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Kinetic solutions of the BOLTZMANN-PEIERLS-Equation and its moment systems

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Abstract

The evolution of heat in crystalline solids is described at low temperatures by the BOLTZMANN-PEIERLS-Equation which is a kinetic equation for the phase density of phonons.

In this study we solve initial value problems for the BOLTZMANN-PEIERLS-Equation with respect to the following questionings: In thermodynamics, a given kinetic equation is usually replaced by its truncated moment systems which in turn is supplemented by a closure principle so that there results a system of PDE's for some moments as thermodynamic variables. A very popular closure principle is the *Maximum Entropy Principle* yielding a symmetric hyperbolic system. In recent times this strategy has lead to serious studies on two problems that might arise. 1. Do solutions of the *Maximum Entropy Principle* exist ? 2. Is the physics which is embodied in the kinetic equation more or less equivalently displayed by the truncated moment system? It was JUNK who proved for the BOLTZMANN equation of gases that *Maximum Entropy* solutions do not exist. The same failure appears for the FOKKER-PLANCK-Equation, which was proved by means of explicit solutions by DREYER/JUNK/KUNIK.

The current study yields a positive existence result. We prove for the BOLTZMANN-PEIERLS-Equation hat the *Maximum Entropy Principle* is well posed and that it can be used to establish a closed hyperbolic moment system of PDE's. Regarding the second question on the equivalence of moments that are calculated by solutions of the BOLTZMANN-PEIERLS-Equation and moments that result from the *Maximum Entropy* system we develop a numerical method that allows a comparison of both solutions. In particular, we introduce a numerical kinetic scheme that consists of free flight periods and two classes of update rules. The first class of rules are the same for the kinetic equation as well as for the *Maximum Entropy* system, while the second class of update rules contain additional rules for the *Maximum Entropy* system.

It is illustrated that if sufficient many moments are taken into account, both solutions converge to each other. However, it is additionally illustrated, that the numerical effort to solve the kinetic equation is less than the effort to solve the *Maximum Entropy* system.

1 A short summary on the kinetic theory of heat conduction

At low temperatures the evolution of heat in crystalline solids is described by the BOLTZMANN-PEIERLS-Equation which is a kinetic equation for the phase density of phonons. Note that the FOURIER theory of heat fails to describe heat conduction processes at low temperatures (see [10] and the references therein). RUGGERI et al. have studied a very interesting hyperbolic system of PDE's of heat conduction, that contains an example where the LAX shock condition is not equivalent to the entropy shock condition (cf. [17]).

The phase density $f \geq 0$ of a gas of phonons evolves according to the BOLTZMANN-PEIERLS-Equation, which can be written in the microscopically two dimensional case as

$$\frac{\partial f}{\partial t}(t,\,\mathbf{x},\,\mathbf{k}) + c_D \frac{k_i}{|\,\mathbf{k}\,|}\frac{\partial f}{\partial x_i}(t,\,\mathbf{x},\,\mathbf{k}) = (Sf)(t,\,\mathbf{x},\,\mathbf{k}). \tag{1}$$

The time is denoted by t and because we consider exclusively two space dimensions, $\mathbf{x} = (x_1,\, x_2)$ denote the space variables and $\mathbf{k} = (k_1,\, k_2)$ is the microscopic wave vector. The positive constant c_D is the DEBYE speed. The quantity S abbreviates the collision operator which will be defined below. The three dimensional BOLTZMANN-PEIERLS-Equation was studied in detail by DREYER/STRUCHTRUP in [10]. However, it is due to the simple form of the group velocity $c_D\mathbf{k}/\,|\,\mathbf{k}\,|$ that nothing is lost qualitatively if one restricts to the two dimensional case.

The moments of the phase density f reflect the kinetic processes on the scale of continuum physics. For any integrable function $m = m(\mathbf{k})$, we define a corresponding moment map u that acts on any phase density f depending on $\mathbf{k}$ via

$$u(f) := \int\limits_{\mathbb{R}^2} m(\mathbf{k}) f(\mathbf{k})\, d\mathbf{k}. \tag{2}$$

We call m the moment weigth of u. Note that f may also depend on t and $\mathbf{x}$, and in turn $u(f)$ depends on t and $\mathbf{x}$, too.

The special moments

$$e(f) = \hbar c_D \int\limits_{\mathbb{R}^2} |\,\mathbf{k}\,|\, f(\mathbf{k})\, d\mathbf{k}, \quad Q_i(f) = \hbar {c_D}^2 \int\limits_{\mathbb{R}^2} k_i f(\mathbf{k})\, d\mathbf{k}, \tag{3}$$

$$p_i(f) = \hbar \int\limits_{\mathbb{R}^2} k_i f(\mathbf{k})\, d\mathbf{k}, \quad N_{ij}(f) = \hbar c_D \int\limits_{\mathbb{R}^2} \frac{k_i k_j}{|\,\mathbf{k}\,|} f(\mathbf{k})\, d\mathbf{k}, \tag{4}$$

have an immediate physical interpretation. The fields e, $\mathbf{p} = (p_1,\, p_2)$, $\mathbf{Q} = (Q_1,\, Q_2)$ and the matrix $\mathbf{N} = (N_{ij})$ are the energy density, the momentum density, the heat flux and the momentum flux, respectively. Note that $\mathbf{Q} = c_D^2\mathbf{p}$.

Phonons are classified as BOSE particles, and the corresponding entropy density-entropy flux pair $(h,\, \Phi_i)$, is thus given by

$$h(f) \;:=\; y \int\limits_{\mathbb{R}^2} \Big((1+\frac{f}{y}) \ln{(1+\frac{f}{y})} - \frac{f}{y} \ln{(\frac{f}{y})} \Big) \mathbf{k}\, d\mathbf{k}, \tag{5}$$

$$\Phi_i(f) \;:=\; y c_D \int\limits_{\mathbb{R}^2} \frac{k_i}{|\,\mathbf{k}\,|} \Big((1+\frac{f}{y}) \ln{(1+\frac{f}{y})} - \frac{f}{y} \ln{(\frac{f}{y})} \Big) \mathbf{k}\, d\mathbf{k}. \tag{6}$$

Here y abbreviates the positive constant $\frac{3}{8}\pi^3$.

