Unsteady ballistic heat transport in infinite harmonic crystals

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Abstract

We study thermal processes in infinite harmonic crystals having a unit cell with arbitrary number of particles. Initially particles have zero displacements and random velocities, corresponding to some initial temperature profile. Our main goal is to calculate spatial distribution of kinetic temperatures, corresponding to degrees of freedom of the unit cell, at any moment in time. An approximate expression for the temperatures is derived from solution of lattice dynamics equations. It is shown that the temperatures are represented as a sum of two terms. The first term describes high-frequency oscillations of the temperatures caused by local transition to thermal equilibrium at short times. The second term describes slow changes of the temperature profile caused by ballistic heat transport. It is shown, in particular, that local values of temperatures, corresponding to degrees of freedom of the unit cell, are generally different even if their initial values are equal. Analytical findings are supported by results of numerical solution of lattice dynamics equations for diatomic chain and graphene lattice. Presented theory may serve for description of unsteady ballistic heat transport in real crystals with low concentration of defects. In particular, solution of the problem with sinusoidal temperature profile can be used for proper interpretation of experimental data obtained by the transient thermal grating technique.

Keywords: ballistic heat transport; heat transfer; harmonic crystal; harmonic approximation; polyatomic crystal lattice; complex lattice; kinetic temperature; transient processes; temperature matrix; unsteady heat transport.

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1 Introduction

At macro scale, heat transport in solids is usually diffusive and well-described by the Fourier law. The law states that heat flux is proportional to temperature gradient with proportionality coefficient refereed to as the thermal conductivity. Recent experiments for materials with low defect concentration have show that at micro and nano scale heat propagates ballistically [11, 14, 27, 57]. In particular, it is demonstrated for many materials including nanowires [2, 27], nanotubes [13], graphene [5, 53, 68], silicon membranes [31] etc. that thermal conductivity strongly depend on sample size and the Fourier law is violated. Therefore development of theoretical models describing ballistic heat transport is required.

Several approaches for derivation of equations describing ballistic heat transport are available in literature. In continuum theories, the equations are usually formulated using phenomenological approach. One of the phenomenological equations, describing wave nature of heat transport is the hyperbolic heat transfer equation, also refereed to as the Maxwell-Cattaneo-Vernotte equation [15, 65]. Development of phenomenological models is limited by small amount of available experimental data on unsteady ballistic heat transport. Another approach is based on Boltzmann transport equation (BTE), formulated for distribution function of phonons [40, 54]. Given known the distribution function, the temperature field can be calculated. The BTE is usually simplified using the relaxation time approximation [8, 34, 40] for the collision term. It allows to solve the BTE numerically [28, 49, 59] and to derive heat conduction equations [12, 38, 52, 67]. In both cases, additional approximations are introduced [62]. In particular, contribution of optical vibrations to heat transport is often neglected. Comprehensive review on application of the BTE to simulation of thermal transport can be found, e.g. in review papers [11, 45, 62].

In the present paper, we use another approach for description of ballistic heat transport. The expression for evolution of temperature field is derived directly from lattice dynamics equations in harmonic approximation. This approach allows to describe heat transport in ballistic limit taking into account all important features of discrete system.

Analysis of heat transport in discrete systems is usually carried out in the so-called nonequilibrium steady-state. In this case, a material is kept between two thermostats with different temperatures. Given known the difference of temperatures, distance between thermostats, and a heat flux, one can calculate the effective heat conductivity of a material. This statement of the problem is widely used in both analytical studies [6, 58, 46] and computer simulations [17, 32, 45, 66] of heat transport. Comprehensive reviews of results obtained in steady-state formulation are given e.g. in papers [10, 16, 45] Calculating heat conductivity as a function of a sample length, one can determine conditions corresponding to ballistic and diffusive heat transport regimes. However, the steady-state formulation does not address the issue of temperature field evolution. Additionally, results of steady-state simulations significantly depend on the type of thermostat being used [25, 32]. Therefore in the present paper we consider unsteady ballistic heat transport.

One of the goals of unsteady heat transport simulations is to describe time evolution of initial temperature profile. The initial profile field can be prescribed by assigning random initial velocities to particles. Then no thermostat is needed. The heat transport
calculations are usually carried out numerically using, for example, molecular dynamics method [22, 47, 39, 55, 64]. The method allows to use realistic interatomic potentials and to consider effect of nonlinearity (anharmonicity), defects, interfaces, and other features of real systems, which are hard to describe analytically. Though numerical modeling is a powerful tool for investigation of heat transport, many issues can not be addressed numerically. In particular, for crystals with several branches of dispersion relation, in numerical simulations it is hard to distinguish between contributions of acoustic and optical vibrations to the heat transport. Therefore analytical studies of unsteady heat transport are of great importance.

A promising model for investigation of ballistic heat transport is a harmonic crystal, i.e. a set of material points forming a perfect crystal lattice and interacting via linearized forces. In this model, harmonic waves do not interact with each other and therefore the heat transport is purely ballistic. Unsteady ballistic heat transport in harmonic crystals is investigated e.g. in papers [4, 20, 21, 23, 36, 43, 48, 61]. In paper [36], an equation, refereed to as the ballistic heat equation, describing evolution of temperature field in a one-dimensional chain with interactions of the nearest neighbors is derived. The equation is also valid [4] for one-dimensional chain with harmonic on-site potential (elastic foundation). An expression for temperature field in scalar lattices with one degree of freedom per unit cell is derived in paper [43]. Similar results are obtained by entirely different means in papers [23, 48]. In realistic systems, each unit cell usually has several degrees of freedom. To our knowledge, no closed-form expressions describing evolution of temperature field in crystals with several degrees of freedom per unit cell are available in literature. Therefore such expression is derived in the present paper.

The paper is organized as follows. In section 2, equations of motion for harmonic crystals are represented in a general form valid for one-, two-, and three-dimensional lattices with arbitrary number of particles per unit cell. Random initial conditions corresponding to an initial temperature profile are formulated. In section 4 an exact solution of equations of motion is derived. The solution is used for calculation of temperatures, corresponding to different degrees of freedom. The temperatures are defined in section 5. In section 6, an exact expression describing temporal and spatial evolution of the temperatures is derived. In section 7, simple approximate formula for the temperatures is derived. In section 8, analysis of specific initial temperature profiles is presented. In particular, decay of a spatially sinusoidal profile of initial temperature is considered in section 8.5. This problem is important, because it is closely related to experimental technique refereed to as the transient thermal grating (TTG) [31, 60, 29]. In the framework of TTG, a sinusoidal initial temperature profile is generated using the interference of two laser pulses. Decay of temperature profile yields information about thermal properties of a material. Results obtained in sections 4-8 are applicable to crystals with an arbitrary lattice. In sections 9, 10 the general theory is employed for analysis of two particular cases, namely one-dimensional diatomic chain and graphene lattice. Analytical results are compared with numerical solution of lattice dynamics equations.
2 Equations of motion of a crystal

We consider infinite crystals in $d$-dimensional space, $d = 1, 2, 3$. Unit cell of a crystal contains arbitrary number of particles. In this section, we represent equations of motion of the unit cell in a matrix form \[44\], convenient for analytical derivations.

Unit cells of the lattice are identified by their position vectors, $x^1$, in the undeformed state. Each unit cell has $N$ degrees of freedom $u_i(x), i = 1, \ldots, N$, corresponding to components of particle displacements $^2$. The displacements form a column:

$$u(x) = \begin{bmatrix} u_1 & u_2 & \ldots & u_N \end{bmatrix}^\top,$$

where $\top$ stands for the transpose sign.

Remark. Here and below matrices are denoted by bold italic symbols, while invariant vectors, e.g. position vector, are denoted by bold symbols.

Particles from the cell $x$ interact with each other and with particles from neighboring unit cells, numbered by index $\alpha$. Vector connecting the cell $x$ with neighboring cell number $\alpha$ is denoted $a_\alpha$. Centers of unit cells always form a simple lattice $^3$, therefore numbering can be carried out so that vectors $a_\alpha$ satisfy the identity:

$$a_\alpha = -a_{-\alpha}.$$  

Here $a_0 = 0$. Vectors $a_\alpha$ for a sample lattice are shown in figure 1.

![Figure 1: Example of a complex two-dimensional lattice with three sublattices. Particles forming sublattices have different color and size.](image)

In the present paper, an infinite crystal is considered as a limiting case of a crystal under periodic boundary conditions. A periodic cell contains $n^d$ unit cells ($n$ cells in each direction). Displacements of particles satisfy periodic boundary conditions:

$$u(x) = u \left( x + \sum_{j=1}^{d} C_j n b_j \right),$$

$^1$For analytical derivations, position vectors are more convenient than indices, because number of indices depends on space dimensionality.

$^2$\(N\) is equal to number of particles in the unit cell multiplied by number of degrees of freedom per particle.

$^3$A lattice is referred to as simple lattice, if it coincides with itself under shift by a vector connecting any two particles.
where \( b_j \) are primitive vectors of the lattice; \( C_j \) are integers. Further analytical derivations are carried out for \( n \to \infty \), while in computer simulations \( n \) is finite.

