

RÓBERT SÁNDOR KOVÁCS
FINAL PROJECT

BUDAPEST UNIVERSITY OF TECHNOLOGY AND ECONOMICS
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Solutions and experimental analysis of the non-equilibrium
thermodynamics of heat conduction equations

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Summary

In the first part of the present thesis we discussed the derivation of the hierarchical system and its connection with the kinetic theory in details. We proved the hyperbolicity properties of each system and determined the characteristic speed of signal propagation. It followed by the analysis of dispersion relations to discover the roles of the parameters in depth with focusing to the signal propagation speeds. These properties are used to discuss the characteristic properties of the solutions. We have seen that the ballistic-diffusive model can reproduce the solutions of the Fourier, MCV, GK and GN equations. Furthermore, it contains the ballistic kind propagation which has very important role in nanosystems.

We analyzed the numerical scheme, its stability and convergence is proved. Further possibility is the improvement of the scheme, the elimination of artificial numerical errors, such as dispersion. In this manner less space and time steps would be needed, so the computational cost would be decreased. The accuracy of the scheme (and the speed of convergence) would be better, too.

In the part of possible application areas, we analyzed the low temperature experiments of NaF. Dreyer's and Struchtrup's result can be exactly reproduced. However, our model does not give back the same propagation speeds in the case of Yanbao's model. It requires further examinations because Ma use a different description and the material parameters are not necessarily the same in two different models. The boundary conditions of the real experiment are ambiguous, nothing is told about the rear side boundary. The cooling effect can significantly modify the temperature distribution.

By the evaluation of the BUTE-DEE-experiment, we can say that the GK equation can be a realistic model to describe heat conduction in heterogeneous materials. The propagation speed is well-handled and we can obtain more realistic result than with the Fourier equation. We can model the small hump (although it is so small) with the help of ballistic-diffusive equation. It can be the first macroscopic observation of ballistic propagation. It cannot be caused by second sound. It requires further experiments and theoretical analysis in this way. We need a more accurate scheme to eliminate the oscillations and make better fitting with this equation.

The main application area of the ballistic-diffusive equation is the appropriate modeling of nanodevices. The thermoelectric effect, the mechanical deformation has influence to the heat conduction, the ballistic propagation. Further research possibility is to analyze its connection with mechanical models, i.e. couple to the deformations, thus we would be able to describe acoustical, relaxation and rheological phenomena. In parallel, the description of the thermal stresses would be also different [1, 2, 3].

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CHAPTER 1

Introduction

Thanks to the technological developments, the age of nano-scale devices has begun where the characteristic time and length of processes is very small. Development and application of lasers with characteristic time of attoseconds [4] (equipment of ELI-ALPS can be used to follow chemical reactions on atomic scale); the nanotechnological improvements requires nano-engineers. Well-known property of the micro-scale structure is the macro-scale laws are not necessarily applicable for such a structure due to the very small characteristic lengths and to the lack of isotropic properties. One must apply some other approach to describe the transport processes.

The present thesis is about heat conduction as a transport mechanism. We will not discuss the different heat propagation phenomena such as radiation and convection, nor the application possibilities of heat conduction models in these transport methods. Although the existence of the temperature wave ("second sound") is proved by experiments on superfluid¹ Helium [5, 6], so far no one could show this kind of propagation under usual environmental conditions in usual materials. There exists no unified continuum model that can describe these low-temperature or nano-scale phenomena in an appropriate way. One can derive a continuum model by using the kinetic theory of phonons via momentum series expansion, but this approach is not adequate from several points of view – although it is the best model to explain the ballistic kind of heat propagation. The most important weakness of the kinetic theory description is the speed of propagation. One must use a coupled system of 30 equations – where the equations contains growing tensorial order variables so the last equation has 30th order tensorial variable – to reproduce the appropriate speed of propagation.

One of the most important property of the Fourier equation is the parabolic type of the heat conduction equation which, rises the paradox of infinite signal propagation speed by heat conduction [7]. The first modification was the Maxwell–Cattaneo–Vernotte equation (MCV) [8], which is a hyperbolic² one, hence it predicts finite propagation speed. Barletta, Zanchini, Dedeurwaerdere et al. draw attention to that the MCV equation is not compatible with the frame of irreversible thermodynamics when using local equilibrium description because, during approaching the equilibrium, entropy will decrease [9, 10, 11]. Nevertheless, this problem can be solved by using generalized entropy [12, 13]. However, despite of the feature of modeling applicability to second sound, it cannot explain the longitudinal and transversal ballistic propagation. Guyer and Krumhansl have derived a phonon hydrodynamic equation by linearizing the Boltzmann equation [14]. This model provides a feature – called the window condition – that corresponds to the temperature domain to predict the phenomenon of second sound.

¹It requires at very low temperatures (around 1-3 K), when the viscosity in the fluid is much lower than at room temperature. To explain this phenomenon, quantum mechanics can be used.

²The analysis of hyperbolicity will be discussed later.

In 1996, Tzou recommended the single phase-lag model [15], but this approach has a concern only in time domain as a memory effect and is not enough to describe the ballistic propagation, because of the lack of a nonlocal part of the model. Chen used an approximation for the Boltzmann equation to derive a ballistic-diffusive equation, and he analyzed in detail the behavior of equations of Fourier, MCV and Boltzmann with various Knudsen numbers [16]. He was able to demonstrate that the MCV equation causes an artificial oscillation in heat flux so this model can not be applied for nanostructures. Cimmelli et al. concentrates on the description of nonlocal nonequilibrium phonon transport in nanosystems [17, 18, 19]. Wang and Guo derived a non-Fourier equation with the help of heat-mass theory [20, 21, 22]. This was inspired by Tolman's theory, which states the existence of heat - mass duality in the frame of general relativity, which means that heat propagation also has some kind of inertia [23]. Despite of the quantity of models, one still cannot clearly describe ballistic propagation. One of the most important difficulties is:

- Heat propagation is described by 3 modes (the “eigendirections” of the propagation), one for the longitudinal and two for the transversal directions, thus ballistic propagation is anisotropic, i.e. depends on the directions. Yanbao Ma draws attention to there are models which that do not distinguish these modes [24].

On the basis of Landau's complex viscosity theory [25], Rogers derived such a phonon gas model [26] that is able to describe the natural transition between the first and second sound in context of low-temperature laser pulse experiments. It's disadvantage is that it does not distinguish the longitudinal and transversal modes. Ma introduced a hybrid model that uses complex viscosity as well and applies a phenomenological extension to model longitudinal phonon propagation [24, 27]. Within the framework of irreversible thermodynamics, theories could derive only the MCV equation in a consistent way of irreversible thermodynamics [28, 13], and the Guyer-Krumhansl equation with dissipative extension [29, 30]. Ballistic propagation does not have (or has not had until now) an irreversible thermodynamical background.

Our goal is to introduce a unified group of models, based on one condition of second law of thermodynamics, hence, on the positivity of entropy production. By comparing several models, we will choose the one that can describe the analyzed phenomena in a credible way. We seek for the characteristic non-Fourier properties in the solutions of each model, which could be detected by macro-level experiments, in such manner we seek for the clue of non-Fourier propagation. The equations are tested via the numerical simulation of the laser pulse experiment. This work started last year in my Scientific Student article [31], and this thesis is a significant improvement.

The thesis consist of two main parts. In the first part, we introduce the background, the framework of irreversible thermodynamics and the derivation of the most important models. One has to use detailed mathematical analysis to solve practical problems and discover the main properties of such models. For this reason, we will discuss the characteristic propagation speed of each model in the chapters of hyperbolicity and dispersion relations. In the second part, the solutions are discussed, and we present the numerical scheme, too. The stability analysis is necessary

to prove the convergence of the numerical scheme. Experiments made at the Department of Energy Engineering, BUTE and NaF experiments are presented. Finally, we summarize the results and discuss the possible application areas.

CHAPTER 2

The generalization of heat conduction equations

The purpose of the generalization is to introduce higher order quantities into the constitutive equations. What does this mean? Constitutive equations formulate for the material laws with using strictly material parameters and objective quantities. Our physical sense tells us that the properties of a point in the medium depend somehow on the surroundings, but we do not know how. Furthermore, we can assume that these properties depend on time as well so one has to consider the states of the medium in previous time instants. These are the so-called memory and nonlocal effects. Let us see it in details.

2.1. Memory and nonlocal effects

In reality, if something is excited – for example with a heat flux pulse – then the disturbance will have finite propagation speed in the medium. For illustration purposes, let us see the example of the Fourier equation. The system¹ is parabolic (loosely saying, it misses one time derivative) causing the infinite speed of propagation. On the macroscopic level, Fourier’s equation is applicable for most of the engineering problems, the system is simple, and the solution methods are well-developed. It provides satisfactory solution for such cases, because usually the higher order terms (of time and space derivatives) are not dominant and the diffusive mechanism is the relevant one.

On the other side, spatial nonlocality is also important. As we said, the idea is similar, but now we extend the model in space, considering the states of the neighboring points as well. Several methods exist to obtain such kind of extension, the most important ones are:

- (1) Theory of internal variables: based on the introduction of a new variable.
- (2) Theory of strong nonlocality: based on memory functionals and space integrals. It is less common and is difficult to use.
- (3) Theory of weak nonlocality: based on the introduction of higher order space and time derivatives than in the classical description.

We will use the unification of the first and third approaches. The following chapter is based on the sources [12, 28, 32, 33, 34, 30].

2.2. Generalization: the hierarchical system

For simplicity, let us assume a rigid and isotropic material. During the derivation we apply the index notation with Einstein’s summation convention. Let it begin with the balance equation of internal energy:

$$\rho \dot{e} + \partial^i q^i = 0, \quad (1)$$

¹It means the balance equation of internal energy plus the constitutive equation(s).

where ρ is mass density, e denotes specific internal energy which is $e = cT$ in the case of constant specific heat, where c and T are the isochoric specific heat and the temperature. The space derivative is denoted by ∂^i , q^i is the conductive part of the flux density of the internal energy, namely the heat flux. The dot means the substantial time derivative. The initial assumption – the medium being rigid – causes that the substantial time derivative is to the partial time derivative and there is no convective part of the flux density.

We used an internal variable as a vector [31] to extend the classical theory. Why we used it in a vector form? In the framework of internal variables, there is no restriction about the order of an internal variable. Let us check the terms of Fourier equation, the gradient of the temperature field is a vector, and the heat flux is also a vector and we would like to extend this equation. It is straightforward to do this with a vector. The internal variable disappears in equilibrium, so it describes the deviation from the equilibrium. Based on this reason, it can be called a dynamical degree of freedom [35]. Now we present another way of the extension.

Let us define the entropy function on a different way than in [30, 36, 31] literatures; we can reach the compatibility with the kinetic theory and irreversible thermodynamics [7, 12] in a simpler way by the consideration below [37]. In this case we are using the heat flux instead of the internal variable and it is quadratic in the new term, so the heat flux is a basic variable.

$$s(e, q^i, Q^{ij}) = \hat{s}(e) - \frac{m_1}{2} q^i q^i - \frac{m_2}{2} Q^{ij} Q^{ij} . \quad (2)$$

Let the flux density of entropy be

$$J^i = B^{ij} q^j + C^{ijk} Q^{jk} . \quad (3)$$

The first term is known, the second one is important now; Q^{ij} is higher order quantity than the heat flux and it is introduced as an internal variable. Let it be noted that the deviation from the equilibrium is minimal, but thermodynamically compatible [38]. Furthermore, the role of the C^{ijk} is very similar to B^{ij} , it is a constitutive function, too. In this way, we can reach the hierarchical extension of the heat conduction equations. Let us substitute into the balance equation of entropy

$$\rho \dot{s} + \partial^i J^i = \sigma \geq 0, \quad (4)$$

thus we get the inequality of the entropy production, i. e.

$$\begin{aligned} \partial^i q^j \left(B^{ij} - \frac{1}{T} \delta^{ij} \right) &+ B^{ij} (\partial^i q^j) + q^j (\partial^i B^{ij} - m_1 \dot{q}^i) \\ &+ Q^{jk} (\partial^i C^{ijk} - m_2 \dot{Q}^{ij}) + C^{ijk} (\partial^i Q^{jk}) \geq 0. \end{aligned} \quad (5)$$

	Classical	Extended	Internal variable I	Internal variable II
Fluxes	$\dot{q}^i - \partial^i B^{ij}$	$B^{ij} - \frac{1}{T} \delta^{ij}$	$\dot{Q}^{jk} - \partial^i C^{ijk}$	C^{ijk}
Forces	q^i	$\partial^i q^j - Q^{ij}$	$\partial^j q^k - Q^{jk}$	$\partial^i Q^{jk}$

TABLE 1. The thermodynamical forces and fluxes in the hierarchical system.

At this point, we can define the connections between the thermodynamical forces and fluxes, the fluxes are on the left hand side of the equalities, the forces are on

the right hand side:

$$m_1 \dot{q}^i - \partial^i B^{ij} = -l_1 q^i, \quad (6)$$

$$m_2 \dot{Q}^{jk} - \partial^i C^{ijk} = -k_1 Q^{jk} + k_{12} \partial^j q^k, \quad (7)$$

$$B^{ij} - \frac{1}{T} \delta^{ij} = -k_{21} Q^{ij} + k_2 \partial^i q^j, \quad (8)$$

$$C^{ijk} = n \partial^i Q^{jk}. \quad (9)$$

To fulfill the inequality of second law require:

$$l_1, k_1, k_2, n \geq 0, \quad (10)$$

$$K = k_1 k_2 - k_{12} k_{21} \geq 0. \quad (11)$$

We find a simpler form via the elimination of the constitutive functions B^{ij} and C^{ijk} over and above the Q^{ij} tensorial internal variable. It results - one space dimension - in:

$$\begin{aligned} m_2 \partial_{xt} \frac{1}{T} - n \partial_x^3 \frac{1}{T} + k_1 \partial_x \frac{1}{T} = \\ m_1 m_2 \partial_{tt} q + (m_2 l_1 + m_1 k_1) \partial_t q - (m_2 k_2 + n m_1) \partial_{xxt} q + \\ + n k_2 \partial_{xx}^4 q - (K + n l_1) \partial_{xx} q + k_1 l_1 q. \end{aligned} \quad (12)$$

The following assumptions lead us to well-known constitutive equations.

- **Fourier equation:** The simplest and most widely used model in engineering applications; $n = m_1 = m_2 = k_2 = 0$ and $k_{12} = 0$ yields:

$$l_1 q = \partial_x \frac{1}{T}. \quad (13)$$

By the differentiation of the reciprocal temperature on the right hand side and divide it by l_1 :

$$q = -\frac{1}{l_1 T^2} \partial_x T, \quad (14)$$

where one can define the Fourier thermal conductivity as $\lambda = \frac{1}{l_1 T^2}$, it also holds to the other models.

- **Maxwell–Cattaneo–Vernotte equation:** This model is valid at very low temperature – at the order of 10 K – and it can represent the phenomenon of second sound, i.e. the wave nature of heat propagation. In 1977, Gyarmati have written the recommendation about this kind of extension [12]. If $n = k_2 = m_2 = k_{12} = 0$ stands:

$$m_1 \partial_t q + l_1 q = \partial_x \frac{1}{T}. \quad (15)$$

Compared to the Fourier case, there is a new parameter, the relaxation time for the heat flux, i.e. $\tau_q = \frac{m_1}{l_1}$.

- **Guyer–Krumhansl equation:** It has an interesting feature, it can reproduce the solutions of Fourier and MCV equations and there is a further domain of the solutions where they are considerably different; the GK equation arises when $n = m_2 = 0$:

$$-K \partial_{xx} q + m_1 k_1 \partial_t q + k_1 l_1 q = k_1 \partial_x \frac{1}{T}. \quad (16)$$

After the same steps of the rearrangement of parameters, one can define the dissipation coefficient as $a = \frac{K}{k_1 l_1}$.

- **Jeffreys-type thermodynamical equation:** if $n = m_1 = k_2 = k_{12} = 0$ stands:

$$m_2 l_1 \partial_t q + l_1 k_1 q = k_1 \partial_x \frac{1}{T} + m_2 \partial_{xt} \frac{1}{T}. \quad (17)$$

It must be noted that the relaxation time in this case is different from the one before, because $\tau = \frac{m_2}{k_1}$ is not identical to τ_q . The meaning of τ will be discussed in the section about kinetic theory and it has a role in the ballistic-diffusive equation. In this paper, we will not discuss this constitutive equation.

- **Green–Naghdi equation:** Two variations exist, the general one and the simple one. The common feature is that both requires to assume Casimirc reciprocity relation. Here we discuss only the simple GN equation which can be derived with the parameters of $n = m_2 = l_1 = 0$,

$$-K \partial_{xx} q + m_1 k_1 \partial_t q = k_1 \partial_x \frac{1}{T}. \quad (18)$$

The parameters are the same as in the GK equation. A further interesting feature is that in reversible case – when entropy production is zero – it can reproduce Fourier heat propagation when using the $J^i = \frac{q^i}{T}$ classical formula for the entropy flux.

- **Cahn–Hilliard equation:** if $n = m_1 = m_2 = 0$ holds, (12) gives:

$$k_1 l_1 q - K \partial_{xx} q = k_1 \partial_x \frac{1}{T}. \quad (19)$$

We will not study this type of equation.

- **Generalized equation:** if $n = m_1 = 0$ holds, we obtain the generalized equation according to [30]:

$$m_2 l_1 \partial_t q - m_2 k_2 \partial_{xxt} q - K \partial_{xx} q + l_1 k_1 q = k_1 \partial_x \frac{1}{T} + m_2 \partial_{xt} \frac{1}{T}. \quad (20)$$

- **Ballistic-diffusive equation:** taking $n = k_2 = 0$, we get the system below:

$$m_1 \dot{q}^i - \partial^i B^{ij} = -l_1 q^i, \quad (21)$$

$$m_2 \dot{Q}^{jk} = -k_1 Q^{jk} + k_{12} \partial^j q^k, \quad (22)$$

$$B^{ij} - \frac{1}{T} \delta^{ij} = -k_{21} Q^{ij}, \quad (23)$$

and the constitutive equation reads

$$m_2 \partial_{xt} \frac{1}{T} + k_1 \partial_x \frac{1}{T} = m_1 m_2 \partial_{tt} q + (m_2 l_1 + m_1 k_1) \partial_t q - K \partial_{xx} q + k_1 l_1 q. \quad (24)$$

Entropy production requires $K = -k_{12} k_{21} \geq 0$, which can be fulfilled with k_{12} and k_{21} having opposite sign. For this reason, we introduce the notation $\tilde{k}_{12} = -k_{12} > 0$. This model has a central role in this work.

We have showed that this generalization method covers all of the models from [30], but we have more than this. The system (6)–(9) is able to describe the ballistic heat propagation mechanism as well.

