International Journal of Heat and Mass Transfer 194 (2022) 123019

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/hmt

Discrete and continuum fundamental solutions describing heat conduction in a 1D harmonic crystal: Discrete-to-continuum limit and slow-and-fast motions decoupling

Serge N. Gavrilov

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

ARTICLE INFO

Article history:
Received 16 January 2022
Revised 4 May 2022
Accepted 9 May 2022
Available online 26 May 2022

Keywords:
Ballistic heat transfer
Harmonic crystal
Asymptotics
The method of stationary phase

ABSTRACT

In the recent paper by Sokolov et al. (Int. J. of Heat and Mass Transfer 176 (2021) 121442) ballistic heat propagation in a 1D harmonic crystal is considered and the properties of the exact discrete solution and the continuum solution of the ballistic heat equation are numerically compared. The aim of this note is to demonstrate that the continuum fundamental solution can be formally obtained as the slow time-varying component of the large-time asymptotics for the exact discrete solution on a moving point of observation.

1. Introduction

In recent paper [1] ballistic heat propagation in a 1D harmonic crystal is considered, and the properties of the exact discrete solution for the kinetic temperature and the approximate continuum solution are numerically compared. The discrete solution and the continuum one can be obtained as the convolutions (see Section 2) of the initial conditions with the corresponding fundamental solutions. The exact discrete fundamental solution is [2–4]

$$\tilde{T}_n(t) \stackrel{\text{def}}{=} 2J_{2n}^2(2t). \tag{1}$$

The continuum fundamental solution [5–7]

$$\tilde{T}(x,t) \stackrel{\text{def}}{=} \frac{H(t-|x|)}{\pi\sqrt{t^2-x^2}} \tag{2}$$

satisfies a partial differential equation called the ballistic heat equation [6]. Here $J_{2n}(\cdot)$ is the Bessel function of the first kind of integer order $2n$, n is a particle number, $H(\cdot)$ is the Heaviside function, t is the dimensionless time, x is the dimensionless spatial co-ordinate ($x = n$ for any integer x). The ballistic heat equation was introduced by Krivstov [5], who considered the infinite system of differential-difference equations for covariance variables and applied the procedure of continualization.

The aim of this note is to demonstrate that the continuum fundamental solution (2) can be formally obtained as the slow time-varying component of the large-time asymptotics for the exact discrete solution (1) on a moving point of observation.

2. Mathematical formulation

In this section we briefly formulate the problem concerning an initial random excitation for a 1D harmonic crystal in the framework of the two approaches to introduce the fundamental solutions, which we plan to compare.

2.1. The discrete (exact) approach

Both solutions (1) and (2) describe the propagation of the kinetic temperature in the same infinite mechanical system, governed by the following equations and initial conditions:

$$\ddot{u}_n = u_{n+1} - 2u_n + u_{n-1}, \tag{3}$$

$$u_n(0) = 0, \qquad \dot{u}_n(0) = \rho_n. \tag{4}$$

Here $n \in \mathbb{Z}$, ρ_n are uncorrelated random quantities such that

$$\langle \rho_n \rangle = 0, \qquad \langle \rho_n \rho_k \rangle = \sigma_n \delta_{nk}; \tag{5}$$

overdot denotes the derivative with respect to dimensionless time t, δ_{nk} is the Kronecker delta, the angle brackets denote the mathematical expectation. The kinetic temperature is conventionally introduced by the following formula

$$T_n \stackrel{\text{def}}{=} 2k_B^{-1}\langle K_n \rangle, \tag{6}$$

E-mail address: serge@pdmi.ras.ru

https://doi.org/10.1016/j.ijheatmasstransfer.2022.123019
0017-9310/

where $K_n(t) = \frac{\dot{u}_n^2(t)}{2}$ is the kinetic energy of the particle with number n, k_B is the (dimensionless) Boltzmann constant.