We represent equations of motion in a quite general form, applicable to one-, two-, and three-dimensional lattices with arbitrary number of degrees of freedom per unit cell. In harmonic crystals, the total force acting on each particle is represented as a linear combination of displacements of all other particles. Using this fact, we write equations of motion in the form [44, 48]:

\[
M \dot{v}(x) = \sum_{\alpha} C_\alpha u(x + a_\alpha), \quad C_\alpha = C_{-\alpha}^\top, \tag{4}
\]

where \( v = \dot{u}; \ u(x + a_\alpha) \) is a column of displacements of particles from unit cell \( \alpha \); \( M \) is diagonal \( N \times N \) matrix composed of particles’ masses; coefficients of matrix \( C_\alpha \) determine stiffnesses of springs connecting particles from unit cell \( x \) with particles from neighboring cell \( \alpha \); matrix \( C_0 \) describes interactions of particles inside the unit cell \( x \). Summation is carried out with respect to all unit cells \( \alpha \), interacting with unit cell \( x \) (including \( \alpha = 0 \)).

**Remark.** Relation \( C_\alpha = C_{-\alpha}^\top \) guarantees that dynamical matrix of the lattice (10) is Hermitian (see section 4 for more details).

Formula (4) describes motion of monoatomic and polyatomic crystals in one-, two-, and three-dimensional cases. For \( N = 1 \) (one degree of freedom per unit cell), equation (4) governs dynamics of the so-called scalar lattices\(^5\), considered, for example, in papers [23, 43, 48]. Monoatomic two- and three-dimensional lattices are covered if we put \( N = d \) and \( C_\alpha = C_{\alpha}^\top \) in formula (4). In the present paper, for illustration we consider polyatomic lattices with two particles per unit cell, namely one-dimensional diatomic chain (section 9) and out-of-plane motions of graphene lattice (section 10).

### 3 Initial conditions

In this section, we specify initial conditions for particles, corresponding to initial temperature profile.

The following initial conditions, typical for molecular dynamics modeling [1], are used:

\[
\begin{align*}
  u(x) &= 0, & \quad v(x) &= v_0(x),
\end{align*}
\tag{5}
\]

Here \( v_0(x) \) is a column of random initial velocities of particles from unit cell \( x \) such that

\[
\langle v_0(x) \rangle = 0, \quad \langle v_0(x)v_0(y) \rangle = B(x)\delta_D(x - y),
\tag{6}
\]

where \( \langle ... \rangle \) stands for mathematical expectation\(^6\); \( \delta_D(0) = 1; \ \delta_D(x - y) = 0 \) for \( x \neq y \).

In other words, components of \( v_0(x) \) are random numbers with zero mean\(^7\) and generally

---

\(^4\)Additionally, matrix \( C_0 \) can include stiffnesses of harmonic on-site potential.

\(^5\)In scalar lattices each particle has only one degree of freedom. This model is applicable to monoatomic one-dimensional chains with interactions of arbitrary number of neighbors and to out-of-plane motions of monoatomic two-dimensional lattices.

\(^6\)In computer simulations, mathematical expectation is approximated by average over realizations with different random initial conditions.

\(^7\)In this case mathematical expectations of all velocities are equal to zero at any moment in time.
different variances given by diagonal elements of matrix $B(x)$. Off-diagonal elements of matrix $B(x)$ are equal to covariances of initial velocities, corresponding to different degrees of freedom of unit cell, $x$. Initial velocities of particles from different unit cells are statistically independent.

From macroscopic point of view, initial conditions (5), (6) specify some initial temperature profile (see formulas (17), (18)) and zero initial heat fluxes. Examples of initial conditions (5), (6) are given by formulas (46), (60). Initial conditions (5), (6) can be considered as a result of heating of a crystal by an ultrashort laser pulse [29, 30, 31, 56, 60].

In the following section, an exact solution of equations of motion (4) with initial conditions (5) is obtained. The solution is employed for description of thermal processes, such as the ballistic heat transport.

4 Exact solution of equations of motion

In this section, we derive an exact solution of equation (4) with initial conditions (5), (6) using the discrete Fourier transform with respect to components of position vector $x$.

Position vector, $x$, of a unit cell is represented as

$$x = \sum_{j=1}^{d} z_j b_j, \quad (7)$$

where $b_j, j = 1, \ldots, d$ are primitive vectors of the lattice; $z_1, \ldots, z_d$ are integer indices of the unit cell; $d$ is space dimensionality. Direct and inverse discrete Fourier transforms with respect to variables $z_1, \ldots, z_d$ for an infinite lattice are defined as

$$\hat{u}(k) = \sum_{x} u(x) e^{-i k \cdot x}, \quad k = \sum_{j=1}^{d} p_j \tilde{b}_j, \quad (8)$$

$$u(x) = \int_{k} \hat{u}(k) e^{i k \cdot x} dp_1 \ldots dp_d.$$  

Here $\hat{u}(k)$ is Fourier image of $u$; $i^2 = -1$; $k$ is wave vector; $\tilde{b}_j$ are vectors of the reciprocal basis, i.e. $b_i \cdot \tilde{b}_j = \delta_{ij}$, where $\delta_{ij}$ is the Kronecker delta. For brevity, the following notation is used:

$$\int_k \ldots dk \overset{\text{def}}{=} \frac{1}{(2\pi)^d} \int_0^{2\pi} \ldots \int_0^{2\pi} \int_{-\infty}^{+\infty} \ldots \int_{-\infty}^{+\infty} dp_1 \ldots dp_d, \quad \sum_{x} \ldots \overset{\text{def}}{=} \sum_{z_1 = -\infty}^{+\infty} \ldots \sum_{z_d = -\infty}^{+\infty} \quad (9)$$

Applying the discrete Fourier transform (8) to formulas (4), (5), (6), yields equation

$$M^{\frac{1}{2}} \ddot{\hat{u}} = -\Omega \hat{u}, \quad \Omega(k) = -\sum_{\alpha} M^{-\frac{1}{2}} C_{\alpha} M^{-\frac{1}{2}} e^{i k \cdot a_{\alpha}}, \quad (10)$$
with initial conditions 
\[
\begin{align*}
\dot{\mathbf{u}} &= 0, \\
\dot{\mathbf{u}} &= \dot{\mathbf{v}}_0 = \sum_x \mathbf{v}_0(x)e^{-ikx}.
\end{align*}
\] (11)

Matrix \( \mathbf{\Omega} \) in formula (10) is the dynamical matrix of the lattice [18].

To simplify equation (10), we use the fact that dynamical matrix \( \mathbf{\Omega} \) is Hermitian, i.e. it is equal to its own conjugate transpose. Then it can be represented as
\[
\mathbf{\Omega} = \mathbf{P}\Lambda\mathbf{P}^\dagger, \quad \Lambda_{ij} = \omega_j^2 \delta_{ij},
\] (12)
where \( \omega_j^2, j = 1, \ldots, N \) are eigenvalues of matrix \( \mathbf{\Omega} \) and \( \omega_j(k) \) are branches of dispersion relation for the lattice (below we consider only nonnegative frequencies, i.e. \( \omega_j(k) \geq 0 \)); * stands for complex conjugate; matrix \( \mathbf{P} \) is composed of normalized eigenvectors of matrix \( \mathbf{\Omega} \). The eigenvectors are referred to as the polarization vectors [18].

**Remark.** We assume that branches of dispersion relation do not intersect with each other, i.e. all eigenvalues of the dynamic matrix \( \mathbf{\Omega} \) are distinct. The case of intersecting branches should be considered separately.

We substitute formula (12) into equation (10), multiply both parts by \( \mathbf{P}^\dagger \) and introduce new variable \( \mathbf{w} = \mathbf{P}^\dagger \mathbf{M}^{\frac{1}{2}} \dot{\mathbf{u}} \). Then we obtain a system of decoupled equations for elements \( w_j \) of vector \( \mathbf{w} \):
\[
\ddot{w} = -\Lambda \mathbf{w} \iff \ddot{w}_j = -\omega_j^2 w_j.
\] (13)
Solving these equations with initial conditions (11) we obtain the following expression for \( \dot{w} \):
\[
\dot{w}_j = \{ \mathbf{P}^\dagger \mathbf{M}^{\frac{1}{2}} \dot{\mathbf{v}}_0 \}_j \cos(\omega_j t) \iff \dot{w} = \mathbf{D}\mathbf{P}^\dagger \mathbf{M}^{\frac{1}{2}} \dot{\mathbf{v}}_0, \quad D_{ij}(k, t) = \cos(\omega_j(k) t) \delta_{ij}.
\] (14)
Here \( \{ \ldots \}_j \) stands for \( j \)th element of a column. Then using definition of \( \mathbf{w} \), we represent Fourier-images of velocities in the form
\[
\dot{\mathbf{v}} = \mathbf{M}^{-\frac{1}{2}} \mathbf{D}\mathbf{P}^\dagger \mathbf{M}^{\frac{1}{2}} \dot{\mathbf{v}}_0.
\] (15)
Applying the inverse discrete Fourier transform to formula (15), yields the following expression for particle velocities:
\[
\mathbf{v}(x) = \mathbf{M}^{-\frac{1}{2}} \int_k \mathbf{D}\mathbf{P}^\dagger \mathbf{M}^{\frac{1}{2}} \dot{\mathbf{v}}_0 e^{ikx} dk,
\] (16)
where \( \dot{\mathbf{v}}_0 \) is defined by formula (11).

Thus formula (16) is an exact solution of equation (4) with initial conditions (5). In the following sections, spatial distribution of temperature is calculated using solution (16).

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10 Matrix \( \mathbf{P} \) is unitary, i.e. \( \mathbf{PP}^\dagger = \mathbf{E} \), where \( \mathbf{E} \) is unit matrix
5 Kinetic temperature. Temperature matrix

Since initial conditions (5), (6) are random then particle velocities given by formula (16) are also random. Following [35, 36, 37] we consider an infinite number of realizations of initial conditions (5), (6). It allows to introduce statistical characteristics such as kinetic temperature.

