this important issue is addressed below.

The aim of the present paper is to link lattice dynamics and kinetic theory descriptions of heat transfer. We consider the simplest model of a crystal, namely a harmonic chain. In Sect. 2, equations of motion and initial conditions, corresponding to the initial temperature distribution, are formulated. In Sect. 3, an exact expression for the kinetic temperature is derived. In Sect. 4, the transition from the exact solution to a continuum limit is carried out. The transition yields wave packets, which can be interpreted as quasi-particles. The properties of the quasi-particles are discussed. Additionally, in Sect. 4, we derive an approximate expression describing the changes in the temperature due to the equilibration of kinetic and potential energies. To compare with the kinetic theory, we present the derivation and solution of the collisionless Boltzmann equation in Sect. 5. This solution is compared with results from Sect. 4. In the concluding Section, we discuss the limitations of the kinetic description.

## 2 Statement of the problem

In this Section, we formulate an unsteady heat transfer problem for a one-dimensional harmonic chain. We present the equations of motion and initial conditions, corresponding to some temperature distribution and zero initial heat fluxes.

<sup>3</sup> Sometimes, it is stated that the word “phonon” was introduced by I.E. Tamm. However, in papers by Tamm, we were only able to find the notion of “elastischen Quanten” [26], while Frenkel was using the word “phonon” in his book [27].

We consider a one-dimensional chain consisting of  $N$  identical particles<sup>4</sup> of mass  $m$ , connected by linear springs. The equations of motion are written in the form<sup>5</sup>

$$m\dot{v}_i = \sum_{j=-n}^n C_j(u_{i+j} - u_i) - C_0u_i, \quad v_i = \dot{u}_i, \quad (1)$$

where  $C_j = C_{-j}$  is the stiffness of the spring connecting a particle with its  $j$ th neighbor,  $C_0$  is the stiffness of the elastic foundation, and  $2n$  is the total number of neighbors connected to the particle. Equation (1) is solved under periodic boundary conditions  $u_i = u_{i+N}$ .

Initially, the particles have random velocities and zero displacements:

$$u_{i0} = 0, \quad v_{i0} = \alpha_i \sqrt{\frac{k_B T_i^0}{m}}, \quad \langle \alpha_i \rangle = 0, \quad \langle \alpha_i \alpha_j \rangle = \delta_{ij}, \quad (2)$$

where  $\alpha_i$  are uncorrelated random numbers with zero mean and unit variance,  $T_i^0$  is the initial kinetic temperature of the particle (see Definition (3)),  $k_B$  is the Boltzmann constant,  $\langle \dots \rangle$  stands for the mathematical expectation, and  $\delta_{ij}$  is the Kronecker delta. We note that under conditions (2) the initial heat flux is equal to zero at each point of the chain. The initial conditions (2) can be considered as a result of the heating of a crystal by an ultrashort laser pulse [28, 29].

We consider an infinite number of realizations of system (1), with random initial conditions (2). The main quantity of interest is the kinetic temperature defined as [10]

$$k_B T_i = m \langle v_i^2 \rangle. \quad (3)$$

In the literature, different definitions of temperature (e.g., kinetic temperature, configurational temperature, etc.) are used. These definitions usually coincide only at (or close to) thermal equilibrium. We refer to paper [30] for a detailed investigation of the differences between the temperatures in nonequilibrium simulations. We use the kinetic temperature because it has clear physical meaning and is easy to compute.

### 3 An exact solution of the heat transfer problem

In this Section, we derive an exact expression for the kinetic temperature by using a solution of the initial value problem (1) and (2).

#### 3.1 An exact solution of the dynamic equations

The solution of problem (1) and (2) is derived using the discrete Fourier transform, defined as

$$\hat{u}_p = \sum_{i=0}^{N-1} u_i e^{-i\frac{2\pi ip}{N}}, \quad u_i = \frac{1}{N} \sum_{p=0}^{N-1} \hat{u}_p e^{i\frac{2\pi ip}{N}}, \quad (4)$$

where  $\hat{u}_p$  is the Fourier image of the displacements and  $i^2 = -1$ . Applying the discrete Fourier transform (4) to the dynamics Eq. (1), we obtain

$$\dot{\hat{v}}_p = -\omega_p^2 \hat{u}_p, \quad \omega_p^2 = \frac{C_0}{m} + 4 \sum_{j=1}^n \frac{C_j}{m} \sin^2 \frac{\pi pj}{N}. \quad (5)$$

Here,  $\omega_p = \omega_{N-p}$  is the  $p$ th eigenfrequency of the chain.

<sup>4</sup> Further, we consider an infinite crystal as a limiting case, where  $N$  tends to infinity.

<sup>5</sup> Choosing parameters  $C_j$  in (1), one can describe any linear pairwise interactions in the chain.