Remark 1. In this paper we discuss mostly the fundamental solutions and consider a slightly different and simpler problem formulation than the one used in [1]. In [1], following to [4], both the kinetic and the potential energy were initially equally excited, and, therefore, both initial conditions (4) were non-zero.

Consider the particular case for ρ_n, namely, a random point excitation:

$$\rho_n = \rho_0 \delta_{n0}. \tag{7}$$

The exact expression for the particle velocity is [2–4]

$$\dot{u}_n = \rho_0 J_{2n}(2t). \tag{8}$$

Accordingly, the exact expression for the mathematical expectation of the kinetic energy is

$$\langle K_n(t)\rangle = \frac{1}{2}\langle \dot{u}_n^2\rangle = \mathscr{E}_0 J_{2n}^2(2t), \tag{9}$$

where

$$\mathcal{E}_0 \stackrel{\text{def}}{=} \sum_{n=-\infty}^{\infty} \langle K_n(0)\rangle = \frac{\sigma_0}{2} \tag{10}$$

is the mathematical expectation for the initial kinetic (as well as the total) energy for the whole crystal in the case of point excitation. Thus, since

$$J_{2n}^2(0) = \delta_{n0}, \tag{11}$$

formulas (6) and (9) result in

$$T_n(t) = k_B^{-1}\mathscr{E}_0 \tilde{T}_n(t), \tag{12}$$

where $\tilde{T}_n(t)$ (the discrete fundamental solution) is defined by Eq. (1). For $t = 0$ the last formula reads

$$T_n(0) = 2k_B^{-1}\mathscr{E}_0\delta_{n0} = k_B^{-1}\sigma_0\delta_{n0}. \tag{13}$$

In more general case (5), the solution of problem (3)–(5) can be expressed in the form of the discrete spatial convolution:

$$T_n(t) = \frac{k_B^{-1}}{2}\sigma_n \star \tilde{T}_n(t) \stackrel{\text{def}}{=} \frac{k_B^{-1}}{2}\sum_{k=-\infty}^{\infty}\sigma_k \tilde{T}_{n-k}(t). \tag{14}$$

It is known [3,8,9] that in the case $\sigma_n = \text{const}$ exact solution (14) of problem (3)–(5) describes the process of thermal equilibration of the kinetic energy $K \equiv K_n$ and the potential one

$$\Pi \equiv \Pi_n = \frac{1}{2}\big\langle (u_{n+1} - u_n)^2\big\rangle. \tag{15}$$

Namely, in the last case, according to (14) one has [3,8,9]

$$\mathcal{L} = K - \Pi = O\big(t^{-1/2}\big), \tag{16}$$

where $\mathscr{L}$ is the Lagrangian.

2.2. The continuum (approximate) approach

The kinetic temperature propagation in the system described by Eqs. (3)–(4) can be approximately described by the ballistic heat equation [5,6]:

$$\ddot{T}(x,t) + \frac{1}{t}\dot{T}(x,t) = T''(x,t). \tag{17}$$

Here $T(x,t)$ is the kinetic temperature per unit length (a continuum quantity), prime denotes the spatial derivative with respect to x. The corresponding initial conditions are

$$T(x,0) = T_0(x), \qquad \dot{T}(x,0) = 0. \tag{18}$$

The initial temperature $T_0(x)$ is assumed to be a slowly varying function. The solution of Eqs. (17)–(18) can be expressed in the form of a spatial convolution [5,6]:

$$T(x,t) = T_0(x) * \tilde{T}(x,t) \stackrel{\text{def}}{=} \int_{-\infty}^{+\infty} T_0(\xi)\tilde{T}(x-\xi,t)\,\mathrm{d}\xi, \tag{19}$$

where $\tilde{T}$ is the continuum fundamental solution. Consider the case of a point excitation, i.e., the solution of the ballistic heat equation with initial conditions

$$T(x,0) = T_0^0\delta(x), \qquad \dot{T}(x,0) = 0. \tag{20}$$

The mathematical expectation for the initial kinetic energy of the whole crystal in the framework of the continuum approach is

$$\frac{k_B}{2}\int_{-\infty}^{\infty} T_0(x)\,\mathrm{d}x = \frac{k_B T_0^0}{2}. \tag{21}$$