While there is only one collision mechanism for ordinary gas atoms, phonons may interact by two different collision processes, which are called R-processes and N-processes. The latter describe phonon-phonon interactions, while R-processes take care for interactions of phonons and lattice impurities. The N-processes conserve energy as well as momentum, while the R-processes conserve only the energy. The CALLAWAY approximation of the collision operator 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 separately. We write

$$Sf = S_R(f) + S_N(f), \quad S_\alpha f = \frac{1}{\tau_\alpha} \Big(P_\alpha f - f \Big), \quad \alpha \in \Big\{ R,\, N \Big\}. \tag{7}$$

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

$$h(P_R f) \;=\; \max_{f'} \Big\{ h(f) \;:\; e(f') = e(f) \Big\}, \tag{8}$$

$$h(P_N f) \;=\; \max_{f'} \Big\{ h(f) \;:\; e(f') = e(f),\, \mathbf{p}(f') - \mathbf{p}(f) \Big\}. \tag{9}$$

These maximization problems can be solved by means of LAGRANGE multipliers Λ_R^0 and Λ_N^0, Λ_N^1, Λ_N^2. There result

$$P_R f(\mathbf{k}) \;=\; \frac{y}{-1 + \exp \Sigma_R(e(f),\, \mathbf{k})}, \tag{10}$$

$$P_N f(\mathbf{k}) \;=\; \frac{y}{-1 + \exp \Sigma_N(e(f),\, \mathbf{p}(f),\, \mathbf{k})}, \tag{11}$$

where

$$\Sigma_R(e,\, \mathbf{k}) \;=\; \hbar c_D \,|\,\mathbf{k}\,|\, \Lambda_R^0(e), \tag{12}$$

$$\Sigma_N(e,\, \mathbf{p},\, \mathbf{k}) \;=\; \hbar c_D \,|\,\mathbf{k}\,|\, \Lambda_N^0(e,\, \mathbf{p}) + \hbar k_i \Lambda_N^i(e,\, \mathbf{p}). \tag{13}$$

From (8) and (9) the LAGRANGE multipliers can be calculated explicitly. They are given by

$$\Lambda_R^0 = \gamma\Big(\frac{1}{3e}\Big)^{\frac{1}{3}}, \quad \Lambda_N^0 = \gamma\Big(\frac{F}{e}\Big)^{\frac{1}{3}}(3-6F)^{-\frac{5}{6}}, \tag{14}$$

$$\Lambda_N^i = c_D^2 \frac{\gamma}{4}\Big(\frac{F}{e}\Big)^{\frac{4}{3}}(3-6F)^{-\frac{5}{6}} p_i, \quad i = 1,\, 2, \tag{15}$$

$$F = \frac{2}{3+\sqrt{9-8c_D^2\mathbf{p}^2 e^{-2}}}, \quad \gamma = \Big(\frac{12\pi y\zeta(3)}{c_D^2\hbar^2}\Big)^{\frac{1}{3}}, \tag{16}$$

where ζ is the RIEMANNian ζ-function.

Next we derive balance equations from the BOLTZMANN-PEIERLS-Equation (1). We obtain for the physically important moments

$$\frac{\partial\, e(f)}{\partial\, t} + \frac{\partial\, Q_j(f)}{\partial\, x_j} \;=\; 0, \tag{17}$$

$$\frac{\partial\, p_i(f)}{\partial\, t} + \frac{\partial\, N_{ij}(f)}{\partial\, x_j} \;=\; -\frac{1}{\tau_R} p_i(f), \tag{18}$$

for any solution f of (1). However, there exist an infinite number of further balance equations, because there follows for any vector $\vec{m}(\mathbf{n})$ of moment weights

$$\frac{\partial\, \vec{u}(f)}{\partial\, t} + \frac{\partial\, \vec{F}_j(f)}{\partial\, x_j} \;=\; \vec{u}(Sf). \tag{19}$$

Here, $\vec{u}$ and $\vec{F}_1$, $\vec{F}_2$ are the vectors of densities and fluxes, repectively. They are defined by

$$\vec{u}(f) = \int\limits_{\mathbb{R}^2} \vec{m}(\mathbf{k}) f(\mathbf{k})\, d\mathbf{k}, \quad \vec{F}_j(f) = \int\limits_{\mathbb{R}^2} k_j \vec{m}(\mathbf{k}) f(\mathbf{k})\, d\mathbf{k}, \quad j = 1,\, 2. \tag{20}$$

Furthermore, the kinetic equation (1) implies an entropy inequality, i.e. any solution f of (1) satisfies

$$\frac{\partial\, h(f)}{\partial\, t} + \frac{\partial\, \Phi_j(f)}{\partial\, x_j} \;\geq\; 0. \tag{21}$$

2 The Maximum Entropy Principle and the Strategy of Extended Thermodynamics

This section is devoted to a general discussion of the *Maximum Entropy Principle* (MEP) and its application in *Extended Thermodynamics*. The objective of *Extended*

Thermodynamics is to solve initial and boundary value problems for truncated moment systems instead of solving the underlying kinetic equation. To this end only the first N equations of the infinite hierarchy of moment equation are used, and the MEP serves to close the truncated system.

For the formulation of the MEP we start with a fixed vector $\vec{m}$ of moment weights of N components. The given $\vec{m}$ induces a vector $\vec{u}$ of densities. In the following we call the pair $(\vec{m}, \vec{u})$ a moment pair of dimension N. The *Maximum Entropy Principle* corresponding to $(\vec{m}, \vec{u})$ can be formulated as follows.

For any given phase density f_0 we seek a phase density f_M that maximizes the entropy, i.e.

$$h(f_M) = \max_f \{h(f) : \quad \vec{u}(f) = \vec{u}(f_0)\}. \tag{22}$$

In order to indicate that f_M depends obviously on f_0, we write $f_M = P_M f_0$. The MEP assumes, that for any phase density f_0 there always exists a phase density $f_M = P_M f_0$ that maximizes the entropy according to (22). Thus, the MEP ends up with an operator P_M. If (!) P_M exists, it has the following properties

1. P_M is a nonlinear projector, i.e. $P_M^2 = P_M$.
2. $P_M f_0$ depends exclusively on $\vec{u}(f_0)$, i.e.

$$\vec{u}(f_1) = \vec{u}(f_2) \quad \Rightarrow \quad P_M \vec{u}(f_1) = P_M \vec{u}(f_2). \tag{23}$$

We call the operator P_M the *MEP projector coressponding to the moment pair* $(\vec{m}, \vec{u})$. The existence of the MEP projector is a very subtle problem, in particular, because several counterexamples are known, where the MEP projector does not exist.

Before we start a discussion on the existence of P_M, let us first describe how the operator P_M can be calculated formally and how the closure problem of *Extended Thermodynamics* is solved. Since (22) is an optimization problem with constraints, we introduce for given f_0 the LAGRANGE multipliers $\vec{\Lambda}_M$ that depend on the moments $\vec{u}(f_0)$, so that

$$P_M f_0 = \frac{y}{-1 + \exp \Sigma_M}, \quad \Sigma_M = \vec{\Lambda}_M \cdot \vec{M}, \quad \vec{\Lambda}_M = \vec{\Lambda}_M\Big(\vec{u}(f_0)\Big). \tag{24}$$

The multipliers $\vec{\Lambda}_M$ are determined by the constraints, and this means that we have to solve the nonlinear equation

$$\vec{u}(P_M f_0) = \vec{u}(f_0). \tag{25}$$

Thus for any given f_0 the following two statements are equivalent

1. There exists $P_M f_0$.
2. The equation (25) has a solution.

According to their definition (8) and (9), the operators P_R and P_N appearing in the CALLAWAY ansatz are also MEP projectors.

