Heat transfer in infinite one-dimensional crystal considering the third coordination sphere

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Abstract. The work focuses on the analytical description of unsteady thermal processes in low-dimensional structures. The object of study is an infinite one-dimensional harmonic crystal with interactions up to the third coordination sphere. The paper explains how a variation in bond stiffness between particles of different coordination spheres affects the behaviour of the system. The fundamental solution to the heat propagation problem has been constructed and investigated. It is shown that the initial thermal perturbation evolves into several consecutive thermal waves propagating with finite velocities. The number, the velocities, and the intensity coefficients of these waves are determined by the bond stiffnesses.

Keywords: harmonic crystal, third coordination sphere, unstationary heat transfer, heat waves, fundamental solution

Acknowledgements*. This work is supported by Russian Science Support Foundation (Grant No. 21-11-00378).*
The authors thank E. Podolskaya and D. Tsvetkov for useful discussions throughout the conducted research.

Citation: Rubinova RV, Loboda OS, Krivtsov AM. Heat transfer in infinite one-dimensional crystal considering the third coordination sphere. *Materials Physics and Mechanics*. 2022;xx(x): xxx-xxx. DOI: 10.18149/MPM.xxx2022_x.

1. Introduction

In most macro-scale objects, heat propagation can be described by the Fourier law, in which the linear relationship between heat flow and temperature gradient is assumed. However, deviations from the law can be observed at the micro/nano-level [1-2] where ballistic and anomalous processes of energy transfer take place. Dynamics of the crystal lattice is widely used in studies of various processes at micro- and macro-levels including thermal [3-9].

The non-diffuse thermal conductivity has been analytically [10-18] and experimentally [19-23] investigated during the last years. Extensive research on unsteady ballistic heat transfer processes was conducted by our scientific group [24-32]. An area of particular interest, where anomalies can be observed the most, is heat transport in harmonic crystals.

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The behaviour of such systems can be described by statistical characteristics. For some of them such as kinetic temperature analytical expression can be obtained [25].

An important area of research is heat transport in polyatomic systems or systems with non-neighbouring interactions. Considerable progress has been made in the analysis of the harmonic diatomic crystals as well as the harmonic crystals with the second coordination sphere [33-35]. In this paper, a crystal with interactions up to the third coordination sphere is discussed.

The crystalline model and its equation of motion are analysed to obtain expressions for the dispersion relation and group velocities. Based on a previously developed model of ballistic heat transfer, a fundamental solution is obtained and the influence of non-neighbouring interactions is investigated.

2. Statement of the Problem

A one-dimensional harmonic crystal is a chain of material points linearized along deformation by forces. The system studied consists of equal masses m that interact with their neighbours up to the third coordination sphere (Fig. 1). Equation of motion

$$m\ddot{u}_n = c_1(u_{n+1} - 2u_n + u_{n-1}) + c_2(u_{n+2} - 2u_n + u_{n-2}) + c_3(u_{n+3} - 2u_n + u_{n-3}) \quad (1)$$

describes the system's behaviour where u_n is the displacement of the n-th particle; c_1, c_2, and c_3 are the stiffnesses of couplings between the nearest, second nearest, and third nearest neighbours respectively.

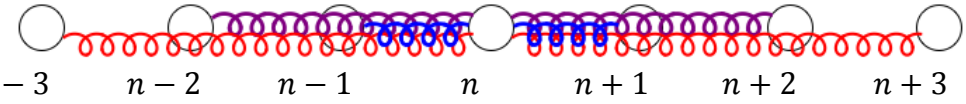


Fig. 1. One-dimensional harmonic crystal considering the third coordination sphere

In [34] the case $c_3 = 0$ was studied. The modified stiffness

$$c_{12} = c_1 + 4c_2 \quad (2)$$

was introduced to emphasize the second-order difference for the particles of the second coordination sphere. To ensure that the model presented in this paper is aligned with previous research, the same procedure was followed. Eq. (1) takes the form:

$$m\ddot{u}_n = c_{12}(u_{n+2} - 2u_n + u_{n-2})/4 - c_1(u_{n+2} - 4u_{n+1} + 6u_n - 4u_{n-1} + u_{n-2})/4 + c_3(u_{n+3} - 2u_n + u_{n-3}). \quad (3)$$

To solve equation (3) initial conditions for displacements and velocities should be specified. In case of instantaneous temperature perturbation, velocities are set to non-zero independent random values:

$$u_n|_{t=0} = 0, \dot{u}_n|_{t=0} = v_n. \quad (4)$$

Expressions (3) and (4) form the stochastic Cauchy problem which can be solved analytically for some crystalline systems.

