A reduction of the Boltzmann-Peierls Equation *

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Abstract. This paper is concerned with the solutions of initial value problems of the Boltzmann-Peierls equation (BPE). This integro-differential equation describes the evolution of heat in crystalline solids at very low temperatures. The BPE describes the evolution of the phase density of a phonon gas. The corresponding entropy density is given by the entropy density of a Bose-gas. We derive a reduced three-dimensional kinetic equation which has a much simpler structure than the original BPE. Using special coordinates in the one-dimensional case, we can perform a further reduction of the kinetic equation. Making a one-dimensionality assumption on the initial phase density one can show that this property is preserved for all later times. We derive kinetic schemes for the kinetic equation as well as for the derived moment systems. Several numerical test cases are shown in order to validate the theory.

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1 Introduction

In 1929, Peierls [13] proposed his celebrated theoretical model based on the Boltzmann equation. According to him the lattice vibrations responsible for the heat transport can be described as an interacting gas of phonons. The Boltzmann-Peierls approach is one of the milestones of the theory of thermal transport in solids, especially at very low temperatures. It is important to mention that Fourier theory of heat flow fails to describe heat conduc tion processes at low temperatures, see for example Dreyer and Struchtrup [9] and references therein.

Dreyer, Herrmann and Kunik [8] have used a kinetic scheme in order to solve the microscopically two-dimensional Boltzmann-Peierls equation (BPE). In this paper we present the kinetic solutions of the microscopically three-dimensional BPE. In order to solve the one-dimensional discrete form of the BPE numerically, we utilize the idea that we automatically obtain kinetic flux vector splitting under a CFL condition. Flux vector splitting is a technique for achieving upwinding bias in numerical flux function, which is a natural consequence of regarding a fluid as an ensemble of particles. Since particles can move forward or backward, this automatically splits the fluxes of energy and heat flux into forward and backward fluxes within each cell. The intial data to the scheme is a discrete matrix of the phase density in phase-space . The present scheme is more efficient and faster than the scheme used in [8], because the kinetic scheme used there is discrete in time but continuous in space, therefore an interpolation polynomial was needed in order to calculate the free-flight phase density.

The Boltzmann-Peierls equation is a kinetic equation for the phase density of phonons. This equation describes the evolution of the phase density $f(t, \mathbf{x}, \mathbf{k})$, where $f(t, \mathbf{x}, \mathbf{k})d^3x d^3k$ is interpreted as the number of phonons at time t in an infinitesimally small phase cell element $d^3x d^3k$ centered at $(\mathbf{x}, \mathbf{k})$. Here $\hbar\mathbf{k}$ denote the momentum, $\mathbf{k}$ the phonon wave vector and $\hbar$ is Planck's constant, see [13, 9] for further details. The microscopically three dimensional Boltzmann-Peierls equation can be written as

$$\frac{\partial f}{\partial t} + c\frac{k_i}{|\mathbf{k}|}\frac{\partial f}{\partial x_i} = \zeta(f)\,, \tag{1.1}$$

where c is the Debye constant, time is denoted by t and the quantity ζ is the collision operator which will be defined below.

The moments of the phase density f reflect the kinetic processes on the scale of continuum physics. The most important moments are

$$e(t,\mathbf{x}) = \hbar c \int\limits_{-\infty}^{\infty} |\mathbf{k}|\, f(t,\mathbf{x},\mathbf{k})\, d^3k\,, \tag{1.2}$$

$$Q_i(t,\mathbf{x}) = \hbar c^2 \int\limits_{-\infty}^{\infty} k_i f(t,\mathbf{x},\mathbf{k})\, d^3k\,, \tag{1.3}$$

$$N_{ij}(t,\mathbf{x}) = \hbar c \int\limits_{-\infty}^{\infty} \frac{k_i k_j}{|\mathbf{k}|} f(t,\mathbf{x},\mathbf{k})\, d^3k\,, \quad i,j = 1,2,3\,. \tag{1.4}$$

The fields e, $\mathbf{Q} = (Q_1, Q_2, Q_3)$ and the Matrix $\mathbf{N} = (N_{ij})$ are the energy density, heat flux and momentum flux, respectively.

Phonons are classified as Bose particles [13, 9], and the corresponding entropy density-entropy flux pair (h, φ) is given by

$$h(f) := y \int\limits_{\mathbb{R}^3} \left[\left(1 + \frac{f}{y}\right) \ln\left(1 + \frac{f}{y}\right) - \frac{f}{y} \ln\left(\frac{f}{y}\right) \right] d^3k\,, \tag{1.5}$$

$$\varphi_i(f) := yc \int\limits_{\mathbb{R}^3} \frac{k_i}{|\mathbf{k}|} \left[\left(1 + \frac{f}{y}\right) \ln\left(1 + \frac{f}{y}\right) - \frac{f}{y} \ln\left(\frac{f}{y}\right) \right] d^3k\,, \tag{1.6}$$

where $y = \frac{3}{8\pi^3}$, see [9] .

In contrast to the ordinary gas atoms, the phonons may interact by two different collision processes, called R- and N-processes. R-processes include interactions of phonons with lattice impurities which destroy the periodicity of the crystal, while N-processes can be interpreted as phonon-phonon interactions which are due to the deviations from harmonicity of the crystal forces. N-processes conserve both, energy and momentum, while R-processes only conserve energy. The Callaway approximation of the collision operator [3, 9] is a suitable simplification of the actual interaction processes. The Callaway collision operator is written as the sum of two relaxation operators modelling the R- and N-processes seperately. We write

$$\zeta(f) = \zeta_R(f) + \zeta_N(f)\,, \qquad \zeta_\alpha = \frac{1}{\tau_\alpha}\left(P_\alpha f - f\right)\,, \quad \alpha \in \{R, N\}\,. \tag{1.7}$$

The positive constants τ_R and τ_N are the relaxation times, while P_R and P_N are two nonlinear projectors. Here $P_R f$ and $P_N f$ represent the phase densities in the limiting case when the relaxation time tends to zero. Explicitly, we define $P_R f$ and $P_N f$ as the solutions of two optimization problems, namely

$$h(P_R f) = \max_{f'} \{h(f) \ : \ e(f') = e(f)\} \,, \tag{1.8}$$

$$h(P_N f) = \max_{f'} \{h(f) \ : \ e(f') = e(f), \, \mathbf{Q}(f') = \mathbf{Q}(f)\} \,, \tag{1.9}$$

where $e(f)$, $\mathbf{Q}(f)$ are given by (1.2),(1.3).