In harmonic crystals, kinetic temperatures, corresponding to degrees of freedom of the unit cell, are generally different (see e.g. figures 3, 4, 5). Therefore in order to characterize thermal state of the unit cell, \( x \), we use \( N \times N \) matrix, \( T(x) \), further referred to as the temperature matrix [44]:

\[
k_B T(x) = M^\frac{1}{2} \left\langle v(x) v(x)^\top \right\rangle M^\frac{1}{2} \quad \iff \quad k_B T_{ij} = \sqrt{M_i M_j} \left\langle v_i v_j \right\rangle,
\]

where \( M^\frac{1}{2} M^\frac{1}{2} = M \); \( M_i \) is \( i \)-th element of matrix \( M \), equal to a mass corresponding to \( i \)-th degree of freedom of the unit cell; \( k_B \) is the Boltzmann constant; brackets \( \left\langle .. \right\rangle \) stand for mathematical expectation\(^{11}\). Diagonal element, \( T_{ii} \), of the temperature matrix is refereed to as kinetic temperature, corresponding to \( i \)-th degrees of freedom of the unit cell. Off-diagonal elements, \( T_{ij} \), characterize correlation between components, \( i, j \), of velocity column, \( v(x) \).

We also use conventional kinetic temperature, \( T \), proportional to the total kinetic energy of the unit cell:

\[
T(x) = \frac{1}{N} \text{tr}(T(x)), \tag{18}
\]

where \( N \) is a number of degrees of freedom per unit cell, \( \text{tr}(..) \) stands for the trace (sum of diagonal elements). If initial kinetic energy is uniformly distributed among degrees of freedom of the unit cell then kinetic temperatures, corresponding to all degrees of freedom of the unit cell, are equal to \( T \).

6 Exact formula for the temperature matrix

In this section, we derive an exact expression for the temperature matrix using the solution (16) of lattice dynamics equation.

To calculate temperature matrix, we substitute solution (16) into definition (17)\(^ {12}\):

\[
k_B T(x) = \int_{k_1} \int_{k_2} P_1 D_1 P_1^\top M^\frac{1}{2} \left\langle \hat{v}_0(k_1) \hat{v}_0(k_2)^\top \right\rangle M^\frac{1}{2} P_2 D_2 P_2^\top e^{i(k_1-k_2)\cdot x} dk_1 dk_2.
\]

Here and below \( P_j = P(k_j) \), \( D_j = D(k_j) \), \( j = 1, 2 \).

Initial conditions (5), (6) are such that initial velocities of any pair of unit cells \( y_1, y_2 \) are uncorrelated. Therefore the following identity is satisfied

\[
\left\langle v_0(y_1) v_0(y_2)^\top \right\rangle = M^{-\frac{1}{2}} k_B T_0(y_1) \delta_D(y_1 - y_2) M^{-\frac{1}{2}}, \tag{20}
\]

\(^{11}\)In computer simulations, mathematical expectation is approximated by average over realizations with different random initial conditions.

\(^{12}\)Here the following identities were used: \( \int_k F(k) dk \int_k F^\top(k) dk = \int_{k_1} \int_{k_2} F(k_1) F^\top(k_2) dk_1 dk_2 \) and \( \mathbf{v} = \mathbf{v}^* \).
Here $T_0$ is the initial temperature matrix, which is calculated by substituting initial velocities, $v_0(x)$, into formula (17); $\delta_D$ is defined after formula (6). Using identity (20), we make the following transformations:

$$
\langle \hat{v}_0(k_1)\hat{v}_0(k_2)^\top \rangle = \sum_{y_1,y_2} \langle v_0(y_1)v_0(y_2)^\top \rangle e^{-i(k_1\cdot y_1-k_2\cdot y_2)} = k_B \sum_y M^{-\frac{1}{2}}T_0(y)M^{-\frac{1}{2}}e^{-i(k_1-k_2)y}.
$$

(21)

Then substitution of formula (21) into (19), yields

$$
T(x,t) = \int_{k_1} \int_{k_2} \sum_y P_1D_1P_1^\top T_0(y)P_2D_2P_2^\top e^{i(k_1-k_2)\cdot (x-y)d\k_1d\k_2}.
$$

(22)

Formula (22) is an exact expression for the temperature matrix.

**Remark.** Formula (22) for the temperature matrix is symmetric with respect to time, i.e. invariant with respect to substitution $t$ by $-t$. This fact follows from the same property of equations of motion (4).

The temperature matrix can be exactly represented as a sum of “fast” and “slow” terms:

$$
T = T_F + T_S, \quad T_F(x) = \int_{k_1} \int_{k_2} \sum_y P_1T_F^y P_2^\top e^{i(k_1-k_2)\cdot (x-y)d\k_1d\k_2},
$$

$$
T_S(x) = \int_{k_1} \int_{k_2} \sum_y P_1T_S^y P_2^\top e^{i(k_1-k_2)\cdot (x-y)d\k_1d\k_2},
$$

$$
\{T_F\}_{ij} = \frac{1}{2}\{P_1^\top T_0(y)P_2\}_{ij} \left[\cos((\omega_i(k_1) + \omega_j(k_2))t) + (1-\delta_{ij})\cos((\omega_i(k_1) - \omega_j(k_2))t)\right],
$$

$$
\{T_S\}_{ij} = \frac{1}{2}\{P_1^\top T_0(y)P_2\}_{ij} \delta_{ij} \cos((\omega_j(k_1) - \omega_i(k_2))t).
$$

(23)

Here $\{\ldots\}_{ij}$ is element $i,j$ of the matrix. The representation (23) is based on the observation that $T_F$ and $T_S$ have different characteristic time scales. The difference of time scales is most clearly demonstrated by example, considered in section 8.5. Physical meaning of $T_F$ and $T_S$ is discussed in the next section.

It is seen that exact formulas (22), (23) for the temperature matrix are quite complicated and require intensive calculations (double integration with respect to wave vectors $k_1, k_2$ and summation with respect to all unit cells). Therefore in the following section we present a simple approximate formula for the temperature matrix.
7 Approximate formula for the temperature matrix. Fast and slow thermal processes

The main result of the present paper is the following approximate formula for the temperature matrix (derivation is presented in the Appendix):

\[ T = T_F + T_S, \quad T_F \approx \int_k P \tilde{T}_F P^* \, dk, \quad T_S \approx \int_k P \tilde{T}_S P^* \, dk, \]

\[
\{\tilde{T}_F\}_{ij} = \frac{1}{2} \left\{ P^* T_0(x) P \right\}_{ij} \left[ \cos((\omega_i + \omega_j)t) + (1 - \delta_{ij}) \cos((\omega_i - \omega_j)t) \right],
\]

\[
\{\tilde{T}_S\}_{ij} = \frac{1}{4} \left\{ P^* (T_0(x + v^j_g t) + T_0(x - v^j_g t)) P \right\}_{jj} \delta_{ij}.
\]

Here \( P = P(k) \); \( v^j_g \) is the group velocity corresponding to \( j \)-th branch of dispersion relation, \( \omega_j \): \[ v^j_g = \frac{d\omega_j}{dk} = \sum_{i=1}^{d} \frac{\partial \omega_j}{\partial p_i} b_i, \quad k = \sum_{i=1}^{d} p_i \hat{b}_i. \]

Since formula (24) contains only a single integral with respect to \( k \), it is significantly more convenient for analysis and calculations than exact expression (23).

Remark. Function \( T_0 \) is originally defined on a discrete set of position vectors, \( x \), of unit cells (see formula (17)), while argument of this function \( x \pm v^j_g t \) changes in space continuously. Therefore further we assume that \( T_0 \) can be defined for the whole space in such a way that at points \( x \) is coincides with values given by formula (17).

The first term, \( T_F \), in formula (24) describes short time behavior of the temperature matrix (fast process [35, 43]). At short times, the temperature matrix oscillates. The oscillations are caused by redistribution of energy among kinetic and potential forms and redistribution of energy among degrees of freedom of the unit cell. These oscillations at different spatial points are independent. At large time scale \( T_F \) tends to zero.

The second term, \( T_S \), in formula (24) describes large time behavior of the temperature matrix (slow process [36, 37, 43]). At large time scale, changes of the temperature matrix are caused by ballistic heat transport. The temperature matrix is represented as a superposition of waves traveling with group velocities \( v^j_g(k) \). Shapes of the waves are determined by initial temperature profile \( T_0 \).

Remark. Approximate formula (24) for the temperature matrix have the same property as the exact formula (22). It is symmetric with respect to time, i.e. substitution \( t \) by \(-t\). At the same time, analysis of formula (24) and results of numerical simulations suggest that thermal processes in infinite harmonic crystals are irreversible.

Remark. According to formula (23), the temperature matrix at the unit cell \( x \) depends on initial temperatures at all other unit cells. This fact is a consequence of infinite propagation speed of disturbances in discrete systems described by equations of motion (4). In contrast, approximate formula (24) does not have this artifact. According to formula (24), temperature matrix of the unit cell \( x \) at time \( t \) depends on initial temperature matrices of unit cells which are not farther from cell \( x \) than \( \max_{k,j} (|v^j_g t|) \).

\[13\] For each value of the wave vector, \( k \), and for each branch, \( j \), there are positive and negative frequencies (except \( \omega_j = 0 \)). In formula (24), positive frequencies \( \omega_j, j = 1, ..., N \) are used.
Remark. Comparison of formula (24) with results of paper [44] shows that $T_S(x)$ at $t = 0$ is equal to the equilibrium value of the temperature matrix in the uniformly heated crystal with initial temperature matrix $T_0(x)$.

