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Unsteady heat transfer in harmonic scalar lattices

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Abstract

An approach for analytical description of unsteady heat transfer in harmonic lattices is presented. Evolution of initial temperature field in infinite lattice is investigated. Dynamics equations for scalar lattices are written in a form valid for longitudinal and transverse vibrations of chains and for out-of-plane vibrations of two-dimensional lattices. The description of heat transfer is based on analysis of velocity covariances for all pairs of particles. The general solution of the unsteady heat transfer problem is obtained in integral form. The solution shows that temperature is represented as a superposition of waves having a shape of initial temperature distribution. The waves propagate with group velocities depending on the wave vector. The heat front propagates with constant speed equal to the maximum group velocity. The general solution is reversible with respect to time, i.e. it is invariant with respect to substitution t by $-t$. Closed-form fundamental solutions for one- and two-dimensional lattices are obtained. The problem of thermal contact of two half-spaces having different initial temperatures is considered. It is shown that effective heat conductivity linearly diverges with length for all harmonic scalar lattices. This fact is consistent with results obtained in literature for stationary heat transfer problem. An example of unsteady heat transfer in a stretched square lattice performing out-of-plane vibrations is given. Analytical solutions of problems with stepwise and sinusoidal spatial distributions of initial temperature are presented. Numerical simulations show that presented theory describes the unsteady heat transfer in harmonic scalar lattices with high accuracy.

1 Introduction

At macrolevel, heat propagation is usually diffusive and well-described by Fourier's law. The law assumes linear dependence between the heat flux and temperature gradient with proportionality coefficient refereed to as the heat conductivity. Phonon theory relates the heat conductivity coefficient with the phonon mean free path [1, 2]. It is assumed that the Fourier law is valid if the mean free path is much smaller than characteristic size of the system. At micro- and nanolevel, this condition may be violated. In particular, it is shown experimentally that the mean free path can be as large as several microns [3]. In this case, the heat transport is ballistic [4, 5, 6] and can not be described by the Fourier

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law. In particular, the effective heat conductivity is size-dependent [4, 5, 6] and it can not be regarded as a material constant. This phenomenon leads to a variety of practical applications of heat transport in micro- and nanosystems (see e.g. a review paper [7]). On the other hand, derivation of macroscopic heat transport equations from lattice dynamics equations is a serious challenge for theoreticians [8].

One of the convenient models for investigation of heat transport in solids is a harmonic crystal. A harmonic crystal is a set of particles forming a lattice and interacting via linearized (harmonic)[1] forces. Heat transport in harmonic crystals is usually investigated in a steady-state regime. Stationary temperature distribution between two reservoirs with different temperatures[2] is considered. For example, in a pioneering work by Reider, Lebowitz and Lieb [9], anomalies of the heat transport in one-dimensional harmonic chain with nearest neighbor interactions are demonstrated and an analytical solution of the steady-state heat transport problem is derived. The solution shows that thermal resistance of the chain[3] is independent on its length. Therefore the effective heat conductivity diverges with length and the Fourier law is not applicable. Anomalous heat transport is also observed in more complicated harmonic systems. Generalization of results obtained in paper [9] for the multidimensional case is carried out in papers [10, 11]. Harmonic chains with alternating masses are considered in papers [12]. The effect of disorder on heat transport in harmonic crystals is studied in papers [13, 14]. The influence of volumetric heating on nonequilibrium steady-state is investigated in papers [15, 16]. Solution of the steady-state problem for an arbitrary harmonic network is obtained in paper [17]. Specific feature of the stationary heat transfer problem considered in the above mentioned papers is that the results strongly depend on the type of thermostat [18, 19, 20]. For example, in paper [20] it is shown that a specific choice of the thermostat leads to Fourier heat conduction in harmonic crystals. Note that the influence of thermostat is also observed in nonlinear systems [21].

In the present paper, we consider unsteady heat transport in an infinite lattice with nonuniform distribution of initial temperature. It allows to investigate properties of the lattice rather than properties of the thermostat. In literature, unsteady heat transport in solids is usually studied numerically [22, 23, 24, 25, 26, 27, 28, 29]. Several analytical solutions are obtained only in one-dimensional case [30, 31, 32, 33]. In paper [30], the decay of sinusoidal temperature distribution in a harmonic one-dimensional chain with on-site potential is considered. It is shown using asymptotic analysis that the amplitude of the temperature distribution decays according to a power law, while diffusive and hyperbolic heat transfer equations [34, 35] predict exponential decay. An alternative form of heat transfer equation has been proposed in papers [31, 32].

An approach for analytical description of the unsteady heat transfer in one-dimensional chains is proposed in papers [31, 32]. The approach is based on the analysis of velocity covariances for all pairs of particles. An equation for dynamics of covariances is derived. The equation describes two types of thermal processes: (i) fast oscillations of kinetic temperature caused by redistribution of energy among kinetic and potential parts [36, 37,

[1] Harmonic forces linearly depend on particle displacements.

[2] Here and below kinetic temperature is considered.

[3] Thermal resistance is the inverse of the heat conductivity.

38, 39] and (ii) slow evolution of spatial distribution of temperature [31, 32]. The later process is associated with the heat transfer. In some cases the approach yields a closed differential equation for kinetic temperature. For example, in a harmonic chain with nearest-neighbor interactions the kinetic temperature satisfies the following equation [31], [32][4]:

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

where t is time, c is the sound speed, prime denotes spatial derivative. Equation (1) describes evolution of spatial temperature distribution in an infinite chain with high accuracy [31, 32]. In particular, in contrast to diffusive (Fourier) and hyperbolic heat transfer equations, formula (1) correctly predicts the power law decay of sinusoidal temperature distribution described above. In paper [33] it is shown that equation (1) is valid for a chain with harmonic on-site potential, provided that c is changed by the maximum group velocity.

The present paper focuses on generalization of the approach proposed in papers [31, 32] for multidimensional case. The paper is organized as follows. In section 2, equations of motion in harmonic approximation are written in a general form. In the one-dimensional case, the equations are valid for longitudinal and transverse vibrations of chains. In the two-dimensional case, the equations are valid for linearized out-of-plane vibrations of square and triangular latices. Pair and multibody interactions with arbitrary number of neighbors and harmonic on-site potential can also be considered. In the above-mentioned cases, motion of each particle is described by a single scalar equation. Therefore the notion "scalar lattice" [40, 41, 42, 43] is used. In section 3, covariances of particle velocities are introduced. Equations in terms of covariances describing thermal processes in a crystal are derived. In section 5, a formula describing oscillations of kinetic temperature caused by redistribution of energy among kinetic and potential parts is derived. In section 6, the general solution of the unsteady heat transfer problem is presented. Closed-form fundamental solutions for one- and two-dimensional lattices are derived. In section 7, several problems for scalar square lattice with different initial temperature distributions are solved analytically and numerically.

2 Equations of motion and initial conditions

Consider an infinite harmonic lattice with simple structure[5] in d-dimensional space, where $d = 1, 2$. Each particle has one degree of freedom, i.e. particles move along parallel lines. Displacement of a particle is described by scalar function $u(\mathbf{x})$, where $\mathbf{x}$ is the radius vector of the particle in the undeformed state. The particle interacts with its neighbors numbered by index α. Vectors $\mathbf{a}_\alpha$, connecting the particle with its neighbors, satisfy relation[6]

$$\mathbf{a}_\alpha = -\mathbf{a}_{-\alpha}. \tag{2}$$

[4]Equation (1) is derived assuming that initial particle displacements are equal to zero and therefore time derivative of kinetic temperature is equal to zero.

[5]Unit cell of the lattice contains only one particle.

[6]Then $\mathbf{a}_0 = 0$.

Since the lattice is harmonic, then the total force acting on the particle is a linear combination of displacements of the neighboring particles. Therefore the equations of motion have the form

$$\ddot{u}\left(\mathbf{x}\right) = \mathcal{L}u\left(\mathbf{x}\right), \qquad \mathcal{L}u\left(\mathbf{x}\right) = \omega_*^2 \sum_{\alpha} b_\alpha u(\mathbf{x}+\mathbf{a}_\alpha), \quad b_\alpha = b_{-\alpha}, \tag{3}$$

where ω_* is a characteristic frequency (see e.g. formulas (4), (5)); $\mathcal{L}$ is a linear difference operator[7].

Equations of motion (3) are valid for a variety of one- and two-dimensional lattices. For example, the simplest one-dimensional lattice described by equation (3) is a chain with nearest-neighbor interactions. In this case

$$\begin{aligned} &\mathcal{L}u\left(\mathbf{x}\right) = \omega_*^2\Big(u(\mathbf{x}+\mathbf{a}_1) - 2u(\mathbf{x}) + u(\mathbf{x}+\mathbf{a}_{-1})\Big) \quad \Rightarrow \\ &\Rightarrow \quad \omega_* = \sqrt{\tfrac{C}{M}}, \qquad \mathbf{a}_{\pm1} = \pm a\mathbf{i}, \qquad b_{\pm1} = 1, \quad b_0 = -2. \end{aligned} \tag{4}$$

where $\mathbf{i}$ is a unit vector directed along the chain; a is an equilibrium distance between neighboring particles; C is bond stiffness; M is particle mass. Note that equation (4) with appropriate choice of ω_* also describes linearized transverse vibrations of a stretched chain with pair interactions [44, 45] and a chain with angular interactions [46, 47]. The simplest two-dimensional system described by equations of motion (3) is a stretched square lattice with nearest-neighbor interactions performing out-of-plane vibrations. In this case

$$\begin{aligned} &\mathcal{L}u\left(\mathbf{x}\right) = \omega_*^2\Big(u(\mathbf{x}+\mathbf{a}_1) + u(\mathbf{x}+\mathbf{a}_2) - 4u(\mathbf{x}) + u(\mathbf{x}+\mathbf{a}_{-1}) + u(\mathbf{x}+\mathbf{a}_{-2})\Big) \quad \Rightarrow \\ &\Rightarrow \quad \omega_* = \sqrt{\tfrac{F}{Ma}}, \quad \mathbf{a}_{\pm1} = \pm a\mathbf{i}, \quad \mathbf{a}_{\pm2} = \pm a\mathbf{j}, \quad b_{\pm1} = b_{\pm2} = 1, \quad b_0 = -4. \end{aligned} \tag{5}$$

where $\mathbf{i}$, $\mathbf{j}$ are orthogonal unit vectors; F is the magnitude of stretching force in equilibrium. This lattice is considered in detail in section 7.