Solving Eq. (5) with initial conditions corresponding to (2), and applying the inverse discrete Fourier transform, we obtain the exact expression for the particle velocities<sup>6</sup>,

$$v_i = \frac{1}{N} \sum_{j,p=0}^{N-1} v_{j0} \cos(\omega_p t) e^{i \frac{2\pi(i-j)p}{N}}. \tag{6}$$

Formula (6) shows that all particles with nonzero initial velocity contribute to the velocity of particle  $i$ . The contribution of each particle is represented by a superposition of harmonic waves<sup>7</sup>  $\exp[i(\omega_p t + 2\pi(i-j)p/N)]$ . The energies of these harmonic waves are usually associated with phonons [26, 27]. We note again that harmonic waves (and phonons) are not localized in the physical space. Therefore, we seek another candidate for the role of the quasi-particle used in the kinetic description. The question arises of whether it is possible to find a localized object in the formula (6) for the velocities. We have no definite answer to this question and so we will seek the localized object in the exact expression for the kinetic temperature, which is derived in the following Section.

### 3.2 An exact expression for the kinetic temperature

An exact expression for the kinetic temperature is derived as follows. Substitution of the exact solution (6) into the definition of the temperature (3) yields<sup>8</sup>

$$k_B T_i = \frac{m}{N^2} \sum_{j,p,k,s=0}^{N-1} \langle v_{j0} v_{k0} \rangle \cos(\omega_p t) \cos(\omega_s t) e^{i \frac{2\pi(i-j)p}{N}} e^{-i \frac{2\pi(i-k)s}{N}}. \tag{7}$$

Using the identity  $m \langle v_{j0} v_{k0} \rangle = k_B T_j^0 \delta_{jk}$ , which follows from the initial conditions (2), we obtain

$$T_i = \frac{1}{N^2} \sum_{j,p,s=0}^{N-1} T_j^0 \cos(\omega_p t) \cos(\omega_s t) \cos\left(\frac{2\pi}{N}(i-j)(p-s)\right). \tag{8}$$

Formula (8) is an exact solution of the heat transfer problem for a periodic crystal.

For an infinite crystal ( $N \rightarrow \infty$ ), the values  $2\pi p/N$  and  $2\pi s/N$  can be replaced by  $k_1, k_2 \in [0; 2\pi)$ . Replacing the sums with respect to  $p, s$  in (8) by integrals with respect to  $k_1, k_2$ , we obtain:<sup>9</sup>

$$T_i = \frac{1}{4\pi^2} \sum_{j=-\infty}^{+\infty} T_j^0 \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \cos(\omega(k_1)t) \cos(\omega(k_2)t) \cos((i-j)\Delta k) dk_1 dk_2, \tag{9}$$

$$\omega^2(k) = \frac{C_0}{m} + 4 \sum_{j=1}^n \frac{C_j}{m} \sin^2 \frac{jk}{2}, \quad \Delta k = k_1 - k_2,$$

where  $\omega(k)$  is the dispersion relation.

Thus, the exact solution of the heat transfer problem for an infinite chain is given by formula (9), and the majority of further results are derived from this formula. The formula shows that the contribution of particle  $j$  to the temperature of particle  $i$  is determined by the double integral. In this expression, the integrand yields the contribution of the two waves with wave numbers  $k_1, k_2$ . Since the contributions of different waves are not strictly positive, there may be some cancelation. Further, it is shown that in the continuum limit the main contribution comes from waves with close values of the wave number  $k_1 \approx k_2$ , i.e., wave packets.

<sup>6</sup> Since the velocity is real, the exponent in formula (6) can be replaced by the cosine function.

<sup>7</sup> To prove this statement, one can replace the cosine by complex exponents.

<sup>8</sup> Here, the relation  $\langle v_i v_i^* \rangle = \langle v_i^2 \rangle$  was used, where  $*$  stands for the complex conjugate.

<sup>9</sup> Since the expression in (8) is periodic, summation can be carried out over the interval, which is symmetric with respect to zero. In the limit of an infinite crystal, the interval becomes a set of integers.

## 4 Heat transfer in the continuum limit

The exact expression (9) for the temperature is hard to use, since it involves summation over all the particles and a double integral. Additionally, the formula contains an artifact: all particles, no matter how far, contribute to the temperature of particle  $i$  at all times. This is a consequence of the infinite speed of propagation of disturbances in discrete systems. Therefore, in this Section, we derive a simple approximate formula for temperature in the continuum limit. This derivation yields an expression for wave packets, which may be interpreted as quasi-particles.

### 4.1 Main hypotheses

In this Section, we formulate the main hypotheses used in the transition from the exact expression (9) to the continuum limit.

We assume that the initial temperature distribution  $T_i^0$  slowly changes in space. To formulate this hypothesis more precisely, we separate the chain into intervals, each containing  $2\Delta N$  particles (see Fig. 1).

For each group  $s$ , we denote the central particle by  $j_s$  (in this case  $j_{s+1} = j_s + 2\Delta N$ ). The assumption formulated above is then equivalent to the following relations:

$$T_i^0 \approx T_{j_s}^0, \quad i \in [j_s - \Delta N + 1; j_s + \Delta N], \quad (10)$$

$$a\Delta N \ll L, \quad (11)$$

$$\Delta N \gg 1, \quad (12)$$

where  $L$  is the macroscopic length scale. In other words, we assume that the function  $T_i^0$  is nearly constant at distances of the order  $a\Delta N$ , which is small compared to the macroscopic length  $L$ . We also assume that the number of particles  $\Delta N$  in each interval is large.