In addition, one can see that the system (6)–(9) contains the Fourier equation three times [2, 39]:

- green denotes the original Fourier equation,

- red is the time derivative of the Fourier equation, and
- blue is the second space derivative of the Fourier equation:

$$\begin{aligned}
& \textcolor{red}{m_2} \partial_{xt} \frac{1}{T} - n \partial_x^3 \frac{1}{T} + \textcolor{green}{k_1} \partial_x \frac{1}{T} = \\
& m_1 m_2 \partial_{tt} q + (\textcolor{red}{m_2} l_1 + \textcolor{red}{m_1} k_1) \partial_t q - (m_2 k_2 + n m_1) \partial_{xxt} q + \\
& + n k_2 \partial_x^4 q - (K + n l_1) \partial_{xx} q + \textcolor{green}{k_1} l_1 q .
\end{aligned} \tag{25}$$

It must be noted that we solve this hierarchical system with parameters of $n = k_2 = 0$ (ballistic-diffusive equation) to eliminate the most of the damping. These parameters are exclude one of the Fourier equation from the system (the blue one). Let us pay attention to the second time derivative of the heat flux, to which there is no corresponding term among the temperature quantities on the left hand side. It means that we cannot reproduce clearly the solution of Fourier equation, but only approximate with “small” parameters. We can see examples for this behavior in the chapter of solutions. The following section summarizes shortly the kinetic theory of ballistic kind heat transport, then we can compare the two models.

2.3. The kinetic theory of heat conduction

Several methods exist to describe the heat conduction phenomenon, among which is the one that is based on the interaction between phonons [7, 40]. This sort of approach does not follow the continuum theory, but puts the emphasis on the statistical physics. First of all, it defines the phonons as quasi-particles² as real point particles and analyses the interactions among them. The first model was a system with mass points which are connected by springs, but the exact solution [42, 25] for such a system gives nondissipative description with infinite propagation speed. Landau draw attention [43] to the anharmonical vibrations of an atom in crystal lattice that these kinds of vibrations are should be considered in the description of heat conduction, based on the works of Debye and Born. According to Ashcroft and Mermin, the strictly harmonic crystals have infinite thermal conductivity and the anharmonic vibrations cause finite speed of energy propagation [44].

One can distinguish two kinds of processes concerning interactions³ between the phonons (this section is based on [7, 45]).

- Normal (N) processes: the total momentum of phonons is conserved during the interaction,
- Resistive (R) processes: the opposite of N processes, total momentum is not conserved.

Common in both processes is that the energy is conserved during the interactions. The thermal conductivity is in connection with R processes and their frequencies $\frac{1}{\tau_R}$, i.e.

$$\kappa = \frac{c^2}{3} c_v \tau_R, \tag{26}$$

²Quasi-particles do not exist in reality. Phonons has important role to describe the phenomenas of heat propagation and electrical conductivity [41].

³A third type – called Umklapp processes – exists, where the energy nor the momentum are conserved [45].

where c is the Debye speed⁴ of phonons, c_v is the isochoric specific heat, and τ_R is the characteristic time of the R processes. In this approach, Fourier's law can be applied only when the R processes are significantly dominant, which results in the diffusive kind heat propagation. However, if we decrease temperature, then N processes become dominant and the wave nature of heat conduction (called "second sound") reveals itself. The Fourier's law can be modified to obtain the MCV equation [7]:

$$\frac{\partial Q_i}{\partial t} + \frac{c^2}{3} c_v \frac{\partial T}{\partial x_i} = -\frac{1}{\tau_R} Q_i. \quad (27)$$

Let it be noticed that the third mechanism of heat transport – the energy transport by ballistic phonons – is not explained yet. The main property of a ballistic phonon is that it goes through the crystal without any interaction. Jackson, Walker and McNelly [46, 47] made experiments on NaF, the result of which can be seen in figure 2.1.

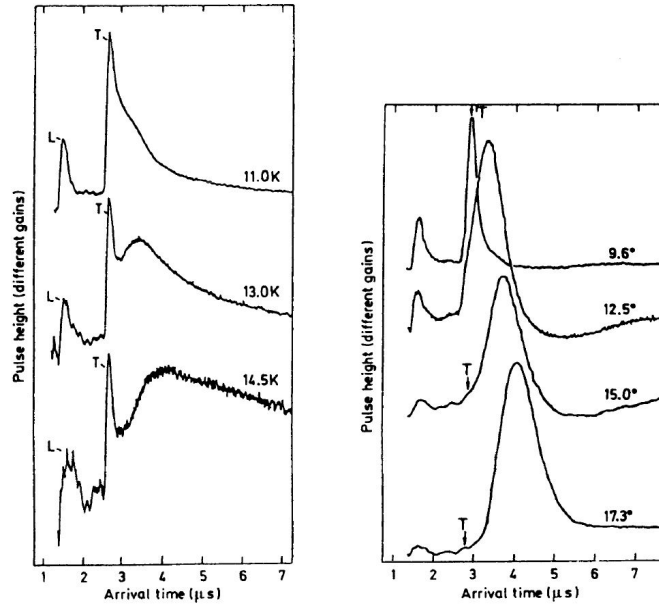


FIGURE 2.1. Phonon propagation in NaF. Left: case of pure NaF crystal [46]. Right: case of very pure NaF crystal [47]. Ballistic propagation; L is the longitudinal and T is the transversal signal.

In these experiments, NaF material is used at 10 to 15 K. Around such a low temperature, the dissipation effects are weak and the wave nature of the heat propagation can be demonstrated.

In figure 2.1, T denotes the arrival time of transversal ballistic phonons. This phenomenon is described by the kinetic theory of the phonon gas model. One needs to distinguish the phase density for the R and N processes⁵. The resistive processes tends to the function f_R and the normal processes tends to the distribution function

⁴The mean value of the transversal and longitudinal speed of sound [7].

⁵The Callaway model combines the distribution functions by weighting with the relaxation times.

f_N :

$$f_R = \frac{y}{\exp\left(\frac{hck}{k_B T}\right) - 1}, \quad (28)$$

$$f_N = \frac{y}{\exp\left\{\frac{hck}{k_B T} \left(1 - \frac{3}{4} \frac{cp_i n_i}{aT^4}\right)\right\} - 1}. \quad (29)$$

This model assumes that the energy density of phonons is defined by the temperature T :

$$e = aT^4; \quad a = \frac{4\pi^5}{5} \frac{k_B^4}{h^3 c^3}, \quad (30)$$

where h is the Planck constant, k_B is the Boltzmann constant and k denotes the wavenumber. One can calculate the momentum equations of the distribution functions and introduce new quantities⁶ this way:

$$u_{\langle i_1 i_2 \dots i_N \rangle} = \int k n_{\langle i_1 \dots i_n \rangle} f dk. \quad (31)$$

The first momentum is the energy density, the second one is the momentum density, the third one is the energy flux and the fourth one is the deviatoric part of the pressure tensor, i.e.

$$e = hcu; \quad p_i = hu_i; \quad Q_i = hc^2 u_i; \quad N_{\langle ij \rangle} = hcu_{\langle ij \rangle}. \quad (32)$$

Let us notice that, by introducing the momentum equations, that one must solve the problem of closure [48]. It means that every momentum equation introduces a new quantity which is defined by the next momentum equation, hence, one needs to do it again and again⁷ and the system becomes infinitely complicated. This problem can be solved by closing the series and it is the so-called “problem of closure”. The simplest solution is that the new highest order (“ $N+1$ ”th) quantity is considered as zero, this method is called truncation. It results the system below:

$$\frac{\partial u_{\langle n \rangle}}{\partial t} + \frac{n^2}{4n^2 - 1} c \frac{\partial u_{\langle n-1 \rangle}}{\partial x} + c \frac{\partial u_{\langle n+1 \rangle}}{\partial x} = \begin{cases} 0 & n = 0 \\ -\frac{1}{\tau_R} u_{\langle 1 \rangle} & n = 1 \\ -\left(\frac{1}{\tau_R} + \frac{1}{\tau_N}\right) u_{\langle n \rangle} & 2 \leq n \leq N \end{cases} \quad (33)$$

One has to apply $N = 30$ equations to get back the appropriate propagation speed of phonons. Naturally, such a system is too difficult to solve for practical problems, but $N = 3$ equations give an acceptable approximation while one must remember that the predicted value of the propagation speed is not correct. The “ $N=3$ ” case contains only two parameters, which is less than in our ballistic-diffusive equation so it is an advantage of this system. The kinetic theory describes the phenomena with this system below:

$$\begin{aligned} \frac{\partial e}{\partial t} + c^2 \frac{\partial p}{\partial x} &= 0, \\ \frac{\partial p}{\partial t} + \frac{1}{3} \frac{\partial e}{\partial x} + \frac{\partial N}{\partial x} &= -\frac{1}{\tau_R} p, \\ \frac{\partial N}{\partial t} + \frac{4}{15} c^2 \frac{\partial p}{\partial x} &= -\left(\frac{1}{\tau_R} + \frac{1}{\tau_N}\right) N. \end{aligned} \quad (34)$$

⁶One can not interpret all of the momenta as real physical quantities. For example, in the topic of computational fluid dynamics, there is a method called Lattice-Boltzmann Method, which applies the kinetic theory. In this method, only the first three momenta have real physical meaning.

⁷In practical applications, three momentum equations are enough.

If we consider $n = k_2 = 0$ in our continuum model – thus most of the dissipative terms are zero – the ballistic-diffusive system is reproduced with equivalent structure of kinetic theory with parameters:

$$q = c^2 p; \quad Q = N; \quad \frac{1}{\tau} = \left(\frac{1}{\tau_R} + \frac{1}{\tau_N} \right) \rightarrow \tau_q = \tau_R; \quad \tau_Q = \tau, \quad (35)$$

$$\lambda = \frac{\tau_R}{3} \rho \hat{c} c^2 \rightarrow c^2 = \frac{3\lambda}{\tau_q \rho \hat{c}}; \quad \tilde{k}_{12} k_{21} = \frac{4}{15} \tau_q \tau_Q c^2, \quad (36)$$

where $\hat{c}$ denotes specific heat to distinguish it from the speed of sound c . Therefore our system is in this form:

$$\begin{aligned} \rho \hat{c} \frac{\partial T}{\partial t} + \frac{\partial q}{\partial x} &= 0, \\ \tau_q \frac{\partial q}{\partial t} + \lambda \frac{\partial T}{\partial x} + k_{21} \frac{\partial Q}{\partial x} &= -q, \\ \tau_Q \frac{\partial Q}{\partial t} + \tilde{k}_{12} \frac{\partial q}{\partial x} &= -Q. \end{aligned} \quad (37)$$

By the comparison of the coefficients and variables of the two models, one can identify the internal variable Q as the current density of the heat flux. These systems are hyperbolic and give finite propagation speed, which will be proved after the following section.

2.4. Dimensionless form of the equations

The set of equations can be brought into a scale-free form, called dimensionless form. Let us define the dimensionless parameters [49, 37] as

$$\begin{aligned} \hat{T} &= \frac{T - T_0}{T_{\text{end}} - T_0}; \quad \text{temperature,} \\ T_{\text{end}} &= T_0 + \frac{1}{\rho \cdot c \cdot L} \cdot \int_0^{t_p} q_0(t) dt; \quad \text{equilibrium temperature,} \\ \bar{q}_0 &= \frac{1}{t_p} \cdot \int_0^{t_p} q_0(t) dt; \quad \hat{q} = \frac{q}{\bar{q}_0}; \quad \text{average of the heat flux and heat flux} \end{aligned} \quad (38)$$

$$\begin{aligned} \alpha &= \frac{\lambda}{\rho \cdot c}; \quad Fo = \frac{\alpha \cdot t}{L^2}; \quad \text{thermal diffusivity, Fourier number (time)} \\ \xi &= \frac{x}{L}; \quad \text{space coordinate,} \\ \hat{\tau}_q &= \frac{\alpha \cdot \tau_q}{L^2}; \quad \hat{\tau}_Q = \frac{\alpha \cdot \tau_Q}{L^2}; \quad \text{relaxation times,} \\ \tau_\Delta &= \frac{\alpha \cdot t_p}{L^2}; \quad \hat{Q} = \sqrt{\frac{k_{12}}{k_{21}}} \bar{q}_0 Q; \quad \text{impulse length; current density of the heat flux,} \\ \hat{\kappa} &= \frac{\sqrt{\tilde{k}_{12} k_{21}}}{L}; \quad \text{coupling coefficient.} \end{aligned}$$

After substitute these parameters, we obtain the dimensionless form of the equations. It's main advantage is we have a system with fewer parameters than in the original system, the situation becomes simpler in this respect, and is much easier to

fit calculated results to measurement data. Obviously, it contains all of the necessary information to get back the original ones. Before we rewrite the equations in dimensionless form, let us simplify the notations. It is easier to memorize them if we leave the notations as introduced, so the time will be denoted by t and not by Fo , and we prefer x for space coordinate as well. We omit the hat from the relaxation times τ . It is very important that we deal only with scale-free equations from now on. Then, we summarize the constitutive equations:

- **ballistic-diffusive model:**

$$\begin{aligned}\tau_q \frac{\partial q}{\partial t} + q + \tau_\Delta \frac{\partial T}{\partial x} + \kappa \frac{\partial Q}{\partial x} &= 0, \\ \tau_Q \frac{\partial Q}{\partial t} + Q + \kappa \frac{\partial q}{\partial x} &= 0.\end{aligned}\tag{39}$$

- **Fourier equation:** the $\kappa = \tau_q = 0$ case of the previous model,

$$q + \tau_\Delta \frac{\partial T}{\partial x} = 0,\tag{40}$$

and Q is decoupled so it need not be followed.

- **Maxwell–Cattaneo–Vernotte equation:** the $\kappa = 0$ case,

$$\tau_q \frac{\partial q}{\partial t} + q + \tau_\Delta \frac{\partial T}{\partial x} = 0.\tag{41}$$

- **Guyer–Krumhansl equation:** $\tau_Q = 0$ and we use the dissipation parameter $\kappa^2 = \hat{a}$:

$$\tau_q \frac{\partial q}{\partial t} + q + \tau_\Delta \frac{\partial T}{\partial x} - \hat{a} \frac{\partial^2 q}{\partial x^2} = 0.\tag{42}$$

- **Green–Naghdi equation:** special case, we are not require that the heat flux q should be zero, because all the terms disappear,

$$\tau_q \frac{\partial q}{\partial t} + \tau_\Delta \frac{\partial T}{\partial x} - \hat{a} \frac{\partial^2 q}{\partial x^2} = 0.\tag{43}$$

One must couple any of the equations above to the balance equation of internal energy:

$$\tau_\Delta \frac{\partial T}{\partial t} + \frac{\partial q}{\partial x} = 0.\tag{44}$$

Let us draw the attention to the parameters, we will see in the chapter of solution that nonzero parameters can also reproduce the solution of the Fourier equation.

CHAPTER 3

Partial differential equations

In theoretical descriptions, partial differential equations have a very important role, these are vital to understand modern physics and engineering sciences. In contrast to ordinary differential equations, here we have functions with more than one variable. In fact, it can be very difficult to solve such equations or systems, even one cannot be sure that the solution exist. It is useful to collect here the most important properties of such equations from the aspect of numerical solutions. It is known that one can classify partial differential equations such as:

- **Elliptic** equations: the solution is analytical¹, it is typical for boundary value problems and gives stationary solutions. The functions are “global”, these are depend on the whole domain. Typical examples are the Laplace, Helmholtz and Poisson equations. From the aspect of numerical solutions, elliptical equations are not difficult to solve. We will not deal with such equations.
- **Hyperbolic** equations: their specialty is that they allow such solutions that are not continuous; from numerical aspects, these can be very difficult to deal with. Furthermore, they give finite speed for propagation without relativistic frame². Usually, the dissipation free wave equations are hyperbolic, for example the Sommerfeld equation and the equation of a vibrating string. We can mention a further physical topic as well, the Klein-Gordon equation from relativistic quantum mechanics is also hyperbolic. This type of equations has an important role in the present thesis, for instance, the dissipation free GN equation, the MCV and the ballistic-diffusive equations belongs to this class. About the mathematical, numerical and physical background of such equations one can find detailed information in the works [50, 51].
- **Parabolic** equations: similarly for the elliptical equations, the solutions are smooth and continuous. One must consider that the characteristic speed of propagation is infinite, which is contradictory to our physical experience. They are typical for diffusive and dissipative systems, for example the Fourier equation or the dissipative GN and GK equations.

3.1. Hyperbolicity

We will compare the signal propagation speed of the introduced systems and we will determine which systems are hyperbolic and which parabolic. By definition [52] we need to rewrite the systems into the canonical form (45) and calculate the

¹The functions that can be differentiable infinite times, and it's Taylor series reproduces the function on an arbitrary domain.

²The Fourier equation has infinite propagation speed by parabolic characteristic, but this can be circumvented by relativistic approach.

eigenvalues of coefficient matrix A^{ij} . Let the system is in the form:

$$\partial_t u^i + A^{ij} \partial_x u^j + B^{ij} u^j = F, \quad (45)$$

where u^i denotes the vector of variables and F is an arbitrary piecewise continuous function. If the $n \times n$ sized coefficient matrix A^{ij} can be diagonalized and its eigenvalues are real then the system is hyperbolic. If all of the eigenvalues are different then the system is strictly hyperbolic; if the matrix A^{ij} is symmetric, the system is called symmetrical hyperbolic. To achieve the canonical form, the balance equation of the internal energy is already in a convenient form, but some of the constitutive equations must be rewritten.

- **Fourier equation:** in this case the variables are $u_1 = T$ and $u_2 = q$, but one time derivative is missing from the constitutive equation, so we extend it with the help of an auxiliary ε parameter:

$$\begin{aligned} \tau_\Delta \partial_t T + \partial_x q &= 0, \\ \varepsilon \partial_t q + q + \tau_\Delta \partial_x T &= 0. \end{aligned} \quad (46)$$

The coefficient matrix is: $A = \begin{pmatrix} 0 & \frac{1}{\tau_\Delta} \\ \frac{\tau_\Delta}{\varepsilon} & 0 \end{pmatrix}$, which eigenvalues are $\pm \frac{1}{\sqrt{\varepsilon}}$.

When ε is sent to zero, the eigenvalues tend to infinite, so the system is parabolic as we expected.