The value of T_0^0 should be chosen in order to make problem (17)–(18) physically equivalent to (3), (4), (7). This requirement is essential to get the approximate continuum solution (19) close to the exact solution (14). The continuum approach implicitly assumes that

- process of thermal equilibration in the case of slowly varying $T_0(x)$ is close to one observed in the case of constant $T_0(x)$ (see (16));
- the ballistic heat equation (17) becomes valid only for large times after equilibration, when $\mathscr{L} \simeq 0$.

Accordingly, for the same physical problem *the initial kinetic energy for the whole crystal, calculated in the framework of the continuum approach should be equal to a half of the initial kinetic energy of the whole crystal observed in the framework of the exact discrete approach.* In particular, considering the case of a random point excitation (7) in the framework of the continuum approach, we need to take initial conditions in the form of (20), where T_0^0 is such that $\frac{k_B T_0^0}{2} = \frac{\mathscr{E}_0}{2}$. Thus, the continuum solution, which corresponds to the discrete solution (12), is

$$T(x,t) = T_0^0\tilde{T}(x,t) = k_B^{-1}\mathscr{E}_0\tilde{T}(x,t). \tag{22}$$

Looking at Eqs. (12) and (22) one can see that to compare the solutions obtained in the frameworks of the discrete and continuum approaches one needs to compare the fundamental solutions (1) and (2). Note that since the initial temperature in the form of the first equation in (20) is not a slowly varying function, the continuum approach is not applicable for a point source, and the solutions, generally speaking, are not close to each other. Indeed, in the case of point excitation, the local energy equilibration co-exists with energy transport, and we can speak about the energy equilibration for the whole crystal only.

3. Asymptotics

Now we want to show that $\tilde{T}(x,t)$ can be formally obtained as a slow component of large-time asymptotics of the corresponding exact discrete solution on a moving point of observation, and looks in some sense like a spatial average of $\tilde{T}_n(t)$. The discrete solution (1) has a physical meaning only for $n \in \mathbb{Z}$. Thus, we can express (1) in terms of the Anger function $\mathbf{J}_n(t)$[1] [11]:

$$\mathbf{J}_n(t) = J_n(t), \quad n \in \mathbb{Z}, \tag{23}$$

$$\mathbf{J}_n(t) \stackrel{\text{def}}{=} \frac{1}{2\pi}\int_{-\pi}^{\pi}\exp \mathrm{i}(t\sin\omega - n\omega)\,\mathrm{d}\omega, \quad n \in \mathbb{R}. \tag{24}$$

[1] The question what is the best continuum approximation for a solution defined only at integer values of a spatial co-ordinate is discussed in book by Kunin [10].