The maximization problems can be solved by means of Lagrange multipliers Λ_R^0 and Λ_N^0, Λ_N^1, Λ_N^2, Λ_N^3. and we get

$$P_R f(\mathbf{k}) = \frac{y}{-1+\exp(\Sigma_R)} \,, \qquad P_N f(\mathbf{k}) = \frac{y}{-1+\exp(\Sigma_N)} \,, \tag{1.10}$$

where

$$\Sigma_R(t,\mathbf{x},\mathbf{k}) = \hbar c \, |\mathbf{k}| \, \Lambda_R^0 \,, \tag{1.11}$$

$$\Sigma_N(t,\mathbf{x},\mathbf{k}) = \hbar c \, |\mathbf{k}| \, \Lambda_N^0(t,\mathbf{x}) + \hbar \, k_i \, \Lambda_N^i(t,\mathbf{x}) \,. \tag{1.12}$$

From (1.8) and (1.9) the Lagrange multipliers can be calculated explicitly. They are given by, see [6], [8],

$$\Lambda_R^0 = \left(\frac{10\hbar^3 c^3}{\pi^2} e\right)^{-\frac{1}{4}} \,, \quad \Lambda_N^0 = \gamma \frac{\left(\frac{F}{e}\right)^{\frac{1}{4}}}{(4-F)^{\frac{3}{4}}} \,, \quad \Lambda_R^i = -\frac{\gamma}{4} \frac{\left(\frac{F}{e}\right)^{\frac{5}{4}}}{(4-F)^{\frac{3}{4}}} Q_i \,, \tag{1.13}$$

$$F = \frac{6}{1+\sqrt{1-\frac{3}{4}\left(\frac{|\mathbf{Q}|}{ce}\right)^2}} \,, \quad \gamma = \left(\frac{4\pi^5 y}{45\hbar^3 c^3}\right)^{\frac{1}{4}} . \tag{1.14}$$

When the thermodynamic state is described by four fields e and Q_i only, then we can derive the following balance equations from the Boltzmann-Peierls equation (1.1) and the maximum entropy principle, see [6],

$$\frac{\partial e}{\partial t} + \frac{\partial Q_i}{\partial x_i} = 0 \,, \tag{1.15}$$

$$\frac{\partial Q_i}{\partial t} + \frac{\partial \left(c^2 N_{ij}\right)}{\partial x_j} = -\frac{1}{\tau_R} Q_i \,, \quad i,j = 1,2,3, \tag{1.16}$$

$$N_{ij} = \frac{1}{3} e \, \delta_{ij} + \frac{1}{2} e(3\chi - 1) \left(\frac{Q_i Q_j}{|\mathbf{Q}|^2} - \frac{1}{3}\delta_{ij}\right) \,, \tag{1.17}$$

where χ is the so called Eddington-factor:

$$\chi = \frac{5}{3} - \frac{4}{3}\sqrt{1 - \frac{3}{4}\left(\frac{|\mathbf{Q}|}{ce}\right)^2} . \tag{1.18}$$

Note that in above equations (1.16) the τ_N term do not appear on the right hand side, therefore the applicability of these equations is restricted to the relaxation limit $\tau_N \to 0$.

Taking the integral-moments of the BPE, one can generate an infinite number of further balance equations, because there follows for any vector $\mathbf{m}(\mathbf{n})$ of moment weights

$$\frac{\partial \mathbf{u}(f)}{\partial t} + \frac{\partial \mathbf{F}_i(f)}{\partial x_i} = \mathbf{u}(\zeta(f)), \qquad i = 1, 2, 3. \tag{1.19}$$

Here, $\mathbf{u}$ and $\mathbf{F}_i$ are the vectors of densities and fluxes, respectively. They are defined as

$$\mathbf{u}(f) = \int_{\mathbb{R}^3} \mathbf{m}(\mathbf{k}) f(\mathbf{k})\, d^3k\,, \qquad \mathbf{F}_i(f) = \int_{\mathbb{R}^3} \frac{k_i}{|\mathbf{k}|} \mathbf{m}(\mathbf{k}) f(\mathbf{k})\, d^3k\,. \tag{1.20}$$

Furthermore, the kinetic equation (1.1) implies an entropy inequality, i.e., any solution f of (1.1) satisfies

$$\frac{\partial h(f)}{\partial t} + \frac{\partial \varphi_i(f)}{\partial x_i} \geq 0\,. \tag{1.21}$$

It is well known that the balance-laws (1.19) can be reduced to a hyperbolic moment system by using the maximum entropy principle like in (1.8), (1.9) and (1.15)-(1.18), see [8].

This article has three main contributions to the theory of kinetic solutions of the Boltzman-Peierls equation (BPE). The first one is the kinetic solutions of the microscopically three-dimensional BPE, while previously only the microscopically two-dimensional BPE was solved, see [8]. The second contribution is the use of special coordinates in the macroscopically one-dimensional case in order to perform a further reduction of the kinetic equation. We show by three lemmas that this reduction is valid for all times. The third contribution is the use of a kinetic flux-vector splitting scheme at a numerical approximation. We use the average values of the initial phase density over phase-space cells as a initial data for the scheme. This scheme is much faster than the kinetic scheme used by [8] which is discrete in time but continuous in space.

Now we give a short overview of this paper:

In Section 2, we derive a reduced kinetic equation for a reduced kinetic phase density. Moreover, we give a reduced form of the reduced entropy density-entropy flux pair. The time integral form of the reduced kinetic equations is obtained by using Duhamel's principle, while the time discrete form of this time integral form is obtained by using Riemann sums.

In Section 3, we further reduce the already reduced kinetic equation by using a special coordinate transformation in the spatially one-dimensional case. In three lemmas we show that this reduction is valid for all times. We solve the discrete kinetic equation by using a KFVS scheme. The initial data for the scheme are the average values of the phase density on phase-space cells and we obtain the average values of the phase density at the next time step. In order to obtain the values of the fields we use Riemann sums.

2 Reduced Boltzmann-Peierls Equation

In this section we intend to recall results from [8] in order to derive a reduced kinetic equation for a reduced phase density. This procedure relies on the observation that for any solution f of (1.1) there exists a corresponding solution of a reduced equation that determines all physically important moments of f. Additionally we give the expression for the reduced entropy density-entropy flux pair, as it was done in [8].

The phase density f depends on the wave vector $\mathbf{k} \in \mathbb{R}^3$, therefore we can calculate the reduced phase density according to the radial integration in polar-coordinates:

$$\Psi(\mathbf{n}) = \hbar c \int_0^\infty |\mathbf{k}|^3 \, f(|\mathbf{k}| \, \mathbf{n}) \, d|\mathbf{k}| \, . \tag{2.1}$$

Note that Ψ only depends on the unit vector $\mathbf{n} = (n_1, n_2, n_2) = \dfrac{\mathbf{k}}{|\mathbf{k}|}$.