- **Maxwell–Cattaneo–Vernotte equation:** this is a very simple situation because we need to consider $\varepsilon = \tau_q$ from the example of Fourier equation thus the eigenvalues are finite and different so the system is hyperbolic.
- **Guyer–Krumhansl equation:** in this case, we have a second order space derivative as well in the constitutive equation,

$$\begin{aligned} \tau_\Delta \partial_t T + \partial_x q &= 0, \\ \tau_q \partial_t q + q + \tau_\Delta \partial_x T - \hat{a} \partial_{xx} q &= 0. \end{aligned} \quad (47)$$

To rewrite the system into the canonical form, let us introduce a new variable, i.e. $u_1 = T, u_2 = q, u_3 = \partial_x q$. Introducing an auxiliary ε again:

$$\begin{aligned} \partial_t u_1 + \frac{1}{\tau_\Delta} \partial_x u_2 &= 0, \\ \partial_t u_2 + \frac{1}{\tau_q} u_2 + \frac{\tau_\Delta}{\tau_q} \partial_x u_1 - \frac{\hat{a}}{\tau_q} \partial_x u_3 &= 0, \\ \varepsilon \partial_t u_3 + u_3 - \partial_x u_2 &= 0. \end{aligned}$$

Then the coefficient matrix is $A = \begin{pmatrix} 0 & \frac{1}{\tau_\Delta} & 0 \\ \frac{\tau_\Delta}{\tau_q} & 0 & -\frac{\hat{a}}{\tau_q} \\ 0 & -\frac{1}{\varepsilon} & 0 \end{pmatrix}$, its eigenvalues are

0, and $\pm \frac{\sqrt{\varepsilon + \hat{a}}}{\sqrt{\varepsilon \tau_q}}$. If ε tends to zero we get infinite eigenvalues thus this system is parabolic.

- **Green–Naghdi equation:** similar to the case of the GK equation, we need a new variable. If the dissipation parameter $\hat{a}$ is zero then the system will be hyperbolic (because it will be a simple second order wave equation) with the phase velocity of the MCV equation, otherwise it is parabolic.

- **Ballistic-diffusive equation:** this has a very convenient form and the variables are straightforward: $u_1 = T$; $u_2 = q$; $u_3 = Q$. The set of equations are:

$$\begin{aligned}\tau_\Delta \partial_t T + \partial_x q &= 0, \\ \tau_q \partial_t q + q + \tau_\Delta \partial_x T + \kappa \partial_x Q &= 0, \\ \tau_Q \partial_t Q + Q + \kappa \partial_x q &= 0.\end{aligned}\tag{48}$$

Accordingly, the coefficient matrix is: $A = \begin{pmatrix} 0 & \frac{1}{\tau_\Delta} & 0 \\ \frac{\tau_\Delta}{\tau_q} & 0 & \frac{\kappa}{\tau_q} \\ 0 & \frac{\kappa}{\tau_Q} & 0 \end{pmatrix}$, which has the

eigenvalues 0 and $\pm \frac{\sqrt{\kappa^2 + \tau_Q}}{\sqrt{\tau_q \tau_Q}}$. One can see the two different propagation speed caused by the coupling parameter. When this coupling disappears, the situation reduces to the MCV equation.

A further remark is that if the matrix B^{ij} in (45) is zero then the system is homogeneous. The system remains linear if B^{ij} depends on the variables u^i linearly [52].

3.2. Dispersion relations

Dispersion relations appear on areas where one needs to analyze the behavior of waves, and their main application areas are optics, quantum mechanics³ and electrodynamics. The dispersion relation⁴ describes the relation between the frequency and the wavenumber of a plane wave. Let us assume the solution in a form of a plane wave, i.e.

$$\chi = A e^{i(kx - \omega(k)t)},\tag{49}$$

where A is the wave amplitude, k is the wavenumber and $\omega(k)$ is the frequency of the wave which depends on the wave number. The phase velocity of a wave is $v_p = \frac{\omega}{k}$ and the group velocity is given by the relation $v_g = \frac{d\omega}{dk}$. The phase velocity corresponds to the speed of the same points of the wave. The group velocity corresponds to the superposition of multiple waves; the different waves has different phase speeds, so a wave packet moving in space, has a “composite velocity”, the group velocity [54]. When the function of $w(k)$ is nonlinear, these 2 speeds are different. It needs to be noted that the dispersion relation gives a useful utility to stability analysis. When the real part of the exponent is negative, the exponential function tends to a finite number.

From the energy aspects, when a system is conservative then the group velocity is equal to the speed of energy transport, i.e. $v_g = v_e = \frac{\bar{F}}{\bar{E}}$, where $\bar{F}$ is the average of energy current and $\bar{E}$ is the average of mechanical energy. If the medium is absorbing, then the speed of group velocity and energy transport is not equal, and the group velocity becomes complex valued function; in usual the central wavenumber of the

³The dispersion relation had a very important role to analyze the wave-particle duality of photons. In 1924, de Broglie used the dispersion relations to define his hypothesis.

⁴In mathematical sense, it is a complex function. There exists an integral relation between the real and imaginary parts, the so-called Kramers-Kronig relation. In the case of light, it gives connection between the refraction index (real) and the absorptive (imaginary) parts [53].

wave packet is not constant and from the energy aspect one cannot find a clear answer [55].

In this section, we analyze the dispersion relations of the considered heat conduction equations to learn more about the effects of the parameters in the equations. It must be noted that in the dimensionless formulation frequency and group velocity are also dimensionless.

3.2.1. Fourier equation: The system is in the form

$$\tau_\Delta \partial_t T + \partial_x q = 0, \quad (50)$$

$$q + \tau_\Delta \partial_x T = 0. \quad (51)$$

Let us substitute the form of solution (49) into the fields of temperature and heat flux, then we obtain an algebraic system of equations. We need to analyze coefficient matrix M

$$M = \begin{pmatrix} -\omega\tau_\Delta & k \\ ik\tau_\Delta & 1 \end{pmatrix}$$

$$\det M = 0 \rightarrow k^2 = i\omega \quad (52)$$

The result is that the phase speed is pure imaginary, has no direct physical interpretation.

3.2.2. Guyer–Krumhansl equation: This system reads

$$\tau_\Delta \partial_t T + \partial_x q = 0, \quad (53)$$

$$\tau_q \partial_t q + q + \tau_\Delta \partial_x T - \hat{a} \partial_{xx} q = 0. \quad (54)$$

Making the calculations in the same way as before, the coefficient matrix is:

$$M = \begin{pmatrix} -\omega\tau_\Delta & k \\ ik\tau_\Delta & 1 - i\omega\tau_q + \hat{a}k^2 \end{pmatrix}$$

$$\det M = 0 \rightarrow k = \sqrt{-\frac{i\omega^2\tau_q + \omega}{\omega\hat{a} + i}} \quad (55)$$

Due to the complex values, it is not convenient to take the square root in this form, so transform it:

$$k^2 = \frac{1}{\omega^2\hat{a}^2 + 1} \left(\omega^2(\tau_q - \hat{a}) + i(\omega^3\tau_q\hat{a} + \omega) \right). \quad (56)$$

Let k^2 be written as a $z = x + iy$ complex number, where

$$x = \frac{\omega^2(\tau_q - \hat{a})}{\omega^2\hat{a}^2 + 1}; \quad y = \frac{\omega^3\tau_q\hat{a} + \omega}{\omega^2\hat{a}^2 + 1}. \quad (57)$$

Then one can rewrite the z complex number in a form of $z = re^{i\phi}$, where $r = \sqrt{x^2 + y^2}$ and $\phi = \arctan(y/x)$. Now we can easily perform the operation of square root, i.e. $\sqrt{z} = \sqrt{r}e^{i\frac{\phi}{2}}$ so the argument is divided by two, thus we get the function of $k(\omega)$. It's real part is:

$$\text{Re}\{k(\omega)\} = \sqrt[4]{\frac{\omega^4\tau_q^2 + \omega^2}{\omega^2\hat{a}^2 + 1}} \cos\left(\frac{1}{2} \arctan\left(\frac{\omega^2\hat{a}\tau_q + 1}{\omega(\tau_q - \hat{a})}\right)\right). \quad (58)$$

In the case of a complex valued dispersion relation, the group velocity is given by the derivative of the real part of the function $\omega(k)$, i.e.

$$v_g = \frac{dRe\{\omega\}}{dk}. \quad (59)$$

We can see that we do not know the function $\omega(k)$, although we know $k(\omega)$, so we can deal with its derivative by the relation of $\frac{dRe\{\omega(k)\}}{dk} = \left(\frac{dRe\{k(\omega)\}}{d\omega}\right)^{-1}$. Thus the group velocity is:

$$v_g = 1 / \left(\frac{\omega(1 + \tau_q^2 \omega^2 (2 + \hat{a}^2 \omega^2)) \cos(\frac{1}{2} \arctan(\frac{1 + \hat{a} \tau_q \omega^2}{\hat{a} \omega - \tau_q \omega}))}{2(1 + a^2 \omega^2)^2 (\frac{\omega^2 + \tau_q^2 \omega^4}{1 + \hat{a}^2 \omega^2})^{\frac{3}{4}}} + \frac{(-\hat{a} + \tau_q) \omega^2 (-1 + \hat{a} \tau_q \omega^2) \sin(\frac{1}{2} \arctan(\frac{1 + \hat{a} \tau_q \omega^2}{\hat{a} \omega - \tau_q \omega}))}{2(1 + a^2 \omega^2)^2 (\frac{\omega^2 + \tau_q^2 \omega^4}{1 + \hat{a}^2 \omega^2})^{\frac{3}{4}}} \right). \quad (60)$$

This formula seems to be quite complicated but it can be useful, so let us investigate it.

- **Fourier case:** if $\hat{a} = \tau_q = 0$ then it reproduces the results of Fourier equation.
- **MCV case:** if $\hat{a} = 0$ then it reduces to the MCV equation which gives:

$$k^2 = \omega^2 \tau_q + i\omega. \quad (61)$$

Hence the real part of the function $k(\omega)$ by using (58) is

$$Re\{k(\omega)\} = \sqrt[4]{\omega^4 \tau_q^2 + \omega^2} \cos\left(\frac{1}{2} \arctan\left(\frac{1}{\omega \tau_q}\right)\right). \quad (62)$$

Let us consider two types of approximation.

- (1) Let τ_q be small, i.e. $\tau_q \ll 1$. Then one can say that $\tau_q^2 \approx 0$ and the function $\arctan$ tends to $\frac{\pi}{2}$, thus the term of $\cos$ tends to $\frac{1}{\sqrt{2}}$. The frequency is strictly positive, so the expression under the square root is simplified $\sqrt[4]{\omega^2} \rightarrow \sqrt{\omega}$. By using these considerations

$$Re\{k(\omega)\} \cong \sqrt{\frac{\omega}{2}}. \quad (63)$$

Simple calculation can show us that $\tau_q \leq 0.001$ is valid, then until frequency of 100 Hz the error remains under 5 %. In this respect, the phase velocity is $v_p = 2k$ and the group velocity is $v_g = 4k$, so they are proportional to the real part of the wavenumber.

- (2) Let τ_q be a big parameter, so $\tau_q^2 \gg 1$ and let the frequency be $\omega > 1$, thus $\omega^4 \gg \omega^2$ is valid. By similar calculation, the function of $k(\omega)$ simplifies to

$$Re\{k(\omega)\} \cong \omega \sqrt{\tau_q}. \quad (64)$$

The relationship between the wavenumber and frequency is linear, thus the phase and group velocity are equal, $v_p = v_g = \frac{1}{\sqrt{\tau_q}}$ which is identical to the result of the hyperbolic propagation speed. We can observe that higher values of τ_q result in slower propagation.

- **GK case:** this time none of the parameters are zero, furthermore, the functions phase and group velocity are not linear, so we should make a lot of approximations to tell more about these relations but there is a more interesting property of the GK equation. Let us see the case when the parameters $\hat{a}$ and τ_q are equal. Then the dispersion relation simplifies to the case of Fourier equation, and the group velocity is $v_g = \sqrt{8\omega}$.

It must be noted that in the case of the GK equation the group velocity cannot be complex valued, since the constants are positive semidefinite because of the second law of thermodynamics. Let us notice that the group velocity is increasing by higher values of parameter $\hat{a}$, therefore the signal transfer speed is also increasing (Fig. 3.2); one can observe this property in the chapter of solutions and BUTE–DEE-experiments.

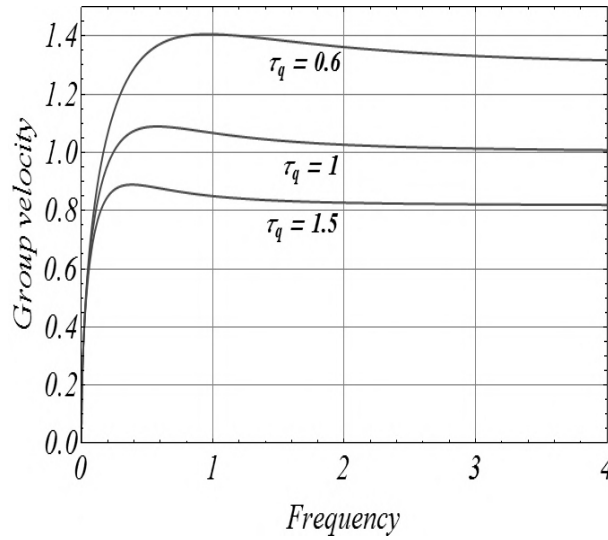


FIGURE 3.1. The characteristic group velocity of the GK equation with various values of τ_q as the function of frequency, where the dissipation parameter $\hat{a} = 0.001$.

In Figure 3.1, one can see the graph of the group velocity function in frequency domain. For low frequencies the function shows nonlinear characteristic and it has an extrema as well. As one increases the frequency, the nonlinearities disappear and group velocity converges to a constant value that depends on the material parameters.

3.2.3. Green–Naghdi equation: This situation is similar to the case of the GK equation, however we cannot derive the formulas by simple parameter substitution because of the constitutive equation:

$$\tau_\Delta \partial_t T + \partial_x q = 0, \quad (65)$$

$$\tau_q \partial_t q + \tau_\Delta \partial_x T - \hat{a} \partial_{xx} q = 0. \quad (66)$$

Using the same method for the calculations, the dispersion relation is found:

$$M = \begin{pmatrix} -\omega \tau_\Delta & k \\ ik \tau_\Delta & -i\omega \tau_q + \hat{a} k^2 \end{pmatrix}$$

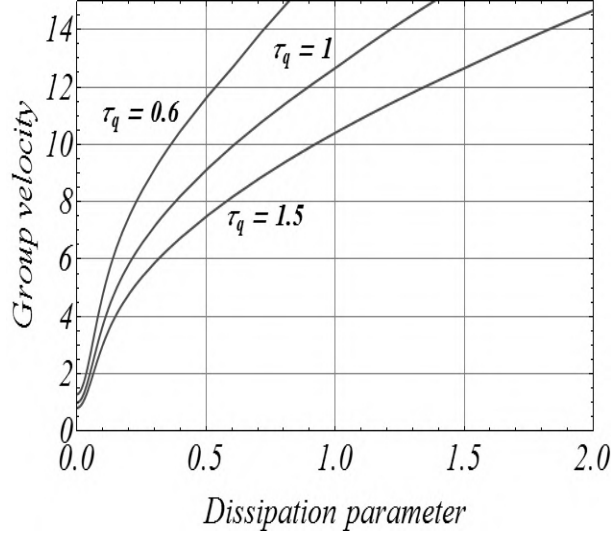


FIGURE 3.2. The characteristic group velocity of the GK equation with various values of τ_q as the function of the dissipation parameter $\hat{a}$, when the frequency is constant.

$$\det M = 0 \rightarrow k^2 = \frac{i\omega^2\tau_q}{\omega\hat{a} + i} \quad (67)$$

- **Dissipation free case:** then $\hat{a} = 0$ holds so we obtain a second order wave equation for temperature, which has the same $\frac{1}{\sqrt{\tau_q}}$ phase speed and group velocity of the MCV equation.
- **GN case:** the real part of the function $k(\omega)$ is

$$\text{Re}\{k(\omega)\} = \sqrt[4]{\frac{\omega^4\tau_q^2}{\omega^2\hat{a}^2 + 1}} \cos\left(\frac{1}{2} \arctan(\hat{a}\omega)\right). \quad (68)$$

Let us notice that the wave amplitude is decreasing by smaller values of $\hat{a}$, it is similarly to the GK equation. The group velocity is

$$v_g = \frac{2(\omega + \hat{a}^2\omega^3)}{\sqrt[4]{\frac{\omega^4\tau_q^2}{\omega^2\hat{a}^2 + 1}}((2 + \hat{a}^2\omega^2) \cos(\frac{1}{2} \arctan(\hat{a}\omega)) - \hat{a}\omega \sin(\frac{1}{2} \arctan(\hat{a}\omega)))}. \quad (69)$$

The properties are very similar as for the GK equation, it increases for higher values of the dissipation parameter. We will show an example for the case when the solution of Fourier equation can be approximated by the GN equation when the parameters τ_q and $\hat{a}$ are high and equal. One can analyze this property for the group velocity, which gives back the case of Fourier equation, $v_g = \sqrt{8\omega}$.

It is interesting to see in Figure 3.3 that the group velocity is constant in the frequency domain in connection of relaxation time. In Figure 3.4, one can see the characteristics of the group velocity as the function of the dissipation parameter, it is same as the case of the GK equation.

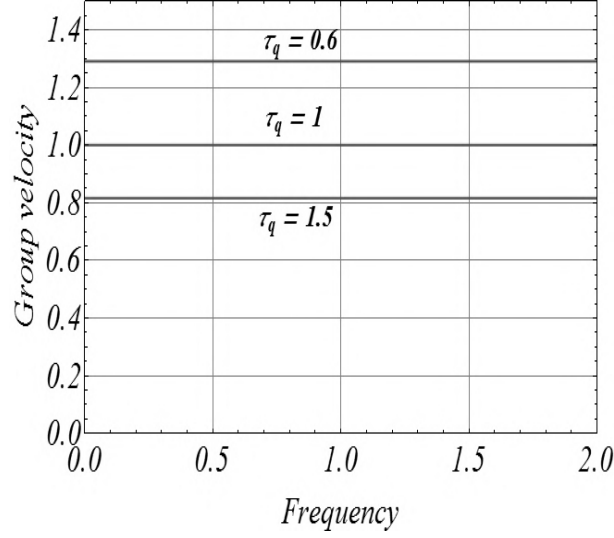


FIGURE 3.3. The characteristic group velocity of the GN equation with various values of τ_q as the function of frequency, where the dissipation parameter $\hat{a} = 0.001$.