In general, an appropriate choice of parameters $\mathbf{a}_\alpha$ and b_α in (3) allows to consider linearized vibrations of one- and two-dimensional scalar lattices. Pair and multibody interactions with arbitrary number of neighbors and harmonic on-site potential can be considered.[8]

We consider the following initial conditions typical for molecular dynamics simulations:

$$u(\mathbf{x}) = 0, \qquad v(\mathbf{x}) = v_0\left(\mathbf{x}\right), \tag{6}$$

where $v = \dot{u}$; initial velocities $v_0\left(\mathbf{x}\right)$ are uncorrelated, centered random numbers with zero mean. Note that no assumptions about distribution function for velocities are made. Evolution of the distribution function and its convergence to the Gaussian distribution are discussed e.g. in papers [49, 50, 51]. Initial conditions (6) correspond to some instantaneous distribution of kinetic temperature in a lattice.

[7] From mathematical point of view, formula (3) is a differential-difference equation or an infinite set of coupled ODE's of the second order.

[8] Out-of-plane vibrations of lattices with torque interactions [48] can also be considered provided that rotational degrees of freedom are fixed.

Equations of motion (3) with initial conditions (6) can be solved analytically. The solution yields random particle displacements and velocities. In contrast, description of macroscopic thermal processes usually focuses on statistical characteristics such as a kinetic temperature. An equation describing evolution of kinetic temperature is derived in the following section.

3 Covariances of velocities and kinetic temperature

In the present section, we derive an equation for covariances of particle velocities. Solution of this equation exactly describes evolution of kinetic temperature. A covariance of velocities for particles with radius-vectors $\mathbf{x}$ and $\mathbf{y}$ is defined as

$$\kappa(\mathbf{x},\mathbf{y}) = \Big\langle v(\mathbf{x})v(\mathbf{y}) \Big\rangle. \tag{7}$$

Here and below angle brackets $\Big\langle ... \Big\rangle$ stand for mathematical expectation[9]. Number of covariances (7) is equal to the number of different particle pairs in the lattice. The velocity covariance is related to kinetic temperature T by the following formula:

$$k_B T(\mathbf{x}) = M\Big\langle v(\mathbf{x})^2 \Big\rangle = M\kappa|_{\mathbf{x}=\mathbf{y}}, \tag{8}$$

where k_B is the Boltzmann constant.

Differentiation of covariances (7) with respect to time taking into account equations of motion (3), yields the following equation (see appendix 10 for more details):

$$\dddot{\kappa} - 2\left(\mathcal{L}_x + \mathcal{L}_y\right)\ddot{\kappa} + \left(\mathcal{L}_x - \mathcal{L}_y\right)^2 \kappa = 0, \tag{9}$$

where

$$\mathcal{L}_x\kappa = \omega_*^2 \sum_\alpha b_\alpha \kappa(\mathbf{x}+\mathbf{a}_\alpha,\mathbf{y}), \quad \mathcal{L}_y\kappa = \omega_*^2 \sum_\alpha b_\alpha \kappa(\mathbf{x},\mathbf{y}+\mathbf{a}_\alpha). \tag{10}$$

Initial conditions for equation (9), corresponding to initial conditions for particle velocities (6), have the form:

$$\kappa = \kappa_0\delta_D(\mathbf{x}-\mathbf{y}), \quad \dot{\kappa} = 0, \quad \ddot{\kappa} = \left(\mathcal{L}_x + \mathcal{L}_y\right)\left(\kappa_0\delta_D(\mathbf{x}-\mathbf{y})\right), \quad \dddot{\kappa} = 0. \tag{11}$$

where $\kappa_0(\mathbf{x}) = \Big\langle v_0^2(\mathbf{x}) \Big\rangle$; function $\delta_D(\mathbf{x}-\mathbf{y})$ is equal to unity for $\mathbf{x}=\mathbf{y}$ and it is equal to zero for $\mathbf{x}\neq\mathbf{y}$. The first formula form (11) follows from the fact that initial velocities of different particles are uncorrelated random numbers (see formula (6)).

Equation (9) *exactly* describes evolution of kinetic temperature (8) in harmonic scalar lattices. In contrast to formula (6), initial conditions (11) for equation (9) are *deterministic*.

Equation (9) can be solved analytically using, for example, discrete Fourier transform. However the solution is cumbersome even in the one-dimensional case. Therefore in the following section, several simplifications are used.

[9]In numerical simulations, the mathematical expectation can be approximated by an average over realizations with different initial conditions (see e.g. section 7.4).

4 Continualization. Fast and slow thermal processes

In the present section, we simplify equation (9) using continualization with respect to spatial variable [31, 52]. We introduce new variables:

$$(\mathbf{x}, \mathbf{y}) \to (\mathbf{r},\, \mathbf{x}-\mathbf{y})\,, \qquad \mathbf{r} = \frac{\mathbf{x}+\mathbf{y}}{2}. \tag{12}$$

From now on, covariance of velocities is represented in the form $\kappa(\mathbf{r}, \mathbf{x}-\mathbf{y})$. Continualization of equation (9) is carried out with respect to variable $\mathbf{r}$. We assume that function κ is slowly changing with $\mathbf{r}$ at distances of order of $|\mathbf{a}_\alpha|$. Then operators $\mathcal{L}_x, \mathcal{L}_y$ can be approximated by the power series expansion with respect to $\mathbf{a}_\alpha$ (see. appendix 11):

$$\begin{gathered}
\mathcal{L}_x \approx \mathcal{L} + \boldsymbol{\mathcal{R}} \cdot \nabla, \qquad \mathcal{L}_y \approx \mathcal{L} - \boldsymbol{\mathcal{R}} \cdot \nabla, \\
\mathcal{L} = \omega_*^2 \sum_\alpha b_\alpha \mathcal{S}_\alpha, \quad \boldsymbol{\mathcal{R}} = \frac{\omega_*^2}{2} \sum_\alpha \mathbf{a}_\alpha b_\alpha \mathcal{S}_\alpha, \quad \mathcal{S}_\alpha \kappa = \kappa\left(\mathbf{r}, \mathbf{x}-\mathbf{y}+\mathbf{a}_\alpha\right),
\end{gathered} \tag{13}$$

where $\nabla = \frac{\partial}{\partial \mathbf{r}}$ is nabla-operator. Substitution of formula (13) into equation (9) yields:

$$\dddot{\kappa} - 4\mathcal{L}\ddot{\kappa} + 4\left(\boldsymbol{\mathcal{R}} \cdot \nabla\right)^2 \kappa = 0. \tag{14}$$

Here and below arguments $\mathbf{r}, \mathbf{x}-\mathbf{y}$ of function κ are omitted for brevity. Equation (14) is differential with respect to continuum variables $\mathbf{r}$, t and difference with respect to discrete-valued variable $\mathbf{x}-\mathbf{y}$.

Numerical simulations and analysis of equation (14) show that there are two thermal processes. At $t \sim \tau_*, \tau_* = 2\pi/\omega_*$, the value $\kappa|_{\mathbf{x}=\mathbf{y}}$ oscillates and tends to $\kappa_0/2$. At this time-scale the last term in equation (14) is small compared to the first two and can be neglected. Then for $t \sim \tau_*$ dynamics of covariances is governed by the equation

$$\dddot{\kappa} - 4\mathcal{L}\ddot{\kappa} = 0. \tag{15}$$

Equation (15) describes, in particular, oscillations of kinetic temperature caused by redistribution of energy among kinetic and potential parts. This phenomenon is usually observed in molecular dynamics simulations [10]. However to our knowledge, analytical description of this phenomenon for scalar lattices described by equation (3) is not presented in literature.[10] Solution of equation (15) is obtained in the next section.

For $t \gg \tau_*$, changes of κ are caused by the heat transfer. This process is much slower than oscillations of temperature described above. In this case the fourth time-derivative in equation (14) can be neglected:

$$\mathcal{L}\ddot{\kappa} - \left(\boldsymbol{\mathcal{R}} \cdot \nabla\right)^2 \kappa = 0. \tag{16}$$

Hence at $t \gg \tau_*$, dynamics of covariances is described by differential-difference equation (16), which is equivalent to a system of coupled wave equations. Solution of equation (16) gives temperature distribution at every moment of time (see formula (8)). Therefore it can be regarded as a heat transfer equation for harmonic scalar lattices. Solution of equation (16) is obtained in section 6.

Note that equations (14), (15), (16), describing thermal processes in scalar lattices are time reversible, i.e. they are invariant with respect to the substitution $t \to -t$.

[10] Oscillations of temperature in one-dimensional chains and two-dimensional triangular lattice is presented in papers [36, 37] and [38, 39] respectively.