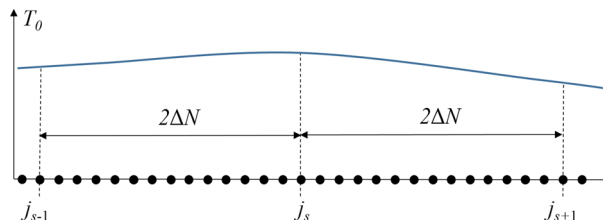
Formulae (10)–(12) are employed below for transition from the exact formula (9) to the continuum limit.

### 4.2 Discrete and continuum fundamental solutions of the heat transfer problem

In this Section, we derive a relation between the discrete and continuum fundamental solutions of the heat transfer problem.

In papers [10–13], it has been shown that thermal processes in crystals with initial conditions (2) have several timescales. At short times of the order of several atomic periods, the temperature oscillates with a high frequency. These oscillations are caused by the equilibration of the kinetic and potential energies. At large times, changes in temperature are caused by heat transfer. We use the following separation of these “fast” and “slow” processes, as proposed in [13]:

$$\begin{aligned} T_i &= T_i^F + T_i^S, \quad T_i^F = \sum_{j=-\infty}^{\infty} T_j^0 F_{i-j}, \quad T_i^S = \sum_{j=-\infty}^{\infty} T_j^0 S_{i-j}, \\ F_{i-j} &= \frac{1}{8\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \cos((\omega(k_1) + \omega(k_2))t) \cos(\Delta k(i - j)) dk_1 dk_2, \\ S_{i-j} &= \frac{1}{8\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \cos((\omega(k_1) - \omega(k_2))t) \cos(\Delta k(i - j)) dk_1 dk_2. \end{aligned} \quad (13)$$



**Fig. 1** Initial distribution of temperature in the chain

Here,  $T_i^F$  describes oscillations of temperature due to the equilibration of energies (fast process), while  $T_i^S$  describes heat transfer (slow process). We note that initially  $T_i^S = T_i^F = T_i^0/2$ .

Using assumption (10), we neglect changes in  $T_i^0$  within each interval of length  $2\Delta N$ . Formula (13) for  $T_i^S$  can then be rewritten as

$$T_i^S = \sum_{s=-\infty}^{+\infty} \sum_{j=j_s-\Delta N+1}^{j_s+\Delta N} T_j^0 S_{i-j} \approx \sum_{s=-\infty}^{+\infty} T_{j_s}^0 g(i - j_s, \Delta N) 2a\Delta N, \tag{14}$$

$$g(i - j_s, \Delta N) = \frac{1}{2a\Delta N} \sum_{l=-\Delta N+1}^{\Delta N} S_{i-j_s-l}.$$

Function  $g(i - j_s, \Delta N)$  determines the contribution of the neighborhood of point  $j_s$  to the temperature at point  $i$ . It is convenient to use one more approximation in (14):

$$T_i^S \approx \sum_{s=-\infty}^{+\infty} T_{i-j_s}^0 g(j_s, \Delta N) 2a\Delta N, \tag{15}$$

where formulae (14) and (15) coincide in the continuum limit (see formula (17)).

We use assumption (11), stating that  $a\Delta N$  is much smaller than the macroscopic length scale  $L$ , and introduce functions  $T_S(x)$ ,  $T_0(x)$ ,  $g_c(x)$ , defined for all real  $x$  such that

$$T_S(ai) = T_i^S, \quad T_0(ai) = T_i^0, \quad g_c(ai) = \lim_{\frac{a\Delta N}{L} \rightarrow 0} g(i, \Delta N). \tag{16}$$

Strictly speaking, formula (16) defines the continuum temperature field only at particle positions. However, since the temperature changes slowly, the values at other points can be obtained by interpolation.

For  $a\Delta N/L \rightarrow 0$ , the sums in formulae (14) and (15) are replaced by the integrals

$$T_S(x) = \int_{-\infty}^{\infty} T_0(y) g_c(x - y) dy = \int_{-\infty}^{\infty} T_0(x - y) g_c(y) dy, \tag{17}$$

where the function  $g_c$  is the fundamental solution of the heat transfer problem in the continuum limit.

Thus, formulae (14) and (16) show that the continuum fundamental solution is obtained by spatial averaging of the discrete fundamental solution over the interval of length  $2\Delta N$ .

### 4.3 Transition to the continuum limit and emergence of wave packets

In this Section, we derive an expression for the continuum fundamental solution  $g_c$  (see formula (16)), under the assumptions  $\Delta N \gg 1$  and  $a\Delta N \ll L$ . We show that the solution is represented by a superposition of wave packets.