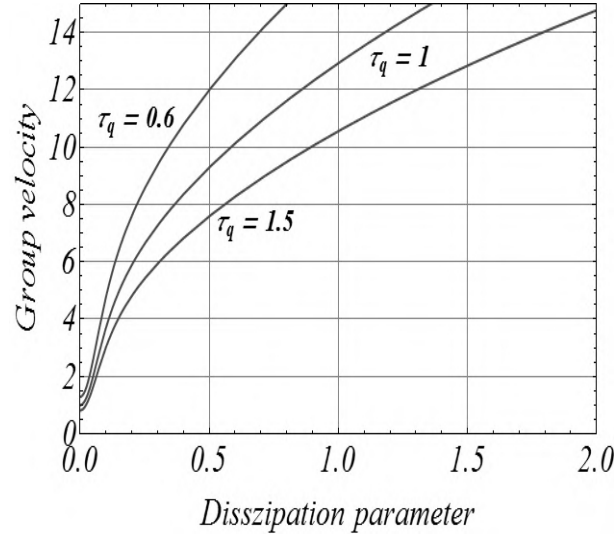


FIGURE 3.4. The characteristic group velocity of the GN equation with various values of τ_q as the function of the dissipation parameter $\hat{a}$, the frequency is constant.

3.2.4. Ballistic-diffusive model: First of all, let us see the system of equations:

$$\tau_{\Delta} \partial_t T + \partial_x q = 0, \quad (70)$$

$$\tau_q \partial_t q + q + \tau_{\Delta} \partial_x T + \kappa \partial_x Q = 0, \quad (71)$$

$$\tau_Q \partial_t Q + Q + \kappa \partial_x q = 0. \quad (72)$$

By the substitution of the plane wave solution, one can derive the coefficient matrix and the dispersion relation as

$$M = \begin{pmatrix} -\omega\tau_\Delta & k & 0 \\ k\tau_\Delta & -\omega\tau_q - i & k\kappa \\ 0 & k\kappa & -\omega\tau_Q - i \end{pmatrix}$$

$$\det M = 0 \rightarrow k^2 = \frac{\omega^2\tau_q + i\omega}{1 + \frac{\kappa^2\omega}{\omega\tau_Q + i}} \quad (73)$$

After separation of the real and imaginary parts, we found

$$k^2 = \frac{1}{\omega^2(\tau_Q + \kappa^2)^2 + 1} \left(\omega^4(\tau_Q^2\tau_q + \tau_Q\tau_q\kappa^2) + \omega^2(\tau_q - \kappa^2) + i[\omega^3(\tau_Q^2 + \tau_Q\kappa^2 + \tau_q\kappa^2) + \omega] \right). \quad (74)$$

Let us begin with the subcases.

- **MCV case:** if the coupling parameter κ is zero, the constitutive equations will be independent of each other and the system reduces to the MCV equation, and the dispersion relation reduces correspondingly.
- **Fourier case:** just continue the last case, furthermore, consider that τ_q is zero, so we obtain the Fourier equation. There exists an other way to approximate the Fourier equation, consider the parameters κ and τ_q as small parameters, but this is only an approximation.
- **GK case:** let $\kappa^2 = \hat{a}$ and $\tau_Q = 0$, then we reproduce the GK equation with its dispersion relation.
- **Ballistic-diffusive case:** the real part of the function $k(\omega)$ is

$$\begin{aligned} \text{Re}\{k(\omega)\} &= \sqrt[4]{\frac{\omega^2(1 + \tau_q^2\omega^2)(1 + \tau_Q^2\omega^2)}{1 + \omega^2(\tau_Q + \kappa^2)^2}} \times \\ &\times \cos\left(\frac{1}{2} \arctan\left(\frac{1 + \omega^2(\tau_Q^2 + \kappa^2(\tau_q + \tau_Q))}{\omega(\tau_q - \kappa^2) + \omega^3\tau_q\tau_Q(\tau_Q + \kappa^2)}\right)\right) \end{aligned} \quad (75)$$

This form can be used only to calculate the group velocity. If one omits the imaginary terms after the calculation of the determinant, it results in the same relation of hyperbolic signal propagation for the phase speed, i.e.

$$v_p = \sqrt{\frac{\kappa^2 + \tau_Q}{\tau_q\tau_Q}}. \quad (76)$$

Let us notice that when τ_q and τ_Q are small parameters and $\kappa > 1$ holds, furthermore $\tau_q\omega = \tau_Q\omega = 1$ is also valid, the the whole function of $\text{Re}\{k(\omega)\}$ can be approximated with $\frac{1}{\kappa}$ which is much simpler function; it gives for the phase speed $\kappa\omega$. The function of the group velocity is too lengthy to write here. It's function is also real valued. The graphs are illustrative how it depends on the parameters (Figs. 3.5 and 3.6).

It is important to note that in the Figure 3.5, one can see the nonlinear property of the function $v_g(\omega)$ which maybe refers to the window condition but this requires more detailed analysis. The group velocities tend to the constant value of GN case and it remains constant in frequency domain. An interesting property of this case that the group velocity is increasing (Fig. 3.6) by the parameter κ but it produces different characteristics from GK and GN equations.

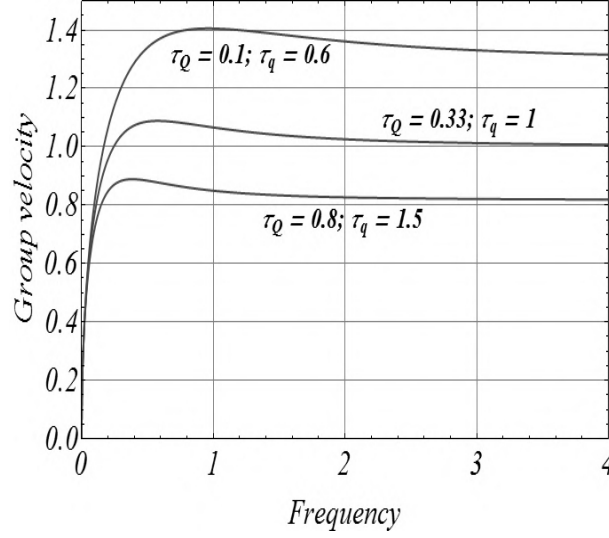


FIGURE 3.5. The characteristic group velocity of the ballistic-diffusive equation with various values of τ_q and τ_Q as the function of frequency, for the dissipation parameter is $\kappa = 0.001$. The characteristics are the same as for the GK equation.

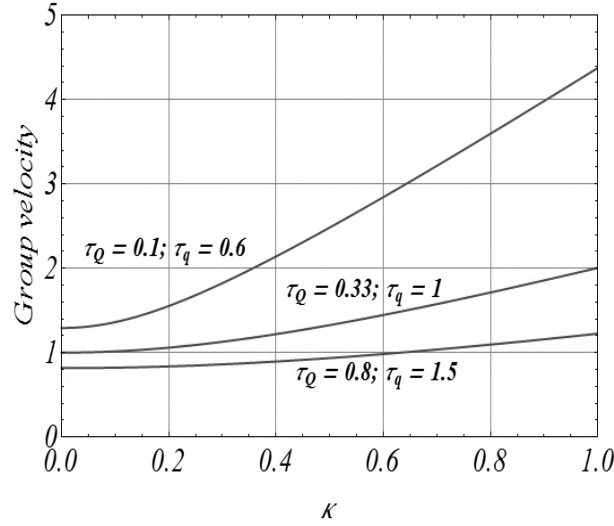


FIGURE 3.6. The characteristic group velocity of the ballistic-diffusive equation with various values of τ_q and τ_Q as the function of the dimensionless parameter κ , the frequency is constant.

In the ballistic domain⁵, the frequency dependence shows more complicated characteristics and the meaning of the extrema values are not well defined.

The goal of this chapter is fulfilled, we have the base for a comprehensive analysis about the parameters, furthermore, managed to learn more about how the parameters modifies the solutions. We have seen there are higher order terms of frequency in the dispersion relations which means dissipation and dispersion. These phenomenas has important role in the numerical solutions, they cause numerical errors which

⁵For parameters, see the chapter of solutions, Figure 6.22

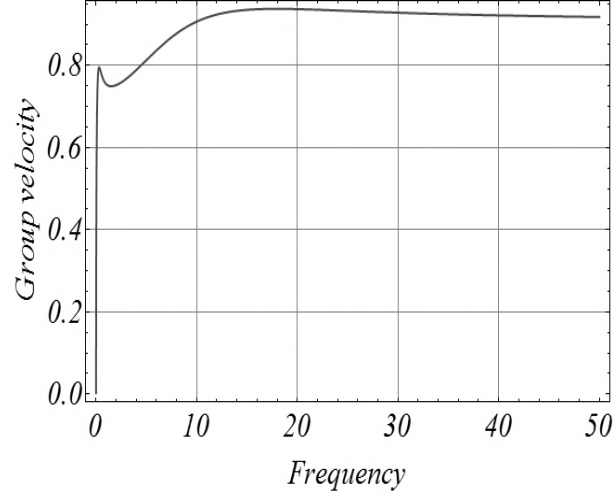


FIGURE 3.7. The characteristic group velocity of the ballistic-diffusive equation with parameters of $\tau_q = 1.9$, $\tau_Q = 0.07$ and $\kappa = 0.2$ in frequency domain.

must be kept bounded during the time evolution calculations. The boundedness property comes from the stability conditions. The stability analysis is important from the aspect of convergence as well.

CHAPTER 4

The laser flash experiment

We can test the introduced heat conduction models with the help of the laser flash experiment. This method is used to measure the thermo-physical properties of materials (heat diffusivity and thermal conductivity). There are several reasons why we choose it:

- The laser flash method is used more than 50 years, well-developed, it is under continuous improvement.
- It is a well-known method in the engineering practice, the measurement is simple and easily reproducible, widely used method.
- The most important property for us is that it may be the most applicable method to show non-Fourier heat conduction by the very small characteristic time of heat pulse.

During the measurement, the temperature is measured on the rear side of the sample. The thermo-physical properties are calculated by this curve, so we will analyze the temperature on the same place. The arrangement of the measurement can be seen in the Figure 4.1.

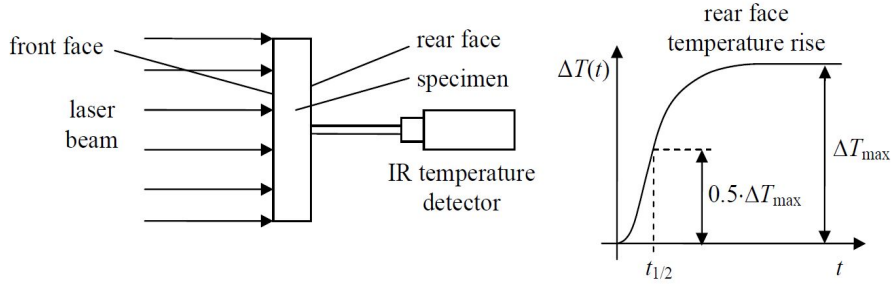


FIGURE 4.1. The arrangement of the laser flash experiment.

4.1. Initial and boundary conditions

We assumed homogeneous fields for the initial conditions which means zero values for all fields. The boundary conditions are not so simple. In the case of most of the models we work with the fields of temperature and heat flux, but in the case of ballistic-diffusive equation, we have a third one, the current density of heat flux. Let us start with the assumption that the laser pulse is heat flux, so we can define the boundaries of this field. We do not deal with the cooling of the sample, so the heat flux will be zero (adiabatic) on the boundaries.

One can rearrange the equations to the form which contains only the temperature field and one can assume that the number of boundary conditions is equal with the order of highest space derivative in the equation. In usually, it is true but not so easy to define the boundary condition when the heat flux is given because we have

no explicitly the heat flux expressed in this form of equations thus the application of the constitutive equations are inevitable. For the weakly nonlocal equations (e.g. GK and GN equations) it is necessary to use the field of heat flux, to be more precise the “one-sided” derivative is necessary. In the work [31] one can see that it can yield serious problems in the solutions, these can be nonphysical.

The situation is more complicated in the case of the ballistic-diffusive equation because one needs to know the third derivative of the temperature on the boundary. This problem can be significantly simplified by consider only the boundary of the field of heat flux which is straightforward in the case of laser flash experiment. The method of this step will be discussed in the following chapter. We define the boundary condition only for the heat flux field in a way [49]:

$$q_{x=0} = \begin{cases} 1 - \cos(2\pi \cdot \frac{t}{t_p}) & \text{if } 0 < t \leq t_p \\ 0 & \text{if } t > t_p \end{cases}$$

Its graph can be seen in Figure 4.2.

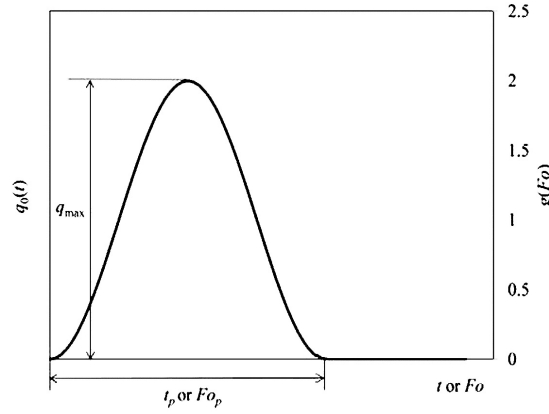


FIGURE 4.2. Boundary condition of the laser pulse.

It must be noted that this function starts smoothly, so its time derivative in the initial time instant is zero. It is important from the aspect of the numerical solution. The nonzero derivative can cause numerical disturbances and errors. It can be illustrated on the heaviside (unit step) function. The sudden change in the function causing such errors which cannot be handled by finite differences.

In real experiments, the shape of the pulse is not the same as here. We do not discuss the dependence of the shape of the pulse, this is enough for qualitative analysis. The length of the pulse is very short in comparison of the time interval of the experiment thus the exact shape is expected to be not so important.

CHAPTER 5

Numerical method

To solve the equations, the finite difference method is used. It has some advantages and disadvantages:

- The discretization is simple, the accuracy can be well-estimated and it can be used independently from the boundary conditions. Easy to programming.
- The possibility of artificial numerical phenomenas, oscillations and phase error. Difficult to handle such suddenly changed solutions.

Our goal was to write such an explicit scheme which can be used for similar structures of equations and can be easily extended. These heat conduction equations have a very similar structure, so it is a very important property. The scheme is explicit then it is conditionally stable. The calculation of such conditions is inevitable. By the Lax-Richtmyer theorem [56], the consistency of a scheme must be proved to ensure the convergence¹. The accuracy and the speed of the convergence can be estimated by the consistency analysis.

5.1. Discretization

We applied shifted fields in our scheme, the Figure 5.1 represents this structure.

One of the fields goes from zero to one, so it covers the whole space domain, the others are shifted by $\frac{\Delta x}{2}$. Let us imagine the space domain consists of little continuum pieces so we calculate the interaction between these continuum cells. By this kind of discretization one can distinguish surface-like and volume-like quantities. The one which covers the whole domain is surface-like quantity, its points are on the cell's boundary, on the other hand the points of shifted fields are on the middle of the cells, these are called volume-like quantities, and represents an average value for a cell. We do not need to define boundary conditions for the volume-like quantities thus the boundary condition of the heat flux field is enough for the whole system in this case. It must be noted that this choice is arbitrary, one can define for instance, the temperature as space-like quantity, it depends on the problem.

The balance equation of internal energy is necessary and the same for all models, it is the evolution equation for the temperature, its discretized form is

$$T_j^{n+1} = T_j^n - \frac{\Delta t}{\tau_\Delta \Delta x} (q_{j+1}^n - q_j^n). \quad (77)$$

Let us continue with the constitutive equations.

- **Fourier equation:**

$$q_j^{n+1} = -\frac{\tau_\Delta}{\Delta x} (T_j^n - T_{j-1}^n). \quad (78)$$

¹Liu [57] draw attention to the need of the analysis of a numerical scheme. Different schemes has different properties (accuracy, speed of the convergence and so on).

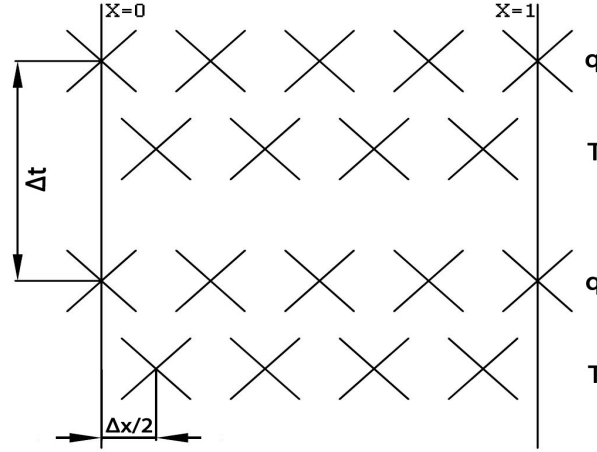


FIGURE 5.1. Discretization method.

- **Guyer–Krumhansl equation:**

$$q_j^{n+1} = q_j^n - \frac{\Delta t}{\tau_q} q_j^n - \frac{\tau_\Delta \Delta t}{\tau_q \Delta x} (T_j^n - T_{j-1}^n) + \frac{\hat{a} \Delta t}{\tau_q \Delta x^2} (q_{j+1}^n - 2q_j^n + q_{j-1}^n). \quad (79)$$

It can be reduced for the MCV equation via the substitution $\hat{a} = 0$.

- **Green–Naghdi equation:**

$$q_j^{n+1} = q_j^n - \frac{\tau_\Delta \Delta t}{\tau_q \Delta x} (T_j^n - T_{j-1}^n) + \frac{\hat{a} \Delta t}{\tau_q \Delta x^2} (q_{j+1}^n - 2q_j^n + q_{j-1}^n). \quad (80)$$

- **Ballistic-diffusive equation:**

$$q_j^{n+1} = q_j^n - \frac{\Delta t}{\tau_q} q_j^n - \frac{\tau_\Delta \Delta t}{\tau_q \Delta x} (T_j^n - T_{j-1}^n) - \frac{\kappa \Delta t}{\tau_q \Delta x} (Q_j^n - Q_{j-1}^n), \quad (81)$$

$$Q_j^{n+1} = Q_j^n - \frac{\Delta t}{\tau_Q} Q_j^n - \frac{\kappa \Delta t}{\tau_Q \Delta x} (q_{j+1}^n - q_j^n). \quad (82)$$

In the ballistic-diffusive model, not only the temperature is represented as shifted fields but the current density of the heat flux as well. The scheme is very simple, it is forward in time and backward in space. It is important to see that it is true only from the aspect of the indices, in fact it is central in space due to the discretization. The main disadvantage is the accuracy of the scheme, it is just first order, however it has very small computation requirements.

5.2. Consistency

A numerical scheme is consistent when the space and time steps $\Delta x, \Delta t$ tend to zero then the numerical solution tend to the exact solution. To prove this property we need to write the appropriate terms in Taylor series and substitute back to the scheme. It yields the numerical (“discrete”) operators for each field. The last step is to send the step sizes to zero and subtract from the original, continuous operators and the result must be zero.