5 Oscillations of temperature (fast process)

In the present section, we solve equation (15), describing oscillations of kinetic temperature caused by equilibration of kinetic and potential energies. According to equation (15), the oscillations in different spatial points are independent. Therefore in the present section the dependence of κ on $\mathbf{r}$ is omitted, i.e. $\kappa = \kappa(\mathbf{x}-\mathbf{y})$. Double integration of equation (15) with respect to time with initial conditions (11), yields:

$$\ddot{\kappa} - 4\mathcal{L}\left(\kappa - \frac{\kappa_0}{2}\delta_D(\mathbf{x}-\mathbf{y})\right) = 0. \tag{17}$$

The initial conditions for equation (17) corresponding to initial conditions (11) are as follows

$$\kappa = \kappa_0\delta_D(\mathbf{x}-\mathbf{y}), \quad \dot{\kappa} = 0. \tag{18}$$

Note that equation (17) is similar to the equation of lattice dynamics (3). Hence there is an analogy between lattice dynamics problem and oscillations of kinetic temperature. Temperature oscillations are described by the same equation and initial conditions as vibrations of the lattice, where one particle has initial displacement and zero initial velocity (displacements and velocities of other particles are equal to zero). This analogy holds for all scalar lattices with equations of motion (3). Similar analogies are mentioned in papers [36, 37, 39, 38].

Equation (17) is solved using the discrete Fourier transform (see Appendix 12 for definition). Since the lattice has simple structure, then vectors $\mathbf{x}-\mathbf{y}$ are represented in the form

$$\mathbf{x}-\mathbf{y} = a\sum_{j=1}^{d} z_j\mathbf{e}_j, \tag{19}$$

where $\mathbf{e}_j$, $j = 1..d$ are unit vectors directed along basis vectors of the lattice; d is space dimensionality; a is an equilibrium distance; z_j are integer numbers. Applying the discrete Fourier transform to equation (17) with respect to z_j, yields

$$\ddot{\hat{\kappa}} - 4\hat{\mathcal{L}}\left(\hat{\kappa} - \frac{\kappa_0}{2}\right) = 0, \qquad \hat{\mathcal{L}} = \omega_*^2\left(b_0 + 2\sum_{\alpha>0} b_\alpha\cos\left(\mathbf{k}\cdot\mathbf{a}_\alpha\right)\right), \tag{20}$$

where $\hat{\kappa}$ is a Fourier image of κ; $\mathbf{k}$ is wave vector; formula for $\hat{\mathcal{L}}$ is derived in appendix 12. Initial conditions for equation (20), corresponding to (11), has the form $\hat{\kappa} = \kappa_0$, $\dot{\hat{\kappa}} = 0$. Then solving equation (20) with the initial conditions and applying the inverse discrete Fourier transform, yields the following expression for kinetic temperature (see appendix 12):

$$T = \frac{T_0}{2}\left(1 + \frac{1}{(2\pi)^d}\int_{-\pi}^{\pi}\cos\bigl(2\omega(\mathbf{k})t\bigr)\mathrm{d}p_1...\mathrm{d}p_d\right), \qquad \mathbf{k} = \frac{1}{a}\sum_{j=1}^{d} p_j\tilde{\mathbf{e}}_j. \tag{21}$$

Here T_0 is the initial temperature; p_j are dimensionless components of the wave vector $\mathbf{k}$ in the reciprocal basis[11] $\tilde{\mathbf{e}}_j$, $j = 1...d$; $\omega(\mathbf{k})$ is the dispersion relation for the lattice (see

[11] Vectors of the reciprocal basis $\tilde{\mathbf{e}}_j$ are defined as $\mathbf{e}_j\cdot\tilde{\mathbf{e}}_k = 1$ for $j = k$ and $\mathbf{e}_j\cdot\tilde{\mathbf{e}}_k = 0$ for $j \neq k$.

Appendix 12):

$$\omega = \omega_* \sqrt{-b_0 - 2\sum_{\alpha>0} b_\alpha \cos\left(\mathbf{k}\cdot\mathbf{a}_\alpha\right)}. \tag{22}$$

For example, consider one-dimensional chain with nearest-neighbor interactions. Substituting parameters (4) into formula (21) after integration, we obtain

$$T = \frac{T_0}{2}\Big(1 + J_0(4\omega_* t)\Big), \tag{23}$$

where J_0 is the Bessel function of the first kind. Formula (23) shows that kinetic temperature in the chain with initial conditions (6) tends to the stationary value $T_0/2$. Deviation from the stationary value decays inversely proportional to the square root of time[12]. Formula (23) coincides with results obtained in paper [36].

Thus oscillations of kinetic temperature in scalar lattices are described by integral (21). Integrand in formula (21) changes sign and oscillates with frequency proportional to time. Therefore the integral tends to zero[13], while temperature tends to the stationary value $T_0/2$. The latter fact also follows from the virial theorem [53]. However in contract to formula (21), the virial theorem does not describe the transition to the stationary state. Analysis of this transient process for stretched square lattice performing out-of-plane vibrations is presented in section 7.

6 Unsteady heat transfer (slow process)

6.1 The general solution

Heat transfer in scalar lattices is described by equation (16). In the present section, we solve this equation for arbitrary initial temperature distribution. The following initial conditions for covariances are considered:

$$\kappa = \frac{k_B}{M} T_0(\mathbf{r})\delta_D(\mathbf{x}-\mathbf{y}), \quad \dot\kappa = 0, \tag{24}$$

where $T_0(\mathbf{r})$ is spatial distribution of temperature after the transient processes described in the previous section[14].

Applying the discrete Fourier transform to equation (16) with respect to $\mathbf{x}-\mathbf{y}$, yields:

$$\hat{\mathcal{L}}\ddot{\hat\kappa} - \Big(\hat{\boldsymbol{\mathcal{R}}}\cdot\nabla\Big)^2 \hat\kappa = 0, \qquad \hat{\boldsymbol{\mathcal{R}}} = i\omega_*^2 \sum_{\alpha>0} b_\alpha \mathbf{a}_\alpha \sin\left(\mathbf{k}\cdot\mathbf{a}_\alpha\right). \tag{25}$$

where i is the imaginary unit, $\hat{\mathcal{L}}$ is given by formula (20). The initial conditions for $\hat\kappa$ follows from (24):

$$\hat\kappa = \frac{k_B}{M} T_0(\mathbf{r}), \qquad \dot{\hat\kappa} = 0. \tag{26}$$

[12]This fact follows from the asymptotic representation of Bessel function J_0.

[13]Rigorous proof of this fact is beyond the scope of the present paper. Investigation of integrals of this type can be carried out using asymptotic methods [54].

[14]Temperature T_0 at every point is equal to a half of the temperature corresponding to initial velocities of particles (6).

Solution of equation (25) is represented as a linear combination of solutions of the following equations:

$$\dot{\hat{\kappa}} + \mathbf{c} \cdot \nabla \hat{\kappa} = 0, \qquad \dot{\hat{\kappa}} - \mathbf{c} \cdot \nabla \hat{\kappa} = 0, \qquad \mathbf{c} = \frac{\mathrm{Im}\hat{\boldsymbol{\mathcal{R}}}}{\sqrt{-\hat{\mathcal{L}}}}. \tag{27}$$

Here Im(...) denotes the imaginary part. In appendix 12, it is shown that $\mathbf{c}$ coincides with vector of group velocity for the lattice:

$$\mathbf{c} = \frac{\mathrm{d}\omega}{\mathrm{d}\mathbf{k}} = \frac{\omega_* \sum\limits_{\alpha>0} b_\alpha \mathbf{a}_\alpha \sin\left(\mathbf{k} \cdot \mathbf{a}_\alpha\right)}{\sqrt{-b_0 - 2\sum\limits_{\alpha>0} b_\alpha \cos\left(\mathbf{k} \cdot \mathbf{a}_\alpha\right)}}, \tag{28}$$

where $\omega(\mathbf{k})$ is the dispersion relation for the lattice given by formula (22). Solving equations (27) with initial conditions (24)[15], applying the inverse discrete Fourier transform, and using the expression for temperature (8), yields:

$$T = \frac{1}{2(2\pi)^d} \int_{-\pi}^{\pi} \Big(T_0\left(\mathbf{r} + \mathbf{c}(\mathbf{k})t\right) + T_0\left(\mathbf{r} - \mathbf{c}(\mathbf{k})t\right) \Big) \mathrm{d}p_1 ... \mathrm{d}p_d, \qquad \mathbf{k} = \frac{1}{a} \sum_{j=1}^{d} p_j \tilde{\mathbf{e}}_j. \tag{29}$$

Formula (29) is the general solution of the unsteady heat transfer problem for scalar lattices. Note that the solution is time reversible, i.e. invariant to the substitution $t \to -t$.

For example, consider one-dimensional chain with nearest-neighbor interactions. Substitution of formulas (4) into expression for group velocity (28), yields

$$c = \omega_* a \cos\frac{p}{2} \operatorname{sign} p. \tag{30}$$

Then the general solution has form

$$T = \frac{1}{\pi} \int_0^{\frac{\pi}{2}} \Big(T_0(x + c_* t \cos p) + T_0(x - c_* t \cos p) \Big) \mathrm{d}p, \qquad c_* = \omega_* a. \tag{31}$$

Formula (31) coincides with analytical solution obtained in paper [31].

Thus the evolution of kinetic temperature in scalar lattices is described by the integral (29). Formula (29) shows that spatial distribution of temperature is represented as the superposition of waves traveling with group velocities $\mathbf{c}(\mathbf{k})$ and having a shape of initial temperature distribution T_0. This is the main result of the present paper.

6.2 Length-dependence of the effective heat conductivity

From formulas (29), (37) it follows that the heat transfer in scalar lattices is ballistic and it can not be described by the Fourier law. In this case the notion of heat conductivity is ambiguous. Therefore the heat conductivity can be defined differently in different problems. In literature, the heat conductivity is usually calculated for problem of stationary heat transfer between two reservoirs with different temperature [9, 13, 11, 17]. In papers [11], [17] it is shown that the heat conductivity in harmonic crystals linearly depend

[15]The general solution for equations of this kind is given, for example, in book [55].

on the length of the system (distance between the reservoirs). In the present section, the heat conductivity is calculated for an unsteady problem.