The concept of kinetic temperature is an essential tool when describing thermal processes at the nanoscale. It depicts the energy transfer taking place through the interactions between the particles and is defined as

$$k_B \mathrm{T_i} \stackrel{\text{def}}{=} m\langle \dot{u}^2{}_i \rangle, \quad (5)$$

where $\mathrm{T_i}$ – kinetic temperature, k_B – Boltzmann constant, $\langle ... \rangle$ – covariance. As shown in [25], the evolution of the temperature field can be described as a superposition of fast and slow processes. The fast processes describe high-frequency oscillations caused by the redistribution of energy among potential and kinetic energy components. The slow processes correspond to the redistribution of energy between particles. This study focuses on the slow processes only.

Given an initial temperature field $T_0(x)$, the temperature at a given time and point is

$$T(x,t) = \frac{1}{8\pi}\int_{-\pi}^{\pi}\Big(T_0\big(x + c_{gr}(ak)t\big) + T_0\big(x - c_{gr}(ak)t\big)\Big)\,d(ak), \quad (6)$$

where k is the wavenumber, $c_{gr}(ak)$ is the group velocity, and a is the lattice constant corresponding to the distance between the nearest particles in the equilibrium state.

3. Dispersion Relation

The dispersion relation describes the waves that can propagate in the system. It is obtained via substitution of the wave function

$$u_n = Ae^{i(akn+\Omega t)} \quad (7)$$

into the equation of motion (3):

$$\Omega^2 = 4\left(sin^2\left(\frac{ak}{2}\right)\left(\omega_1^2\, sin^2\left(\frac{ak}{2}\right) + \omega_{12}^2\, cos^2\left(\frac{ak}{2}\right)\right) + \omega_3^2\, sin^2\left(\frac{3ak}{2}\right)\right), \quad (8)$$

where Ω is the wave frequency, ω_1, ω_{12} and ω_3 are constants introduced as follows:

$$\omega_1 \overset{\text{def}}{=} \sqrt{c_1/m},\ \omega_{12} \overset{\text{def}}{=} \sqrt{c_{12}/m} = \sqrt{(c_1+4c_2)/m},\ \omega_3 \overset{\text{def}}{=} \sqrt{c_3/m}. \quad (9)$$

For real values of the wave frequency, constants ω_1^2, ω_{12}^2 and ω_3^2 should be positive, therefore the system will be stable only for stiffnesses:

$$c_1 > 0,\ c_1 > -4c_2,\ c_3 > 0. \quad (10)$$

Frequencies $\omega_1, \omega_{12}, \omega_3$ can be depicted as Cartesian coordinates in the three-dimensional space of possible configurations and converted to the spherical coordinates:

$$\omega_1 \overset{\text{def}}{=} \omega\sqrt{2}\cos\gamma\cos\left(\beta+\frac{\pi}{4}\right),\ \omega_{12} \overset{\text{def}}{=} \omega\sqrt{2}\cos\gamma\sin\left(\beta+\frac{\pi}{4}\right), \omega_3 \overset{\text{def}}{=} \omega\sqrt{2}\,sin\,\gamma, \quad (11)$$

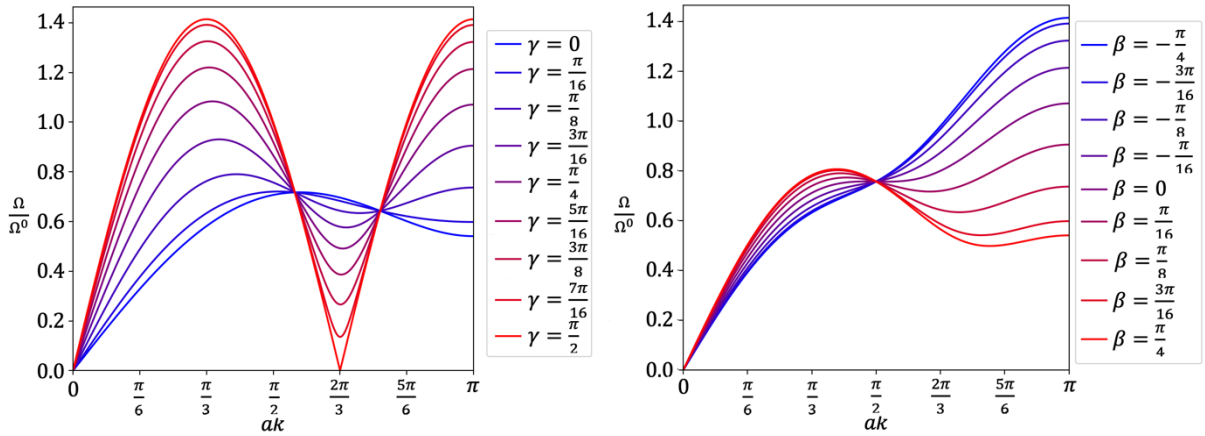
where $\beta \in (-\pi/4; \pi/4)$, $\gamma \in (0; \pi/2)$ and ω is positive. Parameter β describes the transition from interactions between the nearest neighbours to the second coordination sphere, while the third coordination sphere is introduced by parameter γ.