Next we consider the closure problem of *Extended Thermodynamics.* To this end, let us here assume that $P_M f_0$ exists. The strategy of *Extended Thermodynamics* is then as follows. We start from a finite number of balance equations derived from the kinetic equation. As in the last section, we denote the corresponding vectors of densities and fluxes by $\vec{u}$ and $\vec{F}_j$, respectively, see (20). The densities are considered as the independent variables, and because in general the fluxes $\vec{F}_j$ do not depend on the densities $\vec{u}$, there arises the so called closure problem. The closure problem is solved by a reasonable ansatz that provides the fluxes, and in general also the productions, as functions of the densities.

A very popular closure ansatz in *Extended Thermodynamics* is the MEP leading to the so called MEP moment system, which is achieved from (19) by a formal replacement of the actual phase density that solves the kinetic equation by the MEP density $P_M f$:

$$\frac{\partial \vec{u}\,(P_M f)}{\partial t} + \frac{\partial \vec{F}_j\,(P_M f)}{\partial x_j} = \vec{u}\,(S P_M f)\,. \tag{26}$$

Since $P_M f$ depends on f exclusively via the densities $\vec{u}$, the system (26) is in fact a closed system with respect to the variables $\vec{u}$.

Recall that we have assumed, without justification, that the MEP density exists. If this happens, the MEP moment system is hyperbolic and can additionally be brought into a symmetric hyperbolic form, because there is an entropy density-entropy flux pair with a concave entropy density. The entropy density-entropy flux pair depends also exclusively on the variables $\vec{u}$. For more details we refer the reader to the standard textbook on *Rational Extended Thermodynamics* by MÜLLER/RUGGERI, [11].

Now we will pose and answer two questions regarding the *Maximum Entropy Principle* and its application in *Extended Thermodynamics.*

The first and most important question was already posed:

1. Which are the conditions so that the MEP density $P_M f$ does actually exist ?

The second question regards the equivalence between the MEP moment system and the underlying kinetic equation.

2. *How many components must be included in the moment vector $\vec{u}$ so that the MEP moment system and the underlying kinetic equation lead to the same results ?*

It was JUNK, see [13] and [14], who has observed, that for the most prominent case, which is the moment system of the Boltzmann equation, the MEP density $P_M f$ does not exist. JUNK's proof of nonexistence was mathematically accepted, however, it was argued that it is not relevant in physical applications, because the region, where the MEP fails will never be meet in physical processes.

The FOKKER-PLANCK-Equation for BROWNian motion was used by DREYER/ JUNK/ KUNIK in order to illustrate that JUNK's arguments are most serious ones against the *Maximum Entropy Principle* as a general useable closure principle of the truncated moment system of a kinetic equation. These authors calculated in [5] for RIEMANN initial data, the moments of the exact FOKKER-PLANCK solution. These are used in order to show that even for arbitrarily small jumps, so that the initial data are near to equilibrium, the exact solution of the FOKKER-PLANCK-Equation exhibits moment vectors which are not admissible in the MEP moment method. In particular it was shown that the linearized system behaves completely different from the original MEP moment system in equilibrium. The authors could identify the reason for failure which is a singularity appearing in the highest flux in equilibrium. Furthermore it was shown, that the *Maximum Entropy* solution behaves very different from the exact solution of the underlying kinetic problem.

These studies reveal that a rigorous justification of the application of the *Maximum Entropy Principle* as a closure principle in *Extended Thermodynamics* is mandantory.

Our current study on the BOLTZMANN-PEIERLS-Equation equation and its moment system will rigorously prove and illustrate (i) that the MEP phase does really exist in this case, see chapter 4, and (ii) that about eighty components of the moment vector must be included, so that the MEP moment system behaves more or less similiar to the kinetic equation, see Section 7.

We have thus established that it may happen, that the MEP can be used to replace a kinetic equation by a truncated moment system. However, on the other hand we have illustrated in the current case, that it is easier here to solve the kinetic equation directly, because the solution of the more ore less equivalent moment system requires much more mathematical effort.

3 The reduced BOLTZMANN-PEIERLS-Equation

In this section we derive a reduced kinetic equation for a reduced phase density. This procedure relies on the observation that for any solution f of (1) there exists a corresponding solution of the reduced equation that determines all physical important moments of f. Additionally we introduce a definition of a reduced entropy density-entropy flux pair.

From the phase density f which depends on the wave vector $\mathbf{k} \in \mathbb{R}^2$ we calculate the *reduced phase density* φ_f *of* f according to

$$\varphi_f(\mathbf{n}) \;:=\; \int_0^\infty k^2 f(k\mathbf{n})\,dk. \tag{27}$$

Note that φ_f depends only on a normal vector $\mathbf{n} \in \mathbf{S^1}$.

Let m be a homogenous moment weight of degree 1, i.e. $m(\lambda\mathbf{k}) = \lambda m(\mathbf{k})$ for all $\lambda \geq 0$, and let u be the corresponding moment map. We calculate

$$\begin{aligned} u(f) = \int\limits_{\mathbb{R}^2} m(\mathbf{k}) f(\mathbf{k})\, d\mathbf{k} &= \int\limits_{S^1} \int\limits_0^\infty k^2 m(\mathbf{n}) f(k\mathbf{n})\, dk\, d\mathbf{n} \\ &= \int\limits_{S^1} m(\mathbf{n}) \varphi_f(\mathbf{n})\, d\mathbf{n}. \end{aligned} \tag{28}$$

The moment u of f is thus given by the corresponding moment of φ_f. In order to avoid too many symbols, we shall use the same symbol u for a moment of $f = f(\mathbf{k})$ as well as for the corresponding moment of $\varphi_f = \varphi_f(\mathbf{n})$.

Note that all moments with physical interpretation (cf. (3), (4)) are formed by homogenous moment weights of degree 1.

In particular, we have

$$e(f) = e(\varphi_f), \quad \mathbf{p}(f) = \mathbf{p}(\varphi_f) \tag{29}$$

where

$$e(\varphi) = \hbar c_D \int\limits_{S^1} \varphi(\mathbf{n})\, d\mathbf{n}, \quad \mathbf{p}(\varphi) = \hbar \int\limits_{S^1} \mathbf{n}\varphi(\mathbf{n})\, d\mathbf{n}. \tag{30}$$

Next we define the *reduced* collision operators Ψ, Ψ_R and Ψ_N by

$$\Psi_\alpha \varphi = \frac{1}{\tau_\alpha}(\Theta_\alpha \varphi - \varphi), \quad \alpha \in \{R, N\}, \quad \Psi\varphi = \Psi_R\varphi + \Psi_N\varphi, \tag{31}$$

where

$$(\Theta_R\varphi)(\mathbf{n}) = \frac{2y\zeta(3)}{\Sigma_R^3(e(\varphi), \mathbf{n})}, \tag{32}$$

$$(\Theta_N\varphi)(\mathbf{n}) = \frac{2y\zeta(3)}{\Sigma_N^3(e(\varphi), \mathbf{p}(\varphi), \mathbf{n})}. \tag{33}$$