Let m be a homogeneous moment weight of degree 1, i.e. $m(\lambda \mathbf{k}) = \lambda m(\mathbf{k})$ for all $\lambda \geq 0$. Also let $\mathbf{u}$ be the corresponding moment function, then we have

$$\mathbf{u}(f) = \hbar c \int_{\mathbb{R}^3} m(\mathbf{k}) f(\mathbf{k}) \, d\mathbf{k} = \hbar c \oint_{\partial B(0,1)} \int_0^\infty |\mathbf{k}|^3 \, m(\mathbf{n}) f(|\mathbf{k}| \, \mathbf{n}) \, d|\mathbf{k}| \, dS(\mathbf{n}) \tag{2.2}$$

$$= \oint_{\partial B(0,1)} m(\mathbf{n}) \Psi(\mathbf{n}) \, dS(\mathbf{n}) \, . \tag{2.3}$$

The moment $\mathbf{u}$ of f is thus given by the corresponding moments of Ψ. All the moments with physical interpretation cf. (1.2), (1.3), (1.4) are formed by homogeneous moment weights of degree 1. In particular we have

$$e(f) = e(\Psi) \, , \quad Q_i(f) = Q_i(\Psi) \, , \quad N_{ij}(f) = N_{ij}(\Psi) \, , \tag{2.4}$$

where

$$e(\Psi) = \oint\limits_{\partial B(0,1)} \Psi(\mathbf{n})\, dS(\mathbf{n})\,, \quad Q_i(\Psi) = c \oint\limits_{\partial B(0,1)} n_i \Psi(\mathbf{n})\, dS(\mathbf{n})\,, \tag{2.5}$$

$$N_{ij}(\Psi) = \oint\limits_{\partial B(0,1)} n_i n_j \Psi(\mathbf{n})\, dS(\mathbf{n})\,. \tag{2.6}$$

Similarly the reduced collision operators Φ, Φ_R and Φ_N are given by, see [8],

$$\Phi_\alpha = \frac{1}{\tau_\alpha}\left(\Theta_\alpha \Psi - \Psi\right)\,, \quad \alpha \in \{R, N\}\,, \quad \Phi = \Phi_R + \Phi_N\,, \tag{2.7}$$

where

$$\Theta_R \Psi = \frac{e}{4\pi}\,, \quad \Theta_N \Psi = \frac{3}{4\pi} \frac{e(4-F)^3}{F\left(1 - \frac{F\, n_i\, Q_i}{4\, c\, e}\right)^4}\,, \quad F = \frac{6}{1 + \sqrt{1 - \frac{3}{4}\left(\frac{|\mathbf{Q}|}{c\, e}\right)^2}}, \tag{2.8}$$

and

$$\hbar c \int\limits_0^\infty |\mathbf{k}|^3\, P_\alpha f(|\mathbf{k}|\, \mathbf{n})\, d|\mathbf{k}| = \Phi_\alpha(\mathbf{n}), \quad \alpha \in \{R, N\}\,. \tag{2.9}$$

We finally conclude that any solution $f(t, \mathbf{x}, \mathbf{k})$ of (1.1) induces a solution $\Psi(t, x, \mathbf{n})$ of the following reduced Boltzmann-Peierls equation

$$\frac{\partial \Psi}{\partial t}(t, \mathbf{x}, \mathbf{n}) + c\, n_i\, \frac{\partial \Psi}{\partial x_i}(t, \mathbf{x}, \mathbf{n}) = \Phi(t, \mathbf{x}, \mathbf{n})\,. \tag{2.10}$$

This reduced kinetic equation can be rewritten in the following time integral form by using Duhamel's principle

$$\Psi(t+\tau, \mathbf{x}, \mathbf{n}) = \Psi(t, \mathbf{x} - c\tau\mathbf{n}, \mathbf{n}) + \sum_{\alpha \in \{R,N\}} \int\limits_0^\tau \Phi_\alpha(s, \mathbf{x} - c(\tau - s)\mathbf{n}, \mathbf{n})\, ds\,, \tag{2.11}$$

where $\Psi(t, \mathbf{x} - c\tau\mathbf{n}, \mathbf{n})$ is the solution at time $t + \tau$ of the collisionless kinetic equation

$$\frac{\partial \Psi}{\partial t}(t, \mathbf{x}, \mathbf{n}) + c\, n_i\, \frac{\partial \Psi}{\partial x_i}(t, \mathbf{x}, \mathbf{n}) = 0\,. \tag{2.12}$$

In particular, $\Psi_0(t, \mathbf{x} - c\tau\mathbf{n}, \mathbf{n})$ is the free-flight solution of (2.12) for initial data Ψ_0.

Finally we introduce an entropy density-entropy flux pair for the reduced equation (2.10). The definition is not so straight forward as before, because in general the entropy density $h(f)$ cannot be determined from Ψ. The following definition is proposed in [8]

$$h(\Psi) = \mu \oint\limits_{\partial B(0,1)} \Psi^{\frac{3}{4}}(\mathbf{n})\, dS(\mathbf{n})\,, \tag{2.13}$$

$$\varphi_i(\Psi) = \mu\, c \oint\limits_{\partial B(0,1)} n_i\, \Psi^{\frac{3}{4}}(\mathbf{n})\, dS(\mathbf{n})\,, \quad \mu = \frac{4\pi}{3}\left(\frac{y}{15}\right)^{\frac{1}{4}}\,, \quad y = \frac{3}{8\pi^3}\,. \tag{2.14}$$

It was shown in [8] that this entropy density definition for the transformed BPE leads to the same results of the original entropy density definition (1.5) for the original BPE.

Time discretization of the reduced kinetic equation:

Now we replace the time integrals in (2.11) by finite Riemann sums

$$\Psi(t+\tau, \mathbf{x}, \mathbf{n}) = \sum_{\alpha\in\{R,N\}} \frac{\tau}{\tau_\alpha}\Theta_\alpha \Psi(t, \mathbf{x} - c\tau\mathbf{n}, \mathbf{n}) + \left(1 - \frac{\tau}{\tau_R} - \frac{\tau}{\tau_N}\right)\Psi(t, \mathbf{x} - c\tau\mathbf{n}, \mathbf{n})\,. \tag{2.15}$$

This gives us the following kinetic scheme which is discrete in time but continuous in the $\mathbf{x}, \mathbf{n}$ reduced phase-space. For more details the reader is refered to the paper of Dreyer et al. [8]. In order to obtain the first term on the right hand side of (2.15), we first calculate the moments from the following free-flight moment integrals with $\Psi_R = \Theta_R\Psi$ and $\Psi_N = \Theta_N\Psi$, see (2.7), as initial phase densities

$$\begin{aligned}
e^R(t+\tau, \mathbf{x}) &= \oint\limits_{\partial B(0,1)} \Psi_R(\mathbf{x} - c\tau\mathbf{n})\, dS(\mathbf{n})\,, \\
e^N(t+\tau, \mathbf{x}) &= \oint\limits_{\partial B(0,1)} \Psi_N(\mathbf{x} - c\tau\mathbf{n})\, dS(\mathbf{n})\,, \\
Q_i^N(t+\tau, \mathbf{x}) &= c \oint\limits_{\partial B(0,1)} n_i \Psi_N(\mathbf{x} - c\tau\mathbf{n})\, dS(\mathbf{n})\,.
\end{aligned} \tag{2.16}$$

Now we use these moments to project back on to the equilibrium phase densities, i.e., to calculate $\Theta_R\Psi(t, \mathbf{x} - c\tau\mathbf{n}, \mathbf{n}) = \Theta_R\Psi(t, e^R, \mathbf{n})$ and $\Theta_N\Psi(t, \mathbf{x} - c\tau\mathbf{n}, \mathbf{n}) = \Theta_N\Psi(t, e^N, Q_i^N, \mathbf{n})$. The second term on the right hand side of (2.15) is a free-flight phase density with initial data $\Psi(t)$ at time t.