First, let us see the balance equation of internal energy, write the original equation and its scheme in form

$$\begin{aligned}\tau_\Delta \partial_t T + \partial_x q &= 0, \\ P_1 &= \tau_\Delta \frac{\partial}{\partial t}; \quad P_2 = \frac{\partial}{\partial x},\end{aligned}\tag{83}$$

where P_1 and P_2 are the operators of temperature and heat flux.

$$\tau_\Delta \frac{T_j^{n+1} - T_j^n}{\Delta t} + \frac{q_{j+1}^n - q_j^n}{\Delta x} = 0\tag{84}$$

Then write into the form of Taylor series the terms T_j^{n+1} and q_{j+1}^n in a way

$$T_j^{n+1} = T_j^n + \Delta t \partial_t T + \frac{\Delta t^2}{2} \partial_{tt} T + O(\Delta t^3),\tag{85}$$

$$q_{j+1}^n = q_j^n + \Delta x \partial_x q + \frac{\Delta x^2}{2} \partial_{xx} q + O(\Delta x^3),\tag{86}$$

and substitute it back into the equation (84)

$$\tau_\Delta \left(\partial_t T + \frac{1}{2} \Delta t \partial_{tt} T + O(\Delta t^2) \right) + \left(\partial_x q + \frac{1}{2} \Delta x \partial_{xx} q + O(\Delta x^2) \right) = P_{1_{\Delta t, \Delta x}} T + P_{2_{\Delta t, \Delta x}} q,\tag{87}$$

where $P_{1_{\Delta t, \Delta x}}$ and $P_{2_{\Delta t, \Delta x}}$ are the discrete operators. Then let the difference terms to tend to zero and subtract from the original equation, the result is zero. It means that the solution of the scheme tend to the exact solution by the steps goes to zero. The order of the consistency is one then the order of the convergence is also one.

We show the proof only for the GK equation because the structure of the equations is the same, it can be easily reduced to the MCV and Fourier equations and very similar to the GN equation. The steps are the same for the ballistic-diffusive equation, the order of the consistency and convergence is also the same for all models.

In this case we have to write in a form of Taylor series the terms below

$$T_{j-1}^n = T_j^n - \Delta x \partial_x T + \frac{1}{2} \Delta x^2 \partial_{xx} T - O(\Delta x^3),\tag{88}$$

$$q_{j-1}^n = q_j^n - \Delta x \partial_x q + \frac{\Delta x^2}{2} \partial_{xx} q - \frac{\Delta x^3}{6} \partial_x^3 q + \frac{\Delta x^4}{24} \partial_x^4 q - O(\Delta x^5),\tag{89}$$

$$q_{j+1}^n = q_j^n + \Delta x \partial_x q + \frac{\Delta x^2}{2} \partial_{xx} q + \frac{\Delta x^3}{6} \partial_x^3 q + \frac{\Delta x^4}{24} \partial_x^4 q + O(\Delta x^5),\tag{90}$$

$$q_j^{n+1} = q_j^n + \Delta t \partial_t q + \frac{1}{2} \Delta t^2 \partial_{tt} q + O(\Delta t^3).\tag{91}$$

Two terms of the heat flux are needed to write further because of the second order derivative in the scheme. Substitute it back into the equation (79):

$$\begin{aligned}\tau_q \left(\partial_t q + \frac{1}{2} \Delta t \partial_{tt} q + O(\Delta t^2) \right) + q_j^n + \tau_\Delta \left(\partial_x T - \frac{1}{2} \Delta x \partial_{xx} T - O(\Delta x^2) \right) + \\ - \hat{a} \left(\partial_{xx} q + \frac{1}{12} \Delta x^2 \partial_x^4 q + O(\Delta x^4) \right).\end{aligned}\tag{92}$$

One can see that the second order derivative has second order accuracy, but the lowest order of the scheme is the relevant one, so the order of the consistency remains one.

Some important remarks about the consistency:

- We proved only the weak consistency (“w-consistent”) of the scheme. In usual – in a conventional way – it used to be interpreted as “consistency”. A consequence of the weak consistency is that the difference equations may not inherit all of the properties of the differential equation [58]. The proof of the strong consistency (“s-consistent”) is more difficult and complicated. For our purposes, the w-consistency is enough.
- The exact definition of the mentioned Lax-Richtmyer theorem: a consistent finite difference scheme of a linear partial differential equation which belongs to an initial value problem is convergent if the scheme is stable. The initial value problem must be well-posed, i.e.
 - (1) the solution is exist,
 - (2) this solution is unique,
 - (3) the solution depends continuously on the initial and boundary conditions,
 where the two points, the existence and uniqueness are consists of the checking the initial and boundary conditions as well.

To ensure the convergence of the numerical scheme, we need to prove and derive the stability conditions. One can easily define well-posed problems for symmetric hyperbolic systems [45]. To further and more detailed mathematical discussion, see [59].

5.3. Stability analysis

The numerical scheme is stable when the error of the approximation remains bounded. The methods of Neumann and Jury will be used in this section. First, let us see the detailed steps of the Neumann method. Assume the solutions of the difference equations in a form

$$\phi_j^n = \xi^n e^{ikj\Delta x}, \quad (93)$$

where i is the imaginary unit, k is the wavenumber, $j\Delta x$ denotes the j th space steps and n is the index of the time step. The scheme will be stable if $|\xi| \leq 1$ stands for the growing factor ξ . If $|\xi| = 1$ then the scheme is conservative. Substitute back into the schemes, let us start with the balance equation of the internal energy

$$-T_j^{n+1} + T_j^n - \frac{\Delta t}{\tau_\Delta \Delta x} (q_{j+1}^n - q_j^n) = 0, \quad (94)$$

$$(\xi - 1)T_0 + \frac{\Delta t}{\tau_\Delta \Delta x} (e^{ik\Delta x} - 1) q_0 = 0. \quad (95)$$

Since we work with the temperature and the heat flux fields thus it results a linear algebraic system of equations. Let us begin with the most simple one, the Fourier equation,

$$\xi q_0 + \frac{\tau_\Delta}{\Delta x} (1 - e^{-ik\Delta x}) T_0 = 0. \quad (96)$$

So the system is obtained in the form

$$\begin{pmatrix} \xi - 1 & \frac{\Delta t}{\tau_\Delta \Delta x} (e^{ik\Delta x} - 1) \\ \frac{\tau_\Delta}{\Delta x} (1 - e^{-ik\Delta x}) & \xi \end{pmatrix} \cdot \begin{pmatrix} T_0 \\ q_0 \end{pmatrix} = 0.$$

When the determinant of the coefficient matrix is zero the system has a nontrivial solution. The characteristic polynom $F(\xi)$ of the coefficient matrix is

$$F(\xi) = \xi^2 - \xi - \frac{\Delta t}{\Delta x^2} (2 \cos(k\Delta x) - 2) = 0. \quad (97)$$

A very important remark is that the polynomial must have a form within the coefficient of highest order term is positive. When the characteristic polynomial is second order, it comes naturally. Only the ballistic-diffusive model has third order polynomial, thus one must pay attention to the coefficient of the highest order term. When the order of the characteristic polynomial is odd, the relation changes in Jury criterion. Furthermore, it should be noted that the Jury criterion is used for discrete systems; the more commonly known method, the Routh-Hurwitz method is also can be used, but the bilinear transformation must be applied [60]. If the stability conditions are fulfilled, the roots of the characteristic polynomial will be within the unit circle on the complex plane then the stability of the difference equation will be asymptotically stable. For a n th order polynomial we have $n + 1$ conditions. Let us recall the Jury criteria:

- (1) $F(\xi = 1) \geq 0$,
- (2) $F(\xi = -1) \geq 0$ if n is even and $F(\xi = -1) \leq 0$ if n is odd,
- (3) $|a_0| \leq a_n$, then if the coefficient of the highest order term is 1, it will ensure that the zeroth order term will not be higher than 1 in the case of a trivial solution.

If these conditions are fulfilled then the scheme is stable and for the growth factor $|\xi| \leq 1$ will be valid. Hereinafter we write only the characteristic polynomial and we refer to the number of the criterion.

- **Fourier equation:** the polynomial has been derived, let us check the conditions:

- (1) $\frac{4\Delta t}{\Delta x^2} > 0$; it is fulfilled in every case.
- (2) $1 + \frac{2\Delta t}{\Delta x^2} > 0$; it is valid for every parameters.
- (3) $\Delta t < \frac{\Delta x^2}{4}$; this third criterion gives a condition for the time step.

- **Guyer-Krumhansl equation:** let us introduce the polynomial in a form $a_2\xi^2 + a_1\xi + a_0 = 0$, where

$$\begin{aligned} a_2 &= 1, \\ a_1 &= \frac{\Delta t}{\tau_q} - 2 - \frac{\hat{a}\Delta t}{\tau_q\Delta x^2} (2 \cos(k\Delta x) - 2), \\ a_0 &= 1 - \frac{\Delta t}{\tau_q} + \frac{\hat{a}\Delta t}{\tau_q\Delta x^2} (2 \cos(k\Delta x) - 2) - \frac{\Delta t^2}{\tau_q\Delta x^2} (2 \cos(k\Delta x) - 2). \end{aligned}$$

The term $\cos(k\Delta x) = -1$ means the extrema value so we deal with this assumption in every case. So the conditions are given:

- (1) $\frac{4\Delta t^2}{\tau_q\Delta x^2} > 0$;
- (2) $\frac{\Delta x^2}{4} \left(\frac{2\tau_q}{\Delta t} - 1 \right) + \frac{\Delta t}{2} > \hat{a}$.
- (3) It gives us two conditions by the absolute value, the first one is $\Delta t - \frac{\Delta x^2}{4} < \hat{a}$.

The other one is $\frac{\Delta x^2}{4} \left(\frac{2\tau_q}{\Delta t} - 1 \right) + \Delta t > \hat{a}$, which is weaker than the one from the second Jury criterion, because $\frac{\Delta t}{2} < \Delta t$.

These conditions can be reduced to the MCV case by $\hat{a} = 0$ substitution.

- **Green–Naghdi equation:** the zeroth order derivative of the heat flux is missing from the constitutive equation, so the parameter $\frac{\Delta t}{\tau_q}$ is also missing from the coefficients of the polynom, i.e.

$$\begin{aligned} a_2 &= 1, \\ a_1 &= -2 - \frac{\hat{a}\Delta t}{\tau_q\Delta x^2} (2\cos(k\Delta x) - 2), \\ a_0 &= 1 + \frac{\hat{a}\Delta t}{\tau_q\Delta x^2} (2\cos(k\Delta x) - 2) - \frac{\Delta t^2}{\tau_q\Delta x^2} (2\cos(k\Delta x) - 2). \end{aligned}$$

Thus the stability conditions are

- (1) $\frac{4\Delta t^2}{\tau_q\Delta x^2} > 0$; this one is identical to the GK case.
- (2) $\frac{\tau_q\Delta x^2}{2\Delta t} + \frac{\Delta t}{2} > \hat{a}$.
- (3) We obtain again two conditions by the absolute value function; the first one is $\Delta t < \hat{a}$ which exclude the case $\hat{a} = 0$, it is in accordance to the thermodynamic conditions as well.

The second one is $\frac{\tau_q\Delta x^2}{2\Delta t} + \Delta t > \hat{a}$; it is weaker because $\Delta t > \frac{\Delta t}{2}$.

- **Ballistic-diffusive equation:** the system consists of three equations thus the characteristic polynom is third order, its coefficients are

$$\begin{aligned} a_3 &= 1 \\ a_2 &= \frac{\Delta t}{\tau_q} + \frac{\Delta t}{\tau_Q} - 3 \\ a_1 &= \frac{\Delta t^2}{\tau_q\tau_Q} + 3 - \frac{2\Delta t}{\tau_q} - \frac{2\Delta t}{\tau_Q} - \left(\frac{\kappa^2\Delta t^2}{\tau_q\tau_Q\Delta x^2} + \frac{\Delta t^2}{\tau_q\Delta x^2} \right) (2\cos(k\Delta x) - 2) \\ a_0 &= \frac{\Delta t}{\tau_q} + \frac{\Delta t}{\tau_Q} - \frac{\Delta t^2}{\tau_Q\tau_q} - 1 + \left(\frac{\kappa^2\Delta t^2}{\tau_q\tau_Q\Delta x^2} - \frac{\Delta t^2}{\tau_q\Delta x^2} \left(\frac{\Delta t}{\tau_Q} - 1 \right) \right) (2\cos(k\Delta x) - 2) \end{aligned}$$

Because of the order of the polynom we need a fourth condition, namely

$|b_0| > |b_2|$, ahol $b_0 = \begin{vmatrix} a_0 & a_3 \\ a_3 & a_0 \end{vmatrix}$ és $b_2 = \begin{vmatrix} a_0 & a_1 \\ a_3 & a_2 \end{vmatrix}$. The conditions becomes more and more complicated because of the order of the polynom, so the numerical evaluation is recommended. Obviously, the formulas can be derived in an analytical way as well, but it will be too difficult to interpret.

This is the end of the stability analysis, the convergence of the schemes is proved.

CHAPTER 6

Solutions and comparisons

In this chapter we will discuss the effect of the parameters in the constitutive equations. It is very important to note that nonzero parameters also can result the solution of the Fourier equation in nonlocal models. We are seeking such qualitative differences from the Fourier's solution that can be showed in experiments. We start with the Fourier equation, it will be our standard characteristic solution.

6.1. Solutions of the Fourier equation

If we rearrange the system to the temperature (eq. (98)), one can see that it does not contains a parameter. The boundary condition contains the only one time parameter of the system (τ_Δ pulse length) in this case.

$$\partial_t T = \partial_{xx} T. \quad (98)$$

We draw attention to the parameter τ_Δ , it contains all of the material parameters via the thermal diffusivity. We choose $\tau_\Delta = 0.04$ value in most of the cases to follow Czél et al. [49], the only one exception is the ballistic-diffusive model. The solutions can be seen in Figures 6.1 and 6.2.

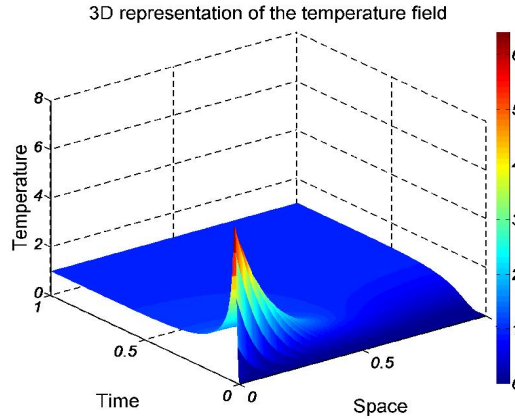


FIGURE 6.1. The 3D representation of the temperature field for the solution of the Fourier equation.

6.2. Solutions of the Maxwell–Cattaneo–Vernotte equation

The Fourier equation is extended by the time derivative of the heat flux, so the solution can represent the wave-kind propagation (called “second sound”),

$$\tau_q \partial_{tt} T + \partial_t T = \partial_{xx} T. \quad (99)$$

As the parameter τ_q tends to zero, the solution tends to the Fourier-type solution. If τ_q is increased then the wave characteristic of the propagation become stronger

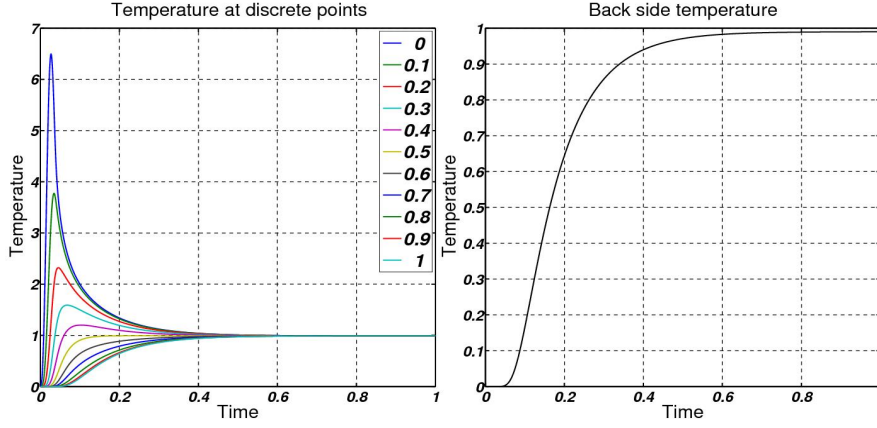


FIGURE 6.2. Solution of the Fourier equation for $\tau_\Delta = 0.04$. The solutions of the other equations will be compared to this one.

(see Figures 6.3, 6.4 and 6.5) and it tends to the solution of a second order wave equation (dissipation free GN equation). A conclusion of the chapter of dissipation relations can be observed, the effect of the parameter τ_q on the propagation speed.

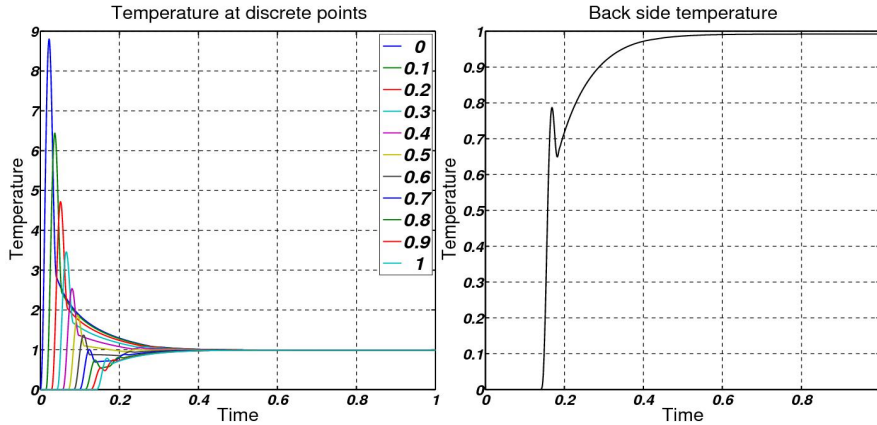


FIGURE 6.3. Solution of the MCV equation for $\tau_\Delta = 0.04$ and $\tau_q = 0.02$. One can see the wave nature of the propagation on the right hand side and we obtain exactly the characteristic propagation speed $\frac{1}{\sqrt{\tau_q}}$ of the system.

6.3. Solutions of the Guyer–Krumhansl equation

As we seen before, $\hat{a} = 0$ leads to the MCV equation, so this case is already discussed. This parameter is responsible for the dissipation in the system, when it is getting higher the damping is increasing (Fig. 6.6). Let us realize that in the form (100) there are two appearance of the Fourier equation, it contains the time derivative of the Fourier equation, too.

$$\tau_q \partial_{tt} T + \partial_t T = \partial_{xx} T + \hat{a} \partial_{txx} T. \quad (100)$$

Consequently, if $\tau_q = \hat{a}$ holds then it leads to the exact solution of the Fourier equation (Fig. 6.7).