Recall that the functions Σ_R, Σ_N are given by (12) and (13). From the integral identity

$$\int\limits_0^\infty \frac{k^2}{-1 + \exp k}\, dk = 2\zeta(3) \tag{34}$$

we conclude

$$\int\limits_0^\infty k^2 (P_\alpha f)(k\mathbf{n})\, dk = (\Theta_\alpha \varphi_f)(\mathbf{n}), \quad \text{i.e.} \quad \Theta_\alpha\varphi_f = \varphi_{P_\alpha f}, \quad \alpha \in \{R, N\}. \tag{35}$$

The equations (27), (31) and (35) imply, that any solution $f(t,\, \mathbf{x},\, \mathbf{k})$ of (1) induces a solution $\varphi_f(t,\, \mathbf{x},\, \mathbf{n})$ of the following *reduced* BOLTZMANN-PEIERLS-Equation

$$\frac{\partial \varphi}{\partial t}(t,\, \mathbf{x},\, \mathbf{n}) + c_D n_i \frac{\partial \varphi}{\partial x_i}(t,\, \mathbf{x},\, \mathbf{n}) = (\Psi\varphi)(t,\, \mathbf{x},\, \mathbf{n}). \tag{36}$$

The identity (35) can be generalized to other MEP projectors P_M. Let $(\vec{m},\, \vec{u})$ be a moment pair so that all components of $\vec{m}$ are homogenous of degree 1. Then we find

$$\int_0^\infty k^2 (P_M f)(k\mathbf{n})\, dk = \frac{2y\zeta(3)}{\Sigma_M^3(\mathbf{n})} \quad \forall\, \mathbf{n} \in S^1, \tag{37}$$

where the function Σ_M is given by (24), i.e. $\Sigma_M = \vec{\Lambda}_M \cdot \vec{m}$.

Finally we introduce an entropy density-entropy flux pair for the reduced equation (36). This definition is not so straight forward as before, because in general the entropy density $h(f)$ is not a function of φ_f. We propose the following definition

$$h(\varphi) \;:=\; \mu \int_{S^1} \varphi(\mathbf{n})^{\frac{2}{3}}\, d\mathbf{n}, \tag{38}$$

$$\Phi_i(\varphi) \;:=\; \mu c_D \int_{S^1} n_i \varphi(\mathbf{n})^{\frac{2}{3}}\, d\mathbf{n}, \quad \mu = \frac{3}{2}\Big(2y\zeta(3)\Big)^{+\frac{1}{3}}. \tag{39}$$

The reasons for and the advantages of these definitions will be discussed in the following section.

4 The Maximum Entropy Principle and the reduced BOLTZMANN-PEIERLS-Equation

Next apply the MEP to the reduced entropy and derive some analytical results. In particular, we will prove, that reduced MEP phase densities do exist, at least for reasonable moments $(\vec{m},\, \vec{u})$. Let $(\vec{m},\, \vec{u})$ be a moment pair of dimension N. We call the pair $(\vec{m},\, \vec{u})$ *admissible*, if

1. All components of $\vec{m}$ are homogenous of degree 1 with respect to $\mathbf{k}$.

2. The energy density e must be among the components of $\vec{u}$.

3. The restrictions of the components of $\vec{m}$ to the sphere S^1 are linearly independent and smooth (at least C^3).

Note that all physical important moment weights m are homogenous of degree 1 with respect to $\mathbf{k}$ and they have smooth restrictions to the sphere.

In the following, we consider exclusively admissible pairs $(\vec{m}, \vec{u})$. For $r \in \{1, \infty\}$ we define

$$L^r_+(S^1) \;=\; \Big\{\varphi \in L^r(S^1) \;:\; \exists\, \delta = \delta(\varphi) > 0 \text{ with } \varphi \geq \delta \text{ a.e.}\Big\}. \tag{40}$$

We may interpret the MEP that corresponds to $(\vec{m}, \vec{u})$ and to the reduced entropy as follows. For any given phase density $\varphi_0 \in L^1_+(S^1)$ we seek a solution φ_M of the following optimization problem with constraints.

Problem 4.1

$$h(\varphi_M) \;=\; \max_{\varphi} \Big\{h(\varphi) \;:\; \varphi \in L^1_+(S^1),\; \vec{u}(\varphi) = \vec{u}(\varphi_0)\Big\}. \tag{41}$$

Our main goal in this section is to prove rigorously, that for any $\varphi_0 \in L^1_+(S^1)$ there exists a corresponding unique solution φ_M of Problem 4.1. To this end we follow the standard approach of convex analysis (see [18]). At first we introduce a functional $h^\star$ according to

$$h^\star(\psi) \;=\; -y\zeta(3) \int\limits_{S^1} \Big(\psi(\mathbf{n})\Big)^{-2} d\mathbf{n}, \tag{42}$$

which gives formally the conjugate functional of h. Note that (42) is well defined at least for $\psi \in L^\infty_+(S^1)$. Using this functional $h^\star$ we formulate the following dual problem of 4.1, namely

Problem 4.2

$$\tilde{h}(\vec{\Lambda}_M) \;=\; \min_{\vec{\Lambda}} \Big\{\tilde{h}(\vec{\Lambda}) \;:\; \vec{\Lambda} \in D_M\Big\}, \tag{43}$$

$$D_M \;:=\; \Big\{\vec{\Lambda} \in \mathbb{R}^n \;:\; \vec{\Lambda}\cdot\vec{m} \in L^\infty_+(S^1)\Big\}, \tag{44}$$

$$\tilde{h}(\vec{\Lambda}) \;=\; -h^\star\Big(\vec{\Lambda}\cdot\vec{m}\Big) + \vec{u}(\varphi_0)\cdot\vec{\Lambda}, \tag{45}$$

which is an optimization problem without constraints. There is a close relation between the Problems 4.1 and 4.2. In particular we show, that the solution $\vec{\Lambda}_M$ of Problem 4.2 gives the LAGRANGE multipliers corresponding to the solution φ_M of Problem 4.1. We summarize our main results in the following theorem.

Theorem 4.3

1. *There exists a unique solution φ_M problem 4.1.*
2. *There exists a unique solution $\vec{\Lambda}_M$ problem 4.2.*

3. There hold the identities

$$\varphi_M \;=\; \frac{2y\zeta(3)}{(\vec{\Lambda}_M\cdot\vec{m})^{\,3}}, \tag{46}$$

$$\vec{u}\Big(\frac{2y\zeta(3)}{(\vec{\Lambda}_M\cdot\vec{m})^{\,3}}\Big) \;=\; \vec{u}(\varphi_0) \tag{47}$$

and

$$\tilde{h}(\vec{\Lambda}_M) = h(\varphi_M). \tag{48}$$

Before we start the proof of Theorem 4.3 we would like to discuss its implications. First there follows the existence of a nonlinear MEP projector

$$\Theta_M \;:\; L^1_+(S^1) \to L^\infty_+(S^1) \tag{49}$$

so that for any φ_0 the phase density $\Theta_M\varphi_0$ is the solution of problem 4.1. Note, that

1. Θ_M depends obviously on $(\vec{m},\,\vec{u})$.
2. $\Theta_M\varphi_0$ depends only on $\vec{u}(\varphi_0)$.
3. Θ_R and Θ_M (cf. (32), (33)) are MEP projectors.