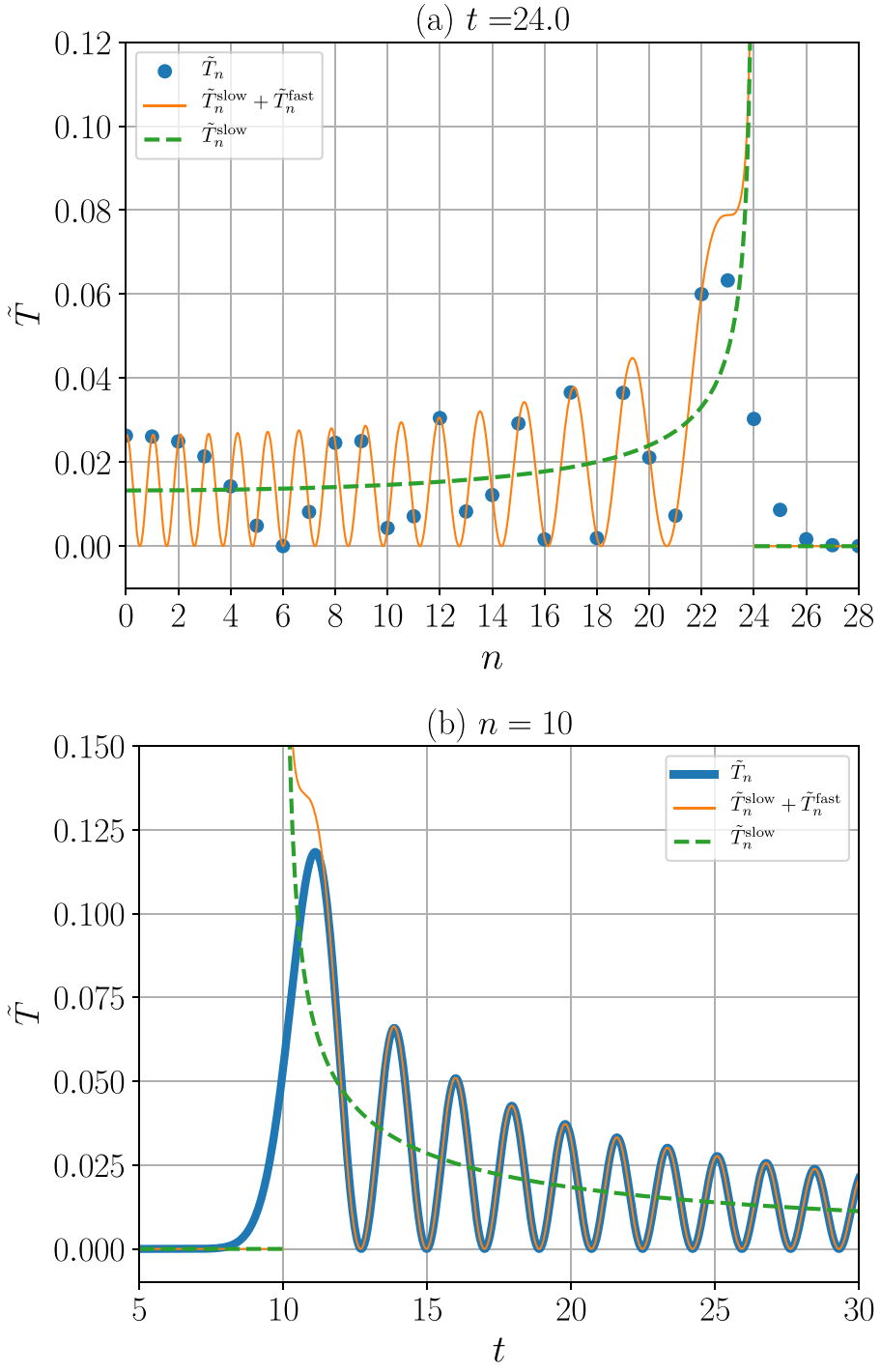

Fig. 1. Comparing the $\tilde{T}_n(t)$, $\tilde{T}_n^{\rm slow}(t)+\tilde{T}_n^{\rm fast}(t)$ and $\tilde{T}_n^{\rm slow}(t)$. (a) The kinetic temperature versus the spatial co-ordinate n, (b) the kinetic temperature versus the time t.

Formula (1) defines an even function of n. Taking into account Eq. (23), we can rewrite formula (1) as follows:

$$\tilde{T}_n(t) = 2\mathbf{J}^2_{2|n|}(2t). \tag{25}$$

Let us calculate the large-time asymptotics of the right-hand side of (25) on the moving front[2]

$$|n| = Vt, \quad V = \text{const}, \quad t \to \infty, \quad t \in \mathbb{R}, \quad n \in \mathbb{R} \tag{26}$$

considering n as a continuum spatial variable. Here the meaning of the quantity $V \geq 0$ is the velocity for the observation point. To estimate the right-hand side of (24) we now use the method of stationary phase [13]. One has