8 Specific profiles of initial temperature

In this section, we apply general solution (24) to several particular initial temperature profiles. The results are valid for all lattices described by equations of motion (4).

8.1 Uniform initial temperature profile

In this subsection, we consider spatially uniform distribution of initial temperature ($T_0$ is independent of $x$). In this case changes of the temperature matrix are caused by two physical processes: redistribution of energy between kinetic and potential forms and redistribution of energy between degrees of freedom. These processes are usually observed in molecular dynamics simulations [1]. Analytical description of these processes for several specific one- and two-dimensional lattices is presented in papers [3, 35, 43, 41, 42]. Generalization for the case of polyatomic crystals is carried out in paper [44]. In these works, the approach, originally proposed in paper [35] and based on analysis of velocity covariances, is used. Here we show that identical results follow from formula (24) derived using solution of lattice dynamics equations.

In the case of spatially uniform distribution of temperature matrix, formula (24) reads

$$T_F = \int_k P\tilde{T}_F P^*\top dk, \quad T_S = \int_k P\tilde{T}_S P^*\top dk,$$

\[
\{\tilde{T}_F\}_{ij} = \frac{1}{2}\{P^* T_0 P\}_{ij} \left[ \cos((\omega_i + \omega_j)t) + (1 - \delta_{ij}) \cos((\omega_i - \omega_j)t) \right]. \quad (26)
\]

\[
\{\tilde{T}_S\}_{ij} = \frac{1}{2}\{P^* T_0 P\}_{jj} \delta_{ij}.
\]

Expressions (26) coincide with exact formulas for the temperature matrix, obtained in paper [44] by entirely different means. In particular, the expression for $T_S$ coincides with equilibrium value of the temperature matrix [44].

Therefore in the case of spatially uniform distribution of temperature, formula (24) is exact.

8.2 Initial equipartition

In this section, we consider the case, when initial kinetic temperatures, corresponding to all degrees of freedom of the unit cell, are equal. Then initial temperature matrix is isotropic\(^\text{14}\), i.e. $T_0 = T_0(x)E$, where $E$ is the unit matrix. Substitution of this expression into formula (24) yields:

$$T_F = \int_k P\tilde{T}_F P^*\top dk, \quad T_S = \int_k P\tilde{T}_S P^*\top dk,$$

\[
\{\tilde{T}_F\}_{ij} = \frac{1}{2}T_0(x)\delta_{ij} \cos(2\omega_j t), \quad \{\tilde{T}_S\}_{ij} = \frac{1}{4} \left( T_0(x + v^j_t) + T_0(x - v^j_t) \right) \delta_{ij}. \quad (27)
\]

\(^{14}\text{Matrix is called isotropic if it is diagonal and all elements on the diagonal are equal.}\)
The kinetic temperature, proportional to trace of the temperature matrix (27), has form
\[ T = T_F + T_S, \quad T_F = \frac{T_0(x)}{2N} \sum_{j=1}^{N} \int_k \cos(2\omega_j t) dk, \]
\[ T_S = \frac{1}{4N} \sum_{j=1}^{N} \int_k (T_0(x + v^i_j t) + T_0(x - v^i_j t)) dk. \] (28)

Remark. For scalar lattices \((N = 1)\), formula (28) coincides with the result obtained in paper [43]. In paper [43] the expression for temperature is derived by approximate solution of equation for covariances of velocities, while in the present paper it is derived from solution of lattice dynamics equations.

Remark. Expression for \(T_S\) in formula (28) is also consistent with results obtained in paper [48] by entirely different means. In paper [48], the expression for the total energy of the unit cell at large times is derived. At large times, kinetic and potential energies equilibrate [44] and therefore behavior of the total energy and kinetic temperature are similar.

Formula (27) shows that the temperature matrix for \(t > 0\) is generally not isotropic, i.e. temperatures, corresponding to degrees of freedom of the unit cell, are different even though initially they are equal. Further this important fact is illustrated by figures 3, 4, 5.

8.3 Fundamental solution

In this subsection, we derive fundamental solution of ballistic heat transport problem.

The following spatial distribution of initial temperature matrix is considered
\[ T_0(x) = A\delta(x)E, \] (29)
where \(\delta(x)\) is Dirac delta function; \(A\) is a constant. Distribution of kinetic temperature at large times is given by formula (28):
\[ T \approx T_S = \frac{A}{4N} \sum_{i=1}^{N} \int_k (\delta(x + v^i_g t) + \delta(x - v^i_g t)) dk. \] (30)

Non-zero contribution to integral (30) comes from values, \(k^*_{ij}\), of wave-vector such that argument of the delta function vanishes:
\[ v^i_g(k^*_{ij}) = \frac{x}{t} \quad \text{or} \quad v^i_g(k^*_{ij}) = -\frac{x}{t}. \] (31)

Here \(j = 1,..,n_i\), where \(n_i\) is the number of real roots of equation (31), for \(i\)th branch or dispersion relation. Then calculation of integrals in formula (30) yields
\[ T = \frac{A}{4N(2\pi)^dtd} \sum_{i=1}^{N} \sum_{j=1}^{n_i} \frac{1}{|\det G^d_i(k^*_{ij})|}, \] (32)
where summation is carried out with respect to all real roots $k^*_{ij}, i = 1, \ldots, N, j = 1, \ldots, n_i$ of equations (31)\(^\dagger\); det stands for determinant of a matrix; $G^i_1$ is the Jacobian matrix in $d$-dimensional case:

$$G^1_i = \frac{\partial v^i_g}{\partial p}, \quad G^2_i = \begin{bmatrix} \frac{\partial v^i_{xg}}{\partial p_1} & \frac{\partial v^i_{yg}}{\partial p_2} \\ \frac{\partial v^i_{yg}}{\partial p_1} & \frac{\partial v^i_{yg}}{\partial p_2} \end{bmatrix}, \quad G^3_i = \begin{bmatrix} \frac{\partial v^i_{xg}}{\partial p_1} & \frac{\partial v^i_{yg}}{\partial p_2} & \frac{\partial v^i_{zg}}{\partial p_3} \\ \frac{\partial v^i_{yg}}{\partial p_1} & \frac{\partial v^i_{yg}}{\partial p_2} & \frac{\partial v^i_{zg}}{\partial p_3} \\ \frac{\partial v^i_{zg}}{\partial p_1} & \frac{\partial v^i_{zg}}{\partial p_2} & \frac{\partial v^i_{zg}}{\partial p_3} \end{bmatrix},$$

(33)

where $v^i_{xg}, v^i_{yg}, v^i_{zg}$ are components of vector of group velocity $v^i_g(k)$.

Since the group velocity is usually bounded then from formulas (31), (32), it follows that the heat front, corresponding to fundamental solution, is a $d$-dimensional sphere given by

$$|x| = t \max_{k,i} |v^i_g|.$$

(34)

In other words, the heat front propagates with maximum group velocity. This fact is illustrated in figure 7.

**Remark.** For one-dimensional and two-dimensional scalar lattices ($N = 1$) fundamental solutions are obtained in papers [36, 43]. These solutions coincide with particular cases of formula (32).

**Remark.** Fundamental solution (32) can be used for calculation of temperature field in a crystal subjected to point heat supply of constant intensity. In paper [20] it is shown that the temperature field is equal to integral of the fundamental solution with respect to time.

### 8.4 Thermal contact of cold and hot half-spaces

Consider thermal contact of two half-spaces with initial temperatures $T_b$ and $T_b + \Delta T$. This problem is important, because it is closely related to classical definition of temperature [26]. By the definition, temperatures of two bodies in thermodynamic equilibrium are equal. The problem considered below demonstrates the transition to thermodynamic equilibrium.

The initial temperature distribution in direction, given by unit vector $e$, has form:

$$T_0 = (T_b + \Delta TH(x)) E, \quad x = x \cdot e,$$

(35)

where $H$ is the Heaviside function. Substituting formula (35) into (27), yields

$$\begin{align*}
\{T_F\}_{ij} &= \frac{1}{2} (T_b + \Delta TH(x)) \delta_{ij} \cos(2\omega_j t), \\
\{\tilde{T}_S\}_{ij} &= \frac{T_b}{2} \delta_{ij} + \frac{\Delta T}{4} \left( H \left( x + v^i_g \cdot et \right) + H \left( x - v^i_g \cdot et \right) \right) \delta_{ij}.
\end{align*}$$

(36)

Computing kinetic temperature by formulas (27), (36) and using the property of Heaviside

\(^\dagger\)Components of $k^*_{ij}$ belong to interval $[0; 2\pi]$. 

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function $H(ax) = H(x)$, yields

$$T = T_F + T_S, \quad T_F = \frac{1}{2N} \left( T_b + \Delta TH(x) \right) \sum_{j=1}^{N} \int_{k} \cos(2\omega_j t) dk,$$

$$T_S \left( \frac{x}{t} \right) = \frac{T_b}{2} + \frac{\Delta T}{4N} \sum_{j=1}^{N} \int_{k} \left( H \left( \frac{x}{t} + v_g^j \cdot \mathbf{e} \right) + H \left( \frac{x}{t} - v_g^j \cdot \mathbf{e} \right) \right) dk.$$  (37)

Formula (37) shows that slow part of the temperature matrix, $T_S$, is \textit{self-similar}, i.e. dependent on $x/t$. This fact is used for comparison with results of numerical solution of equations of motion in sections 9.3, 10.4.