Thus, for any admissible pair $(\vec{m},\,\vec{u})$ we have two MEP projectors: Θ_M and P_M resulting from the MEP, which is either applied to reduced phase densities φ or to phase densities f, respectively. Obviously, up to now P_M exists only formally. The equations (24), (37), (46), and (47) provide

$$\Theta_M\varphi_f = \varphi_{P_M f} \tag{50}$$

for all phase densities f with $\varphi_f \in L^1_+(S^1)$ (cf. (27)). This equation is a generalization of (35).

The identity (50) has two important consequences.

1. For admissible pairs $(\vec{m},\,\vec{u})$ there exist a MEP projector P_M that is defined for all f with $\varphi_f \in L^1_+(S^1)$ according to

   $$P_M f \;=\; \frac{y}{-1+\exp\Sigma_M}, \quad \Sigma_M = \vec{\Lambda}_M\cdot\vec{m}, \tag{51}$$

   where $\vec{\Lambda}_M$ is the solution of the problem 4.2 corresponding to $\Theta_M\varphi_f$.

2. If we consider exclusively admissible pairs and furthermore the MEP as the closure principle, the two moment systems derived from the BOLTZMANN-PEIERLS-Equation and from the reduced equation, respectively, are identical.

These properties are the actual advantages of definition (38).

We return to the proof of Theorem 4.3. The domains of definition $L^1_+(S^1)$ and D_M in the problems 4.1 and 4.2, respectively, have a special structure. In particular, D_M is an open set in $\mathbb{R}^N$, whereas $L^1_+(S^1)$ is neither open nor closed in $L^1(S^1)$. Due to this fact, the existence of solutions of the Problems 4.1 and 4.2 cannot be derived from standard theorems of convex analysis.

The proof of Theorem 4.3 relies on four lemmas.

Lemma 4.4 *The problem 4.1 as well as the problem 4.2 have at most one solution.*

Lemma 4.5 *For all $\varphi \in L^1_+(S^1)$, $\psi \in L^\infty_+(S^1)$ there holds*

$$h(\varphi) + h^\star(\psi) \leq \int\limits_{S^1} \varphi(\mathbf{n})\psi(\mathbf{n})\, d\mathbf{n}. \tag{52}$$

If $\varphi \in L^1_+(S^1)$, $\psi \in L^\infty_+(S^1)$ are two functions that imply in (52) the equality sign, then there holds

$$\varphi \quad = \quad 2y\zeta(3)\psi^{-3}. \tag{53}$$

Lemma 4.6 *Let $\vec{\Lambda}_M$ be a solution of problem 4.2. Then there holds*

1. *$\vec{\Lambda}_M$ solves the nonlinear equation (47).*
2. *The phase density φ_M given by (46) is a solution of problem 4.1 and satisfies (48).*

Lemma 4.7 *There exists a (unique) solution $\vec{\Lambda}_M$ of 4.2.*

Obviously, these lemmas imply Theorem 4.3. Lemma 4.4 follows immediately because the the sets $L^1_+(S^1)$ and D_M are strictly convex and because the functionals h and $h^\star$ are strictly concave. Lemma 4.5 and Lemma 4.6 can be proved with standard methods of convex analysis (we refer the reader again to [18]). The details of the proofs are thus omitted.

There remains the proof of Lemma 4.7. At first we consider the special case $N = 1$, $\vec{m}(\mathbf{k}) = \hbar c_D\, |\mathbf{k}|$, $\vec{u} = e$. With $\vec{\Lambda} = \lambda \in \mathbb{R}$ we conclude

$$D_M \quad = \quad \Big\{\lambda \in \mathbb{R} \,:\, \lambda > 0\Big\}, \tag{54}$$

$$\tilde{h}(\lambda) \quad = \quad 2\pi y\zeta(3)\lambda^{-2} + e(\varphi)\lambda. \tag{55}$$

Thus

$$\lambda_M \quad = \quad \Big(\frac{4y\pi\zeta(3)}{e(\varphi)}\Big)^{\frac{1}{3}}, \quad \tilde{h}(\lambda_M) < \infty, \tag{56}$$

is the unique solution of Problem 4.2.

Proof of Lemma 4.7: The function $\tilde{h}$ is strictly convex and continuous on the convex and open set D_M. We can extend $\tilde{h}$ to a functional $\overline{h}$ defined on the closure of D_M, namely

$$\overline{D}_M \;=\; \left\{\vec{\Lambda} \in \mathbb{R}^N \;:\; \vec{\Lambda}_M \cdot \vec{m} \geq 0 \text{ a.e. on } S^1\right\}. \tag{57}$$

Note, that $\overline{h}$ can achieve the value $+\infty$. $\overline{h}$ is convex and lower semicontinuous due to FATOU's Lemma. The vector $\vec{\Lambda}_R = (\lambda_M,\, 0\,,..,0)$, where λ_M is given by (56), is contained in D_M. Thus, it is sufficient to consider $\overline{h}$ restricted to the convex and closed set

$$\overline{D}_R \;:=\; \left\{\vec{\Lambda} \in \overline{D}_M \;:\; \overline{h}(\vec{\Lambda}) \leq \overline{h}(\vec{\Lambda}_R)\right\}. \tag{58}$$

Next we show, that $\overline{D}_R$ is bounded and therefore compact. Recall that we have assumed the existence of a constant $\delta > 0$, so that $\varphi_0 \geq \delta$ almost everywhere. Consequently we find

$$\overline{h}(\vec{\Lambda_R}) \geq \overline{h}(\vec{\Lambda}) \geq \vec{u}(\varphi_0)\cdot\vec{\Lambda} = \int\limits_{S^1} \vec{\Lambda}\cdot\vec{m}(\mathbf{n})\varphi_0(\mathbf{n})\,d\mathbf{n} > \delta \int\limits_{S^1} \vec{\Lambda}\cdot\vec{m}(\mathbf{n})\,d\mathbf{n} > 0 \tag{59}$$

for all $\vec{\Lambda} \in \overline{D}_R$ with $\vec{\Lambda} \neq 0$. We thus conclude

$$\|\vec{\Lambda}\cdot\vec{m}\|_1 < \delta^{-1}\overline{h}(\vec{\Lambda_R}) < \infty \quad \forall\,\vec{\Lambda} \in \overline{D}_R. \tag{60}$$