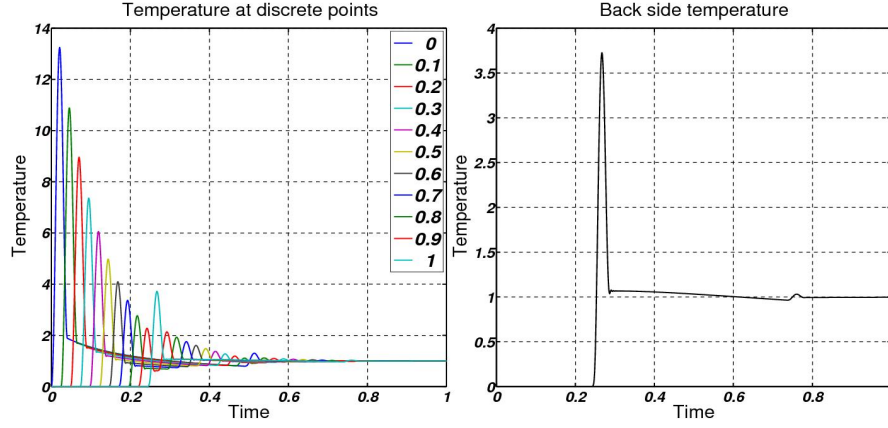


FIGURE 6.4. Solution of the MCV equation for $\tau_\Delta = 0.04$ and $\tau_q = 0.06$.

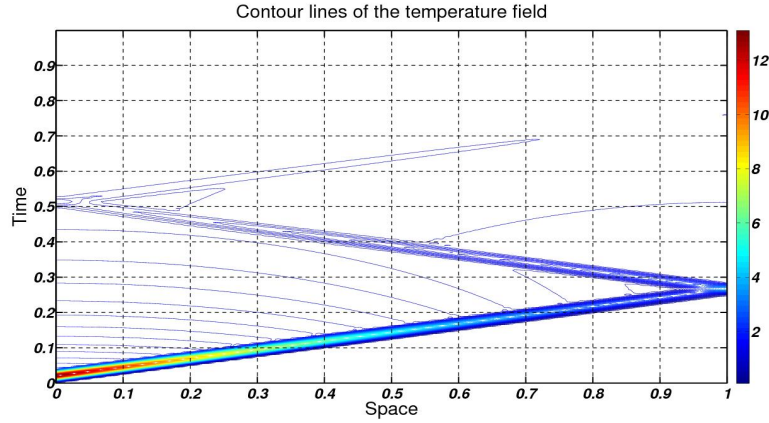


FIGURE 6.5. Solution of the MCV equation for $\tau_\Delta = 0.04$ és $\tau_q = 0.06$ with contour line representation. The heat pulse is reflected back then smoothed out.

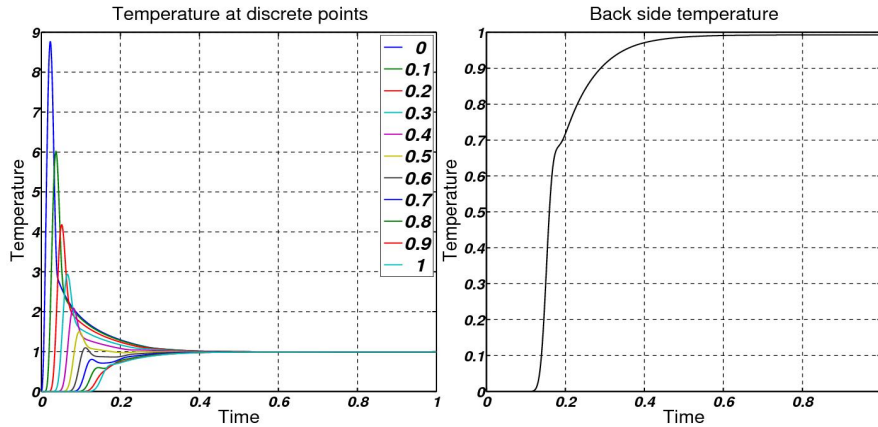


FIGURE 6.6. Underdamped (MCV-kind) solution of the GK equation for $\tau_\Delta = 0.04$; $\tau_q = 0.02$; $\hat{a} = 0.001$.

If we increase further the dissipation parameter then the solution becomes overdamped (or called overdiffusive) and the signal propagation speed will be higher as we saw it in the chapter of dispersion relations (Fig. 6.8).

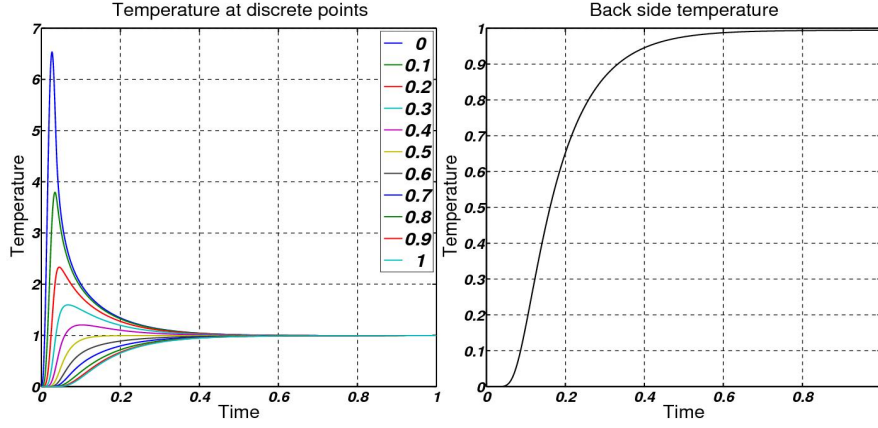


FIGURE 6.7. Fourier-type solution of the GK equation for $\tau_\Delta = 0.04$; $\tau_q = \hat{a} = 0.02$. Then we obtain the same solution as in the Figure 6.2.

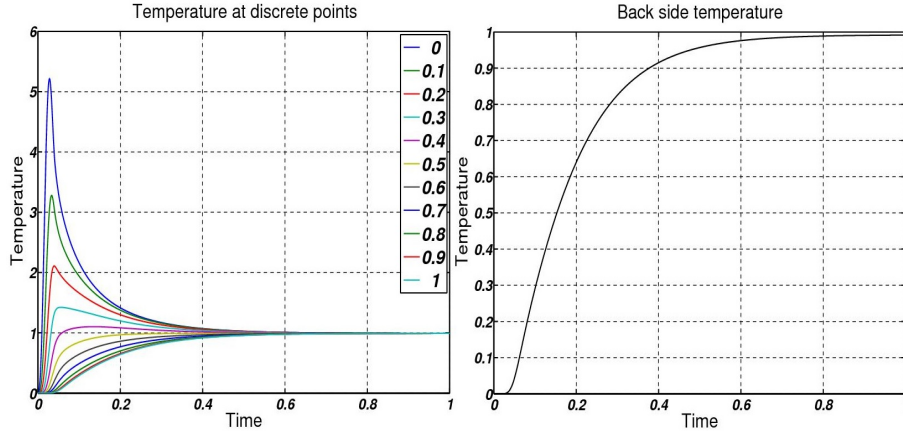


FIGURE 6.8. Overdiffusive solution of the GK equation for $\tau_\Delta = 0.04$; $\tau_q = 0.02$; $\hat{a} = 0.04$. The temperature begin to increase sooner than in the case of Fourier equation (Figs. 6.2 and 6.7).

6.4. Solutions of the Green–Naghdi equation

One can rearrange the system to the form with temperature terms (101) and let us notice that it is a dissipative wave equation. When $\hat{a} = 0$ holds then the system is dissipation free but this case is excluded by thermodynamical conditions. The GN equation reads

$$\tau_q \partial_{tt} T = \partial_{xx} T + \hat{a} \partial_{txx} T. \quad (101)$$

The Figure 6.9 shows a weakly damped solution. The temperature peaks caused by the wave reflections on the boundary, it is illustrated in the Figure 6.10 with contour lines, too.

Visibly, the wave broadens, its energy is dispersed in space as time goes by. When the dissipation is weak, the transient part of the solution will take significantly more time to smooth over. The Figures 6.11 and 6.12 shows such solutions when the dissipation is strong, so the wave will smooth out soon.

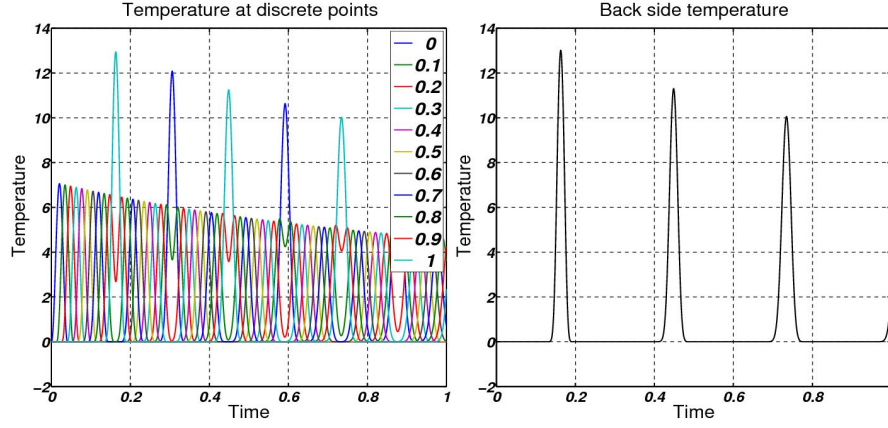


FIGURE 6.9. Solution of the GN equation for $\tau_\Delta = 0.04$; $\tau_q = 0.02$; $\hat{a} = 10^{-4}$. The reflections and attenuation of the wave is clear.

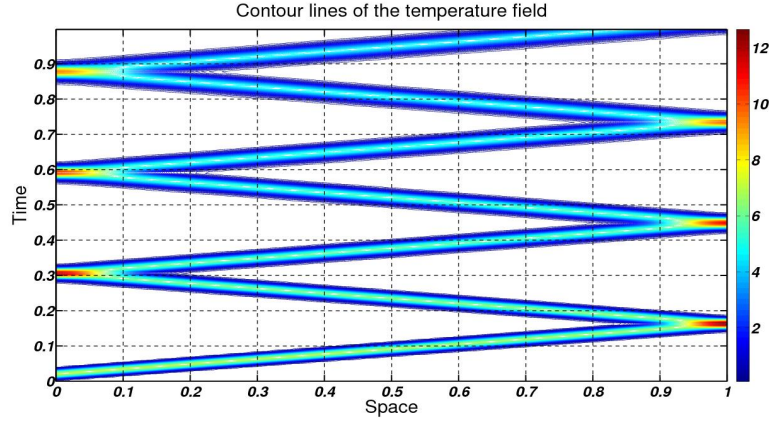


FIGURE 6.10. Contour line representation of the solution of the GN equation for $\tau_\Delta = 0.04$; $\tau_q = 0.02$; $\hat{a} = 10^{-4}$.

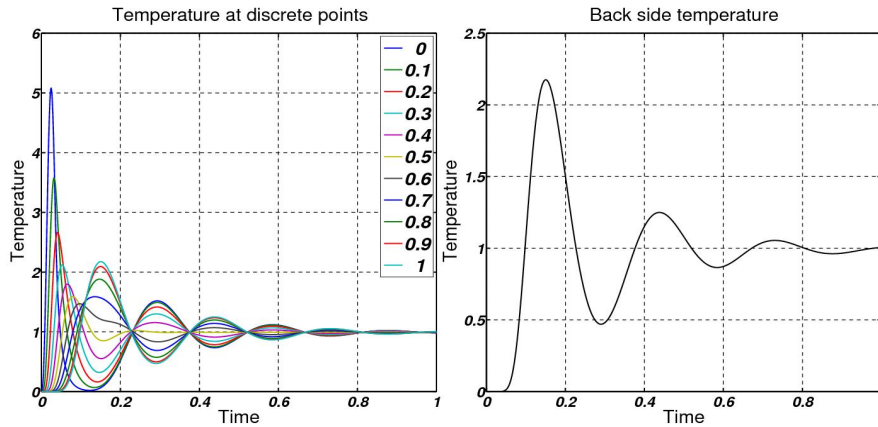


FIGURE 6.11. Solution of the GN equation for $\tau_\Delta = 0.04$; $\tau_q = 0.02$; $\hat{a} = 0.02$.

If we increase the parameters τ_q and $\hat{a}$ in parallel and these are equal with each other then the solution will tend to the Fourier-type solution, it is illustrated in the Figures 6.13 and 6.14.

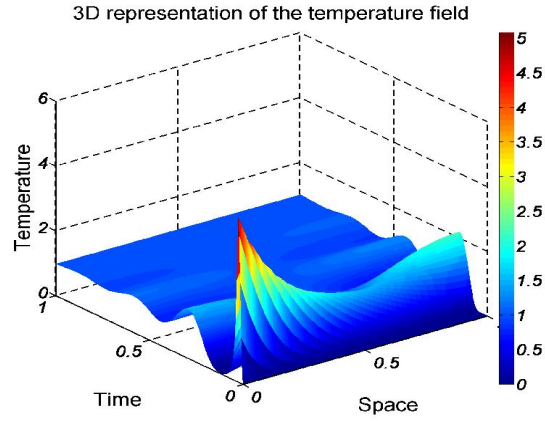


FIGURE 6.12. The 3D representation of the temperature field by the GN equation for $\tau_\Delta = 0.04$; $\tau_q = 0.02$; $\hat{a} = 0.02$.

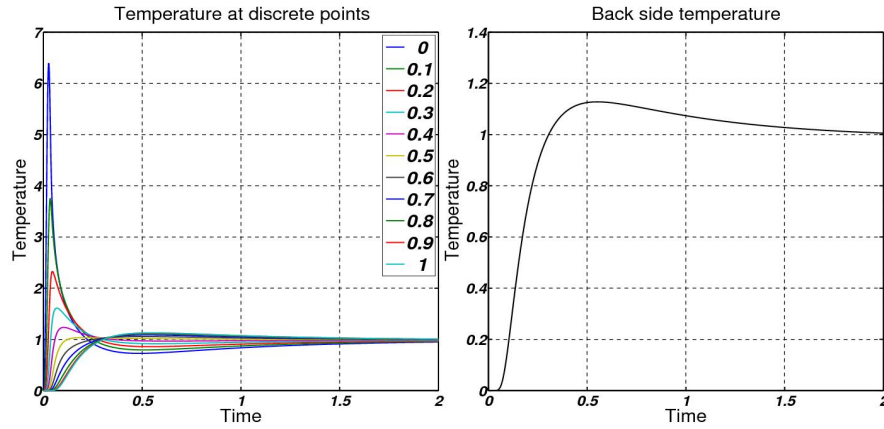


FIGURE 6.13. Solution of the GN equation for $\tau_\Delta = 0.04$; $\tau_q = 0.8$; $\hat{a} = 0.8$.

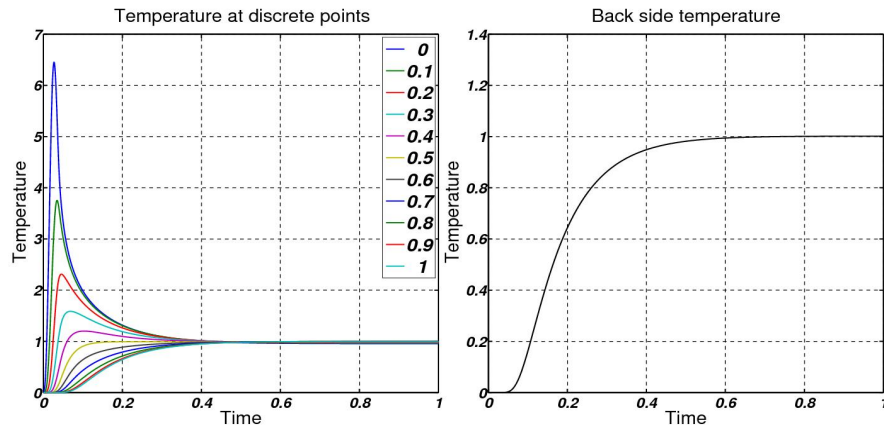


FIGURE 6.14. Fourier-type solution of the GN equation for $\tau_\Delta = 0.04$; $\tau_q = 10$; $\hat{a} = 10$.

When τ_q remains unchanged and $\hat{a}$ is increasing then we obtain a highly over-damped solution which propagates faster and reach the steady state quickly (Fig. 6.15).

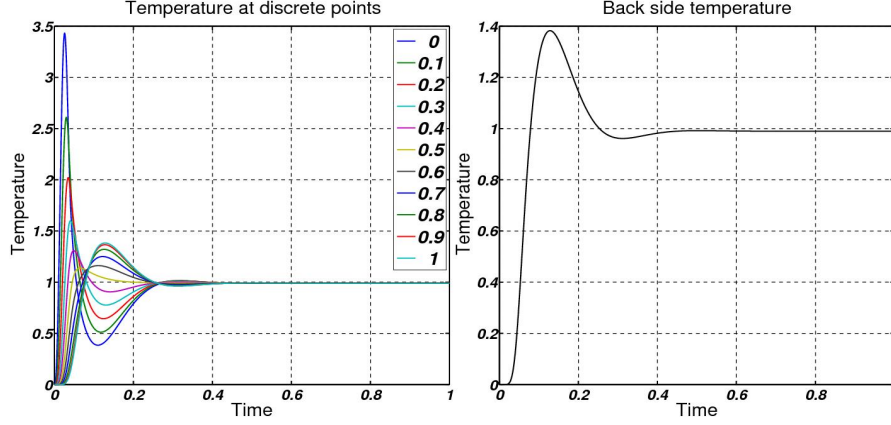


FIGURE 6.15. Solution of the GN equation for $\tau_\Delta = 0.04$; $\tau_q = 0.02$; $\hat{a} = 0.06$.

6.5. Solutions of the ballistic-diffusive equation

It is important to remember that during the derivation of the ballistic-diffusive system, we have simplified the hierarchic system. The equation in the form of temperature terms only is founded

$$\tau_Q \tau_q \partial_{ttt} T + (\tau_Q + \tau_q) \partial_{tt} T + \partial_t T = \partial_{xx} T + (\tau_Q + \kappa^2) \partial_{txx} T. \quad (102)$$

One can realize the Fourier equations two times in this form but we can interpret it as a memory extension of the GK equation. The parameter τ_Q appears in the coefficient of third order time derivative but in the terms of the second order time derivative and in the mixed one as well. Furthermore, it is interesting to see that the role of the coupling parameter is similar to the $\hat{a}$. Therefrom it can be seen that the solutions of the lower order models can be reproduced but not only via simple substitution because of the parameter τ_Q .