According to formula (16), the continuum solution,  $g_c$ , is a limit of function  $g$ , defined by formula (14). We rewrite function  $g$  as

$$g(j, \Delta N) = \frac{1}{8\pi^2 a} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \cos((\omega(k_1) - \omega(k_2))t) \varphi(j, \Delta k, \Delta N) dk_1 dk_2, \tag{18}$$

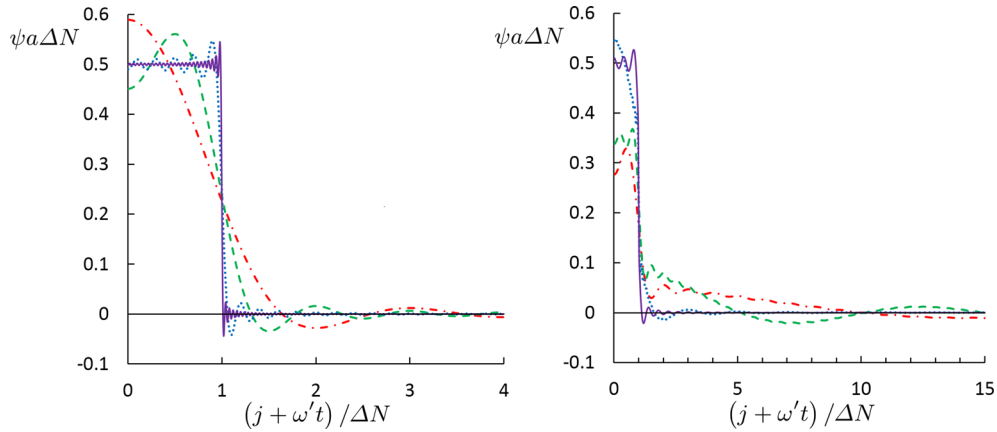
$$\varphi(j, \Delta k, \Delta N) = \frac{1}{2\Delta N} \sum_{l=-\Delta N+1}^{\Delta N} \cos(\Delta k(j - l)).$$

In ‘‘Appendix 2,’’ it is shown that  $\varphi$  is represented by

$$\varphi = \frac{\Delta k}{2} \operatorname{sinc}(\Delta N \Delta k) \left[ \cot \frac{\Delta k}{2} \cos(j \Delta k) + \sin(j \Delta k) \right], \tag{19}$$

where  $\operatorname{sinc} x = \sin x/x$  and  $\cot x = \cos x/\sin x$ .

Further simplification is based on the properties of the function  $\varphi$  for  $\Delta N \gg 1$ . It is equal to one for  $\Delta k = 0$  and  $\Delta k = \pm 2\pi$ , while at all other points it tends to zero as  $\Delta N$  tends to infinity. Therefore, for large  $\Delta N$ , the



**Fig. 2** Wave packet  $\psi$  for  $q_1 = 0$  (left),  $q_1 = 0.9\pi$  (right) and  $\Delta N = 1$  (dash-dotted line), 2 (dashed line), 10 (dotted line), and 50 (solid line). Since  $\psi$  is an even function of  $j + \omega't$ , only positive values of the arguments are considered

main contribution to the integral (18) is given by the points  $\Delta k \approx 0$  ( $k_1 \approx k_2$ ). Using  $\Delta k$  as a small parameter, we make the series expansions

$$\omega(k_1) - \omega(k_2) \approx \Delta k \omega'(k_1), \quad \omega' = \frac{d\omega}{dk}, \quad \varphi \approx \text{sinc}(\Delta N \Delta k) \cos(j \Delta k). \quad (20)$$

Then, employing formula (20) and substituting  $q_1 = k_1$ ,  $q_2 = k_1 - k_2$ , we rewrite formula (18) as<sup>10</sup>

$$g \approx \frac{1}{4\pi} \int_0^\pi [\psi(j + \omega'(q_1)t, \Delta N) + \psi(j - \omega'(q_1)t, \Delta N)] dq_1, \quad (21)$$

$$\psi(j + \omega't, \Delta N) = \frac{1}{2\pi a} \int_{q_1 - \pi}^{q_1 + \pi} \cos[q_2(j + \omega'(q_1)t)] \text{sinc}(q_2 \Delta N) dq_2. \quad (22)$$

Here, the function  $\psi$  is a wave packet, carrying heat with group velocity  $c_g = a\omega'$ . The wave packets arise as a result of the averaging of the discrete fundamental solution over the interval of length  $2\Delta N$ .

The function  $\psi$ , for different values of  $\Delta N$  and wave numbers  $q_1$ , is shown in Fig. 2. It can be seen that the function  $\psi$  converges to the following expression as  $\Delta N$  tends to infinity<sup>11</sup>:

$$\psi(j + \omega't, \Delta N) \approx \begin{cases} \frac{1}{2a\Delta N}, & a|j + \omega't| < a\Delta N, \\ 0, & a|j + \omega't| > a\Delta N. \end{cases} \quad (23)$$

The derivation of (23) is given in “Appendix 2.” Figure 2 shows that the rate of convergence is higher for small values of the wave number  $q_1$ . This faster convergence may be due to the fact that at small wave numbers the waves are less dispersive.

In “Appendix 2,” it is also shown that for  $\Delta N \gg 1$ ,  $a\Delta N \ll L$ , function  $\psi$  tends to the Dirac delta function, i.e.

$$\psi(j + \omega't) \approx \delta(a(j + \omega't)). \quad (24)$$

Then, taking the limit  $a\Delta N/L \rightarrow 0$  in (21) and using definition (16), we obtain the continuum fundamental solution

$$g_c(x) = \frac{1}{4\pi} \int_{-\pi}^\pi \delta(x + c_g(q)t) dq, \quad c_g = a\omega'. \quad (25)$$

Formulae (21) and (25) show that the fundamental solution of the heat transfer problem is represented by a superposition of the wave packets  $\psi$ . In the continuum limit, the wave packets tend to be of delta-like shape

<sup>10</sup> Here, the identity  $\omega'(q_1) = -\omega'(-q_1)$  is used.