Since the norm $\vec{\Lambda} \rightsquigarrow \;\|\,\vec{\Lambda}\cdot\vec{m}\,\|_1$ is equivalent to the standard norm in $\mathbb{R}^N$, we have shown the compactness of $\overline{D}_R$. There exists thus a unique minimum point $\vec{\Lambda}_M$ of $\overline{h}$ in $\overline{D}_R$ that is also a unique minimum point of $\overline{h}$ in $\overline{D}_M$. Recall that $\overline{h}(\vec{\Lambda}_M) \leq \overline{h}(\vec{\Lambda}_R) < \infty$ and $\vec{u}(\varphi_0)\cdot\vec{\Lambda}_M > 0$. Hence

$$0 < \int\limits_{S^1} \left(\vec{\Lambda}_M\cdot\vec{m}(\mathbf{n})\right)^{-2} d\mathbf{n} < \infty. \tag{61}$$

There remains to show, that $\vec{\Lambda}_M$ is an inner point of $\overline{D}_M$. Let us assume, that the function $\Sigma_M = \vec{\Lambda}_M\cdot\vec{m}$ vanishes at some point $\mathbf{n}_0 \in S^1$. If we introduce coordinates x on S^1, we can express Σ by means of a TAYLOR sum, at least locally around x_0 corresponding to $\mathbf{n}_0$, which is always possible due to the smoothness of the components of $\vec{m}$. The TAYLOR sum gives rise to local estimations of Σ, namely

$$\Sigma_M(x) \leq \Sigma_M(x_0) + (x-x_0)\Sigma_M'(x_0) + \frac{1}{2}(x-x_0)^2\,\|\Sigma_M''\|_\infty\,. \tag{62}$$

Since Σ_M is nonnegative and equal to zero at x_0, we find $\Sigma_M(x_0) = 0$, $\Sigma_M'(x_0) = 0$. Thus we conclude

$$\Sigma_M^{-2}(x) \geq \alpha(x-x_0)^{-4}, \quad a > 0, \tag{63}$$

locally around x_0. However, this is a contradiction to the integral condition (61). We conclude that the continuous function Σ_M is strictly positive und that $\vec{\Lambda}_M$ is contained in D_M. $\square$

5 Kinetic solutions for the reduced kinetic equation

In this section we derive kinetic schemes that allow the construction of approximate solutions of (36) in the time interval $[0, \infty)$. In particular, we look for phase densities $\varphi = \varphi(t, \mathbf{x}, \mathbf{n})$, $\varphi \in \mathcal{V}$ with

$$\mathcal{V} := W^{1,1}_{\mathrm{loc}}\Big([0, \infty); V\Big), \tag{64}$$

$$V := \Big\{ f \in L^1_{\mathrm{loc}}(\mathbb{R}^2 \times S^1) \,:\, \exists\, \delta \in \mathbb{R} \text{ s.t. } f \geq \delta > 0 \text{ a.e.} \Big\}, \tag{65}$$

that satisfy (36) in the sense of distributions and that have prescribed initial data $\varphi^0 \in V$ at time $t = 0$.

The solution of the CAUCHY problem of the collisionless kinetic equation

$$\frac{\partial \varphi}{\partial t}(t, \mathbf{x}, \mathbf{n}) + c_D n_i \frac{\partial \varphi}{\partial x_i}(t, \mathbf{x}, \mathbf{n}) = 0 \tag{66}$$

is given by the *free transport group* $T(t)$ acting on V according to

$$\Big(T(t)\varphi\Big)(\mathbf{x}, \mathbf{n}) := \varphi(\mathbf{x} - c_D t\mathbf{n}, \mathbf{n}). \tag{67}$$

In particular, $T(t)\varphi^0$ is a solution of (66) with initial data φ^0. In other words, the group $T(t)$ generates the operator $-c_D n_i \frac{\partial}{\partial x_i}$. $T(t)$ preserves the positivity, i.e. $T(t)V = V$. Furthermore, $T(t)$ conserves the energy in the sense that $T(t)$ maps the set

$$V \cap L^1(\mathbb{R}^2 \times S^1) \tag{68}$$

into itself and preserves the $L^1(\mathbb{R}^2 \times S^1)$-norm. The solution of the CAUCHY problem for the reduced BOLTZMANN-PEIERLS-Equation (36) can be represented by means of DUHAMEL's principle as

$$\varphi(t) = T(t)\varphi^0 + \int_0^t T(t-s)\Psi_R \varphi(s)\, ds + \int_0^t T(t-s)\Psi_N \varphi(s)\, ds. \tag{69}$$

Obviously, the formula (69) is not explicit in $\varphi(t)$. In order to find approximate solutions, we shall replace the integrals in (69) by RIEMANN sums. If we introduce two small parameters $\tilde{\tau}_R > 0$ and $\tilde{\tau}_N > 0$, we find

$$\begin{aligned} \varphi(t) \simeq T(t)\varphi^0 &+ \sum_{i\,:\,0 \leq i\,\tilde{\tau}_R < t} \tilde{\tau}_R T(t - i\tilde{\tau}_R)\Psi_R \varphi(i\tilde{\tau}_R) \\ &+ \sum_{i\,:\,0 \leq i\,\tilde{\tau}_N < t} \tilde{\tau}_N T(t - i\tilde{\tau}_N)\Psi_N \varphi(i\tilde{\tau}_N). \end{aligned} \tag{70}$$

If we replace $\Psi_R\varphi(s)$ and $\Psi_N\varphi(s)$ in (69) by

$$\Psi_{R,\tilde\tau_R}(s)\varphi(s) = \sum_{i=0}^{\infty}\tilde\tau_R\delta_{i\tilde\tau_R}(s)\Psi_R\varphi(s) \quad \text{and} \tag{71}$$

$$\Psi_{N,\tilde\tau_N}(s)\varphi(s) = \sum_{i=0}^{\infty}\tilde\tau_N\delta_{i\tilde\tau_N}(s)\Psi_N\varphi(s), \tag{72}$$

respectively, and if we take care for the identity

$$\int_0^t T(t-s)\delta_{i\tilde\tau_\alpha}(s)\Psi_\alpha\varphi(s)\,ds = \begin{cases} 0 & \text{if } \; t \le i\tilde\tau_\alpha \\ T(t-i\tilde\tau_\alpha)\Psi_\alpha\varphi(i\tilde\tau_\alpha) & \text{if } \; t > i\tilde\tau_\alpha \end{cases} \tag{73}$$

for $i \in \mathbb{N}$ and $\alpha \in \{R, N\}$, we obtain, at least formally, again the right hand side of (70). Therefore we seek for solutions of the following *approximate* equation

$$\begin{aligned}\frac{\partial\varphi}{\partial t}(t, \mathbf{x}, \mathbf{n}) + c_D n_i\frac{\partial\varphi}{\partial x_i}(t, \mathbf{x}, \mathbf{n}) &= \Psi_{R,\tilde\tau_R}(t)\varphi(t, \mathbf{x}, \mathbf{n}) + \\ &\quad \Psi_{N,\tilde\tau_N}(t)\varphi(t, \mathbf{x}, \mathbf{n}).\end{aligned} \tag{74}$$