3 One-dimensional Reduced Kinetic Equation

Here we are interested in reducing the already reduced Boltzmann-Peierls equation (2.10) further. Later on we show by three lemmas that this reduced phase density describes a spatially one-dimensional flow.

In the one dimensional case we have $\mathbf{x} = (x, 0, 0)$, $\mathbf{Q} = (Q(t, x), 0, 0)$ and $e = e(t, x)$. We introduce the new variables $-1 \le \xi \le 1$, $0 \le \vartheta \le 2\pi$ by

$$n_1 = \xi\,, \qquad n_2 = \sqrt{1-\xi^2}\sin\vartheta\,, \qquad n_3 = \sqrt{1-\xi^2}\cos\vartheta\,, \tag{3.1}$$

with the surface element $dS(\mathbf{n}) = d\xi d\vartheta$. Since in the one dimensional case the macroscopic fields inside the phase density $\Psi(t, x, \mathbf{n})$ will not depend on the angle ϑ, we can further reduce Ψ to

$$\psi(t, x, \xi) = \int_0^{2\pi} \Psi(t, x, 0, 0, \mathbf{n})\, d\vartheta = 2\pi\Psi(t, x, \xi). \tag{3.2}$$

The reduced Boltzmann-Peierls equation(2.10) then further reduces to

$$\frac{\partial\psi}{\partial t}(t, x, \xi) + c\,\xi\,\frac{\partial\psi}{\partial x}(t, x, \xi) = \sum_{\alpha\in\{R,N\}} \frac{1}{\tau_\alpha}\left(\Theta_\alpha\psi - \psi\right)(t, x, \xi)\,, \tag{3.3}$$

where

$$\Theta_R\psi = \frac{e}{2}\,, \quad \Theta_N\psi = \frac{3}{2}\frac{e(4-F)^3}{F\left(1-\frac{F\,\xi\,Q}{4\,c\,e}\right)^4}\,, \quad F = \frac{6}{1+\sqrt{1-\frac{3}{4}\left(\frac{Q}{c\,e}\right)^2}}\,. \tag{3.4}$$

We have used the same notation for the projection as in (2.8), but this will not lead to confusion within the context. Also the reduced moments integrals are given by

$$e(t, x) = \int_{-1}^{1} \psi(t, x, \xi)\, d\xi, \quad Q(t, x) = c\int_{-1}^{1} \xi\psi(t, x, \xi)\, d\xi\,, \tag{3.5}$$

$$N(t, x) = N_{11}(t, x) = \int_{-1}^{1} \xi^2\psi(t, x, \xi)\, d\xi. \tag{3.6}$$

In the following three lemmas we are going to show that the above reduction is valid for all later times.

Definition: Let $S_2 := \{\mathbf{n}\in\mathbb{R}^3 \mid \ |\mathbf{n}| = 1\}$ be the unit sphere in $\mathbb{R}^3$. Any function $g : \mathbb{R}^3\times S_2 \to \mathbb{R}$, $g = g(\mathbf{x}, \mathbf{n})$, has **property 1D** if and only if $g(\mathbf{x}, \mathbf{n})$ depends only on $x = x_1$ and $\xi = n_1$, where $\mathbf{x} = (x_1, x_2, x_3) \in \mathbb{R}^3$ and $\mathbf{n} = (n_1, n_2, n_3) \in S_2$.

Assumption
For the next three lemmas, we assume that the initial phase density $\Psi(t_0, \cdot, \cdot) : \mathbb{R}^3\times S_2 \to \mathbb{R}$

at fixed initial time t_0 has property 1D and that all surface-integral moments exist.

Lemma 1: Under the above assumption $\Theta_N\left(\Psi(t_0,\cdot,\cdot)\right)$ and $\Theta_R\left(\Psi(t_0,\cdot,\cdot)\right)$ have also property 1D, furthermore the energy density and heat flux moment vector of $\Psi(t_0,\cdot,\cdot)$ are of the form

$$e(t_0,\mathbf{x}) = e(t_0,x)\,, \quad \mathbf{Q}(t_0,\mathbf{x}) = (Q_1(t_0,x),0,0)\,, \quad x = x_1\,.$$

Proof: Du to the property 1D we can write $\Psi(t_0,x,\xi)$ instead of $\Psi(t_0,\mathbf{x},\mathbf{n})$. We rewrite the surface integrals in (2.5) in terms of the new integration variables ξ,ϑ, also using (3.2) we have

$$\begin{aligned} e(t_0,x) &= \int_{-1}^{1}\int_{0}^{2\pi} \Psi(t_0,x,\xi)d\vartheta d\xi \\ &= \int_{-1}^{1} 2\pi\,\Psi(t_0,x,\xi)d\xi = \int_{-1}^{1} \psi(t_0,x,\xi)d\xi\,, \end{aligned} \tag{3.7}$$

$$\begin{aligned} Q(t_0,x) = Q_1(t_0,x) &= c\int_{-1}^{1}\int_{0}^{2\pi} \xi\Psi(t_0,x,\xi)d\vartheta d\xi \\ &= c\int_{-1}^{1} \xi\, 2\pi\,\Psi(t_0,x,\xi)d\xi = c\int_{-1}^{1} \xi\psi(t_0,x,\xi)d\xi\,, \end{aligned} \tag{3.8}$$

$$Q_2(t_0,x) = c\int_{-1}^{1}\int_{0}^{2\pi} \sin\vartheta\sqrt{1-\xi^2}\,\Psi(t_0,x,\xi)d\vartheta d\xi = 0\,, \tag{3.9}$$

similarly $Q_3(t_0,x)=0$.

Keeping in view (3.7),(3.8) and (3.9) we can see from the definitions (2.8) of $\Theta_R(\Psi)$ and $\Theta_N(\Psi)$ that they are only depending on $e(t_0,x)$, $Q_1(t_0,x)$ and $\xi = n_1$. Therefore they also satisfy property 1D. □

Lemma 2: The time derivative $\dfrac{\partial\Psi}{\partial t}(t_0,\cdot,\cdot)$ has property 1D, if Ψ satisfies the reduced Boltzmann-Peierls equation (BPE) (2.10).

Proof: The reduced BPE (2.10) can be rewritten as

$$\frac{\partial\Psi}{\partial t}(t,\mathbf{x},\mathbf{n}) = \Phi(t,\mathbf{x},\mathbf{n}) \; - c\,n_i\,\frac{\partial\Psi}{\partial x_i}(t,\mathbf{x},\mathbf{n}). \tag{3.10}$$

The first term $\Phi(t, \mathbf{x}, \mathbf{n})$ on the right hand side of (3.10) has property 1D for $t = t_0$ due to the assumption and Lemma 1. Also since $\dfrac{\partial \Psi}{\partial x_2} = \dfrac{\partial \Psi}{\partial x_3} = 0$, the second term on the right hand side of (3.10) also satisfies property 1D. This implies that the left hand side of (3.10) satisfies the property 1D. $\square$

Lemma 3: The free-flight phase density $\Psi_{free}(t_0 + \tau, \mathbf{x}, \mathbf{n}) = \Psi(t_0, \mathbf{x} - \tau\mathbf{n}, \mathbf{n})$ also satisfies the property 1D for all later times $t_0 + \tau$, $\tau > 0$.