$$\mathbf{J}_{Vt}(t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \exp it\phi(\omega)\,\mathrm{d}\omega, \quad t \to \infty; \tag{27}$$

$$\phi(\omega) \stackrel{\rm def}{=} \sin\omega - V\omega. \tag{28}$$

The stationary points for the phase function $\phi(\omega)$ are defined by the condition $\phi' = 0$. There are no stationary points in the case $V > 1$, therefore integral (27) can be roughly estimated as $O(t^{-1})$. In the case $0 \leq V < 1$ the stationary points are solutions of the equation $\cos\omega = V$, or, in the explicit form,

$$\omega_\pm = \pm\arccos V. \tag{29}$$

[2] This approach [12] allows one to describe running waves, wave-fronts, and to describe the wave-field as a whole.

One gets

$$\phi(\omega_\pm) = \sin\omega_\pm - \omega_\pm = \pm\sqrt{1-V^2} - V\arccos V, \tag{30}$$

$$\phi'' = -\sin\omega, \tag{31}$$

$$\phi''(\omega_\pm) = \mp\sqrt{1-V^2}. \tag{32}$$

Now using the formula for contribution from a stationary point [13], in the case $0 < V < 1$ we obtain:

$$\begin{aligned}\mathbf{J}_{V_t}(t) &= \frac{1}{2\pi}\sum_{(\pm)}\sqrt{\frac{2\pi}{t\phi''(\omega_\pm)}}\exp\mathrm{i}\Big(\phi(\omega_\pm)t + \frac{\pi}{4}\,\mathrm{sign}\phi''(\omega_\pm)\Big) + O(t^{-1})\\ &= \sqrt{\frac{2}{\pi t\sqrt{1-V^2}}}\cos\Big((\sqrt{1-V^2} - V\arccos V)t - \frac{\pi}{4}\Big) + O(t^{-1}).\end{aligned} \tag{33}$$

Thus, according to (25), and provided that (26) is true, one has

$$\begin{aligned}\tilde{T}_n(t) &= \frac{2}{\pi t\sqrt{1-V^2}}\cos^2\Big(\Big(\sqrt{1-V^2} - V\arccos V\Big)2t - \frac{\pi}{4}\Big) + O(t^{-3/2})\\ &= \frac{1}{\pi t\sqrt{1-V^2}}\Big(1 + \sin\Big(\big(\sqrt{1-V^2} - V\arccos V\big)4t\Big)\Big) + O(t^{-3/2}).\end{aligned} \tag{34}$$

Now we return to variables n, t, and substitute $V = |n|/t$ into the last expression. This yields

$$\tilde{T}_n(t) \simeq \tilde{T}_n^{\mathrm{slow}}(t) + \tilde{T}_n^{\mathrm{fast}}(t), \quad |n| < t; \tag{35}$$

$$\tilde{T}_n^{\mathrm{slow}}(t) = \frac{1}{\pi\sqrt{t^2-n^2}}, \tag{36}$$

$$\tilde{T}_n^{\mathrm{fast}}(t) = \tilde{T}_n^{\mathrm{slow}}(t)\sin\left(\left(\frac{\sqrt{t^2-n^2}}{t} - \frac{|n|}{t}\arccos\frac{|n|}{t}\right)4t\right). \tag{37}$$

Formula (35) yields the asymptotic decoupling of thermal motions as the sum of the slow and the fast motions. The right-hand side of Eq. (36) coincides with Eq. (2) provided that $n = x$. The comparison between $\tilde{T}_n(t)$, $\tilde{T}_n^{\mathrm{slow}}(t) + \tilde{T}_n^{\mathrm{fast}}(t)$ and $\tilde{T}_n^{\mathrm{slow}}(t)$ is given in Fig. 1.