### 8.5 Sinusoidal initial temperature profile: application to transient thermal grating

In this subsection, we consider spatially sinusoidal profile of initial temperature. This problem is closely related to transient thermal grating technique [31, 60]. In the framework of this experimental technique, the sinusoidal profile in a thin film is generated using the interference of two laser pulses. Amplitude of the temperature profile decays in time due to heat transport. Measurement of the amplitude yields information on thermal properties of a material. Here we present an analytical solution of this problem, corresponding to purely ballistic regime of heat transport.

The initial temperature profile in direction given by unit vector $\mathbf{e}$ has form:

$$T_0(x) = \left( T_b + \Delta T \sin \frac{2\pi x}{L} \right) E, \quad x = x \cdot \mathbf{e},$$  (38)

where $T_b$, $\Delta T$ are constants; $\Delta T < T_b$; $L$ is length of the periodic cell. Note that initial temperatures, corresponding to all degrees of freedom of the unit cell, are equal.

\textbf{Remark.} Heat transport in several scalar lattices with initial temperature distribution (38) is considered in papers [36, 37, 43]. In the present paper, we derive a general solution valid for any lattice described by equations of motion (4).

The temperature matrix at time $t$ is calculated by formula (27). Substitution of initial temperature profile (38) into (27) after some transformations yields

$$T_F = \frac{1}{2} \left( T_b + \Delta T \sin \frac{2\pi x}{L} \right) F(t), \quad T_S = \frac{T_b}{2} E + \frac{\Delta T}{2} S(t) \sin \frac{2\pi x}{L},$$

$$F = \int_{k} \mathbf{P} \tilde{F} \mathbf{P}^*_{\mathbf{P}} dk, \quad S = \int_{k} \mathbf{P} \tilde{S} \mathbf{P}^*_{\mathbf{P}} dk, \quad \tilde{F}_{ij} = \cos(2\omega_j t) \delta_{ij}, \quad \tilde{S}_{ij} = \cos \frac{2\pi v_g^j t}{L} \delta_{ij}.$$  (39)

Here $v_g^j = v_g^j \cdot \mathbf{e}$. Calculating trace in formula (39) we obtain simple expression for kinetic temperature:

$$T = T_F + T_S, \quad T_F = \frac{1}{2N} \left( T_b + \Delta T \sin \frac{2\pi x}{L} \right) \sum_{j=1}^{N} \int_{k} \cos(2\omega_j t) dk,$$

$$T_S = \frac{T_b}{N} + \frac{\Delta T}{2N} \sin \frac{2\pi x}{L} \sum_{j=1}^{N} \int_{k} \cos \frac{2\pi v_g^j t}{L} dk.$$  (40)
Formula (40) shows that temperature profile remains sinusoidal at any moment in time. Therefore we compute amplitude of a sin as a function of time. In real experiment, the amplitude can be measured using the transient thermal grating technique [31, 60]. In one-dimensional case the amplitude is calculated as

\[ A = \frac{2}{L} \int_0^L T(x,t) \sin \frac{2\pi x}{L} \mathrm{d}x, \quad A = \frac{1}{N} \text{tr} A = \frac{2}{L} \int_0^L T(x,t) \sin \frac{2\pi x}{L} \mathrm{d}x, \quad (41) \]

To increase the accuracy, in two-, and three-dimensional cases, results are additionally integrated in directions, orthogonal to \( x \). Substituting expression for temperature (39) into formula (41), yields

\[ A = \Delta T (F(t) + S(t)), \quad A = \frac{\Delta T}{2N} \sum_{j=1}^N \int_k \left( \cos(2\omega_j t) + \cos \frac{2\pi v_j^g t}{L} \right) \mathrm{d}k. \quad (42) \]

Formula (42) shows that time evolution of amplitude \( A \) depends on direction, \( e \), of initial thermal perturbation. Therefore heat transport in two- and three-dimensional lattices is generally anisotropic (see, for example, figure 10).

Formula (39) shows that \( T_F \) and \( T_S \) have different time scales, proportional to \( 1/\omega_j \) and \( L/v_j^g \) respectively. The first time scale is determined by frequencies of vibrations of individual atoms. The second time scale is determined by a time required for a wave to travel distance \( L \). The ratio of these time scales is a large parameter. Therefore time scales of fast and slow thermal processes are well separated.

From formula (42) and the stationary phase method [19] it follows that amplitude, \( A \), of temperature profile in ballistic regime decays as \( 1/t^2 \). Note that solution of analogous problem using Fourier and hyperbolic (Maxwell-Cattaneo-Vernotte [15, 65]) heat transfer equations yields exponential decay of the amplitude.

Thus decay of amplitude of sinusoidal temperature profile in a purely ballistic regime is described by formulas (42). Presented results may serve for interpretation of experimental data obtained by transient thermal grating technique [31, 60]. In particular, in a recent paper [29] it is shown experimentally that decay of a sinusoidal profile in polycrystalline graphite at temperatures about 100K is nonmonotonic. Similar effect is predicted by our formula (42) (see e.g. figure 10).

9 Example. Diatomic chain

In this section, ballistic heat transport in the simplest one-dimensional polyatomic lattice is analyzed. We demonstrate that formulas (24) describe time evolution of a temperature profile with high accuracy. Also we show that during heat transport temperatures, corresponding to two degrees of freedom of the unit cell, are generally different even if their initial values are equal.

9.1 Equations of motion

We consider a diatomic chain with alternating masses \( m_1, m_2 \) and stiffnesses \( c_1, c_2 \) (see fig. 2). The chain consists of two sublattices, one formed by particles with mass \( m_1 \) and another formed by particles with mass \( m_2 \).
Figure 2: Two unit cells of a diatomic chain with alternating masses and stiffnesses. Particles of different size form two sublattices.

We write equations of motion of the chain in matrix form (4). Unit cells, containing two particles each, are numbered by index $j$. Position vector of the unit cell $j$ has form

$$x_j = x_j e, \quad x_j = a \left(j - \frac{n_c}{2}\right),$$

where $a$ is a distance between unit cells; $e$ is a unit vector directed along the chain; $n_c$ is the total number of unit cells in the periodic cell. Each particle has one degree of freedom. Displacements of particles, belonging to the unit cell $j$, form a column

$$u_j = u(x_j) = \begin{bmatrix} u_{1j} & u_{2j} \end{bmatrix}^T,$$

where $u_{1j}, u_{2j}$ are displacements of particles with masses $m_1$ and $m_2$ respectively. Then equations of motion have form

$$M \ddot{u}_j = C_1 u_{j+1} + C_0 u_j + C_{-1} u_{j-1},$$

$$M = \begin{bmatrix} m_1 & 0 \\ 0 & m_2 \end{bmatrix}, \quad C_0 = \begin{bmatrix} -c_1 - c_2 & c_1 \\ c_1 & -c_1 - c_2 \end{bmatrix}, \quad C_1 = C_1^\top = \begin{bmatrix} 0 & 0 \\ c_2 & 0 \end{bmatrix}. (45)$$

Initially particles have random velocities and zero displacements. In this section we consider isotropic initial temperature matrices, i.e. $T_0(x_j) = T_0(x_j) E$. Then initial temperatures of the sublattices are equal ($T_{11}^0 = T_{22}^0 = T_0$). Corresponding initial conditions for the particles have form:

$$u_{1j} = u_{2j} = 0, \quad \dot{u}_{1j} = \beta_j \sqrt{\frac{k_B}{m_1}} T_0(x_j), \quad \dot{u}_{2j} = \gamma_j \sqrt{\frac{k_B}{m_2}} T_0(x_j),$$

where $\beta_j, \gamma_j$ are uncorrelated random values with zero mean and unit variance, i.e. $\langle \beta_j \rangle = \langle \gamma_j \rangle = 0$, $\langle \beta_j^2 \rangle = \langle \gamma_j^2 \rangle = 1$, $\langle \beta_i \gamma_j \rangle = 0$ for all $i, j$.

### 9.2 Dispersion relation and group velocities

In this subsection, we calculate the dispersion relation and matrix $P$ included in formulas (24) for the temperature matrix.

We calculate dynamical matrix, $\Omega$, by formula (10). Substituting expressions (45) for matrixes $M, C_\alpha, \alpha = 0, \pm 1$ into formula (10), we obtain:

$$\Omega = \begin{bmatrix} \frac{c_1+c_2}{m_1} & -\frac{c_1+c_2 e^{-i\kappa}}{\sqrt{m_1 m_2}} \\ \frac{c_1+c_2 e^{i\kappa}}{\sqrt{m_1 m_2}} & \frac{c_1+c_2}{m_2} \end{bmatrix}, \quad k = p \hat{b}, \quad \hat{b} = \frac{e}{a}. (47)$$
where $k$ is a wave vector; $p \in [0; 2\pi]$. Calculation of eigenvalues of matrix $\Omega$, yields the dispersion relation:

$$\omega_{1,2}^2(p) = \frac{\omega_{\text{max}}^2}{2} \left( 1 \pm \sqrt{1 - \frac{16c_1c_2 \sin^2 \frac{p}{2}}{m_1m_2\omega_{\text{max}}^4}} \right), \quad \omega_{\text{max}}^2 = \frac{(c_1 + c_2)(m_1 + m_2)}{m_1m_2}, \quad (48)$$

where index 1 corresponds to plus sign. Functions $\omega_{1}(p), \omega_{2}(p)$ are referred to as optical and acoustic branches of the dispersion relation respectively. Note that $\omega_{1,2}/\omega_{\text{max}}$ equally depend on $m_1/m_2$ and $c_1/c_2$.