This parametrization allows for a decrease in the dimensionality of the problem. The dispersion relation is rewritten as follows:

$$\Omega = \pm\left(\Omega^0/\sqrt{2}\right)\sqrt{\cos^2\gamma\,(1-\cos ak)[1+\cos ak\,\sin 2\beta] + 2\sin^2\gamma\,(1-\cos(3ak))}, \quad (12)$$

where $\Omega^0 = 2\omega$ is the maximal frequency in the case of a one-dimensional monoatomic harmonic chain with nearest interactions only.

With an increase of the parameter γ the number of extrema as well as the frequency range increase (Fig 2(a)). For the crystal where the third coordination sphere is dominant, three extrema are observed and the maximal frequency is $\sqrt{2}$ times as high as Ω^0.



(a) (b)

Fig. 2. Dispersion relation for different values of (a) parameter γ with fixed $\beta = \frac{\pi}{8}$; (b) parameter β with fixed $\gamma = \frac{\pi}{8}$

For large negative values of parameter β, the influence of the third sphere is levelled out by negative stiffness c_2 (Fig. 2(b)). Additionally, the range of possible frequency values is inversely dependent on the parameter β.

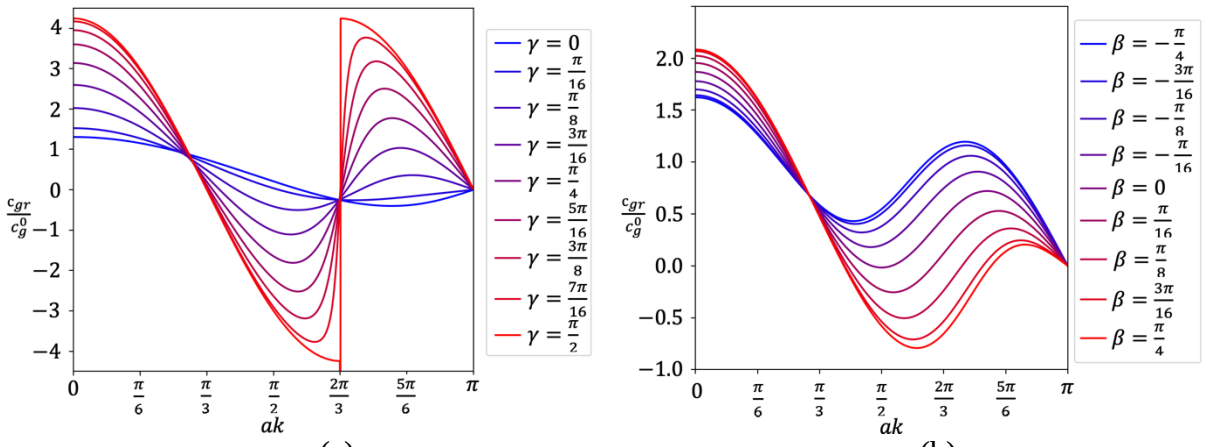
4. Group Velocity

The heat waves propagate in the crystal with group velocities, which can be obtained as a derivative of Eq. (12) with respect to the wavenumber k:

$$c_{gr} = (\Omega^0 c_g^0/2\Omega)[\cos^2\gamma \sin(ak)\,[1 + (2\cos(ak) - 1)\sin(2\beta)] + 6\sin^2\gamma \sin(3ak)], \quad (13)$$

where $c_g^0 = a\omega$ is maximal group velocity in a one-dimensional monoatomic harmonic crystal with nearest interactions only.

The shape and the value range of group velocity curves depend on parameters β and γ (Fig. 3). For the case of non-zero parameter γ, group velocity has three extrema, which is also true for cases when interactions with the second coordination sphere can be neglected ($\beta = 0$, Fig. 3(b)). One extremum is always observed for $ak = 0$, while the second and the third extrema are located in the vicinity of $ak = 2\pi/3$.