Thermal contact of two half-spaces having different initial temperatures is considered. Initial distribution of temperature has the form

$$T_0(x) = T_1 + (T_2 - T_1)H(x), \tag{32}$$

where H is the Heaviside function; T_1, T_2 are initial temperatures of the half-spaces $x < 0$ and $x > 0$ respectively. We define the heat conductivity as follows

$$\lambda = -\frac{\int_{-L}^{L} h(x,t)\mathrm{d}x}{T(L) - T(-L)}, \tag{33}$$

where h is a projection of the heat flux on the x-axis[16]; L is a half-length of averaging interval. If the Fourier law is valid, then equation (33) is satisfied identically and the heat conductivity is independent on length L. We show that for scalar lattices it is not the case.

We calculate the heat flux h using continuum equation of energy balance[17]:

$$\rho\dot{U} = -h', \qquad \rho = \frac{M}{V}, \tag{34}$$

where V is a volume of per particle. The internal energy per unit mass U is calculated using formula[18]:

$$U = \frac{k_B T}{M}. \tag{35}$$

Substituting formula (35) into equation of energy balance (34) yields

$$\frac{k_B}{V}\dot{T} = -h' \tag{36}$$

Formula (36) is used for calculation of the heat flux for given temperature distribution.

In the case of one-dimensional initial temperature distribution $T_0(x)$ in the d-dimensional lattice, the general solution (29) takes the form

$$T = \frac{1}{2(2\pi)^d}\int_{-\pi}^{\pi}\Big(T_0\left(x + c_x t\right) + T_0\left(x - c_x t\right)\Big)\mathrm{d}p_1 ... \mathrm{d}p_d, \qquad c_x = \mathbf{c}\cdot\mathbf{i}, \tag{37}$$

where $\mathbf{i}$ is a unit vector directed along x-axis. Using formula (37) we show that the solution of the problem with initial distribution of temperature (32) is self-similar:

$$T = T_1 + \frac{T_2 - T_1}{2(2\pi)^d}\int_{-\pi}^{\pi}\left[H\left(\frac{x}{t} - c_x\right) + H\left(\frac{x}{t} + c_x\right)\right]\mathrm{d}p_1 ... \mathrm{d}p_d = T\left(\frac{x}{t}\right). \tag{38}$$

Integrating both parts of formula (34) from $-\infty$ to x and assuming that $h(-\infty) = 0$, we obtain:

$$h = -\frac{k_B}{V}\int_{-\infty}^{x}\frac{\mathrm{d}}{\mathrm{d}t}T\left(\frac{z}{t}\right)\mathrm{d}z = \frac{k_B}{V}\int_{-\infty}^{\frac{x}{t}} yT'\left(y\right)\mathrm{d}y \quad \Rightarrow \quad h = h\left(\frac{x}{t}\right). \tag{39}$$

[16]The relation between the heat flux, forces and particle velocities is not used in the present derivations.

[17]Macroscopic mechanical deformation of the lattice and volumetric heat sources in the present model are absent.

[18]From the virial theorem it follows that kinetic and potential energies per particle are equal to $k_B T/2$. Then the total energy per particle is equal to $k_B T$.

Here prime denotes the derivative with respect to x/t. Formula (39) shows that the heat flux is also self-similar.

The heat conductivity is calculated using formula (33). We choose L equal to the distance traveled by the heat front, i.e. $L = c_* t$, where c_* is the speed of the heat front equal to the maximum group velocity[19]. Then $T(L) - T(-L) = T_2 - T_1$. Substituting this expression into the definition of the heat conductivity (33) and taking into account formula (39), yields:

$$\lambda = -\frac{L}{T_2 - T_1} \int_{-1}^{1} h\left(z\right) \mathrm{d}z \quad \Rightarrow \quad \lambda \sim L. \tag{40}$$

Formula (40) shows that the effective heat conductivity linearly diverges with length L. This fact is in agreement with results obtained in papers [11], [17] for the steady-state heat transfer problem. Note that formula (40) is derived for any scalar lattice described by equations of motion (3).

6.3 Fundamental solution for one-dimensional chains. Speed of the heat front

In the present section, we derive fundamental solution of the heat transfer problem for one-dimensional chains described by equations (3). The following initial distribution of temperature is considered

$$T_0(x) = A\delta(x), \tag{41}$$

where δ is the Dirac delta function. The multiplier A is introduced in order to obtain solution in proper units. In this case the solution (29) has the form:

$$T = \frac{A}{2\pi} \int_0^{\pi} \Big(\delta\left(x - ct\right) + \delta\left(x + ct\right) \Big) \mathrm{d}p, \qquad c = \frac{\omega_* a \sum\limits_{\alpha>0} b_\alpha \alpha \sin\left(\alpha p\right)}{\sqrt{-b_0 - 2\sum\limits_{\alpha>0} b_\alpha \cos\left(\alpha p\right)}}. \tag{42}$$

The integral is calculated using the identity [56]:

$$\int \delta\left(\phi(x)\right) \psi(x) \mathrm{d}x = \sum_j \frac{\psi(x_j)}{|\phi'(x_j)|}, \qquad \phi(x_j) = 0. \tag{43}$$

Here summation is carried out over real roots of the equation $\phi(x) = 0$. Calculation of the integral (42) using identity (43), yields the fundamental solution:

$$T = \frac{A}{2\pi t} \sum_j \frac{1}{|c'(p_j)|}, \qquad |c(p_j)| = \frac{|x|}{t}, \qquad c' = \frac{\mathrm{d}c}{\mathrm{d}p}, \tag{44}$$

Here summation is carried out over all real roots of the second equation $p_j \in [-\pi; \pi]$. Function c is defined by formula (28). Formula (44) shows that the temperature tends to infinity at extremes of function $c(p)$.

[19] We prove that the heat front moves with constant speed in the next.

For example, consider the one-dimensional chain with nearest-neighbor interactions. Substitution of expression (30) for the group velocity into equation (44) yields:

$$T = \frac{A}{\pi c_* t \sqrt{1 - \left(\frac{x}{c_* t}\right)^2}}, \qquad c_* = \omega_* a. \tag{45}$$

Formula (45) coincides with analytical solution obtained in paper [31].

Thus formula (44) gives the fundamental solution of the heat transfer problem for one-dimensional chains. The general solution corresponding to the initial temperature distribution $T_0(x)$ has the form:

$$T = \frac{c_*}{2\pi} \sum_j \int_{-1}^{1} \frac{T_0(x + z c_* t)}{|c'(p_j)|} \mathrm{d}z, \qquad |c(p_j)| = c_* |z|. \tag{46}$$

We calculate the speed of heat front propagation in one-dimensional chains. Assume that function $c(p)$ is limited. Therefore there exist a maximum value of $|x|$ such that the second equation from formula (44) has a solution. This value correspond to the heat front. From formulas (44) it follows that the heat front of fundamental solution propagates with finite speed c_*, equal to the maximum group velocity:

$$c_* = \max_p |c(p)|. \tag{47}$$

The general solution corresponding to the initial temperature distribution $T_0(x)$ is given by formula (46). Assume that $T_0(x)$ is nonzero on the interval $[x_{min}; x_{max}]$. Then from formula (46) it follows that at time t the temperature is nonzero on the interval $[x_{min} - c_* t; x_{max} + c_* t]$. Therefore the heat front in one-dimensional chains propagates with constant speed equal to the maximum group velocity. This result was also obtained in paper [30] using asymptotic analysis.

6.4 Fundamental solution for two-dimensional lattices

In the present section, we derive the fundamental solution of the heat transfer problem for two-dimensional scalar lattices. The following distribution of initial temperature is considered:

$$T_0 = A\delta(\mathbf{r}) = A\delta(x)\delta(y), \tag{48}$$

where x,y are Cartesian coordinates. Substitution of the initial conditions (48) into formula (29) yields

$$T = \frac{A}{8\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \Big(\delta\left(\mathbf{r} + \mathbf{c}t\right) + \delta\left(\mathbf{r} - \mathbf{c}t\right) \Big) \mathrm{d}p_1 \mathrm{d}p_2. \tag{49}$$

Radius-vector $\mathbf{r}$ and vector of group velocity $\mathbf{c}$ are represented as

$$\mathbf{r} = x\mathbf{i} + y\mathbf{j}, \qquad \mathbf{c} = c_x\mathbf{i} + c_y\mathbf{j}, \tag{50}$$

where $\mathbf{i}$, $\mathbf{j}$ are unit vectors corresponding to x and y axes. Then changing the integration variables $(p_1, p_2) \to (c_x, c_y)$ in formula (49) and calculating the integral using the identity (43), we obtain

$$T = \frac{A}{8\pi^2 t^2} \sum_j \frac{1}{|G(p_1^j, p_2^j)|}, \qquad G = \frac{\partial c_x}{\partial p_1}\frac{\partial c_y}{\partial p_2} - \frac{\partial c_x}{\partial p_2}\frac{\partial c_y}{\partial p_1},$$
$$\left[\begin{array}{l} c_x = \dfrac{x}{t}, \quad c_y = \dfrac{y}{t}, \\ c_x = -\dfrac{x}{t}, \quad c_y = -\dfrac{y}{t}, \end{array}\right. \tag{51}$$

where G is the Jacobian of the transformation; square bracket stands for logical "or"; summation is carried out over the roots of the last two equations $p_1^j, p_2^j \in [-\pi; \pi]$. Two facts follow from formulas (51). Firstly, the temperature is nonzero at points satisfying the inequality:

$$\left(\frac{x}{c_* t}\right)^2 + \left(\frac{y}{c_* t}\right)^2 \le 1, \qquad c_*^2 = \max_{p_1, p_2} \left(c_x^2 + c_y^2\right). \tag{52}$$

Secondly, the temperature at the central point $x = 0, y = 0$ decays as $1/t^2$.