Group velocities are calculated by definition (25). Projection of group velocities on direction of the chain for $p \in (0; 2\pi)$ have form

$$v_g^j = a \frac{d\omega_j}{dp}, \quad v_g^1 = \frac{c_1c_2a \sin p}{m_1m_2\omega_1(\omega_1^2 - \omega_2^2)}, \quad v_g^2 = \frac{c_1c_2a \sin p}{m_1m_2\omega_2(\omega_1^2 - \omega_2^2)}. \quad (49)$$

Here $\omega_j$ is a non-negative frequency in formula (48). The maximum group velocity is as follows

$$v_* = \max_{p,j} |v_g^j| = a \sqrt{\frac{c_1c_2}{(c_1 + c_2)(m_1 + m_2)}}, \quad (50)$$

We calculate matrix $P$ in equations (24). By the definition, columns of matrix $P$ are equal to normalized eigenvectors of dynamical matrix $\Omega$. Eigenvectors $d_{1,2}$, corresponding to eigenvalues $\omega_1^2, \omega_2^2$, have form:

$$d_{1,2} = \left[ 1 - \frac{m_1}{m_2} \pm \sqrt{\left(1 - \frac{m_1}{m_2}\right)^2 + 4\left|g\right|^2 \frac{m_1}{m_2} - 2g \sqrt{\frac{m_1}{m_2}}} \right]^\top, \quad g = \frac{c_1 + c_2 e^{ip}}{c_1 + c_2}. \quad (51)$$

Normalization of vectors $d_{1,2}$ yields columns of matrix $P$.

In the following sections, formulas (48), (51) are employed for calculation of temperatures of sublattices $T_{11}, T_{22}$.

### 9.3 Thermal contact of cold and hot parts of the chain

In this section, we consider thermal contact of cold and hot parts of the chain and show that temperatures of sublattices in this problem are different even though their initial values are equal.

Initial spatial distribution of temperature matrix has form

$$T_0(x) = T_0(x)E, \quad T_0(x) = T_b + \Delta TH(x). \quad (52)$$

According to formula (52) initial temperatures of sublattices are equal. In our calculations $\Delta T = T_b$. Since the chain is harmonic, the value $\Delta T/T_b$ does not change results qualitatively\(^{16}\).

Analytical solution of this problem is given by formulas (27), (36). Integrals in formulas (27), (36) are evaluated numerically using Riemann sum approximation. Interval of integration is divided into $2 \cdot 10^4$ equal segments.

\(^{16}\)Note that for anharmonic crystals $\Delta T/T_b$ is an important parameter of the problem, which can change results significantly.
To check formulas (27), (36), we compare them with results of numerical solution of equations of motion (45) with initial conditions (46), (52). Numerical integration is carried out using symplectic leap-frog integrator with time-step $5 \cdot 10^{-3} \tau_{\text{min}}$. According to formulas (27), (36) temperature matrix at large times is self-similar, i.e. it depends on $x/t$ only. Therefore it is sufficient to compare numerical and analytical results at a single moment in time. We compare results at $t = 500 \tau_{\text{min}}$, where $\tau_{\text{min}} = 2\pi/\omega_{\text{max}}$, $\omega_{\text{max}}$ is defined by formula (48). The chain consists of $10^4$ unit cells under periodic boundary conditions. During the simulation, kinetic temperatures of sublattices $T_{11}, T_{22}$, at each unit cell, $j$, are calculated as

$$k_B T_{11}(x_j) = m \left\langle \dot{u}_{1j}^2 \right\rangle_r, \quad k_B T_{22}(x_j) = m \left\langle \dot{u}_{2j}^2 \right\rangle_r,$$

where $\left\langle ... \right\rangle_r$ stands for averaging over realizations of random initial conditions. In the present example, number of realizations is equal to $7 \cdot 10^4$. Resulting temperatures of sublattices $T_{11}, T_{22}$ at $t = 500 \tau_{\text{min}}$ for $m_2 = 2m_1, c_1 = c_2$ are shown in figure 3.

![Figure 3: Thermal contact of hot and cold parts of the diatomic chain ($m_2 = 2m_1, c_1 = c_2$). Temperatures of sublattices $T_{11}$ (solid red line and squares) and $T_{22}$ (dashed blue line and circles) at $t = 500 \tau_{\text{min}}$ are shown. Lines correspond to analytical solution (36). Squares and triangles are results of numerical solution of equations of motion.](image)

The figure shows that numerical results are accurately described by our approximate analytical formulas (27), (36). It is seen that temperatures of sublattices in the central part of the plot are different even though initially they are equal everywhere. This fact is predicted by formulas (27), (36).

**Remark.** Difference of temperatures of light and heavy particles has also been observed in steady problems considered in papers [32, 33]. Our results suggest that in unsteady problems light and heavy particles also have generally different temperatures.
9.4 Sinusoidal initial temperature profile

In the present section, we consider decay of sinusoidal temperature profile (38) in a diatomic chain and show that, as in a previous example, temperatures of sublattices, $T_{11}, T_{22}$, at each unit cell are generally different. Decay of amplitude of sign is nonmonotonic.

Initial spatial distribution of temperature matrix has form

$$T_0(x) = T_0(x)E, \quad T_0(x) = T_b + \Delta T \sin \frac{2\pi x}{L},$$

where $L$ is length of a periodic cell; in further calculations $\Delta T = T_b/2$. Note that according to formula (54) initial temperatures of sublattices are equal. Analytical solution of this problem is given by formula (39). The solution shows that spatial distribution remains sinusoidal at any moment in time. Therefore we compute matrix $A$ by formula (41). Elements $A_{11}, A_{22}$ of this matrix correspond to amplitudes of temperatures $T_{11}, T_{22}$.

Analytical expression for $A$ is given by formula (42). Integrals in formula (42) are evaluated numerically using Riemann sum approximation. Interval of integration is divided into $10^3$ equal segments. Below we compare predictions of this formula with results of numerical solution of equations of motion.

In computer simulations, the chain consists of $10^4$ unit cells under periodic boundary conditions. Equations of motion (45) are solved numerically with initial conditions (46), (54). During the simulation matrix $A$ is calculated by formula (41), where integral is replaced by summation with respect to all unit cells. Temperatures of unit cells are calculated by formula (53). Resulting value of $A$ is averaged over $10^2$ realizations with random initial conditions. Note that number of realizations is less than in the previous example, because formula (41) involves additional spatial averaging, increasing the accuracy. Amplitudes $A_{11}, A_{22}$ of temperatures $T_{11}, T_{22}$ for $m_2 = 2m_1, c_1 = c_2$ are shown in figures 4, 5. Figures show that numerical results are accurately described by our approximate analytical formula (42).

Thus, similarly to the previous example, temperatures of sublattices for $t > 0$ are different ($T_{11} \neq T_{22}$), while their initial values are equal. We also note that decay of amplitude of sinusoidal temperature profile is nonmonotonic.

10 Example. Graphene (out-of-plane motions)

In this section, we consider ballistic heat transport in graphene lattice (see fig. 6). Only out-of-plane vibrations are considered. The model describes out-of-plane vibrations of a stretched graphene sheet [5, 9, 24]. In-plane vibrations can be considered separately, since in harmonic approximation in-plane and out-of-plane vibrations are decoupled. The main goal of this section is to show that approximate formulas (24) describe behavior of temperature in two-dimensional lattices with high accuracy. Additionally we demonstrate individual contributions of acoustic and optical vibrations to thermal transport.

10.1 Equations of motion

In this subsection we represent equations of motion for the graphene lattice in a matrix form.
The lattice is shown in figure 6. Unit cells, containing two particles each, are numbered by pair of indices $i,j$. Primitive vectors $\mathbf{b}_1, \mathbf{b}_2$ for the lattice have form

$$
\mathbf{b}_1 = \frac{\sqrt{3}a}{2} \left( i + \sqrt{3}j \right), \quad \mathbf{b}_2 = \frac{\sqrt{3}a}{2} \left( \sqrt{3}j - i \right),
$$

(55)

where $i,j$ are Cartesian unit vectors directed along $x$ and $y$ axes respectively; $a$ is equilibrium distance between the nearest particles. Vector $\mathbf{b}_1$ connects centers of cells $i,j$ and $i+1,j$. Vector $\mathbf{b}_2$ connects centers of cells $i,j$ and $i,j+1$. Position vector of cell $i,j$ is represented in terms of the primitive vectors as

$$
x_{i,j} = i\mathbf{b}_1 + j\mathbf{b}_2.
$$

(56)

Each particle has one degree of freedom (displacement normal to lattice plane). Displacements of a unit cell $i,j$ form a column:

$$
\mathbf{u}_{i,j} = \mathbf{u}(x_{i,j}) = \begin{bmatrix} u_{1,ij}^1 & u_{1,ij}^2 \end{bmatrix}^T,
$$

(57)

where $u_{1,ij}^1, u_{1,ij}^2$ are displacements of two sublattices.