(a) (b)

Fig. 3. Group velocity for different values of (a) parameter γ with fixed $\beta = \frac{\pi}{8}$; (b) parameter β with fixed $\gamma = \frac{\pi}{8}$

5. Fundamental Solution

The initial perturbation corresponding to the single-point heat source takes the form of the delta function $T_0(x) = T_0\delta(x)$, where T_0 is an amplitude. An approximate fundamental solution to the heat transfer problem can hence be written as [35]:

$$T = T_0 \sum_j 1/\left(4\pi t\left|c'_{gr}(ak_j)\right|\right), \quad (14)$$

where k_j are roots of the equation

$$\left|c_{gr}(ak_j)\right| = |x|/t. \quad (15)$$

As time evolves, the initial perturbation is spread across the crystal. The position of the heat front can be derived from the singular point of Eq. (14). For the model under study, the number of fronts is a function of the parameters β and γ and can take integer values from one to three. The velocities of the heat waves have been introduced as $c_{gr}^{extr,1}$, $c_{gr}^{extr,2}$ and $c_{gr}^{extr,3}$ respectively, and are obtained by solving equation:

$$\left|c'_{gr}(ak_j)\right| = 0. \quad (16)$$

To quantify the intensity of the front, an approximation of Eq. (14) near a singular point is constructed as shown in [35]:

$$T(x,t) = T_0 / \left(4\pi t \sqrt{2\left|(\zeta^* - \zeta) c''_{gr}(ak^*)\right|} \right), \quad (17)$$

where ζ^* is group velocity at the singular point, ζ is group velocity in its vicinity. Eq. (17) has a singularity when $\zeta = \zeta^*$. The intensity coefficient for a single wave is then introduced as follows:

$$A = 1 / \left(4\pi t \sqrt{2\left|c''_{gr}(ak^*)\right|} \right). \quad (18)$$

For the case of three waves, normalised intensity coefficients are obtained using the following formula:

$$a_i^2 = A_i^2 / (A_1^2 + A_2^2 + A_3^2),\ i = 1,2,3, \quad (19)$$

where A_i are calculated as shown in Eq. (18). These coefficients allow for comparison of the amount of energy stored by different waves.

Some of the configurations of the system studied are considered in this paper (Table 1). For each set of the parameters β and γ the corresponding stiffnesses, wave velocities, and intensity coefficients have been calculated.

Table 1. Stiffnesses, wave velocities, and wave intensity coefficients

β	γ	c_1	c_2	c_3	c_{gr_1}/c_g^0	c_{gr_2}/c_g^0	c_{gr_3}/c_g^0	a_1	a_2	a_3
$-\pi/8$	$\pi/32$	1.69	-0.35	0.02	0.68	1.15	–	0.65	0.76	–
	$\pi/8$	1.46	-0.30	0.29	1.70	1.06	0.32	0.30	0.69	0.66
	$3\pi/16$	1.18	-0.24	0.62	2.40	1.36	0.42	0.26	0.52	0.82
$3\pi/16$	$\pi/16$	0.07	0.44	0.08	1.60	0.62	–	0.35	0.94	–
	$3\pi/16$	0.05	0.32	0.62	2.60	1.26	1.00	0.24	0.72	0.66
	$\pi/2$	0.00	0.00	2.00	4.24	–	–	1.00	–	–

Wave velocities have been analysed as functions of the parameter γ (Figs. 4 and 5). The values $\beta = -\frac{\pi}{8}$ (Fig. 4) and $\beta = \frac{3\pi}{16}$ (Fig. 5) have been considered. The colour of the curves represents the wave intensity coefficient. The numerical solution of Eq. (6) is depicted in footnotes.

For γ equal or close to zero, two waves (1 and 2) are observed. This corresponds to the crystal considering the second coordination sphere studied in [34,35]. When the parameter γ reaches a certain value in the vicinity of $\pi/16$ a third wave appears. For $\gamma = \pi/2$ three waves propagate with equal velocity and only one heat front is observed.

As γ increases, so do the velocities of the waves. Observations establish the inverse dependency between the intensity coefficient and the velocity: the fastest wave 1 stores the lowest amount of energy.

In the first case considered (Fig. 4) wave 3 propagates in the opposite direction unless the bond with the third coordination sphere begins to prevail. The observed behaviour is a result of the negative stiffness c_2. Therefore, the velocity of the third wave is a non-monotonous function with a global minimum around $\gamma = 5\pi/32$.

In the second case (Fig. 5), all the waves propagate in the same direction for all values of γ. As in the first case, the velocity of the second wave is also a non-monotonous function.

In two cases, the third wave appears differently. In the first case (Fig. 4), wave 1 splits up into waves 1 and 3 propagating close together with finite non-zero velocity. In the second case (Fig. 5), the third wave appears in the vicinity of the initial perturbation. For large γ, both cases exhibit similar behaviour. Hence, the conclusion can be made that for parameter γ equal to or larger than $\pi/4$, the influence of the third coordination sphere starts to prevail.