<sup>11</sup> For finite  $\Delta N$ , the integral in formula (22) can be represented via the sine integral.

and have a definite position in the physical space. The speed of a wave packet is equal to the group velocity, which depends on the wave number. Therefore, the wave packets may be associated with the quasi-particles.

Note that the position of the wave packet is determined to an accuracy of the order of  $a\Delta N$ . The width of the packet in the Fourier space (i.e., range of wave numbers included in the packet) is inversely proportional to  $\Delta N$ . Therefore, the localizations in the physical space and the Fourier space are mutually exclusive.

#### 4.4 Quasi-particle (wave packet) lifetime

Wave packets consist of waves with close (but not equal) wave numbers. We denote the maximum difference of wave numbers in the wave packet by  $\max(\Delta k)$ . Due to dispersion, the speeds of waves in the wave packet are different, and therefore the width of a wave packet grows over time. We introduce the “lifetime,”  $t_*$ , of a wave packet (quasi-particle), which is defined as the time required for a wave packet to increase its width by  $a\Delta N$ . In order to estimate the difference in wave speeds, we consider the first formula of (20). In this formula, a quantity of the order of  $\max(\omega'') \max(\Delta k)^2 t$  was neglected. The neglected difference in the wave speeds is then estimated as  $a \max(\omega'') \max(\Delta k)$ . From formula (19), it can be seen that  $\max(\Delta k) \sim \Delta N^{-1}$ . The lifetime of a quasi-particle is then estimated as

$$t_* \sim \frac{\Delta N}{\max(\omega'') \max(\Delta k)} \sim \frac{\Delta N^2}{\max(\omega'')} \tag{26}$$

In a medium without dispersion, the lifetime is infinite; otherwise, it is proportional to  $\Delta N^2$ . Therefore, the lifetime depends on the rate of change of the initial temperature profile  $T_0(x)$ .

#### 4.5 The general solution of the heat transfer problem

Using the fundamental solution (25), we construct the general solution for an arbitrary initial temperature distribution  $T_0(x)$ . Substitution of formula (25) into the integral (17) yields

$$T_S(x) = \frac{1}{4\pi} \int_{-\pi}^{\pi} T_0(x + c_g(q)t) dq \tag{27}$$

Then, using approximations (10)–(12) in the exact solution (13), we obtain an approximate continuum expression (27) for the temperature. Strictly speaking, formula (27) is valid only for slowly changing temperature profiles, satisfying conditions (10)–(12). However, numerical simulations show that it has reasonable accuracy even for discontinuous functions, e.g., the Heaviside function (see, e.g., papers [10–12]).

The derivation of formula (27) using the kinetic theory is presented below.

#### 4.6 Continuum expression for the “fast” part of the temperature

In this Section, we derive a continuum expression for the “fast” part of the temperature,  $T_i^F$ , describing the equilibration of kinetic and potential energies (see formula (13)).

As in the previous Sections, under assumptions (10)–(12), we introduce continuum functions  $T_F(x)$ ,  $h_c(x)$  such that

$$T_F(ai) = T_i^F, \quad T_F = \int_{-\infty}^{+\infty} T_0(x - y)h_c(y)dy, \quad h_c(aj) = \lim_{\frac{a\Delta N}{L} \rightarrow 0} h(j, \Delta N), \tag{28}$$

$$h(j, \Delta N) = \frac{1}{8\pi^2 a} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \cos((\omega(k_1) + \omega(k_2))t) \varphi(j, \Delta k, \Delta N) dk_1 dk_2. \tag{29}$$

The expression for  $h_c$  is derived in the same way as formula (25) for  $g_c$  (see Sect. 4.3). We use the fact that the main contribution to the integral (29) for large  $\Delta N$  is given by points  $k_1 \approx k_2$ . Then, using the approximate formula (20) for  $\varphi$  and the following expansion:

$$\omega(k_1) + \omega(k_2) \approx 2\omega(k_1), \tag{30}$$



we represent function  $h$  by

$$h \approx \frac{1}{2\pi} \int_0^\pi \cos(2\omega(q_1)t) \psi(j, \Delta N) dq_1. \quad (31)$$

It is seen that, similarly to  $g$  (formula (21)), function  $h$  is represented by a superposition of wave packets  $\psi$ , as defined by formula (22). However, in (31) the wave packets are static, and their amplitudes oscillate over time. These oscillations are caused by exchange of energy among kinetic and potential forms.

Substituting (31) into the definition of  $h_c$  (28), and calculating the limit, we obtain

$$h_c(x) = \frac{\delta(x)}{2\pi} \int_0^\pi \cos(2\omega(q)t) dq. \quad (32)$$

The subsequent substitution of formula (32) into formula (28) yields

$$T_F = \frac{T_0(x)}{2\pi} \int_0^\pi \cos(2\omega(q)t) dq. \quad (33)$$

In the case of interactions between the nearest neighbors, this reduces to

$$T_F = \frac{1}{2} T_0(x) J_0(2\omega_e t), \quad (34)$$

where  $\omega_e = \sqrt{C/m}$  and  $J_0$  is the Bessel function of the first kind.<sup>12</sup>

We now consider the range of applicability of formula (33). Our derivation is based on expansion (30), in which the term  $\omega'' (\Delta k)^2/2$  is neglected. Note that in formula (29) the neglected value is multiplied by time  $t$ , which may be arbitrarily large. Therefore, the approximate formula (33) is only accurate as long as the value  $\omega'' (\Delta k)^2 t/2$  is small. By using the same arguments as in Sect. 4.4, we show that formula (33) is applicable only for  $t < t_*$ , where  $t_*$  is given by formula (26).