Proof: The proof of this lemma is obvious from the definition of $\Psi_{free}(t_0 + \tau, \mathbf{x}, \mathbf{n})$, since due to the assumption that Ψ is only depending on $x = x_1$, therefore Ψ_{free} will maintain this property for all later times. $\square$

3.1 Discrete Kinetic Solution in the One-dimensional Case

Now we want to present a discrete kinetic solution of the reduced kinetic equation (2.11). In the one dimensional case (2.15) can be written as

$$\psi(t+\tau, x, \xi) = \sum_{\alpha \in \{R,N\}} \frac{\tau}{\tau_\alpha} \Theta_\alpha \psi(t, \mathbf{x} - c\tau\xi, \xi) + \left(1 - \frac{\tau}{\tau_R} - \frac{\tau}{\tau_N}\right) \psi(t, x - c\tau\xi, \xi). \quad (3.11)$$

This equation is discrete in time but continuous in the x, ξ reduced phase-space. In order to get a fully discretized piecewise constant solution, we first define a grid in the reduced phase-space consisting on the cells $C_{i,j} = I_i \times J_j$ centered around $(x_i = i\Delta x,\ \xi_j = j\Delta\xi)$,

$$C_{i,j} = \left\{ (x, \xi) \in \mathbb{R}^2 \,\middle|\, |x - x_i| \le \frac{\Delta x}{2} \ , \quad |\xi - \xi_j| \le \frac{\Delta \xi}{2} \right\} ,$$

where $\Delta x = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}$ and $\Delta\xi = \xi_{j+\frac{1}{2}} - \xi_{j-\frac{1}{2}}$. The cell-average of ψ at time $t = t_n$ over the cell $C_{i,j}$ is given by

$$\overline{\psi}_{i,j}(t) = \frac{1}{\Delta x \Delta \xi} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} \psi(t, x, \xi)\, d\xi dx\,. \quad (3.12)$$

With the characteristic function $\chi_{i,j}(x, \xi)$ of the cell $C_{i,j}$ we can write the desired piecewise constant phase density in the form $\sum \overline{\psi}_{i,j}(t_n) \chi_{i,j}(x, \xi)$.

Integrating (3.11) over $\left[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}\right] \times \left[\xi_{j-\frac{1}{2}}, \xi_{j+\frac{1}{2}}\right]$ and dividing by $\Delta x \Delta \xi$, we get for time step $\tau = \Delta t$

$$\begin{aligned} \overline{\psi}_{i,j}(t_n + \Delta t) = {} & \frac{\Delta t}{\tau_R}\, \Theta_R \overline{\psi}_{i,j}(t_n, e_i^R(t_n + \Delta t)) + \frac{\Delta t}{\tau_N}\, \Theta_N \overline{\psi}_{i,j}(t_n, e_i^N(t + \Delta t), Q_i^N(t_n + \Delta t)) \\ & + \left(1 - \frac{\Delta t}{\tau_R} - \frac{\Delta t}{\tau_N}\right) \overline{\psi}^f_{i,j}(t_n)\,, \end{aligned} \quad (3.13)$$

where if the natural CFL condition $\Delta t \leq \frac{\Delta x}{2}$ is satisfied, then

$$\overline{\psi}^f_{i,j}(t_n) = \begin{cases} -c\,\frac{\xi_j}{2}\psi_{i+1,j}(t_n) + (1 + c\,\frac{\xi_j}{2})\,\psi_{i,j}(t_n) & \xi_j \leq 0\,, \\ \\ c\,\frac{\xi_j}{2}\psi_{i-1,j}(t_n) + (1 - c\,\frac{\xi_j}{2})\,\psi_{i,j}(t_n) & \xi_j \geq 0\,. \end{cases} \tag{3.14}$$

Note that this upwind formulation comes naturally by integrating the moment integrals. Futhermore, to calculate projection on the equilibrium phase densities $\Theta_R\psi$ and $\Theta_N\psi$ we use (3.14),(3.4) in (3.5),(3.6)

$$\begin{aligned} e^R_i(t_n + \Delta t) &= \frac{c}{8}\left[\overline{e}_{i-1}(t_n) + -2\overline{e}_i(t_n) + \overline{e}_{i+1}(t_n)\right] + \overline{e}_i(t_n)\,, \\ e^N_i(t_n + \Delta t) &= \frac{1}{2}\left[Q^+_{i-1}(t_n) + Q^-_i(t_n)\right] - \frac{1}{2}\left[Q^+_i(t_n) + Q^-_{i+1}(t_n)\right] + \overline{e}_i(t_n)\,, \\ Q^N_i(t_n + \Delta t) &= \frac{c^2}{2}\left[N^+_{i-1}(t_n) + N^-_i(t_n)\right] - \frac{c^2}{2}\left[N^+_i(t_n) + N^-_{i+1}(t_n)\right] + \overline{Q}_i(t_n)\,. \end{aligned} \tag{3.15}$$

where

$$\begin{aligned} Q^{\pm}_i(t_n) &= \frac{4\,c^3\,e^3_i(t_n)\,[-4 + F_i(t_n)]^3\,[\mp 12\,c\,e_i(t_n) + F_i(t_n)\,Q_i(t_n)]}{F_i(t_n)\,[4\,c\,e_i(t_n) \mp F_i(t_n)\,Q_i(t_n)]^3}\,, \\ \\ N^{\pm}_i(t_n) &= \frac{32\,c^3\,e^4_i(t_n)\,[4 - F_i(t_n)]^3}{F_i(t_n)\,[4\,c\,e_i(t_n) \mp F_i(t_n)\,Q_i(t_n)]^3}\,. \end{aligned} \tag{3.16}$$

The "+" sign in (3.16) means that the integration limits are 0 and 1 for ξ, while "−" sign means that the integration limits are -1 and 0 for ξ. Using the above relations in (3.13), we obtain a discrete matrix of the phase-density at the next time step. In order to get the moments from this phase-space matrix of the phase-density, we use the Riemann sums as given below

$$\begin{aligned} \overline{e}_i(t_n + \Delta t) &= \Delta\xi \sum_{j=1}^{N_\xi} \overline{\psi}_{i,j}(t_n + \Delta t)\,, \\ \\ \overline{Q}_i(t_n + \Delta t) &= c\Delta\xi \sum_{j=1}^{N_\xi} \xi_j\,\overline{\psi}_{i,j}(t_n + \Delta t)\,, \end{aligned} \tag{3.17}$$

where N_ξ is number of elements in the interval $-1 \leq \xi \leq 1$.

4 Numerical Examples

In order to validate our results obtained in the previous sections, we present some numerical test cases.