Thus the fundamental solution of the heat transport problem for two-dimensional scalar lattices is given by formulas (51). The solution has circular front propagating with maximum group velocity c_*. For example, the fundamental solution for stretched square lattice performing out-of-plane vibrations is obtained in section 7.7.

7 Example: out-of-plane vibrations of a square lattice

7.1 General formulas

In the present section, we consider out-of-plane vibrations of a stretched square lattice. Initial radius-vectors of the particles have the form:

$$\mathbf{x}_{n,m} = a\left(n\mathbf{i} + m\mathbf{j}\right), \tag{53}$$

where $\mathbf{i}$, $\mathbf{j}$ are orthogonal unit vectors; a is an initial distance between the nearest neighbors. Particles are connected with the nearest neighbors by linear springs. Equilibrium length of the springs is less than a, i.e. the lattice is stretched[20]. Then linearized equations for out-of-plane vibrations of the lattice have the form[21]:

$$\ddot{u}_{n,m} = \mathcal{L}u_{n,m}, \qquad \mathcal{L}u_{n,m} = \omega_*^2\left(u_{n+1,m} + u_{n,m+1} - 4u_{n,m} + u_{n-1,m} + u_{n,m-1}\right), \tag{54}$$

where $u_{n,m} = u(\mathbf{x}_{n,m})$ is a component of displacement normal to plane of the lattice. It is seen that equation (54) is a particular case of equation (3), where parameters ω_*, $\mathbf{a}_\alpha$, b_α are determined by formula (5).

[20] Otherwise the out-of-plane vibrations of the lattice are nonlinear.

[21] In harmonic approximation, in-plane and out-of-plane vibrations of the lattice are independent. The in-plane vibrations of the lattice are beyond the scope of the present paper.

The dispersion relation and group velocity are calculated using formulas (5), (22), (28):

$$\omega = 2\omega_* \sqrt{\sin^2 \frac{p_1}{2} + \sin^2 \frac{p_2}{2}}, \quad \mathbf{c} = \frac{c_* \left(\sin p_1 \mathbf{i} + \sin p_2 \mathbf{j}\right)}{2\sqrt{\sin^2 \frac{p_1}{2} + \sin^2 \frac{p_2}{2}}}, \quad \mathbf{k} = \frac{1}{a}\left(p_1 \mathbf{i} + p_2 \mathbf{j}\right), \tag{55}$$

where $c_* = \omega_* a$ is the maximum group velocity.

7.2 Oscillations of kinetic temperature

In the present section, we consider the following initial conditions for particles corresponding to uniform distribution of instantaneous temperature T_0:

$$u_{n,m} = 0, \qquad v_{n,m} = v_0, \tag{56}$$

where v_0 is a random quantity with dispersion $\left\langle v_0^2 \right\rangle = k_B T_0 / M$. In this case initial kinetic and potential energies of the system are not equal. Equilibration of energies leads to oscillations of the kinetic temperature. The oscillations are described by formula (21). Substitution of dispersion relation (55) into formula (21), yields:

$$T = \frac{T_0}{2}\Big(1 + \frac{1}{\pi^2} \int_0^\pi \int_0^\pi \cos\left(4\omega_* t \sqrt{\sin^2 \frac{p_1}{2} + \sin^2 \frac{p_2}{2}}\right) \mathrm{d}p_1 \mathrm{d}p_2\Big). \tag{57}$$

In order to check the accuracy of formula (57), we compare the results with numerical solution of equations of motion (54). Leap-frog integration scheme with time-step equal to $0.005\tau_*$, $\tau_* = 2\pi/\omega_*$ is used. Periodic boundary conditions in both directions are used. Square periodic cell contains 10^6 particles. During the simulation the kinetic temperature of the entire system is calculated. The dependence of temperature on time is shown in figure 1. Every point on the plot corresponds to average over 10 realizations with different initial conditions. The standard error of the mean is of order of circle diameter. Figure 1 shows that analytical solution (57) coincides with results of numerical solution of lattice dynamics equations (54).

Temperature oscillations caused by equilibration of kinetic and potential energies decays in time. Characteristic time of the decay is of order of several periods τ_*. Multiplying the temperature by time it can be shown that deviation from the stationary value decays as $1/t$. The same process in one-dimensional chain decays as $1/\sqrt{t}$. Heat propagation is a much slower process. For example, during τ_* the heat front passes the distance equal to $2\pi a$, which is small from macroscopic point of view.

Thus the example considered in the present section shows that oscillations of temperature and heat propagation have different time scales and can be considered separately.

7.3 Fundamental solution of the planar problem

In the present section, we derive the fundamental solution of planar heat transport problem for scalar square lattice. The following initial temperature distribution is considered:

$$T_0(x) = A\delta(x), \tag{58}$$

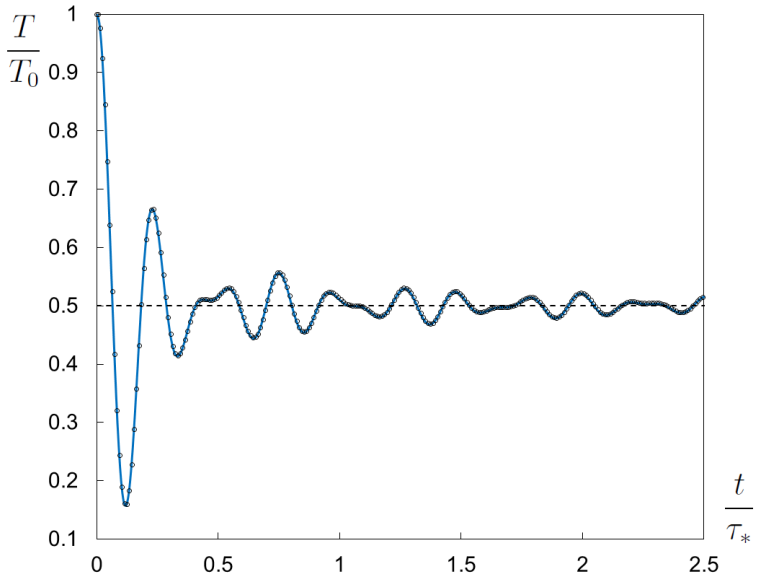

Figure 1: Oscillations of temperature in uniformly heated scalar square lattice. Line — analytical solution (57), circles — numerical solution of lattice dynamics equations (54).

where x is directed along the basis vector $\mathbf{a}_1 = a\mathbf{i}$. Substituting the initial conditions into formula (37) and taking into account formula (55), yields:

$$T = \frac{A}{2\pi^2}\int_0^\pi\int_0^\pi \Big(\delta\left(x - c_x t\right) + \delta\left(x + c_x t\right)\Big)\mathrm{d}p_1\mathrm{d}p_2, \qquad c_x = \frac{c_* \sin p_1}{2\sqrt{\sin^2\dfrac{p_1}{2} + \sin^2\dfrac{p_2}{2}}}, \quad (59)$$

We make a substitution $\beta = \sin^2\frac{p_1}{2}$, $\gamma = \sin^2\frac{p_2}{2}$ and consider the case $t > 0$, $x > 0$. Solution for $x < 0$ is obtained using symmetry of the problem. Then (59) takes the form:

$$T = \frac{A}{2\pi^2}\int_0^1\int_0^1 \frac{\delta\left(\tilde{x} - \sqrt{\frac{\beta(1-\beta)}{\beta+\gamma}}\right)}{\sqrt{\beta\gamma(1-\beta)(1-\gamma)}}\mathrm{d}\beta\mathrm{d}\gamma, \qquad \tilde{x} = \frac{x}{c_* t}. \quad (60)$$

One of the integrals is evaluated using the identity (43). The argument of delta-function in formula (60) has roots given by the following equation

$$\gamma = \frac{\beta}{\tilde{x}^2}\left(1 - \tilde{x}^2 - \beta\right). \quad (61)$$

By the definition $0 \le \gamma \le 1$. Then formula (61) yields the inequalities for β:

$$\beta \le 1 - \tilde{x}^2, \qquad \beta^2 - (1 - \tilde{x}^2)\beta + \tilde{x}^2 \ge 0. \quad (62)$$

Solving the inequality (62) and using the identity (43), we obtain:

$$\begin{aligned} T &= \frac{A}{\pi^2 c_* t|\tilde{x}|}\begin{cases} f(0, 1-\tilde{x}^2), & \sqrt{2}-1 \le |\tilde{x}| \le 1, \\ f(0,\beta_1) + f(\beta_2, 1-\tilde{x}^2), & |\tilde{x}| \le \sqrt{2}-1, \end{cases} \\ \beta_{1,2} &= \frac{1}{2}\left(1 - \tilde{x}^2 \mp \sqrt{(1-\tilde{x}^2)^2 - 4\tilde{x}^2}\right), \\ f(\xi_1,\xi_2) &= \int_{\xi_1}^{\xi_2}\left(\frac{1-\beta}{(1-\tilde{x}^2-\beta)(\tilde{x}^2 - \beta(1-\tilde{x}^2-\beta))}\right)^{\frac{1}{2}}\mathrm{d}\beta, \end{aligned} \quad (63)$$

and $T = 0$ for $|\tilde{x}| \geq 1$. Formula (63) shows that function Tc_*t/A depends only on the self-similar variable $\tilde{x}$ (see figure 2). It is seen from figure 2 that the heat front moves with