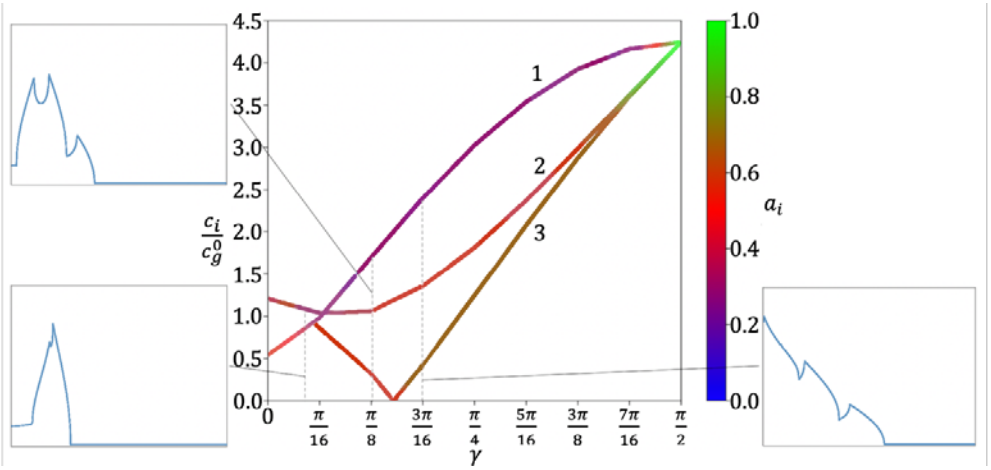


Fig. 4. Velocity and intensity of heat waves as a function of the parameter γ with fixed $\beta = -\frac{\pi}{8}$

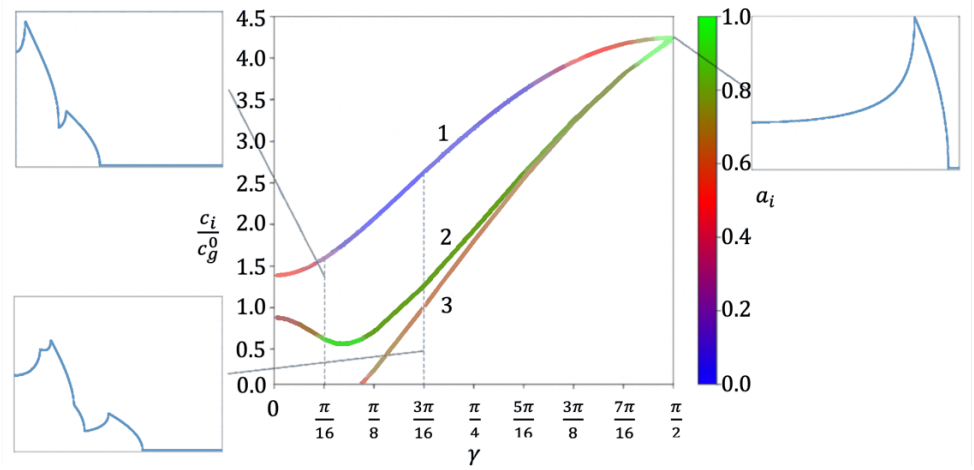


Fig. 5. Velocity and intensity of heat waves as a function of the parameter γ with fixed $\beta = \frac{3\pi}{16}$

6. Conclusion

Heat propagation in a model of a one-dimensional harmonic crystal considering interactions up to the third coordination sphere has been investigated in this study. After the parametrization the system has been described by a function of two dimensionless parameters $\beta \in (-\pi/4; \pi/4)$ and $\gamma \in (0; \pi/2)$. The parameter β characterizes the relative difference in bond stiffnesses of the first and the second coordination spheres. The parameter γ extends the interactions to the third coordination sphere.

The temperature field has been represented as a superposition of several consecutive heat waves propagating with group velocities. There is at least one wave for all stable configurations of the system. When the second coordination sphere is considered, the propagation of two waves with different velocities and intensities is possible. When three coordination spheres are taken into account, up to three heat waves can be observed in the crystal. The second and the third waves occur at certain values of parameters β and γ. In most cases, there is one fast wave accompanied by two slow almost equal velocities waves. The fastest wave as a rule has the lowest intensity coefficient. The deviations can be observed for the border cases when one wave separates into two.

The results can be used for the correct interpretation of experiments on nonstationary ballistic heat transfer in crystals and for further research on crystals with non-neighbouring interactions.

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