Thus, in the continuum approximation, the evolution of the temperature field is described by (27) and (33). In the case of a uniform distribution of initial temperature ( $T_0 = \text{const}$ ), these formulae are exact, while in the nonuniform case they are approximate. The formulae lose accuracy at times of order of  $t_*$ .

## 5 Description of heat transport using the kinetic theory

### 5.1 Collisionless Boltzmann equation

In this Section, we present a simplified formulation of the heat transfer problem in the framework of kinetic theory. In particular, the collisionless Boltzmann equation is derived. Though the equation is well known, we have decided to include this detailed derivation in order to simplify comparison with the results obtained above by the lattice dynamics approach.

In the kinetic theory of heat transfer, it is assumed that the heat in a crystal is carried by quasi-particles moving with some speeds. A portion of the heat carried by a particle is regarded as an unrelated additional scalar characteristic, which does not affect, for example, the particle velocity. Additionally, we assume that each quasi-particle carries the same amount of heat. The temperature of an elementary volume is then proportional to the number of quasi-particles in this volume. In fact, a one-dimensional motion of a gas consisting of collisionless quasi-particles is considered. The temperature is thus assumed to be proportional to the concentration of the quasi-particles.

We introduce the distribution function

$$f(t, x, v) = \lim_{\Delta x, \Delta v \rightarrow 0} \frac{\Delta M}{\Delta x \Delta v}, \quad (35)$$

where  $\Delta M$  is the number of quasi-particles with coordinates and velocities in the intervals  $[x - \frac{1}{2} \Delta x; x + \frac{1}{2} \Delta x]$  and  $[v - \frac{1}{2} \Delta v; v + \frac{1}{2} \Delta v]$ , respectively. Given a known distribution function, the temperature is calculated as

$$T(t, x) = \gamma \int_{-\infty}^{\infty} f(t, x, v) dv, \quad (36)$$

<sup>12</sup> Formulae (33) and (34) were originally derived in the [10, 11] by entirely different means.

where  $\gamma$  is a proportionality coefficient.

We consider the balance of quasi-particles in a two-dimensional phase space of coordinates and velocities. The change in the number of quasi-particles in an elementary phase volume  $dx dv$  from time  $t$  to time  $t + dt$  is given by equation

$$(f(t + dt, x, v) - f(t, x, v))dx dv = (f(t, x, v) - f(t, x + dx, v))v dt dv. \tag{37}$$

Formula (37) shows that the number of particles changes due to flux through boundaries of the elementary phase volume. A series expansion of the function  $f$  in formula (37) with respect to  $dt$  and  $dx$  in the first approximation yields

$$\frac{\partial}{\partial t} f(t, x, v) + v \frac{\partial}{\partial x} f(t, x, v) = 0. \tag{38}$$

Here, formula (38) is the collisionless Boltzmann equation, which can be considered to be an infinite set of independent wave equations. Then, the exact solution of Eq. (38) has the form

$$f(t, x, v) = f_0(x - vt, v), \tag{39}$$

where  $f_0(x, v)$  is the initial distribution function for the quasi-particles.

### 5.2 Evolution of an initial temperature profile

In this Section, we consider the evolution of an initial temperature profile  $T_0(x)$  in the crystal. The temperature profile can be considered to be the result of some excitation of the crystal. We assume that initial heat fluxes are absent and that the initial distributions of velocities at all spatial points are identical. The velocity distribution depends on the properties of the crystal and is independent of excitation characteristics. Then, the initial distribution function is represented by

$$f_0(x, v) = T_0(x) \eta(v) / \gamma, \tag{40}$$

where  $T_0(x)$  is the initial temperature profile and  $\eta(v)$  is the distribution of the quasi-particles' velocities such that

$$\eta(-v) = \eta(v), \quad \int_{-\infty}^{\infty} \eta(v) dv = 1. \tag{41}$$

Here, the first relation guarantees the absence of heat fluxes, while the second relation is a normalization condition.

Substitution of expressions (39) and (40) into the definition of temperature (36) yields

$$T(t, x) = \int_{-\infty}^{\infty} T_0(x - vt) \eta(v) dv = \int_{-\infty}^{\infty} T_0(x + vt) \eta(v) dv. \tag{42}$$

The equivalence of these expressions follows from the fact that  $\eta(v)$  is even (see formula (41)).