6.5.1. Fourier-type solutions.

- Let us choose τ_Q , τ_q , κ to be small parameters such as $\tau_Q = \tau_q = \kappa = 0.001$ so the solution tend to the solution of the original Fourier equation (Fig. 6.16).
- In this case let us choose τ_Q to be significantly higher than in the last case thus it reproduces the Fourier-type solution in a way which is similar to the case of the GK equation, we deal with the time derivative of the Fourier equation beside such parameters (Fig. 6.17).
- When the ballistic-diffusive equation was introduced we noted that the third Fourier-type solution cannot be reproduced¹.

¹For reasons, see the chapter of the generalization of heat conduction equations.

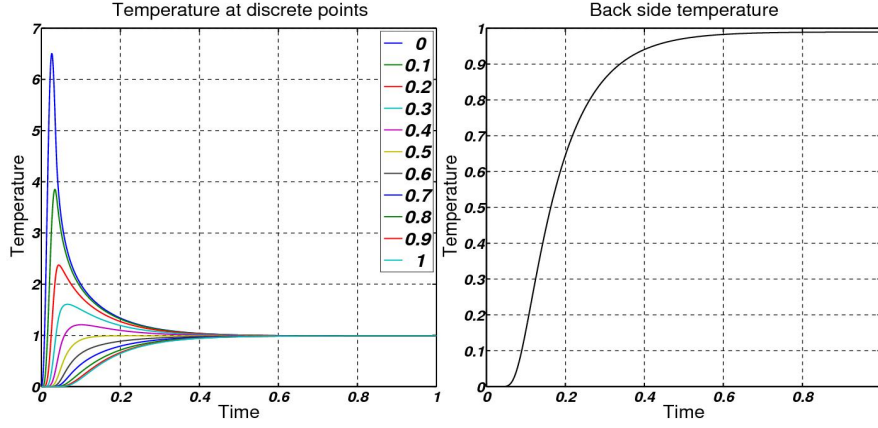


FIGURE 6.16. Fourier-type solution of the ballistic-diffusive equation for $\tau_Q = \tau_q = \kappa = 0.001$.

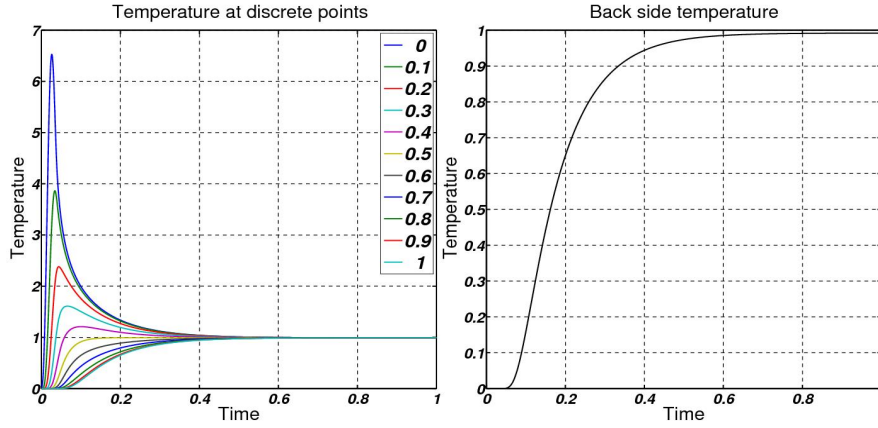


FIGURE 6.17. Fourier-type solution of the ballistic-diffusive equation for $\tau_Q = 1; \tau_q = \kappa = 0.001$.

6.5.2. MCV-type solutions. When the coupling between the constitutive equations is removed (so $\kappa = 0$), the current density of the heat flux and the heat flux itself will be independent from each other, thus the signal propagation will be independent² from the parameter τ_Q and the solutions will be exactly the solutions of the MCV equation (Figure 6.18).

6.5.3. GK-type solutions. Let $\tau_Q \ll \tau_q$ then the coefficient of the third order time derivative will be small, furthermore, let $\kappa = 0.25$ then $\kappa^2 \gg \tau_Q$ holds for the coefficient of the mixed derivative. Since the role of the coupling parameter is similar for the dissipation parameter $\hat{a}$ in the GK equation thus we can approximate this type of characteristics by κ . One can see an overdifusive (or overdamped) solution in Figure 6.19.

One can reproduce other GK-type solution in a similar way.

6.5.4. GN-type solutions. The characteristic wave-kind propagation of the GN equation can be reproduced by parameters $\tau_q = 0.7; \tau_Q = 15; \kappa = 9; \tau_\Delta = 0.04$, the result is illustrated in the Figures 6.20 and 6.21.

²See the chapter of hyperbolicity.

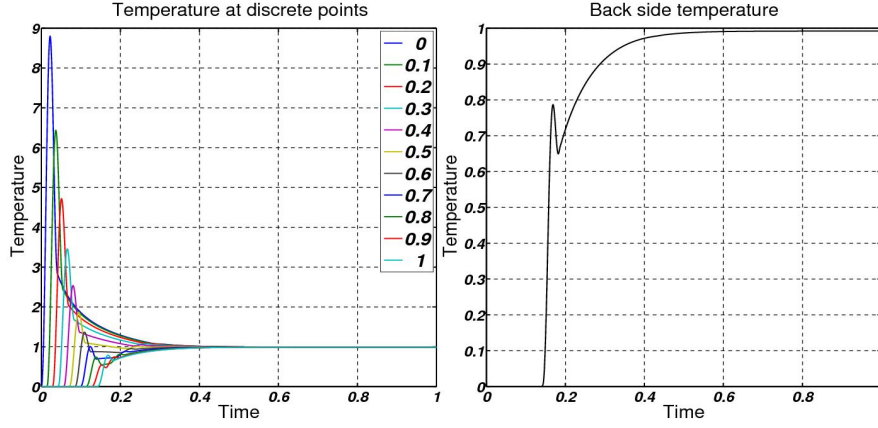


FIGURE 6.18. MCV-type solution of the ballistic-diffusive equation for $\tau_q = 0.02$; $\kappa = 0.001$.

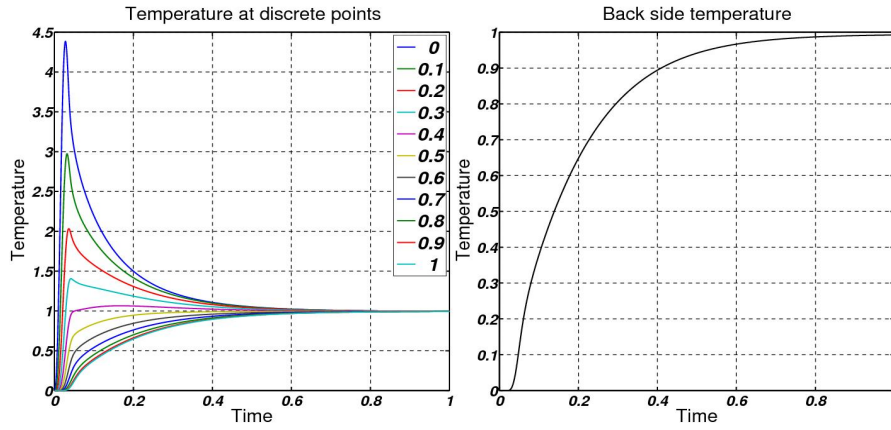


FIGURE 6.19. GK-type solution of the ballistic-diffusive equation for $\tau_q = 0.02$; $\tau_Q = 0.001$; $\kappa = 0.25$.

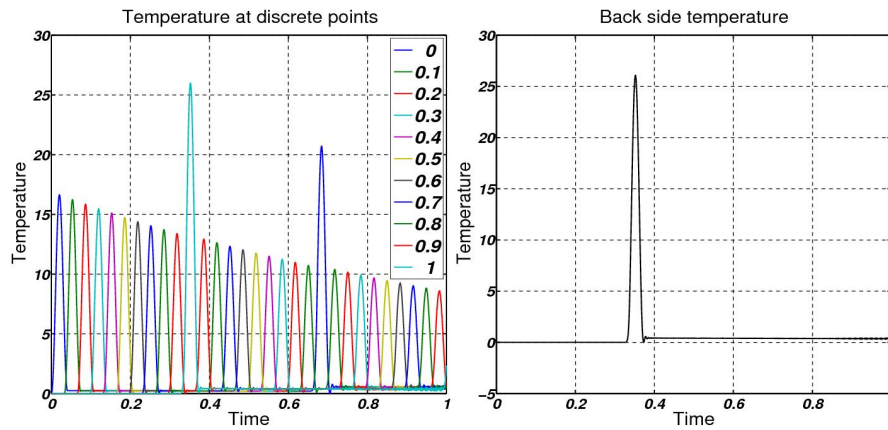


FIGURE 6.20. GN-type solution of the ballistic-diffusive equation for $\tau_q = 0.7$; $\tau_Q = 15$; $\kappa = 9$; $\tau_\Delta = 0.04$.

6.5.5. Ballistic solutions. Our goal is to reproduce such characteristics which can be seen in Figure 2.1, so we seek such a domain where the two different signal

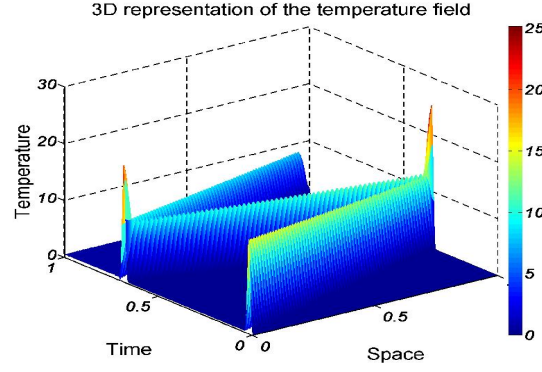


FIGURE 6.21. 3D representation of the temperature field in the case of GN-type solution of the ballistic-diffusive equation for $\tau_q = 0.7$; $\tau_Q = 15$; $\kappa = 9$; $\tau_\Delta = 0.04$.

propagation exist. The length of the laser pulse has an important role, it can significantly modify the solution, the existence of the ballistic signal depends on it; these solutions are represented in Figures 6.22 and 6.23.

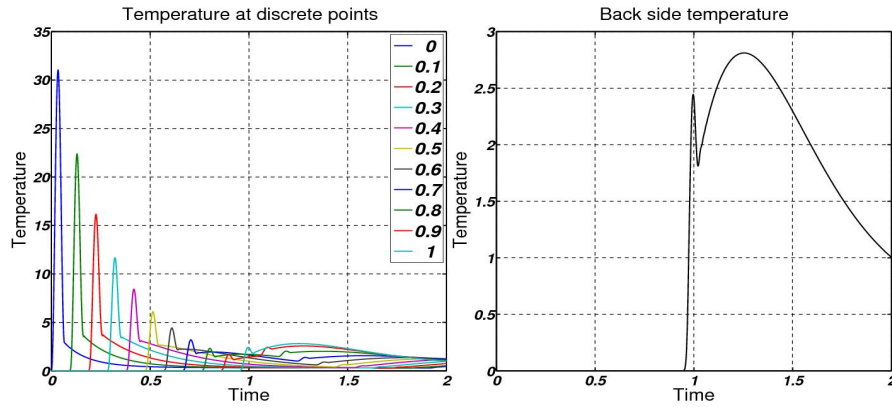


FIGURE 6.22. The ballistic solution of the ballistic-diffusive equation for $\tau_q = 1.9$; $\tau_Q = 0.07$; $\kappa = 0.28$; $\tau_\Delta = 0.065$.

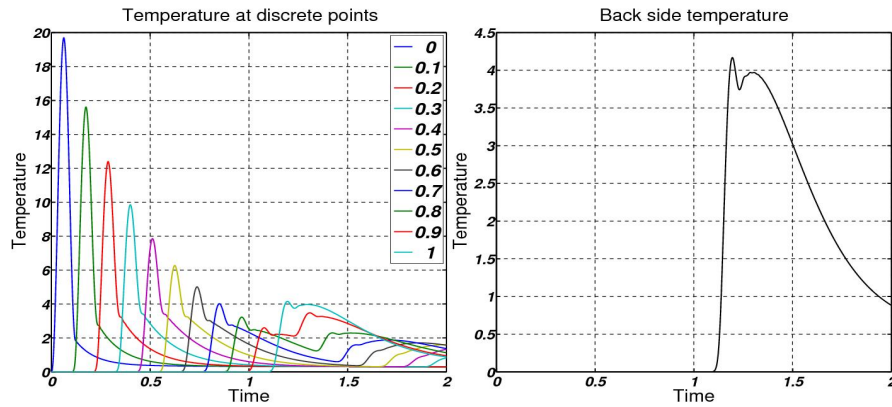


FIGURE 6.23. The ballistic solution of the ballistic-diffusive equation for $\tau_q = 1.9$; $\tau_Q = 0.07$; $\kappa = 0.2$; $\tau_\Delta = 0.12$.

CHAPTER 7

Experiments

7.1. Comparison of ballistic models with experiments

In this subsection we compare three models from the aspect of NaF experiment:

- (1) The kinetic model of Dreyer and Struchtrup [7],
- (2) Complex viscosity model of Yanbao Ma [24, 27],
- (3) Ballistic-diffusive model of continuum thermodynamics [37].

The common property of these models is that they measure the goodness of the model on the NaF experiments however the authors place emphasis on different aspects. Dreyer and Struchtrup concentrates on qualitative representation in contrast of Ma who obtained quantitative match with experiments. The considered material parameters of NaF are valid on 15 K and given by [61], so

$$\rho = 2866 \frac{kg}{m^3}; \quad c = 2.774 \frac{J}{kgK}; \quad \lambda = 20500 \frac{W}{mK}, \quad (103)$$

where ρ is the mass density, c is specific heat and λ denotes the thermal conductivity. Dreyer and Struchtrup used different laser pulse length (Δt_1) and sample length (L_1) from Ma's model (Δt_2 and L_2) to reproduce the results of the Jackson - Walker experiments, but in the same order of magnitude.

$$\Delta t_1 = 10^{-7}s; \quad L_1 = 6.26mm; \quad \Delta t_2 = 2.4 \cdot 10^{-7}s; \quad L_2 = 7.9mm \quad (104)$$

Now we can calculate the dimensionless parameters. The relaxation times are given by the articles and the parameter κ is calculated to obtain the correct signal propagation speed¹. Let us first compare our solution to the kinetic model of Dreyer and Struchtrup. We would like to reproduce the characteristic from the Figure 7.1.

The Figure 7.2 shows our result. By comparison of the kinetic model and our continuum thermodynamically derived system showed us that the speed of sound in dimensional and dimensionless form is

$$c = \sqrt{\frac{3\alpha}{\tau_q}}; \quad \hat{c} = \sqrt{\frac{3}{\hat{\tau}_q}}, \quad (105)$$

where c denotes the dimensional speed of sound and $\hat{c}$ denotes it in dimensionless form, α is the thermal diffusivity which can be calculated from the material parameters, τ_q is the relaxation time which belongs to the heat flux. So the speed of sound is $c = 2724.3 \frac{m}{s}$ and we can adjust the parameter κ to get exactly the same speed for ballistic signal propagation. It is very important to note it again that the kinetic theory also can give the appropriate speed but by using $N = 30$ equations. The right dimensionless time instant where we have to measure the ballistic signal is $Fo = 0.196$. Summarizing our parameters:

$$\tau_q = 0.068; \quad \tau_Q = 0.0137; \quad \kappa = 0.102; \quad \tau_\Delta = 0.0065. \quad (106)$$

¹The significance of the chapter of hyperbolicity is vital.

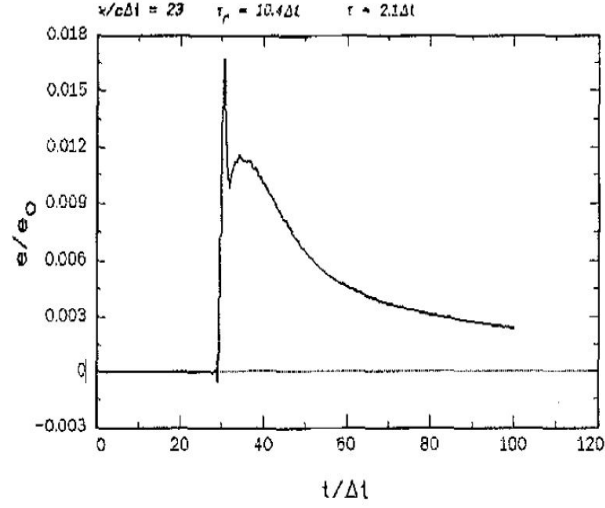


FIGURE 7.1. Solution of the kinetic model which solved by Dreyer and Struchtrup for $\tau_R = 10.4\Delta t$; $\tau = 2.1\Delta t$, where Δt is the pulse length [7].

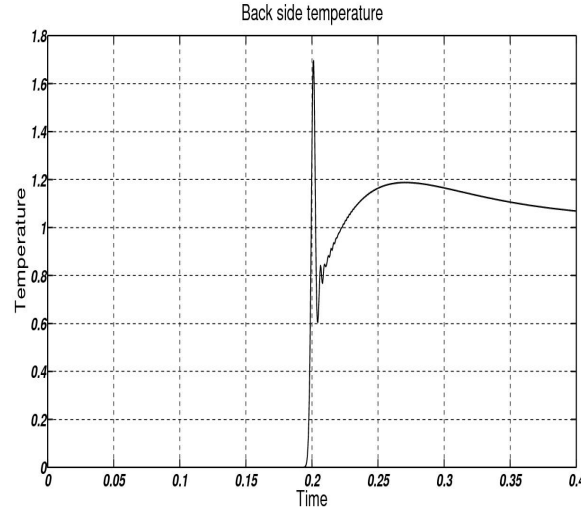


FIGURE 7.2. Solution of our model for $\tau_q = 0.068$; $\tau_Q = 0.0137$; $\kappa = 0.102$; $\tau_\Delta = 0.0065$ dimensionless parameters.

So our model can reproduce the result of Dreyer and Struchtrup [7].

Let us see now the data of Yanbao Ma [27]. He gives the relaxation times and the considered speed of sound:

$$\tau_R = 0.937\mu s; \tau_N = 0.338\mu s; \rightarrow \tau_Q = 0.248\mu s; c = 3187 \frac{m}{s}. \quad (107)$$

The Figure 7.3 shows the results of Ma, among which is the blue one (for 13 K) is the relevant one for us. The fitted results of the ballistic-diffusive equation can be seen on Figure 7.4. The characteristics of this curve is in accordance of the measured one but the propagation speeds are not correct at this point. Our

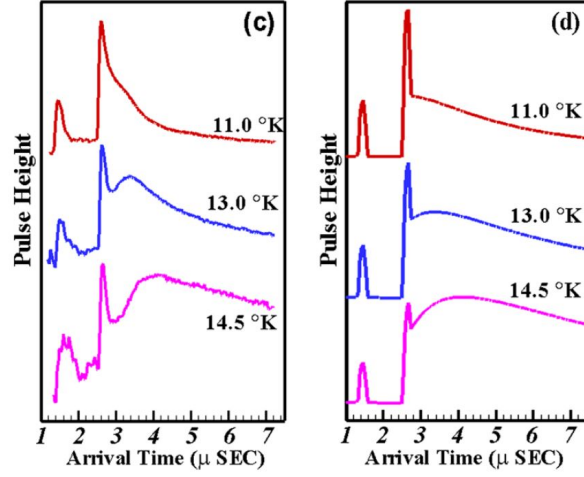


FIGURE 7.3. Fitting of Yanbao Ma; the measured data can be seen on the left hand side, his fitted data is on the right hand side [27]. The important one is belongs to 13 K from these curves. The signal of second sound and ballistic propagation can be clearly identified.