4.1 Energy Pulse

In this example we assume that $\tau_R = \infty$, so that from the physical point of view, we study a phonon gas in a pure crystal at low temperature. Since there are no lattice impurities, diffusion cannot appear. In particular, the propagation of heat behaves like a wave phenomenon. Further we assume that the phase density only depends on $x = x_1$. In order to simulate the problem, we consider the following macroscopic initial data for energy density e and the momentum density Q cf. Figure 1 for the energy density. The initial data are

$$e(0,x) = \begin{cases} 1.5 & \text{if} \quad 0.99 \le x \le 1.01 \\ 1.0 & \qquad\qquad \text{otherwise} \end{cases}, \qquad Q(0,x) = 0.0\,. \tag{4.1}$$

Furthermore, the Debye speed c is set to 0.5.

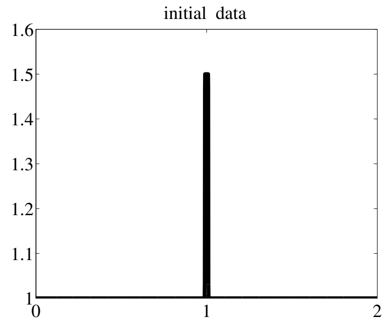

Figure 1: Initial energy pulse

Figures 2 shows the spatial dependence of the energy density, heat flux and momentum flux at different times for the relaxation time $\tau_N = 0.5$. While Figures 5 gives the distribution functions ψ and $\Theta_N\psi$ at time t=1.2.

4.2 Two Interacting Heat Pulses

This test problem demonstrates the interaction of two heat pulses, which leads to a large increase of the energy density at the collision point during a short time interval. The initial data are

$$e(0,x) = \begin{cases} 1\,, & x \le 0.3, \\ 2\,, & 0.3 \le x \le 0.4 \\ 1\,, & 0.4 \le x \le 0.6 \\ 2\,, & 0.6 \le x \le 0.7 \\ 1\,, & x \le 1.0 \end{cases}, \quad Q(0,x) = \begin{cases} 0\,, & x \le 0.3, \\ 1\,, & 0.3 \le x \le 0.4 \\ 0\,, & 0.4 \le x \le 0.6 \\ -1\,, & 0.6 \le x \le 0.7 \\ 0, & x \le 1.0\,. \end{cases} \tag{4.2}$$

We solve the above problem at time $t = 0.2$ for two values of τ_N, i.e., $\tau_N = 1$ and $\tau_N = 0.1$, while $\tau_R = 1.0$. Figure 4 shows the results. From the comparison of the initial and final curves of energy density, we observe a large increase of the energy density e at the collision point $x = 0.5$.

4.3 Initial Phase Density Independent of Space

Here we consider an initial phase density which is independent of the x-coordinate, i.e., $\psi_0 = \psi_0(\xi)$. Furthermore we assume that $\tau_R = \infty$, this implies that the Bolzmann-Peierls equation (3.3) will only contain τ_N and Θ_N. Therefore we have to solve the following simplified Boltzmann-Peierls equation with unit Debye constant, i.e, $c = 1$.

$$\frac{\partial\psi}{\partial t}(t,\xi) + \xi\,\frac{\partial\psi}{\partial x}(t,\xi) = \frac{1}{\tau_N}\left(\Theta_N\psi - \psi\right)(t,\xi)\,. \tag{4.3}$$

The energy density e and the heat flux Q are constant with respect to the time, which is clear from the following conservation laws

$$\frac{\partial e}{\partial t}(t) = \int_{-1}^{1} \frac{\partial\psi}{\partial t} d\xi = \int_{-1}^{1} \frac{\Theta_N\psi - \psi}{\tau_N} d\xi = \frac{1}{\tau_N}\left(e_N - e\right) = 0\,,$$

$$\frac{\partial Q}{\partial t}(t) = c\int_{-1}^{1} \xi\frac{\partial\psi}{\partial t} d\xi = c\int_{-1}^{1} \xi\frac{\Theta_N\psi - \psi}{\tau_N} d\xi = \frac{c}{\tau_N}\left(Q_N - Q\right) = 0\,.$$

Both of the above integrals are zero because of the constraints $e_N = e$ and $Q_N = Q$. Therefore equation (4.3) is simply an ordinary differential equation with initial data $\psi_o = \psi(\xi)$. The explicit solution of this equation is given by

$$\psi_{exact}(t,\xi) = \psi_0(\xi)\,\exp\left(-\frac{t}{\tau_N}\right) + \left(1 - \exp\left(-\frac{t}{\tau_N}\right)\right)\Theta_N\psi_0(\xi)\,. \tag{4.4}$$

Now we consider two examples in which the inital phase density ψ_0 only depend on ξ.

Example 1: Here we consider the initial phase density as a linear function, $\psi_0 = \dfrac{1+\xi}{2}$. Figure $5_{1,2}$ gives the numerical value of phase density ψ at $t = 0.0$ and $t = 1.0$, while Figure 5_3 gives the difference between the exact and numerical solutions.

Example 2: The initial phase density is a shifted hat function

$$\psi_0(\xi) = \begin{cases} \frac{4}{7}(\xi+1)\,, & -1 \le \xi \le \frac{3}{4}\,, \\ 4(-\xi+1)\,, & \frac{3}{4} \le \xi \le 1\,, \end{cases}\,. \tag{4.5}$$

Figure $6_{1,2}$ gives the numerical value of phase density ψ at $t = 0.0$ and $t = 1.0$, while Figure 6_3 gives the difference between the exact and numerical solutions.

4.4 A single shock solution

We consider now a single shock solution. The initial data are

$$(e, Q)(0, x) = \begin{cases} \left(2, \frac{1}{\sqrt{3}}\sqrt{\frac{3\sqrt{2}-1}{\sqrt{2}+1}}\right), & x \leq 0.5, \\ (1, 0), & x \geq 0.5. \end{cases} \tag{4.6}$$

This problem was considered by [6] using Rankine-Hugoniot conditions which were derived in [9]. The computational domain is $0 \leq x \leq 1$. In this example $\tau_R = \infty$, while $\frac{\tau}{\tau_N} = 1$, where τ is the numerical time step. Then the Boltzmann-Peierls equation (3.3) approximates the solution of the hyperbolic four field moments system, see [6]. The x, ξ reduced phase-space is divided by 1000×1000 mesh points. The results are shown in Figure 7.

5 Conclusions

In this paper we have derived a kinetic scheme for the solution of the reduced Boltzmann-Peierls equations as well as for the hyperbolic four-field system. The first reduction of the BPE reduces its moment integrals to surface integrals over the unit sphere. This reduction can be obtained without further assumptions on the intial data and was studied in [8]. In that paper only the microscopically two-dimensional BPE was studied, while we are dealing with the microscopically three-dimensional BPE.

Moreover we have obtained a second reduction of the already reduced BPE which is looking much simplier than the first one, but requires the additional assumption of a one-dimensional flow. Using special coordinates which are adapted for this one-dimensional flow, we can reduce the surface integrals for the moments to simple one-fold integrals ranging over the compact interaval -1 to 1.

The numerical implementation of the kinetic scheme is very easy in our case due to the reduction to one-dimensional moment integrals and due to the discretization of the whole phase-space. A further study is necessary in order to exend the scheme to second order.