In the second integral of (42), we change from variable  $v$  to  $q$  using

$$q = 2\pi \operatorname{sign}(v) \int_{|v|}^{\infty} \eta(u) du \iff v = c_g(q), \tag{43}$$

where  $c_g(q)$  is the inverse function with respect to  $q(v)$ . We note that, by the definition, both functions are odd. Substitution of formula (43) into (42) yields

$$T(t, x) = \frac{1}{2\pi} \int_{-\pi}^{\pi} T_0(x + c_g(q)t) dq. \tag{44}$$

Formula (44) coincides with formula (27), as derived from the solution of the lattice dynamics equations, to the accuracy of the prefactor<sup>13</sup> 1/2. A comparison of these expressions shows that in formula (44) the variable  $q$

<sup>13</sup> The difference is caused by the fast process, which is only present in the lattice dynamics solution (see Sect. 3). The fast process leads to a reduction in the temperature by a factor of 2. The solutions coincide exactly if the initial temperature in the kinetic theory is interpreted as a result of the fast process.

plays the role of a wave number, while  $c_g$  is the group velocity. Therefore, the quasi-particles move with group velocities.

For example, for Hooke's crystal (a chain of identical particles, connected to their nearest neighbors by identical springs) the distributions of velocities and the group velocity have the form

$$\eta(v) = \frac{1}{\pi} \frac{H(c^2 - v^2)}{\sqrt{c^2 - v^2}}, \quad c_g(q) = c \operatorname{sign} q \cos \frac{q}{2}, \quad (45)$$

where  $c$  is the speed of sound in the chain (the long wavelength limit of the phase velocity) and  $H(x)$  is the Heaviside step function ( $H(x) = 1$  for  $x > 0$ , and  $H(x) = 0$  for  $x < 0$ ). Substitution of formulae (45) into expressions (42) and (44) yields two known formulae [31], which describe ballistic heat transfer in Hooke's crystal:

$$T(t, x) = \frac{1}{\pi} \int_{-c}^c \frac{T_0(x - vt)}{\sqrt{c^2 - v^2}} dv = \frac{1}{2\pi} \int_0^{2\pi} T_0\left(x + ct \cos \frac{q}{2}\right) dq. \quad (46)$$

Here, the integration limits have been changed for simplicity.

Thus, the derivation of (44) using the kinetic theory is significantly simpler than the derivation based on lattice dynamics. However, this apparent simplicity can be misleading. Firstly, the change of variables (43) is only valid for crystals with one-to-one correspondence between the wave number  $q$  and the group velocity  $c_g$  (otherwise derivations are more complicated). Secondly, from the lattice dynamics point of view, formula (44) is an approximation, which is applicable only when conditions (10)–(12) are satisfied. These conditions impose certain restrictions on the system size, initial temperature profile, etc. Finally, the concept of the kinetic theory, based on the existence of the quasi-particles (which are not real physical objects), raises many questions. The main question is how to interpret the quasi-particles in terms of some of the other structures and objects which are present in the results of lattice dynamics calculations. In previous Sections, it has been shown that wave packets (22) may play the role of quasi-particles, because the wave packets are localized (to some extent) in both physical and Fourier spaces. However, due to dispersion, the wave packets have finite lifetimes. Therefore, the continuum solution (44) is only valid at finite times.

## 6 Conclusions

We have shown that the transition from the exact expression for the kinetic temperature to the continuum limit is carried out using assumptions (10)–(12). The key assumption is a slow variation of the initial temperature profile at the length scale  $a\Delta N$ , this scale being large compared to the lattice constant  $a$  and small compared to a macroscopic length scale. Neglecting variation of the initial temperature at distances of the order of  $a\Delta N$ , we have shown that the macroscopic fundamental solution is represented by a spatial average of the discrete fundamental solution. This averaging yields wave packets, e.g., groups of harmonic waves with close wave numbers. The wave packets are localized in space and move with group velocities. These facts allow us to consider the wave packets as the quasi-particles used in the kinetic theory.

Two properties of the quasi-particles were demonstrated. Firstly, the position of the quasi-particle is determined with uncertainty of the order of  $a\Delta N$ , and secondly the characteristic width of the wave packet in the Fourier space is inversely proportional to  $\Delta N$ . Therefore, localizations of the quasi-particles in real and Fourier spaces are mutually exclusive. This fact is somewhat similar to the uncertainty principle being used in quantum mechanics. We refer to paper [32] for further discussion of the relationship between classical chain dynamics and quantum phenomena. Secondly, the dispersion leads to an increase in the width of the wave packet over time. Therefore, the kinetic description remains valid for a period of time of the order of the quasi-particle lifetime, which is proportional to  $\Delta N^2$  (see formula (26)).

We believe that the inaccuracy of the kinetic approach will be most pronounced in problems with localized initial temperature distribution  $T_0(x)$ . We refer to paper [16] for a detailed comparison of the extreme case, and notably a comparison of the discrete and continuum fundamental solutions. However, no alternative to the continuum solution (27) has been presented in the literature. The derivation of approximate formulae, describing the behavior of temperature at times much larger than the quasi-particle lifetime, would be an interesting extension of the present work.

We note an important difference between lattice dynamics and kinetic approaches. In lattice dynamics, the properties of the crystal are determined by the equation of motion. In particular, features of the ballistic

heat transport regime are determined by the dispersion relation and corresponding group velocity [11, 13]. The initial conditions specify the temperature field and fluxes, but there is no way to influence the rate of heat transfer via the initial conditions. In contrast, the Boltzmann transport equation, governing motion of the quasi-particles, contains no information about the properties of the crystal (at least in the collisionless case). Motion of the quasi-particles, e.g., their velocities, is completely determined by the initial condition  $f_0(x, v)$ . This fact allows us to partially answer the question, raised in paper [23]: “In fact, upon specifying the complete displacement field, including its velocities, it is not so clear how to extract from it the positions and momenta of the particle-like objects called phonons.” From our reasoning, it follows that the velocities of the quasi-particles cannot be extracted from the displacement field, while we suspect that the spatial distribution of the quasi-particles can be derived from that field. However, the corresponding procedure is yet to be developed.