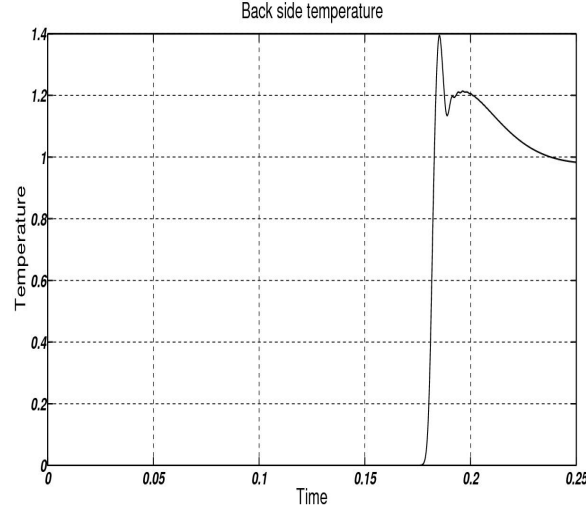


FIGURE 7.4. Fitting of the ballistic-diffusive equation for $\tau_q = 0.039$, $\tau_Q = 0.007$, $\tau_\Delta = 0.01$, $\kappa = 0.04$. The characteristics of this curve is correct, but the speed of ballistic propagation is not, it should be at $Fo = 0.12$.

dimensional parameters are

$$\tau_q = 0.937\mu s; \tau_Q = 0.168\mu s; c = 1849 \frac{m}{s}. \quad (108)$$

The back side boundary condition is not clear at all neither in the model of Dreyer and Struchtrup, nor in Ma's model. It is not clear that which kind of boundary condition could be better to fit the measured results instead of our adiabatic boundary condition.

7.2. Further applications

- The application of the ballistic-diffusive model is not restricted to analyze phenomenas of low temperatures. A very important and continuously improving area is the nanoelectronic devices. The thermoelectric effect changes the thermal conductivity which modifies the efficiency and the operation abilities of such devices [62].
- By comparison with the kinetic theory we conclude that the speed of sound is in connection with the thermal conductivity. It can be more complicated to consider the mechanical part of the modeling, by coupling with the deformations of the medium the viscosity will also play a role [63].
- An interesting way to consider the role of sample length is calculate the dependence of the thermal conductivity from Knudsen number. When the characteristic length of the sample is in the same order of magnitude with the mean free path², then the ballistic propagation plays a role. Alvarez and Jou showed [64] that the MCV equation gives a better description in this way than the usual one. The heat flux oscillations - which is mentioned in the article of Chen [16] - can be eliminated, furthermore the heat flux will be converge to the ballistic-diffusive equation instead of the Fourier equation.

7.3. Evaluation of the BUTE-DEE-experiment

Based on preliminary measurement experiences, on 3. June 2014. Soma Both (measurement), Gyula Gróf (calibration), Péter Ván (sample preparation and measurement) made experiments at the Department of Energy Engineering to detect non-Fourier heat conduction macroscopically.

One can expect deviance from Fourier-type heat conduction in heterogeneous materials as well, not just at very low temperatures [65, 66, 67]. Our models are effective in the sense of material parameters, so it defines the overall properties of a material thus the inhomogeneity is represented, too. Layered samples are made to the experiments, it is easy to fabricate and the components are known.

We consider now the most interesting one; this sample consists of 16 layers, 8 layers made from paper (180 g) and the other 8 layer made from aluminum, the overall length is 3.35 mm. The arrangement of the experiment is in accordance with the numerical simulations. The Figure 7.5 shows the shape of the pulse which is not identical to the one from simulations, but it can be applied by reasons which discussed in the chapter of boundary conditions. The measured temperature can be seen in Figure 7.6 in the respect of time. This curve begins at the point of the trigger signal, so we have to put it to the origin. The next step is to normalize it to the equilibrium temperature, so we need to divide every points of the curve in a way to put the equilibrium temperature to one. Now we can compare it to the simulations.

This measurement is interesting from the aspect of signal propagation, the temperature immediately starts to rise, furthermore there may the small hump can be seen after this immediate temperature rising. This kind of sudden temperature rising is also observed in the case of other samples. We begin with the Fourier equation to determine the thermal diffusivity, the other models will use the same value. We

²The average distance traveled by a particle between two collisions. The Knudsen number is the ratio of the mean free path and the characteristic length of the sample.

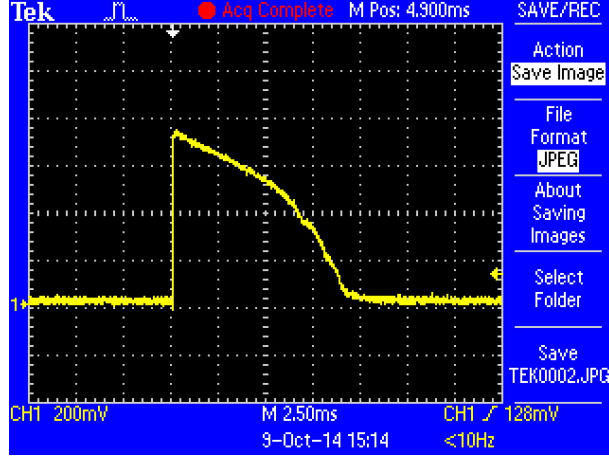


FIGURE 7.5. The signal's shape in the BUTE-DEE-experiment.

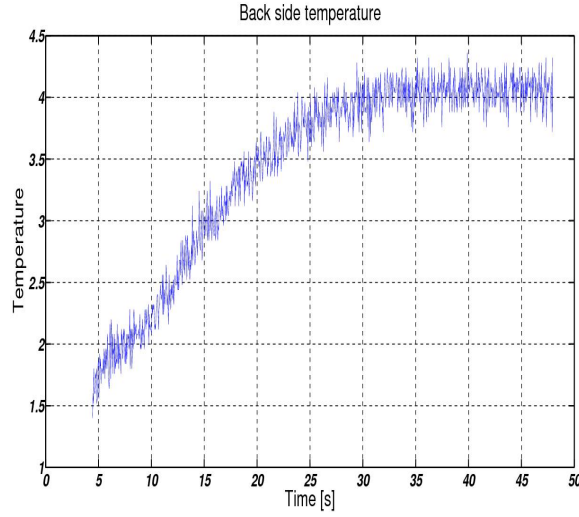


FIGURE 7.6. The measured temperature values on the rear side of the sample as the function of time.

deal with the GK and ballistic-diffusive equations, too. One can modify the signal propagation speed in these models parametrically and it is not valid for the Fourier equation. The MCV and GN equations are not considered here. We will represent the goodness of the fitting with the help of the absolute error and squared deviations.

$$\chi = \sqrt{\sum_i \Delta x_i^2}, \quad (109)$$

where χ denotes the squared deviation, Δx is the difference between the calculated and measured values, the index i corresponds to the measuring points. We summarize it to the all measurement points.

7.3.1. Fitting of the Fourier equation. By the adjustment of the thermal diffusivity, we calculated the dimensionless parameters first, then ran the simulation

to get the temperature distribution. In this case

$$\alpha = 1.59 \cdot 10^{-7} \frac{m^2}{s} \quad (110)$$

seems to be the best result, so we apply it in other models for simplicity.

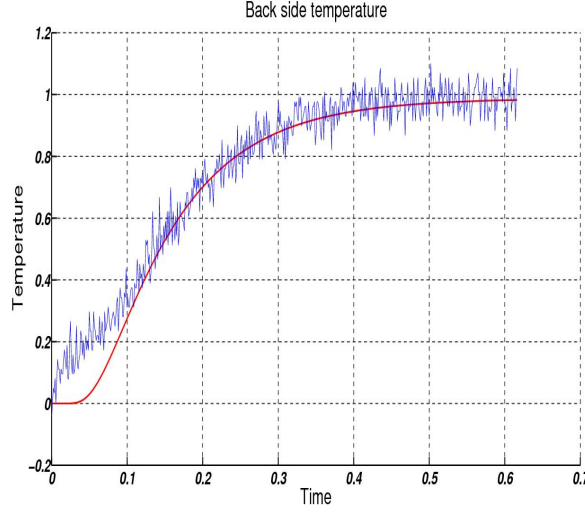


FIGURE 7.7. The measured and calculated temperature distribution on the rear side of the sample in dimensionless form. The red curve shows the calculated values.

The Figure 7.7 shows the result of the fitting. Significant difference can be experienced at the beginning of the measurement, the Fourier equation predicts the temperature rising with some delay in comparison of the measurement data. This difference also can be seen in Figure 7.8.

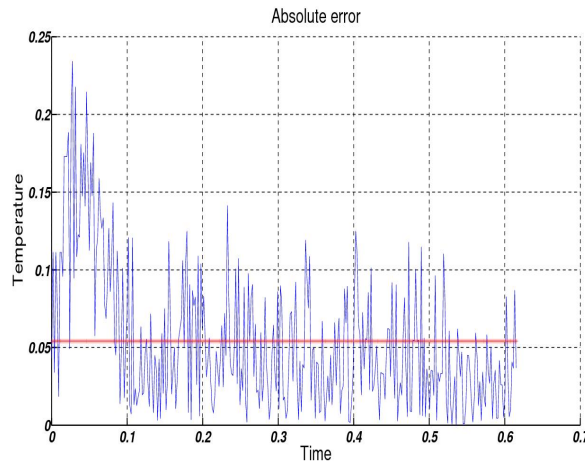


FIGURE 7.8. The absolute difference in each measurement point. The red line shows the average value of the absolute error ($E = 0.054$). The squared deviance is $\chi = 2.254$.

7.3.2. Fitting of the Guyer–Krumhansl equation. We can influence the speed of signal propagation by the adjustment of the dissipation parameter. Then we create such a solution where the temperature is immediately rising on the boundary (Fig. 7.9). The used parameters are

$$\alpha = 1.59 \cdot 10^{-7} \frac{m^2}{s}; \quad \tau_q = 0.141s; \quad a = 2.244 \cdot 10^{-7} m^2. \quad (111)$$

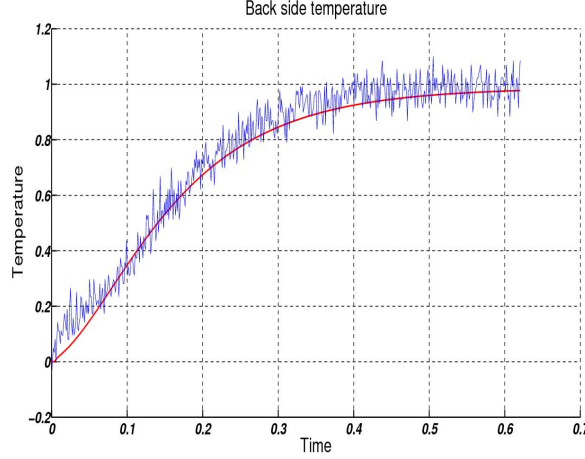


FIGURE 7.9. The measured and calculated temperature distribution on the back side of the sample in dimensionless form. The red curve shows the calculated values.

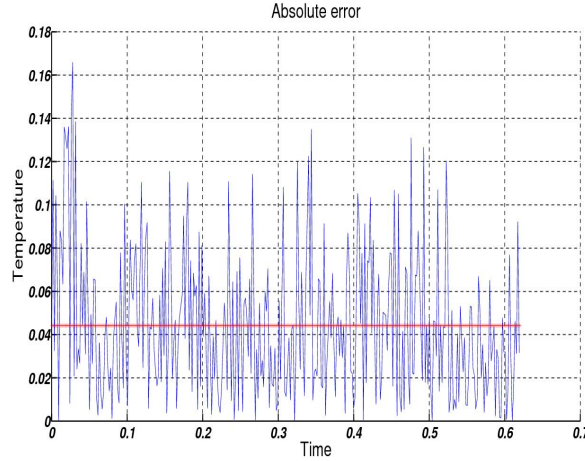


FIGURE 7.10. The absolute difference in each measurement point. The red line shows the average value of the absolute error ($E = 0.0442$). The squared deviance is $\chi = 1.75$.

Let us note that besides such parameters we can not see the “edgy” characteristic property of the GK equation, i.e. the temperature distribution is not so steep [37]. Due to the quick temperature rising the GK equation can be fitted better than the Fourier equation (Fig. 7.10).

7.3.3. Ballistic-diffusive model. Our goal was to reproduce the small hump at the beginning of the measured curve, the other two model is not able to do this. The parameters are

$$\alpha = 1.59 \cdot 10^{-7} \frac{m^2}{s}; \tau_q = 0.21s; \tau_Q = 0.28s; \kappa = 0.155. \quad (112)$$

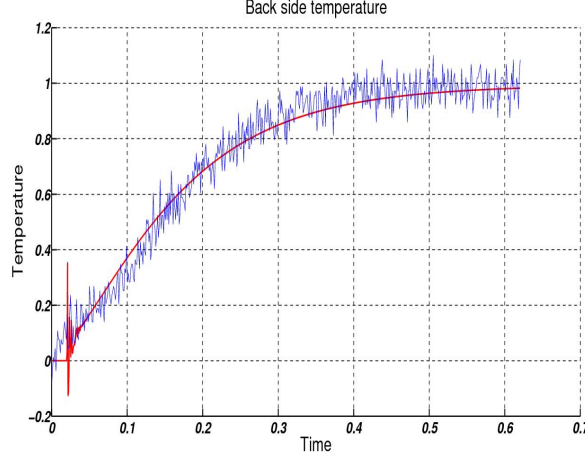


FIGURE 7.11. The measured and calculated temperature distribution on the back side of the sample in dimensionless form. The red curve shows the calculated values.

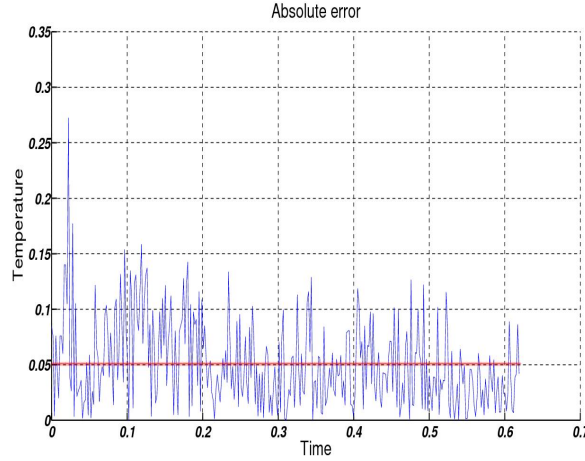


FIGURE 7.12. The absolute difference in each measurement point. The red line shows the average value of the absolute error ($E = 0.0459$). The squared deviance is $\chi = 2.035$.

Although we managed to produce a little hump, the numerical errors and oscillations (caused by narrow pulse) are impairing the result (Fig. 7.11). In this respect, the error distribution is not representing well the real ability of this model. Despite of this numerical phenomenon, the error is almost identical to the case of the GK equation (Fig. 7.12).

CHAPTER 8

Összefoglalás

A dolgozat első felében részletesen ismertettük a hierarchikus rendszer származtatását és kapcsolatát a kinetikus elmélettel. Ellenőriztük az egyes rendszerek hiperbolicitását, a jelterjedési sebességeket is megállapítottuk. További vizsgálatokat végeztünk a diszperziós relációkon keresztül az egyes paraméterek szerepének feltérképezésére, szintén a jelterjedési sebességre fókuszálva. A megállapított tulajdonságokat is felhasználtuk a megoldások elemzésében. Láttuk, hogy a ballisztikus-diffúzív modell képes reprodukálni a Fourier-, a MCV-, a GK- és a GN-egyenletek megoldásait. Ezen felül tartalmazza a ballisztikus hővezetési jelenséget is, melynek különleges jelentősége van nanorendszerek esetén.

Részletesen elemeztük a modellek megoldására alkalmazott numerikus eljárást, bizonyítottuk a stabilitását és a konvergenciáját. További lehetőség a séma fejlesztése, a mesterséges numerikus diszperzió csökkentése lehet. Ezzel csökkenne a szükséges térlépések száma, azaz csökkenne a séma számításigénye. Ezzel szorosan összefügg a séma pontossága, illetve a pontos megoldáshoz való konvergencia sebessége.

Az alkalmazási területeken belül részletesen elemeztük a NaF-on alacsony hőmérsékleten végzett mérési eredményeket. Dreyer és Struchtrup által számolt eredményt pontosan visszakaptuk, azonban láttuk, hogy Yanbao Ma paramétereit felhasználva a terjedési sebességet nem ugyanúgy adja meg. Ez további vizsgálatokat igényel, ugyanis Ma más modellt használ, nem feltétlenül lehet egyenesen megfeleltetni egymásnak az anyagi paramétereket.

Az EGR-kísérlet kiértékelése alapján elmondható, hogy a GK-egyenlet reális modell lehet inhomogén anyagok modellezésére. A jelterjedési sebesség jól kezelhető és reálisabb eredményt kaptunk, mint a Fourier-egyenlet megoldásával. A ballisztikus-diffúzív egyenlettel a megfigyelt (de nem túlságosan kiugró) “púpot” is modellezni tudjuk. Ez a jelenség a makroszkópikus ballisztikus terjedés első megfigyelése lehet. Oka nem lehet a második hang. Természetesen további kísérleti és elméleti vizsgálatokra van szükség ebben az irányban. A mesterséges oszcillációk miatt az illesztés jóságára nem mondhatunk biztosat, pontosabb sémával az éles ugrásoknál jelentkező hibákat előbb meg kell szüntetni.

A ballisztikus-diffúzív modellnek fő alkalmazási területe azonban a nanoeszközök megfelelő modellezése. A hőelektromos hatás, a mechanikai deformáció, mind hatással vannak a hővezetésre, a ballisztikus jelterjedésre. További kutatási lehetőség a mechanikai modellekkel való kapcsolatának részletes feltérképezése, például a deformációkkal való csatolt modell létrehozása, melyben az akusztikai és relaxációs, reológiai jelenségek főszerepet kapnának. Ezzel párhuzamosan változna a hőfeszültségek leírásának módja is [1, 2, 3].

CHAPTER 9

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