4. Conclusion

Up to nowadays it was unclear how to analytically derive the expression (2) for the fundamental solution of the ballistic heat Eq. (17) basing on the fundamental solution (1) of the discrete problem. In the paper we have demonstrated that Eq. (2) can be formally obtained as the slow time-varying component of the large-time asymptotics for the exact discrete solution (1) on a moving point of observation. We also provide the direct procedure to uncouple the slow and the fast thermal motions caused by a point heat source in a 1D harmonic crystal.

We expect that the similar approach can be applied to more complicated and physically significant systems, e.g., to obtain the expression for the slow motion related to unsteady ballistic thermal transport in a 1D harmonic crystal with an isotopic defect (such a model has been used in [14] to describe the Kapitza thermal resistance).

Declaration of Competing Interest

None to declare.

CRediT authorship contribution statement

Serge N. Gavrilov: Conceptualization, Formal analysis, Software, Writing – original draft, Writing – review & editing, Visualization.

Acknowledgements

The author is grateful to A.M. Krivtsov, O.V. Gendelman, A.A. Sokolov, E.V. Shishkina, A.S. Murachev and V.A. Kuzkin for useful and stimulating discussions. This work is supported by Russian Science Support Foundation (Grant No. 21-11-00378).

References

[1] A. Sokolov, W. Müller, A. Porubov, S. Gavrilov, Heat conduction in 1D harmonic crystal: discrete and continuum approaches, Int. J. Heat Mass Transf. 176 (2021) 121442, doi:10.1016/j.ijheatmasstransfer.2021.121442.
[2] E. Schrödinger, Zur dynamik elastisch gekoppelter punktsysteme, Ann. Phys. 349 (14) (1914) 916–934, doi:10.1002/andp.19143491405.
[3] G. Klein, I. Prigogine, Sur la mecanique statistique des phenomenes irreversibles III, Physica 19 (1–12) (1953) 1053–1071, doi:10.1016/S0031-8914(53)80120-5.
[4] P. Hemmer, Dynamic and stochastic types of motion in the linear chain, 1959 Norges tekniske høgskole, Trondheim.
[5] A. Krivtsov, Heat transfer in infinite harmonic one-dimensional crystals, Dokl. Phys. 60 (9) (2015) 407–411, doi:10.1134/S1028335815090062.
[6] A. Krivtsov, The ballistic heat equation for a one-dimensional harmonic crystal, in: H. Altenbach, et al. (Eds.), Dynamical Processes in Generalized Continua and Structures, Advanced Structured Materials 103, Springer, 2019, pp. 345–358, doi:10.1007/978-3-030-11665-1_19.
[7] S. Gavrilov, A. Krivtsov, D. Tsvetkov, Heat transfer in a one-dimensional harmonic crystal in a viscous environment subjected to an external heat supply, Continuum. Mech. Thermodyn. 31 (2019) 255–272, doi:10.1007/s00161-018-0681-3.
[8] A. Krivtsov, Energy oscillations in a one-dimensional crystal, Dokl. Phys. 59 (9) (2014) 427–430, doi:10.1134/S1028335814090080.
[9] S.N. Gavrilov, A.M. Krivtsov, Thermal equilibration in a one-dimensional damped harmonic crystal, Phys. Rev. E 100 (2) (2019) 022117, doi:10.1103/PhysRevE.100.022117.
[10] I. Kunin, Elastic Media with Microstructure I: One-Dimensional Models, Springer-Verlag, Berlin Heidelberg, 1982, doi:10.1007/978-3-642-81748-9.
[11] M. Abramowitz, I. Stegun, Handbook of Mathematical Functions: with Formulas, Graphs, and Mathematical Tables, Dover, New York, 1972.
[12] L. Slepyan, Non-Stationary Elastic Waves, Sudostroenie, Leningrad, 1972.
[13] M. Fedoryuk, The Saddle-Point Method, Nauka, Moscow, 1977.
[14] O.V. Gendelman, J. Paul, Kapitza thermal resistance in linear and nonlinear chain models: isotopic defect, Phys. Rev. E 103 (5) (2021) 052113, doi:10.1103/PhysRevE.103.052113.