Consider equations of motion of unit cell $i,j$. Each particle is connected with three nearest neighbors by linear springs (solid lines in fig. 6). Equilibrium length of the spring is less than initial distance between particles, i.e. the graphene sheet is uniformly stretched.$^{17}$ Stiffness of the spring, determined by stretching force, is denoted by $c$. Then equations of motion have form

$$
\mathbf{M} \ddot{\mathbf{u}}_{i,j} = \mathbf{C}_2 \mathbf{u}_{i+1,j} + \mathbf{C}_1 \mathbf{u}_{i+1,j} + \mathbf{C}_0 \mathbf{u}_{i,j} + \mathbf{C}_{-1} \mathbf{u}_{i-1,j} + \mathbf{C}_{-2} \mathbf{u}_{i,j-1},
$$

$$
\mathbf{M} = mE, \quad \mathbf{C}_0 = \begin{bmatrix} -3c & c \\ c & -3c \end{bmatrix}, \quad \mathbf{C}_1 = \mathbf{C}_2 = \begin{bmatrix} 0 & 0 \\ 0 & c \end{bmatrix},
$$

(58)

$^{17}$In the absence of stretching, out-of-plane vibrations are essentially nonlinear. Nonlinear effects in unstrained graphene are considered e.g. in paper [7].
Here \( C_{-1} = C_1^T, \ C_{-2} = C_2^T; m \) is mass of a particle.

Initially particles have random velocities and zero displacements. In this section we consider isotropic initial temperature matrices:

\[
T_0(x_{i,j}, y_{i,j}) = T_0(x_{i,j}, y_{i,j}) E, \tag{59}
\]

where \( x_{i,j}, y_{i,j} \) are Cartesian coordinates of position vector \( x_{i,j} \). In this case initial temperatures of the sublattices are equal \( (T_{11}^0 = T_{22}^0 = T_0) \). Corresponding initial conditions for the particles have form:

\[
u_{1,j} = \nu_{2,j} = 0, \quad \dot{u}_{1,j}^1 = \beta_{i,j} \sqrt{\frac{k_B}{m} T_0(x_{i,j}, y_{i,j})}, \quad \dot{u}_{1,j}^2 = \gamma_{i,j} \sqrt{\frac{k_B}{m} T_0(x_{i,j}, y_{i,j})}, \tag{60}\]

where \( \beta_{i,j}, \gamma_{i,j} \) are uncorrelated random values with zero mean and unit variance, i.e. \( \langle \beta_{i,j} \rangle = \langle \gamma_{i,j} \rangle = 0, \langle \beta_{i,j}^2 \rangle = \langle \gamma_{i,j}^2 \rangle = 1, \langle \beta_{i,j} \gamma_{s,p} \rangle = 0 \) for all \( i, j, s, p \).

Further we consider time evolution of kinetic temperature \( T = \frac{1}{2} (T_{11} + T_{22}) \).

### 10.2 Dispersion relation and group velocities

In this subsection, we calculate the dispersion relation, matrix \( P \) (see formula (12)), and group velocities.

We calculate dynamical matrix \( \Omega \) using formula (10). Substituting expressions (58) for matrixes \( M, C_\alpha, \alpha = 0; \pm 1; \pm 2 \) into formula (10), yields

\[
\Omega = \omega^2 \begin{bmatrix}
3 & -1 - e^{-ip_1} - e^{-ip_2} \\
-1 - e^{ip_1} - e^{ip_2} & 3
\end{bmatrix}, \quad p_1 = k \cdot b_1, \quad p_2 = k \cdot b_2, \tag{61}
\]

where \( k \) is wave-vector; \( \omega^2 = \frac{c}{m} \); \( p_1, p_2 \in [0; 2\pi] \) are dimensionless components of the wave vector.
Figure 6: Numbering of unit cells in graphene lattice. Here $b_1$, $b_2$ are primitive vectors of the lattice. Particles move along the normal to lattice plane. $x$, $y$ axes correspond to zigzag and armchair directions respectively.

Eigenvalues $\omega_1^2, \omega_2^2$ of matrix $\Omega$ determine dispersion relation for the lattice. Solution of the eigenvalue problem yields:

$$\omega_{1,2}^2 = \omega_*^2 (3 \pm R(p_1, p_2)),$$

where index 1 corresponds to plus sign. Functions $\omega_1(p_1, p_2), \omega_2(p_1, p_2)$ are referred to as optical and acoustic dispersion surfaces respectively. Eigenvectors of matrix $\Omega$ are columns of matrix $P$:

$$P = \frac{1}{\sqrt{||b||^2 + b^2}} \left[ \begin{array}{c} |b| \\ -b \\ b \end{array} \right], \quad b = 1 + e^{ip_1} + e^{ip_2}. \quad (63)$$

Group velocities $v^1_g, v^2_g$ for $p_1, p_2 \in (0; 2\pi)$ are calculated by definition (25) as

$$v^j_g = \frac{\partial \omega_j}{\partial k} = \frac{\partial \omega_j}{\partial p_1} b_1 + \frac{\partial \omega_j}{\partial p_2} b_2,$$

$$\frac{\partial \omega_1}{\partial p_1} = \frac{-\omega_*^2 \sin p_1 \sin (p_1 - p_2)}{2\omega_1 R(p_1, p_2)}, \quad \frac{\partial \omega_1}{\partial p_2} = \frac{-\omega_*^2 \sin p_1 \sin (p_1 - p_2)}{2\omega_1 R(p_1, p_2)}, \quad \frac{\partial \omega_2}{\partial p_1} = \frac{\omega_*^2 \sin p_1 + \sin (p_1 - p_2)}{2\omega_2 R(p_1, p_2)}, \quad \frac{\partial \omega_2}{\partial p_2} = \frac{\omega_*^2 \sin p_1 - \sin (p_1 - p_2)}{2\omega_2 R(p_1, p_2)}. \quad (64)$$

Here $\omega_1 \geq 0, \omega_2 \geq 0$; function $R(p_1, p_2)$ is defined by formula (62); primitive vectors $b_1, b_2$ are given by formula (55).

According to formulas (64), the maximum absolute values of group velocities corresponding to acoustic and optical branches are as follows

$$\max_{p_1, p_2} |v^1_g| \approx 0.448v_*, \quad \max_{p_1, p_2} |v^2_g| \approx 0.897v_*, \quad v_* = \omega_* a. \quad (65)$$

In the following sections, formulas (61), (62), (63), (64) are employed for description of ballistic heat transport.
10.3 Circular initial temperature profile

In this subsection we consider contributions of acoustic and optical vibrations to ballistic heat transport.

Initially the temperature has constant value, \( T_1 \), inside a circle of radius \( R \) and vanishes outside:

\[
T_0(x,y) = \begin{cases} 
T_1, & x^2 + y^2 \leq R^2, \\
0, & x^2 + y^2 > R^2, 
\end{cases} 
\]  

(66)

In our calculations \( R = 10a \). Analytical solution of this problem is calculated using formula (28). Integrals in formula (28) are evaluated numerically using Riemann sum approximation. Integration area is divided into 300 \( \times \) 300 equal square elements.

In computer simulations a square graphene sheet of length \( L = 300a \) is considered. Equations of lattice dynamics (58) with initial conditions (60), (66) are solved numerically using leap-frog integrator with time-step \( 5 \cdot 10^{-3} \tau_* \), \( \tau_* = 2\pi/\omega_* \). Kinetic temperatures of all unit cells \( T(x_i,j,y_i,j) \) at \( t = 20\tau_* \) are calculated as

\[
k_B T(x_i,j,y_i,j) = \frac{1}{2}m\left\langle \left(\dot{u}^1_{i,j}\right)^2 + \left(\dot{u}^2_{i,j}\right)^2 \right\rangle, 
\]  

(67)

where averaging is carried out with respect to realizations of random initial conditions. The moment in time is chosen such that fast relaxation process can be neglected. Resulting temperature fields averaged over 10, 10^2, 10^3, 10^4 realizations are shown in figure 7. With increasing number of realizations, results of numerical solution of equations of motion converges to analytical solution given by formula (28). For 10^4 realizations plots of analytical and numerical solutions are visually indistinguishable.

Figure 7 shows, in particular, that heat front is a circle as predicted by formula (34). At the same time, the temperature field has a symmetry of the lattice, i.e. the heat transport is significantly anisotropic.

According to formula (28), temperature field has contributions from acoustic and optical branches of dispersion relation. The contributions are shown in figure 8. Acoustic waves have larger group velocities than optical waves. Therefore temperature front on the left plot from figure 8 propagates faster.

Thus formula (28) describes temperature distribution in graphene lattice with high accuracy. In contrast to numerical results, formula (28) allows to analyze individual contributions of acoustic and optical vibrations to ballistic heat transport.

10.4 Thermal contact of cold and hot half-planes

In this subsection we consider thermal contact of two half-planes with initial temperatures \( T_b \) and \( 2T_b \) (see formula (35)). Temperatures of sublattices are equal. Since thermal transport in graphene is anisotropic, we consider two problems with temperature distribution in \( x \) and \( y \) directions:

\[
T_0 = T_0(x,y) \mathbf{E}, \quad T_0(x,y) = T_b (1 + H(x)) \quad \text{or} \quad T_0(x,y) = T_b (1 + H(y)). 
\]  

(68)

Analytical solution of this problem is given by formula (37).
Figure 7: Temperature field in graphene at $t = 20\tau^*$ corresponding to circular distribution of initial temperature (66). Results of numerical solution of lattice dynamics equations averaged over $10, 10^2, 10^3, 10^4$ realizations are shown. Color bars show $T/T_1$, where $T_1$ is constant in formula (66).

To check formula (37), we compare them with results of numerical solution of equations of motion. Formula (37) shows that at large times the solution is self-similar. Therefore it is sufficient to consider temperature field at a single moment in time. In our calculations it is equal to $t = 20\tau^*$. Nearly square graphene sheet containing $301 \times 348$ unit cells is considered. Particles have random initial velocities corresponding to initial temperature distributions (68). Initial particle displacements are equal to zero. Periodic boundary conditions in both directions are used. During the simulation, kinetic energy of each unit cell is calculated. In order to calculate temperatures, results are averaged over $1.5 \cdot 10^3$ realizations with random initial conditions. Temperature distributions in $x$ and $y$ directions are shown in figure 9.