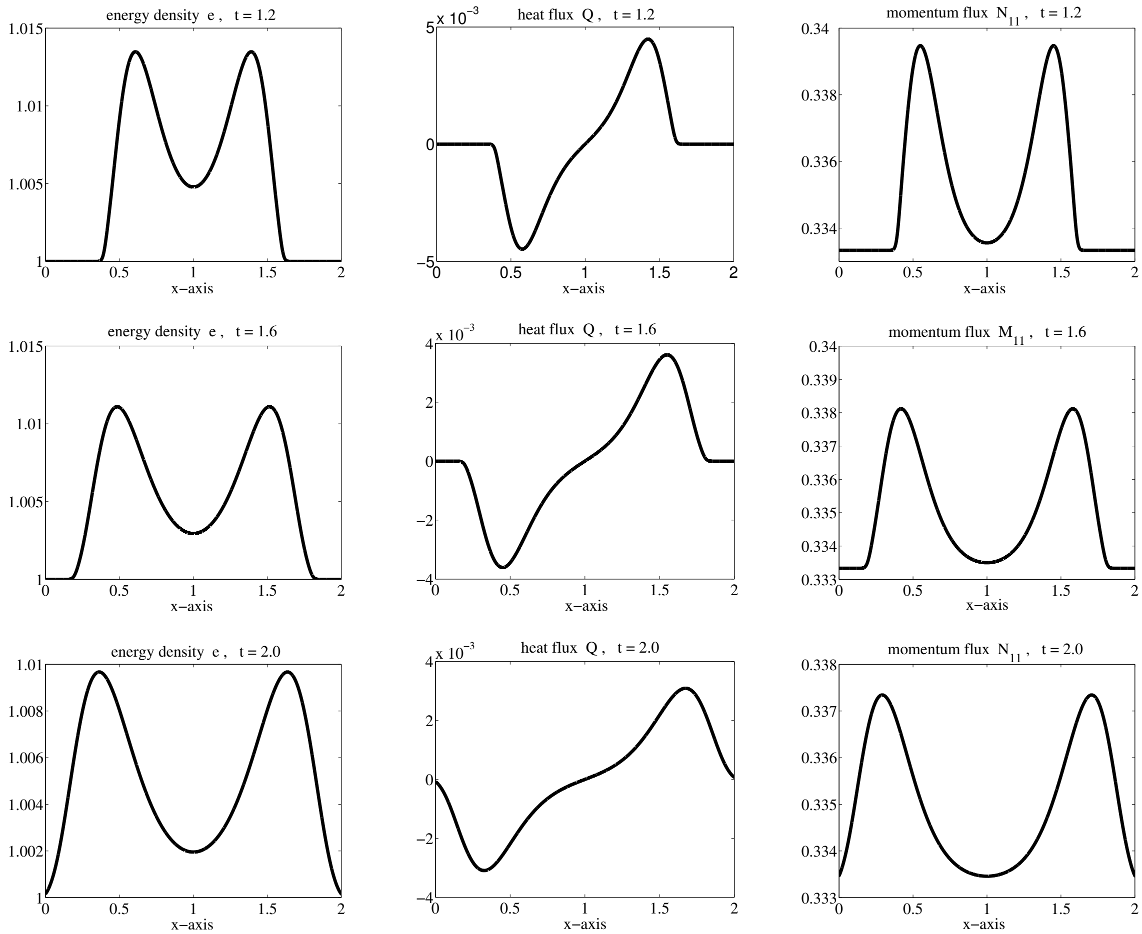

Figure 2: Evolution of energy, heat flux and momentum flux pulses at $\tau_N = 0.5$.

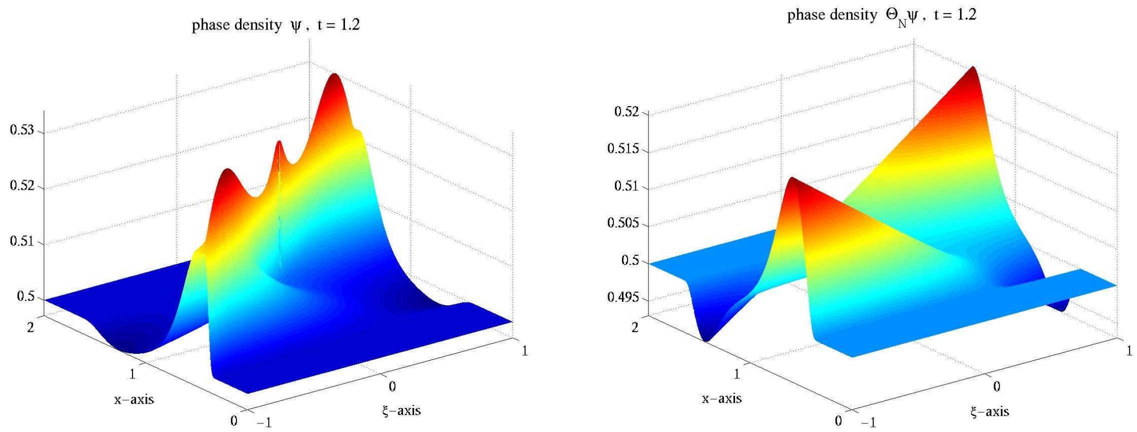

Figure 3: Representation of the phase densities at $\tau_N = 0.5$ and t=1.2.