Solutions of (74) can be calculated explicitly by a kinetic scheme. For simplicity we will consider at first the case $\tilde\tau = \tilde\tau_R = \tilde\tau_N$. Due to the delta-distributions any solution of (74) has discontinuities in time at the multiples of $\tilde\tau$. Thus we have to distinguish between the left hand side and the right hand side limits at these times. Setting

$$\varphi_{i\pm} = \lim_{t\downarrow 0}\varphi(i\tilde\tau \pm t) \quad \text{for} \quad i \ge 0 \tag{75}$$

and $\varphi_{0-} = \varphi^0$ we find by a straight forward calculation, that *exact* solutions of (74) can be calculated by the following kinetic scheme

$$\varphi(i\tilde\tau + t) = T(t)\varphi_{i+}, \quad 0 < t < \tilde\tau, \tag{76}$$

$$\varphi_{i+} = \frac{\tilde\tau}{\tau_R}\Theta_R\varphi_{i-} + \frac{\tilde\tau}{\tau_N}\Theta_N\varphi_{i-} + \Big(1 - \frac{\tilde\tau}{\tau_R} - \frac{\tilde\tau}{\tau_N}\Big)\varphi_{i-}. \tag{77}$$

The time intervals $(i\tilde\tau,\, i\tilde\tau + \tilde\tau)$ are called *transport intervals*, whereas the multiples of $\tilde\tau$ are called *update times.*

For the general case $\tilde\tau_R \ne \tilde\tau_N$ we have to consider nonequidistent transport intervals. Furthermore, there are three different kinds of update time

1. common multiples of $\tilde\tau_R$ and $\tilde\tau_N$,
2. other multiples of $\tilde\tau_R$ and
3. other multiples of $\tilde\tau_N$.

In this case the evolution between two subsequent update times is again determined by the free transport equation. However, at the update times different update rules have to be applied. We find the following rules

$$\begin{aligned}
1.\ \varphi_{i+} &= \frac{\tilde{\tau}_R}{\tau_R}\Theta_R\varphi_{i-} + \frac{\tilde{\tau}_N}{\tau_N}\Theta_N\varphi_{i-} + (1 - \frac{\tilde{\tau}_R}{\tau_R} - \frac{\tilde{\tau}_N}{\tau_N})\varphi_{i-}, \qquad (78)\\
2.\ \varphi_{i+} &= \frac{\tilde{\tau}_R}{\tau_R}\Theta_R\varphi_{i-} + (1 - \frac{\tilde{\tau}_R}{\tau_R})\varphi_{i-}, \qquad (79)\\
3.\ \varphi_{i+} &= \frac{\tilde{\tau}_N}{\tau_N}\Theta_N\varphi_{i-} + (1 - \frac{\tilde{\tau}_N}{\tau_N})\varphi_{i-}, \qquad (80)
\end{aligned}$$

respectively, for the three different kinds of update times.

We mention that in the simple case $\tilde{\tau} = \tilde{\tau}_R = \tilde{\tau}_N$, the kinetic scheme (76)-(77) is equivalent to a standard splitting scheme. This can be shown by transforming the update rule (77) into

$$\varphi_{i+} - \varphi_{i-} = \tilde{\tau}\Psi\varphi_{i-}. \qquad (81)$$

In particular, we can interpret (81) as an EULER step for the reduced kinetic equation.

Lemma 5.1 *For any given initial data $\varphi^0 \in V$ and sufficiently small parameter $\tilde{\tau} = \tilde{\tau}_R = \tilde{\tau}_N$, the kinetic scheme* (76)-(77) *defines an exact solution φ of* (74) *with the following properties*

1. *φ is an element of $L^1_{\mathrm{loc}}\Big((0,\,\infty);\,V\Big)$ and there exist the left hand side limits with respect to time.*
2. *φ satisfies exactly the conservation of energy, that is*
$$\frac{\partial\, e(\varphi)}{\partial\, t} + \frac{\partial\, Q_i(\varphi)}{\partial\, x_i} \;=\; 0. \qquad (82)$$
3. *The entropy production is nonnegative, i.e.*
$$\frac{\partial\, h(\varphi)}{\partial\, t} + \frac{\partial\, \Phi_i(\varphi)}{\partial\, x_i} \;\geq\; 0. \qquad (83)$$

The equation (82) *and the inequality* (83) *are satisfied in the sense of distributions.*

Regarding the proof of this lemma we mention that

1. The first statement follows from basic properties of the free transport operators $T(t)$.

2. The equations (82) and the inequality (83) are trivially satiesfied within any period of free transport ((83) with equality sign). Across the update times energy is conserved and there is a nonnegative entropy production.

Further details are omitted here for shortness. A simliar result holds for the kinetic scheme with $\tilde{\tau}_R \neq \tilde{\tau}_N$.

There remains to show that the kinetic scheme (76)-(77) produces approximative solutions that converge to a solution of the BOLTZMANN-PEIERLS-Equation if $\tilde{\tau} \to 0$. This is the subject of a forthcoming paper. However, in Section 7 we discuss some numerical simulations.

6 Kinetic solutions of moment systems

In this section we shall describe how kinetic schemes can be used in order to solve moment systems of the reduced kinetic equation that are derived by means of the MEP. In particular it will turn out, that there is a close relationship between kinetic schemes for the kinetic equation and kinetic schemes for its moment systems. In the following, we assume that $(\vec{u}, \vec{m})$ is admissible in the sense of Section 4 and we denote by Θ_M the MEP projector corresponding to $(\vec{u}, \vec{m})$ (cf. Section 4). The moment system corresponding to $\vec{u}$ is given by

$$\frac{\partial\, \vec{u}(\Theta_M \varphi)}{\partial\, t} + \frac{\partial\, \vec{F}_j(\Theta_M \varphi)}{\partial\, x_j} \;=\; \vec{u}(\Psi \Theta_M \varphi), \tag{84}$$

cf. (26) and the end of Section 3.

The standard kinetic approach of the CAUCHY problem for this moment system can be summarized as follows.

1. We start with initial data of the form $\Theta_M \varphi^0$ that correspond to the given macroscopic initial data $\vec{u}^0$, i.e. $\vec{u}^0 = \vec{u}(\Theta_M \varphi^0)$.

2. For a small but fixed time τ_M we solve the kinetic equation (36) for $0 \leq t \leq \tau_M$, at least approximately.

3. The resulting phase density will be used to calculate the moments $\vec{u}$.

4. At the time τ_M the phase density $\varphi(\tau_M)$ will be replaced by the corresponding MEP phase density $\Theta_M \varphi(\tau_M)$ and we restart the scheme.

Kinetic schemes of this kind are well known and studied by many authors for moment systems relying on various kinetic equations (see [6], [7], [13] and [16] for moment systems of the BOLTZMANN equation and [8], [9] for a moment system of the BOLTZMANN-PEIERLS-Equation).