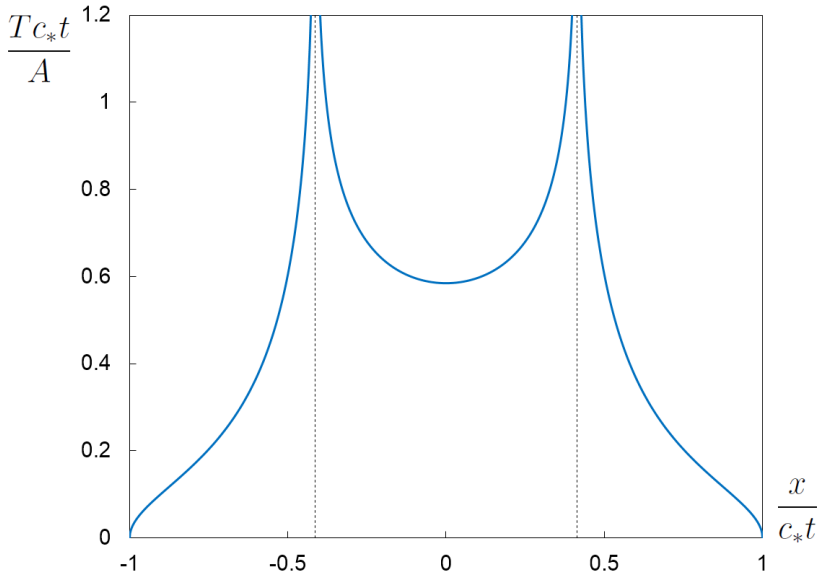

Figure 2: Solution of the heat transfer problem with initial conditions (58). Solid line — formula (63); dashed lines— vertical asymptotes at $|\tilde{x}| = \sqrt{2} - 1$.

constant speed equal to c_*. Temperature have singularities at the points $|\tilde{x}| = \sqrt{2} - 1$. Note that in one-dimensional chain the temperature in similar problem has singularities at the heat front $|\tilde{x}| = 1$ (see formula (45)).

7.4 Thermal contact of hot and cold half-planes

Consider thermal contact of two half-planes of scalar square lattice with initial temperatures T_1 and T_2 (see formula (32)). Substituting initial conditions (32) into the solution (37) and taking into account properties of the Heaviside function and function c_x, yields:

$$T = \frac{T_1 + T_2}{2} + (T_2 - T_1) w\left(\frac{|x|}{t}\right) \operatorname{sign}(x), \qquad w = \frac{1}{2\pi^2}\int_0^\pi \int_0^\pi H\left(|x| - c_x t\right) \mathrm{d}p_1 \mathrm{d}p_2. \quad (64)$$

We make the substitution $\beta = \sin^2 \frac{p_1}{2}$, $\gamma = \sin^2 \frac{p_2}{2}$, then

$$w = \frac{1}{2\pi^2}\int_0^1 \int_0^1 \frac{H\left(|\tilde{x}| - \sqrt{\frac{\beta(1-\beta)}{\beta+\gamma}}\right)}{\sqrt{\beta\gamma(1-\beta)(1-\gamma)}} \mathrm{d}\beta \mathrm{d}\gamma. \quad (65)$$

Integrand in formula (65) is nonzero if the following inequality is satisfied:

$$\gamma \geq \frac{\beta}{\tilde{x}^2}\left(1 - \tilde{x}^2 - \beta\right). \quad (66)$$

The inequality (66) is satisfied identically for $\beta > 1 - \tilde{x}^2$; β also satisfies the second inequality from (62). Then evaluation of the integral with respect to β, yields:

$$w = \frac{1}{4} + \frac{1}{2\pi}\arcsin|\tilde{x}| - \begin{cases} g(0, 1-\tilde{x}^2), & \sqrt{2}-1 \le |\tilde{x}| \le 1, \\ \dfrac{\arcsin\beta_2 - \arcsin\beta_1}{2\pi} + g(0,\beta_1) + g(\beta_2, 1-\tilde{x}^2), & |\tilde{x}| \le \sqrt{2}-1, \end{cases}$$
$$g(z_1, z_2) = \frac{1}{2\pi^2}\int_{z_1}^{z_2} \frac{\arcsin\left(\frac{2\beta}{\tilde{x}^2}(1-\tilde{x}^2-\beta)-1\right)}{\sqrt{\beta(1-\beta)}}\mathrm{d}\beta, \tag{67}$$

where β_1, β_2 are defined by formula (63); $w = \frac{1}{2}$ for $|\tilde{x}| \ge 1$.

Thus solution of the problem is given by formulas (64), (67). It is seen that the solution (67) is self-similar and it depends on $\tilde{x} = x/(c_* t)$.

We check the accuracy of formulas (64), (67) using numerical solution of lattice dynamics equations (54). Without loss of generality we put $T_2 = 2T_1$. In this case, initial conditions for particles has the form:

$$u_{n,m} = 0, \qquad v_{n,m} = \begin{cases} v_0, & n < 0, \\ \sqrt{2}v_0 & n >= 0. \end{cases} \tag{68}$$

where v_0 is a random quantity with dispersion $\left\langle v_0^2 \right\rangle = 2k_B T_1/M$. Periodic boundary conditions are used. The periodic cell contains $4 \cdot 10^6$ particles ($4 \cdot 10^2$ in x direction and 10^4 in y direction). In order to compute temperature, we consider 10^3 realizations with initial conditions (68). Then temperature is computed by formula (8), where mathematical expectation is approximated by an average over realizations. Since the solution is self-similar, then it is sufficient to consider only one moment of time. Temperature distribution at $t = 15\tau_*$ is computed. At this moment oscillations of kinetic temperature described in section 7.2 practically vanish. The temperature distribution is additionally averaged in y direction. Comparison of numerical results with analytical solution (67) is shown in figure 3. Small differences between analytical and numerical solutions are observed in the vicinity of the central point $x = 0$. At this point the temperature has large gradient (initially it is infinite) and therefore the long-wave approximation looses the accuracy. Far from the central point, analytical solution (67) almost coincide with numerical results.

7.5 Rectangular distribution of initial temperature

We demonstrate once again that the heat transfer in scalar square lattice is ballistic. Rectangular distribution of initial temperature is considered:

$$T = T_0\Big(H(x+L) - H(x-L)\Big), \tag{69}$$

where L is a half-length of the interval with nonzero initial temperature. Solution of the problem with initial conditions (69) can be obtained using formula (67) and the superposition principle. The resulting distribution of temperature at several moments of time is shown in figure 4. Figure 4 clearly shows two "thermal waves" traveling in opposite directions.

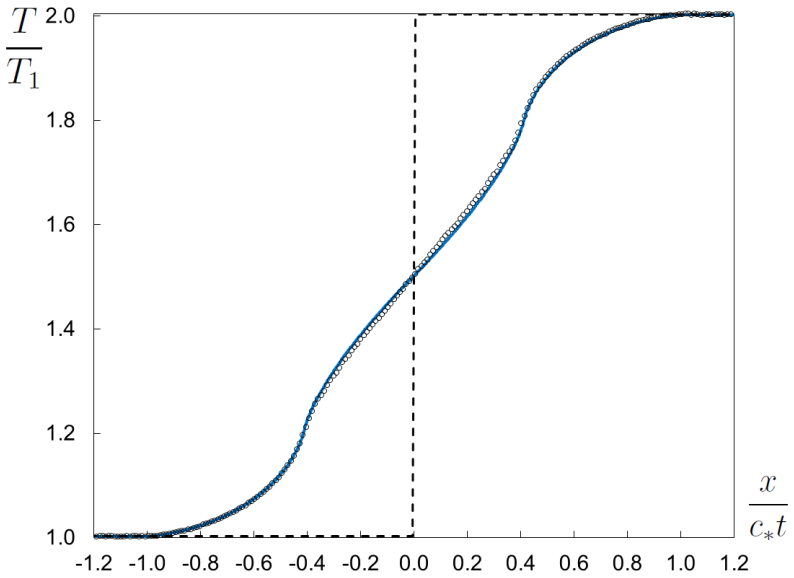

Figure 3: Contact of hot and cold half-planes: self-similar temperature profile. Line — analytical solution (67), circles — numerical solution of lattice dynamics equations (54).

7.6 Sinusoidal distribution of initial temperature

Consider the decay of initial sinusoidal temperature distribution:

$$T_0(x) = B_0 \sin \frac{2\pi x}{L} + B_1, \tag{70}$$

where L is wave-length of initial temperature distribution; $B_1 \geq B_0$. Fourier's law as well as the hyperbolic heat transfer equation [34], [35] predict that amplitude of sin decays exponentially. In this section, we show using analytical solution (37) and numerical simulations that the amplitude decays inversely proportional to time.

Substituting the initial temperature distribution (70) into the general solution (37), yields[22]:

$$T = B(t) \sin \frac{2\pi x}{L} + B_1, \qquad B = \frac{B_0}{\pi^2} \int_0^\pi \int_0^\pi \cos \left(\frac{\pi c_* t \sin p_1}{L \sqrt{\sin^2 \frac{p_1}{2} + \sin^2 \frac{p_2}{2}}} \right) \mathrm{d}p_1 \mathrm{d}p_2. \tag{71}$$

It is seen that amplitude of the sin wave B is a function of dimensionless time $c_* t/L$.