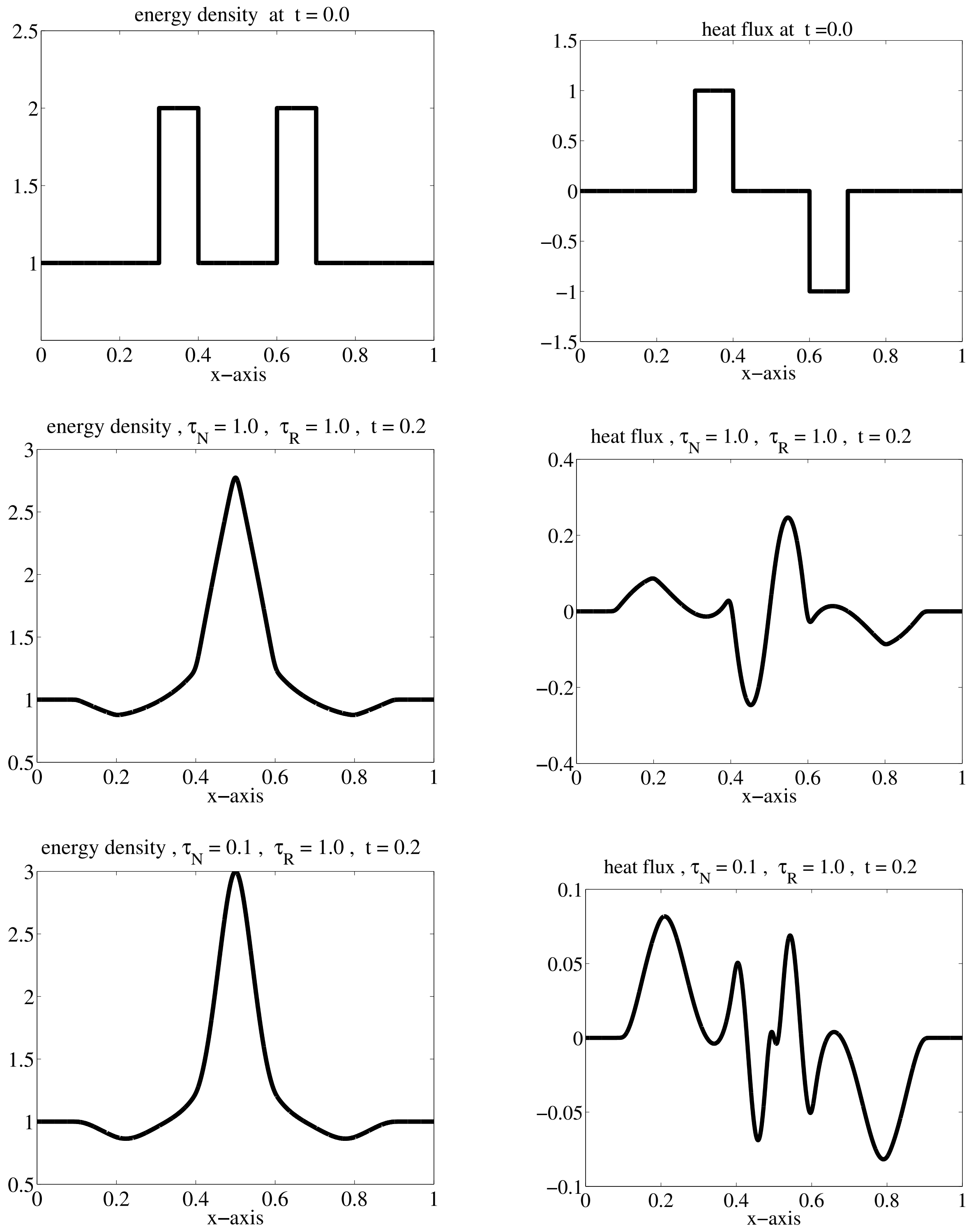

Figure 4: Evolution of energy and heat flux.

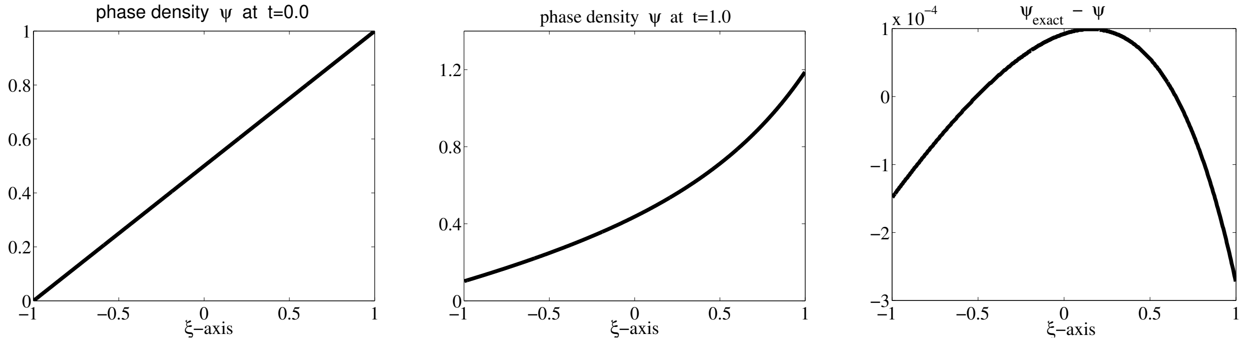

Figure 5: Phase densities and the error difference between exact the numerical values.

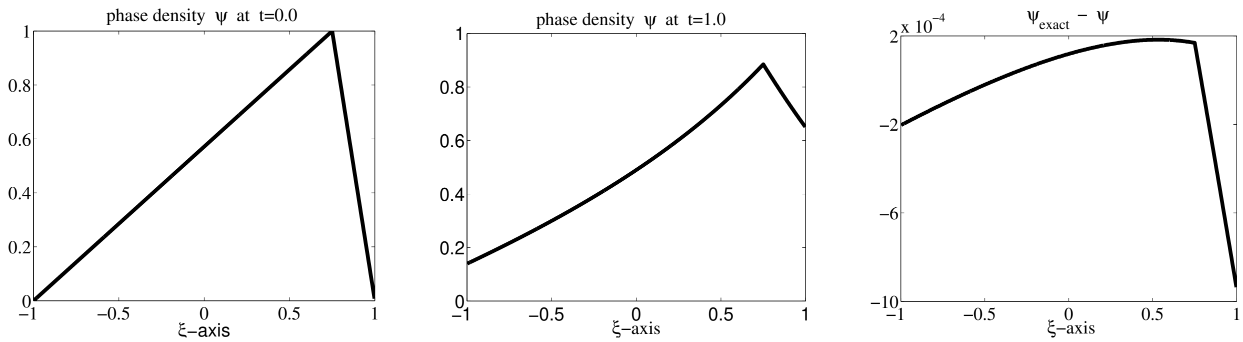

Figure 6: Phase densities and the error difference between exact the numerical values.

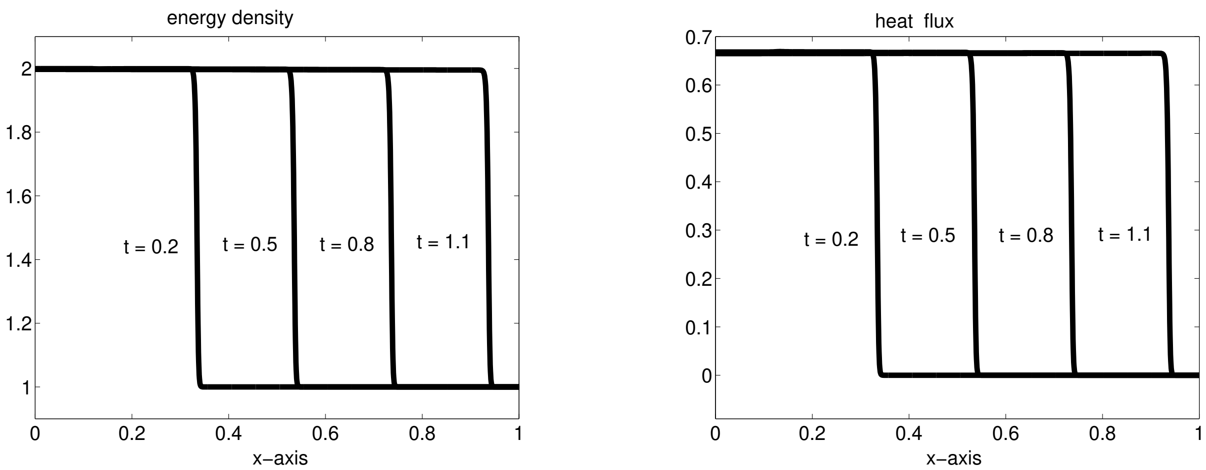

Figure 7: Evolution of a single shock at different times.

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