Additionally, we have shown that the presented approach allows the rigorous separation of two physical processes, namely the equilibration of kinetic and potential energies, and ballistic heat transport. Similar separations have already been carried out in papers [11, 13]. However, in these works, several heuristic assumptions have been made. In this work, we have managed to eliminate those assumptions.

Finally, we note that it would be interesting to explore the interaction of the quasi-particles (wave packets) with defects and interfaces. Important steps in this direction have been performed in the recent paper [33], where the Kapitza interfacial resistances in linear and nonlinear chains were investigated.

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**Compliance with ethical standards**

**Conflict of interest** The authors declare that they have no conflict of interest.

**Appendix 1: Change of the summation limits**

We show that in formula (8) the summation from 0 to  $N - 1$  can be replaced by a summation from  $M - N + 1$  to  $M$  (for  $M < N$ ) as follows:

$$\begin{aligned}
 \sum_{j=0}^{N-1} T_j^0 \cos\left(\frac{2\pi}{N}(i-j)(p-s)\right) &= \sum_{j=0}^M \dots + \sum_{j=M+1}^{N-1} \dots, \\
 &= \sum_{j=0}^M \dots + \sum_{j=M+1}^{N-1} T_{j-N}^0 \cos\left(\frac{2\pi}{N}(i-j+N)(p-s)\right) \\
 &= \sum_{j=0}^M \dots + \sum_{j=M-N+1}^{-1} T_j^0 \cos\left(\frac{2\pi}{N}(i-j)(p-s)\right) \\
 &= \sum_{j=M-N+1}^M T_j^0 \cos\left(\frac{2\pi}{N}(i-j)(p-s)\right). \tag{47}
 \end{aligned}$$

Here, the periodicity of the problem  $T_j^0 = T_{j-N}^0$  is used. Similarly, we show that the following identity is satisfied:

$$\sum_{s,p=0}^{N-1} \cos(\omega_p t) \cos(\omega_s t) \cos\left(\frac{2\pi}{N}(i-j)(p-s)\right) = \sum_{s,p=M-N+1}^M \dots, \quad \omega_p = \omega_{p-N}. \tag{48}$$

## Appendix 2: Derivation of the formula for $\varphi$

Consider the derivation of formula (19) for function  $\varphi$ . By definition,

$$\varphi = \frac{1}{2\Delta N} \sum_{l=-\Delta N+1}^{\Delta N} \cos(\Delta k(j-l)). \quad (49)$$

We make the following transformations at the right side of formula (49):

$$\varphi = \frac{\cos(j\Delta k)}{2\Delta N} \sum_{l=-\Delta N+1}^{\Delta N} \cos(\Delta kl) + \frac{\sin(j\Delta k)}{2\Delta N} \sum_{l=-\Delta N+1}^{\Delta N} \sin(\Delta kl). \quad (50)$$

Substitution of the identities

$$\sum_{l=-\Delta N+1}^{\Delta N} \cos(\Delta kl) = \cot \frac{\Delta k}{2} \sin(\Delta N \Delta k), \quad \sum_{l=-\Delta N+1}^{\Delta N} \sin(\Delta kl) = \sin(\Delta N \Delta k) \quad (51)$$

into (50) yields expression (19) for  $\varphi$ .

## Appendix 3: Derivation of the formula for $\psi$

We derive the approximate expression (24) for  $\psi$  in the limit  $\Delta N \gg 1$ ,  $a\Delta N \ll L$ . We make the following transformations:

$$\begin{aligned} \psi &= \frac{1}{2\pi a} \int_{q_1-\pi}^{q_1+\pi} \cos(q_2(j+\omega't)) \operatorname{sinc}(\Delta N q_2) dq_2 \\ &= \frac{1}{2\pi a \Delta N} \int_{(q_1-\pi)\Delta N}^{(q_1+\pi)\Delta N} \cos \frac{q_2(j+\omega't)}{\Delta N} \operatorname{sinc} q_2 dq_2 \\ &\approx \frac{1}{2\pi a \Delta N} \int_{-\infty}^{+\infty} \cos \frac{q_2(j+\omega't)}{\Delta N} \operatorname{sinc} q_2 dq_2. \end{aligned} \quad (52)$$

Here,  $q_1 \in [0; \pi]$ ,  $\omega' = \omega'(q_1)$ . Calculation of the integral at the right side of formula (52) yields formula (24):

$$\psi \approx \begin{cases} \frac{1}{2a\Delta N}, & a|j+\omega't| < a\Delta N, \\ 0, & a|j+\omega't| > a\Delta N. \end{cases} \quad (53)$$

Here,  $a\Delta N$  is small compared to the macroscopic length scale  $L$ . Therefore, for  $a\Delta N \ll L$ , function  $\psi$  can be replaced by the Dirac delta function.

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