We check the accuracy of formula (71) using numerical solution of lattice dynamics equations (54). Particles have random initial velocities such that after a transient process described in section 7.2, initial conditions (70) are satisfied. Periodic boundary conditions in both directions are used. The periodic cell contains $2 \cdot 10^6$ particles. Size of the periodic cell in x direction is equal to $L = 2 \cdot 10^2 a$. Results are averaged over 10^3 realizations with different initial conditions. The dependence of amplitude B on dimensionless time $c_* t/L$ is shown in figure 5. Every circle on the plot corresponds to average over realizations. Standard error of mean is of order of circle's diameter. Figure 5 shows that analytical

[22]The identity $\sin(x \pm y) = \sin x \cos y \pm \sin y \cos x$ is used for derivation.

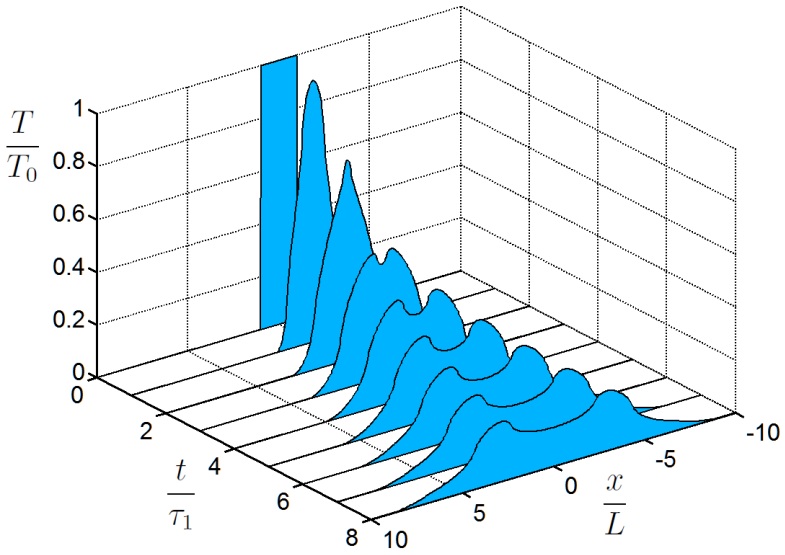

Figure 4: Evolution of rectangular initial temperature distribution in scalar square lattice. Here $\tau_1 = 2\pi L/c_*$.

solution (71) practically coincides with results of numerical solution of lattice dynamics equations (54).

Thus amplitude of sinusoidal distribution of initial temperature in scalar square lattice decays inversely proportional to time. In the one-dimensional chain with nearest neighbor interactions, the same oscillations are described by the Bessel function of the first kind [32, 31], which decays inversely proportional to square root of time.

7.7 Fundamental solution

The fundamental solution of heat transport problem for two-dimensional scalar lattices is given by formula (51). In order to obtain the solution for square lattice, we calculate the Jacobian G using formulas (51) and (55):

$$G = -\frac{c_*^2\left(\cos p_1 \sin^4\frac{p_2}{2} + \cos p_2 \sin^4\frac{p_1}{2}\right)}{4\left(\sin^2\frac{p_1}{2} + \sin^2\frac{p_2}{2}\right)^2}. \tag{72}$$

We make two consecutive substitutions in formulas (51), (72): $s_1 = \sin^2\frac{p_1}{2}, s_2 = \sin^2\frac{p_2}{2}$ and $w = s_1 s_2$, $q = s_1 + s_2$. Then excluding w we obtain:

$$\begin{aligned} &T = \frac{A}{(\pi c_* t)^2}\sum_j \frac{q_j}{|q_j^2 - \tilde{r}^2(q_j+1)|}, \\ &q_j^3 - 2\left(\tilde{r}^2+1\right)q_j^2 + \left((\tilde{r}^2+1)^2 - 4\tilde{x}^2\tilde{y}^2 + 1\right)q_j - 2\tilde{r}^2 = 0. \end{aligned} \tag{73}$$

where $\tilde{r}^2 = 1 - \tilde{x}^2 - \tilde{y}^2$, $\tilde{x} = \frac{x}{c_* t}$, $\tilde{y} = \frac{y}{c_* t}$. Summation is carried out with respect to all real roots q_j of the given cubic equation such that $q_j \in [0; 2]$. Formula (73) shows that the function $Tc_*^2t^2/A$ is self-similar.

Formula (73) gives closed-form fundamental solution for harmonic scalar square lattice. According to formula (73), the temperature is nonzero inside the circle $\tilde{x}^2 + \tilde{y}^2 \le 1$. It

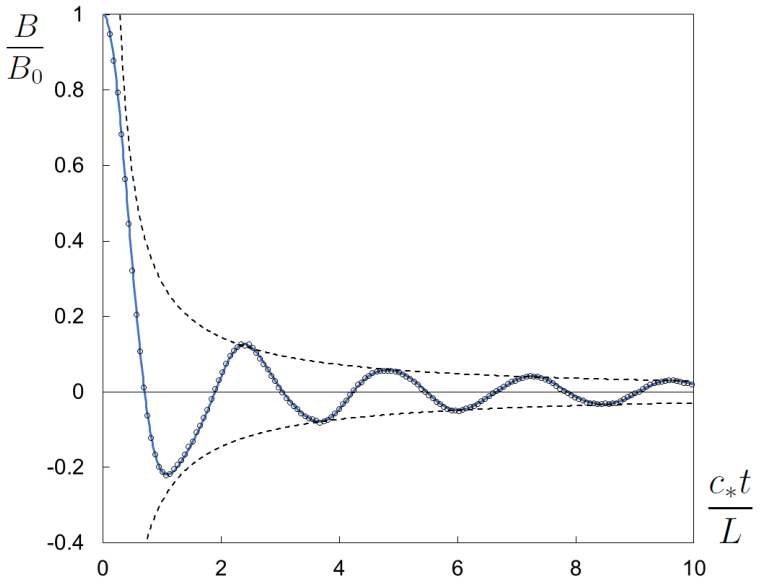

Figure 5: Decay of amplitude of initial sinusoidal temperature distribution. (70). Solid line — analytical solution (71), circles — numerical solution of lattice dynamics equations (54), dashed lines — envelope $\pm 0.29L/(c_* t)$.

has singularity along the line determined by the following system of equations:

$$\tilde{x}^2 + \tilde{y}^2 = 1 - \frac{q^2}{q+1}, \qquad \tilde{x}^2 \tilde{y}^2 = \frac{2 - q^2}{4(q+1)^2}. \tag{74}$$

The line (74) is shown in figure 6. It intersects $\tilde{x}$-axis at the points $\pm(\sqrt{2} - 1)$.

Fundamental solution (73) is symmetrical with respect to axes $\tilde{x}$ and $\tilde{y}$. Solution for positive $\tilde{x}$, $\tilde{y}$ is shown in figure 7. We check the accuracy of fundamental solution (73) as follows. Problems described in sections 7.3, 7.4 are solved using the convolution of the fundamental solution with corresponding initial conditions. It is shown that the resulting temperature distribution coincides with results obtained in sections 7.3, 7.4.

Thus the closed-form fundamental solution of unsteady heat transfer problem for scalar square lattice is given by formula (73). We note the analogy between our result (73) and results obtained in paper [41]. In paper [41], spatial distribution of energy corresponding to the fundamental solution of equations of motion (3) is obtained using Wigner transform. The energy distribution is similar to temperature distribution shown in figure 7. Therefore there is an analogy between deterministic lattice dynamics problem [41] and the unsteady heat transfer problem discussed above. Detailed discussion of the analogy is beyond the scope of the present paper.

8 Conclusions

An analytical description of unsteady heat transfer in infinite harmonic scalar lattices was presented. The heat transfer problem for a lattice with arbitrary initial temperature distribution was solved analytically. Evolution of spatial temperature distribution is described by a superposition of waves having a shape of initial temperature distribution and

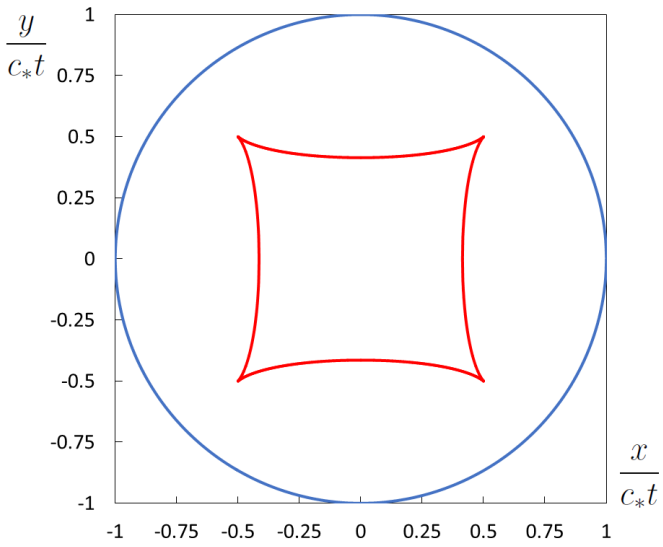

Figure 6: Heat front (circle) and line with infinite temperature (equation (74)) corresponding to the fundamental solution (73).

traveling with group velocity (see formula (29)). Therefore in harmonic scalar lattices the heat propagates ballistically. The heat front propagates with constant speed equal to the maximum group velocity. The solution of heat transfer problem has the same property as the equations of motions: it is time-reversible, i.e. invariant to the substitution $t \to -t$. Therefore Loschmidt's paradox [57] in the present system is absent.

Closed-form fundamental solutions of the unsteady heat transfer problem for one- and two-dimensional scalar lattices were derived. The solutions at the origin $\mathbf{r} = 0$ decay as $1/t^d$, where d is space dimensionality. Analytical solutions of problems with stepwise and sinusoidal distributions of initial temperature for scalar square lattice were presented. Comparison of analytical results with numerical solution of lattice dynamics equations shows that presented theory describes the propagation of heat in harmonic scalar lattices with high accuracy.