The figure 9 shows that numerical results are accurately described by our approximate formulas (24).
Figure 8: Contribution of acoustic (left) and optical (right) vibrations to temperature field in graphene at $t = 20\tau_*$ for circular distribution of initial temperature (66) with $R = 10a$. Color bars show $T/T_1$, where $T_1$ is constant in formula (66). Plus signs mean that the resulting temperature field can be obtained by summation of acoustic and optical contributions.

10.5 Sinusoidal initial temperature profile

In the present section, we consider decay of spatially sinusoidal temperature profile (38) in graphene. We investigate the influence of lattice anisotropy on heat transfer by comparing solutions of two problems with temperature changing zigzag ($x$) and armchair ($y$) directions:

$$T_0(x,y) = T_0 E, \quad T_0(x,y) = T_b + \Delta T \sin \frac{2\pi x}{L} \quad \text{or} \quad T_0(x,y) = T_b + \Delta T \sin \frac{2\pi y}{L}, \quad (69)$$

where $L$ is length of a periodic cell. In our calculations $\Delta T = T_b/2$.

Analytical solution of this problem is given by formula (39). The solution shows that spatial distribution remains sinusoidal at any moment in time. Therefore we compute amplitude of temperature profile (see formula (41)). Analytical expression for $A$ is given by the second formula from (42). Integrals in formula (42) are evaluated numerically using Riemann sum approximation. Interval of integration is divided into $200 \times 200$ equal
Figure 9: Thermal contact of hot and cold parts of graphene. Solutions of two problems with temperature distributions in $x$ (solid red line) and $y$ (dashed blue line) directions at $t = 19.5\tau_*$ are shown. Analytical solution (37) (lines) and results of numerical solution of equations of motion (squares and crosses). Here $v_* = \omega_*/a$.

Below we compare predictions of this formula with results of numerical solution of equations of motion.

We check the accuracy of formula (42) using numerical solution of equations of motion. Particles have random initial velocities corresponding to initial temperature distributions (69). Initial particle displacements are equal to zero. Periodic boundary conditions in both directions are used. The periodic cell contains $200 \times 232$ unit cells. During simulation amplitude, $A$, is calculated using two-dimensional version of formula (41):

$$A = \frac{2}{L^2} \int_0^L \int_0^L T(x,y) \sin \frac{2\pi x}{L} \, dx \, dy \quad \text{or} \quad A = \frac{2}{L^2} \int_0^L \int_0^L T(x,y) \sin \frac{2\pi y}{L} \, dx. \quad (70)$$

Integral in formula (70) is replaced by sum with respect to unit cells.

Dependence of dimensionless amplitude, $A/\Delta T$, on dimensionless time, $c_* t/L$, is shown in figure 10. Every circle on the plot corresponds to average over realizations. Figure 10 shows that analytical solution (42) practically coincides with results of numerical solution of lattice dynamics equations. Results for $x$ and $y$ directions practically coincide for $t \leq L/v_*$, while for $t > L/v_*$ they are significantly different.

Thus our analytical solution (42) shows that decay of amplitude of the sinusoidal profiles in zigzag and armchair directions is nonmonotonic. Similar nonmonotonic behavior has been recently observed experimentally in polycrystalline graphite [29] at temperatures about $T_b \sim 100K$ and length scales $L \sim 1\mu m$. The nonmonotonic behavior shows that at these time and length scales the heat transport in graphite is ballistic.

11 Conclusions

We have shown that time evolution of initial temperature profile in infinite harmonic crystals is described by formula (24) with high accuracy.
Figure 10: Amplitude, $A$, of sinusoidal temperature profile in graphene at short times (left) and large times (right). Solutions of two problems with temperature distributions in zigzag (red line) and armchair (blue line) directions are shown. Analytical solution (42) (lines) and numerical solution of equations of motion (squares and triangles). Here $v_* = \omega_* a$.

It was shown that at short times temperatures, corresponding to degrees of freedom of the unit cell, oscillate and tend to generally different equilibrium values. The oscillations are caused by redistribution of energy between kinetic and potential forms and redistribution of energy between degrees of freedom of the unit cell. In infinite crystals\textsuperscript{18}, the oscillations practically vanish at times of order of 100 periods of atomic vibrations.

Evolution of temperature profile at large times is caused by ballistic heat transport. At large times temperature field is represented as a superposition of waves having a shape of initial temperature distribution and traveling with group velocities depending on the wave vector. Formula (24) has the same property as equations of lattice dynamics, it is invariant with respect to change $t$ by $-t$.

It is noteworthy that temperatures, corresponding to degrees of freedom of the unit cell, at large times are generally neither equal to each other nor equal to their equilibrium values. Therefore thermal state of unit cells reached by thermal waves is strongly nonequilibrium (see e.g. figures 3, 4, 5). It was shown that these analytical findings are in a good agreement with results of numerical solution of equations of motion.

Though formula (24) allows to calculate the temperature profile, it does not yield an equation describing ballistic heat transport. So far the closed equation has been derived only for several particular lattices [4, 36, 37]. Derivation of the general equation valid for all harmonic crystals would be an interesting extension of the present work.

Presented theory may serve for proper statement and interpretation of experiments on unsteady ballistic heat transport in crystals. Analytical solution of the problem with sinusoidal profile of initial temperature can be used for interpretation of results obtained by the transient thermal grating technique [31, 60, 29]. In particular, the solution predicts

\textsuperscript{18}In the case of finite crystals, the phenomenon of thermal echo introduced in paper [51] is observed.
nonmonotonic decay of the temperature profile, which was recently observed experimentally in graphite [29].

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A Approximate formula for the temperature matrix

In this section, approximate formula (24) for the temperature matrix is derived. The derivation is based on the assumption that the main contribution to integrals $T_F, T_S$ comes from the points such that $k_1 \approx k_2$.

The expression for $T_F$ in formula (24) is derived as follows. We introduce new variables in formula (23) for $T_F$:

$$p_1 = k_1, \quad p_2 = k_1 - k_2.$$  \hspace{1cm} (71)

Jacobian of this transformation is equal to unity. Using periodicity of the integrand in formula (23), it can be shown that integration is carried out in the same domain as in formula (9). We assume that the main contribution to the integral (24) comes from the points $p_2 \approx 0$ ($k_1 \approx k_2$). Then integrand is expanded into series with respect to $p_2$. In particular, the following approximate formulas are used:

$$P(p_1 - p_2) \approx P(p_1), \quad \omega_i(p_1) \pm \omega_j(p_1 - p_2) \approx \omega_i(p_1) \pm \omega_j(p_1),$$  \hspace{1cm} (72)

where $i \neq j$. Then formula (23) for $T_F$ reads

$$T_F \approx \int_{p_1} P \int_{p_2} \sum_y \hat{T}_F(y, p_1) e^{i p_2 \cdot (x-y)} dp_2 P^{*\top} dp_1, \quad P = P(p_1),$$

$$\{\hat{T}_F\}_{ij} = \frac{1}{2} \{P^{*\top} T_0(y) P\}_{ij} \left[ \cos((\omega_i(p_1) + \omega_j(p_1))t) + (1 - \delta_{ij}) \cos((\omega_i(p_1) - \omega_j(p_1))t) \right].$$  \hspace{1cm} (73)

According to the definition of the discrete Fourier transform the following identity is satisfied:

$$\int_{p_2} \sum_y \hat{T}_F(y, p_1) e^{i p_2 \cdot (x-y)} dp_2 = \hat{T}_F(x, p_1).$$  \hspace{1cm} (74)

Substituting this identity into formula (73) yields the expression for $T_F$ in formula (24).

To derive approximate expression for $T_S$ in formula (24) we introduce new variables (71) in formula (23). The integrand in formula (23) is expanded into series with respect to $p_2$. In particular, the following approximate formulas are used:

$$P(p_1 - p_2) \approx P(p_1), \quad \omega_j(p_1) - \omega_j(p_1 - p_2) \approx p_2 \cdot v_j(p_1),$$  \hspace{1cm} (75)
where $v^j_2$ is the group velocity defined by formula (24). Then formula (23) for $T_S$ reads

$$T_S \approx \int_{p_1} \int_{p_2} \sum_y P T_S(y) P^{sT} e^{ip^2_2(x-y)} dp_2 dp_1, \quad P = P(p_1),$$

$$\{T_S\}_{ij} \approx \frac{1}{2} \{P^{sT} T_0(y) P\}_{ij} \delta_{ij} \cos(p^2_2 \cdot v^j_2(p_1)t).$$

(76)

Using identity $2 \cos(p^2_2 \cdot v^j_2 t) = e^{ip^2_2 \cdot v^j_2 t} + e^{-ip^2_2 \cdot v^j_2 t}$ and properties of the discrete Fourier transform, we show that

$$\int_{p_2} \sum_y \{P^{sT} T_0(y) P\}_{jj} \cos(p^2_2 \cdot v^j_2 t) e^{ip^2_2 \cdot(x-y)} dp_2 = \frac{1}{2} \{P^{sT} (T_0(x + v^j_2 t) + T_0(x - v^j_2 t)) P\}_{jj}.$$

(77)

Substituting formula (77) into formula (76), yields the expression for $T_S$ in formula (24).

More rigorous derivation of formula (24) is beyond the scope of the present paper. In the present paper, we show that formula (24) has high accuracy by comparison of analytical solutions of several problems with results of numerical solution of lattice dynamics equations (see sections 9, 10).

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