Additionally, the transition of scalar lattice with random initial velocities and zero displacements towards the steady state was discussed. It was shown that the transition is accompanied by high-frequency oscillations of kinetic temperature exactly described by formula (21). The oscillations are caused by redistribution of the total energy between kinetic and potential parts. We refer to papers [36, 37, 38, 39] for further discussion of this transient process in harmonic and anharmonic crystals.

Thus results of the present paper may serve as a theoretical basis for investigation of ballistic heat transfer in one- and two-dimensional materials and structures such as nanowires [3] and graphene [24].

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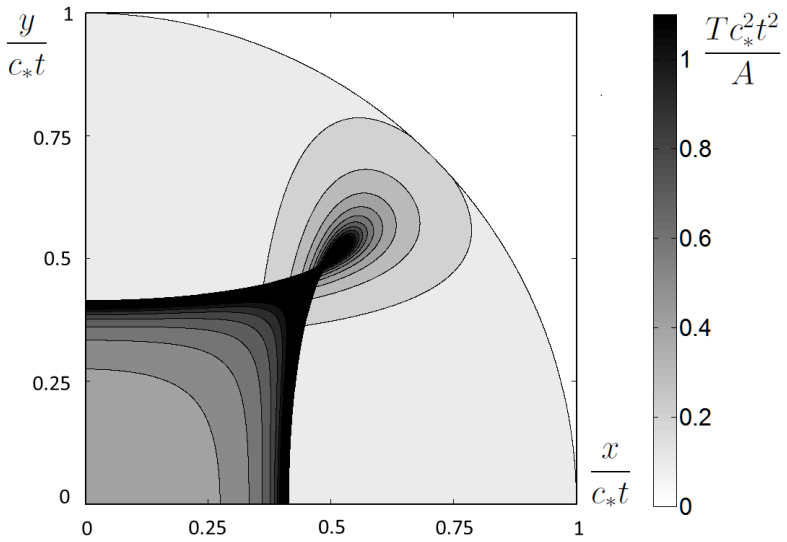

Figure 7: Fundamental solution (73) of the unsteady heat transfer problem for scalar square lattice.

merical simulations have been carried out using facilities of the Supercomputer Center "Polytechnic" at Peter the Great Saint Petersburg Polytechnic University.

10 Appendix A

In the present appendix, we derive equation (9) for velocity covariances. Note that particle velocities satisfy equation of motion (3):

$$\ddot{v}\left(\mathbf{x}\right) = \mathcal{L}v\left(\mathbf{x}\right). \tag{75}$$

We introduce covariance of accelerations

$$\zeta = \Big\langle \dot{v}(\mathbf{x})\dot{v}(\mathbf{y}) \Big\rangle. \tag{76}$$

Differentiating covariances of velocities κ and covariances of accelerations ζ with respect to time and taking into account equations of motion (3), (75), yields:

$$\ddot{\kappa} = \left(\mathcal{L}_x + \mathcal{L}_y\right)\kappa + 2\zeta, \quad \ddot{\zeta} = \left(\mathcal{L}_x + \mathcal{L}_y\right)\zeta + 2\mathcal{L}_x\mathcal{L}_y\kappa. \tag{77}$$

Excluding ζ from system (77) yields equation (9) for velocity covariances.

11 Appendix B

In the present appendix, we describe series expansion of difference operators $\mathcal{L}_x$, $\mathcal{L}_y$. We represent the covariance of particle velocities in the form $\kappa\left(\mathbf{r}, \mathbf{x}-\mathbf{y}\right)$ (see formula (12)). Consider the following expression

$$\mathcal{L}_x\kappa\left(\mathbf{r}, \mathbf{x}-\mathbf{y}\right) = \omega_*^2 \sum_\alpha b_\alpha \kappa\left(\mathbf{r} + \frac{1}{2}\mathbf{a}_\alpha, \mathbf{x}-\mathbf{y}+\mathbf{a}_\alpha\right). \tag{78}$$

Assume that function κ slowly changes with the first argument at distances of order of $|\mathbf{a}_\alpha|$. Then series expansion in the right side of formula (78) with respect to $\mathbf{a}_\alpha$ yields

$$\begin{aligned}
&\mathcal{L}_x\kappa \approx \omega_*^2 \sum_\alpha b_\alpha \mathcal{S}_\alpha \kappa + \frac{\omega_*^2}{2} \sum_\alpha b_\alpha \mathcal{S}_\alpha \mathbf{a}_\alpha \cdot \nabla\kappa = (\mathcal{L} + \boldsymbol{\mathcal{R}} \cdot \nabla)\,\kappa, \\
&\boldsymbol{\mathcal{R}} = \frac{\omega_*^2}{2} \sum_\alpha b_\alpha \mathcal{S}_\alpha \mathbf{a}_\alpha, \qquad \mathcal{L} = \omega_*^2 \sum_\alpha b_\alpha \mathcal{S}_\alpha, \qquad \mathcal{S}_\alpha\kappa = \kappa\left(\mathbf{r}, \mathbf{x} - \mathbf{y} + \mathbf{a}_\alpha\right),
\end{aligned} \tag{79}$$

where $\nabla = \partial/\partial\mathbf{r}$ is nabla-operator. Formulas (79) yield $\mathcal{L}_x \approx \mathcal{L} + \boldsymbol{\mathcal{R}} \cdot \nabla$. Analogously we show that $\mathcal{L}_y \approx \mathcal{L} - \boldsymbol{\mathcal{R}} \cdot \nabla$. Then

$$\mathcal{L}_x - \mathcal{L}_y \approx 2\boldsymbol{\mathcal{R}} \cdot \nabla, \qquad \mathcal{L}_x + \mathcal{L}_y \approx 2\mathcal{L}. \tag{80}$$

Substitution of the expressions (80) into equation (9), yields formula (14).

12 Appendix C

In this appendix, we prove that $\mathbf{c}$ defined by formula (27) coincides with the group velocity for the lattice.

Formula (27) is obtained using the discrete Fourier transform. The transform in d-dimensional space is defined as follows

$$\begin{aligned}
&\hat{\kappa}\left(\mathbf{k}\right) = \Phi\left(\kappa\right) = \sum_{j=1}^{d} \sum_{z_j=-\infty}^{+\infty} \kappa(\mathbf{z}) e^{-i\mathbf{k}\cdot\mathbf{z}}, \qquad \kappa(\mathbf{z}) = \frac{1}{(2\pi)^d} \int_{-\pi}^{\pi} \hat{\kappa}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{z}} \mathrm{d}p_1 ... \mathrm{d}p_d, \\
&\mathbf{k} = \frac{1}{a} \sum_{j=1}^{d} p_j \tilde{\mathbf{e}}_j, \quad \mathbf{z} = \mathbf{x} - \mathbf{y} = a \sum_{j=1}^{d} z_j \mathbf{e}_j, \quad \mathbf{e}_j \cdot \tilde{\mathbf{e}}_k = \delta_{jk}.
\end{aligned} \tag{81}$$

Here a is equilibrium distance, i is the imaginary unit, $\mathbf{e}_j$ are basis vectors for the lattice, $\tilde{\mathbf{e}}_k$ are the reciprocal vectors, δ_{jk} is the Kronecker delta. The discrete Fourier transform has the following property:

$$\Phi\left(\kappa(\mathbf{z} + \mathbf{a}_\alpha)\right) = \Phi\left(\kappa(\mathbf{z})\right) e^{i\mathbf{k}\cdot\mathbf{a}_\alpha}. \tag{82}$$

Using the identity (82), we calculate $\hat{\mathcal{L}}$ and $\hat{\boldsymbol{\mathcal{R}}}$ in formula (27)

$$\Phi\left(\mathcal{L}\kappa\right) = \hat{\mathcal{L}}\hat{\kappa}, \qquad \hat{\mathcal{L}} = \omega_*^2 \sum_\alpha b_\alpha e^{i\mathbf{k}\cdot\mathbf{a}_\alpha}, \qquad \Phi\left(\boldsymbol{\mathcal{R}}\kappa\right) = \hat{\boldsymbol{\mathcal{R}}}\hat{\kappa}, \qquad \hat{\boldsymbol{\mathcal{R}}} = \frac{\omega_*^2}{2} \sum_\alpha b_\alpha \mathbf{a}_\alpha e^{i\mathbf{k}\cdot\mathbf{a}_\alpha}. \tag{83}$$

It can be shown that $\hat{\mathcal{L}}$ and $\hat{\boldsymbol{\mathcal{R}}}$ are related by the following formula:

$$\hat{\boldsymbol{\mathcal{R}}} = -\frac{i}{2} \frac{\partial \hat{\mathcal{L}}}{\partial \mathbf{k}}. \tag{84}$$

Substituting formula (84) into the third formula from (27), we obtain

$$\mathbf{c} = \frac{\partial \sqrt{-\hat{\mathcal{L}}}}{\partial \mathbf{k}}. \tag{85}$$

Consider the dispersion relation for the lattice. Substituting $u(\mathbf{x}) = A\exp(i(\omega t + \mathbf{k}\cdot\mathbf{x}))$ into the equation of motion (3), yields:

$$\omega^2 = -\omega_*^2 \sum_\alpha b_\alpha e^{i\mathbf{k}\cdot\mathbf{a}_\alpha}. \tag{86}$$

Combining the dispersion relation (86) with formulas (83), (85), we obtain the expression for $\mathbf{c}$:

$$\mathbf{c} = \frac{\mathrm{d}\omega}{\mathrm{d}\mathbf{k}}. \tag{87}$$

Therefore, $\mathbf{c}$ is equal to the group velocity. Substitution of the expression (83) for $\hat{\mathcal{L}}$ into formula (85) yields the expression for group velocity (28).

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