In view of this standard approach and in view of the kinetic schemes from Section 5 we consider the following kinetic equation

$$\frac{\partial \varphi}{\partial t}(t, \mathbf{x}, \mathbf{n}) + c_D n_i \frac{\partial \varphi}{\partial x_i}(t, \mathbf{x}, \mathbf{n}) = (\Psi_R\varphi + \Psi_N\varphi + \Psi_M\varphi)(t, \mathbf{x}, \mathbf{n}), \tag{85}$$

where

$$\Psi_M\varphi := \frac{1}{\tau_M}\Big(\Theta_M\varphi - \varphi\Big) \tag{86}$$

is again a relaxation operator with an artificial relaxation time τ_M.

If we apply the moment maps $\vec{u}$ to (85), we obtain formally for the limiting case $\tau_M \to 0$ the system (84). We can thus interpret equation (85) as a kinetic approximation of the moment system (84).

Next we apply the approach from Section 5 to the kinetic equation (85). Introducing only a single small discretization parameter $\tilde{\tau}$, we find the following approximative equation of (85)

$$\frac{\partial \varphi}{\partial t}(t, \mathbf{x}, \mathbf{n}) + c_D n_i \frac{\partial \varphi}{\partial x_i}(t, \mathbf{x}, \mathbf{n}) = (\Psi_{R,\tilde{\tau}}\varphi + \Psi_{N,\tilde{\tau}}\varphi + \Psi_{M,\tilde{\tau}}\varphi)(t, \mathbf{x}, \mathbf{n}). \tag{87}$$

The operators which appear on the right hand side are defined analogously to (71) and (72), namely

$$\Psi_{\alpha,\tilde{\tau}}(s)\varphi(s) \;=\; \sum_{i=0}^{\infty} \tilde{\tau}\delta_{i\tilde{\tau}}(s)\Psi_\alpha\varphi(s), \quad \alpha \in \{R, N, M\}. \tag{88}$$

Now we the identity (73) to find by a straight forward calculation, that exact solutions of the CAUCHY problem of (87) can be calculated by the following kinetic scheme

$$\begin{aligned}
\varphi(i\tilde{\tau} + t) &= T(t)\varphi_{i+}, \quad 0 < t < \tilde{\tau}, &(89)\\
\varphi_{i+} &= \frac{\tilde{\tau}}{\tau_R}\Theta_R\varphi_{i-} + \frac{\tilde{\tau}}{\tau_N}\Theta_N\varphi_{i-} + \frac{\tilde{\tau}}{\tau_M}\Theta_M\varphi_{i-} + \\
&\quad \Big(1 - \frac{\tilde{\tau}}{\tau_R} - \frac{\tilde{\tau}}{\tau_N} - \frac{\tilde{\tau}}{\tau_M}\Big)\varphi_{i-}. &(90)
\end{aligned}$$

Similar to the last section we use at the update times $i\tilde{\tau}$, $i \in \mathbb{N}$, the abbreviations φ_{i+} and φ_{i-} for the right hand side and left hand side limits, respectively. Furthermore we denote the initial data by φ_{0-}. If $\tilde{\tau}$ is sufficiently small, i.e. $3\tilde{\tau} \le \min\{\tau_R, \tau_N, \tau_M\}$, we conclude, that any solution of (87) is positive if we start with positive initial data.

The kinetic scheme (89)-(90) can be generalized by introducing three different and small discretization parameters $\tilde{\tau}_R$, $\tilde{\tau}_N$ and $\tilde{\tau}_M$ corresponding to the three relaxation operators on the right hand side of (85). In this case we end up with nonequidistant intervals of free transport and different kinds of update times. The set $\mathcal{T}$ of update times is given by all multiples of $\tilde{\tau}_R$, $\tilde{\tau}_N$ and $\tilde{\tau}_M$, i.e.

$$\mathcal{T} \;=\; \bigcup_{\alpha\in\{R,\,N,\,M\}} \bigcup_{i\in\mathbb{N}} \{i\tilde{\tau}_\alpha\}. \tag{91}$$

Henceforth we denote the elements of $\mathcal{T}$ by $0 = t_0 < t_1 < ...$
We use again the abbreviations φ_{i+} and φ_{i-} for the right hand side and left hand side limits at the update time t_i, respectively. The resulting general scheme reads then

$$\begin{aligned} \varphi(i\tilde{\tau}+t) \;&=\; T(t)\varphi_{i+}, \quad 0 < t < t_{i+1} - t_i, & (92)\\ \varphi_{i+} \;&=\; \gamma_{i,R}\Theta_R\varphi_{i-} + \gamma_{i,N}\Theta_N\varphi_{i-} + \gamma_{i,M}\Theta_M\varphi_{i-} + \\ &\quad \Big(1 - \gamma_{i,R} - \gamma_{i,N} - \gamma_{i,M}\Big)\varphi_{i-}, & (93) \end{aligned}$$

where $\gamma_{i,\alpha} = \tilde{\tau}_\alpha/\tau_\alpha$ if t_i is a multiple of $\tilde{\tau}_\alpha$, and $\gamma_{i,\alpha} = 0$ otherwise. We proceed with the following remarks.

1. There is an approximate equation similar to (87), so that the scheme (92)-(93) produces exact solutions of this equation.

2. If $\tilde{\tau}_R$, $\tilde{\tau}_N$ and $\tilde{\tau}_M$ are sufficiently small, all assertions of Lemma 5.1 are satisfied by the scheme (92)-(93).

3. If we apply the moment map $\vec{u}$ to phase densities produced by (92)-(93), we obtain good approximate solutions of the moment system (84), at least for small values of τ_M.

The content of the last assertion can be illustrated most easily by setting

$$\tilde{\tau}_M = \tau_M \quad \text{and} \quad \tilde{\tau}_R = \tilde{\tau}_N = \tilde{\tau} \ll \tau_M \tag{94}$$

in (92)-(93). The resulting kinetic scheme agrees, except for the moment integration, with the standard approach for moment systems which we have described above. In particular, we find that

1. a phase density φ will be replaced by $\Theta_M\varphi$ at the multiples of τ_M,

2. the kinetic equation is solved within the time intervals $(i\tau_M,\, i\tau_M + \tau_M)$ by the scheme (76)-(77) defined in the last section.

Finally, we summarize the last two sections as follows.

1. The equation (85) is a kinetic approximation of the MEP moment system (84), so that (85) and the original kinetic equation (36) have (i) the same transport term on the left hand side and (ii) a sum of relaxation operators on the rights hand side.

2. There are kinetic schemes both for the kinetic equation and for the moment system and all schemes have the same formal structure.

3. The common structure of all schemes can be described as follows. Intervals of free transport are interrupted by update times. At any update time, a free transport phase density will by replaced by a convex combination of the phase density itself and of three corresponding MEP phase densities. The weights appearing in the convex combinations depend in general on the update time.

Recall that these properties rely on the CALLAWAY collision operator and the MEP as closure principle. A generalization to other kinetic equations may fail due to more complicated collision operators or due to the nonapplicability of the MEP, which happens for the BGK-model of the BOLTZMANN equation. However, we think, that the reduced BOLTZMANN-PEIERLS-Equation is a good model in order to study the relationship between a kinetic equation and its moment systems. Analytical investigations are still to be completed. Nevertheless, in the next section we discuss some numerical results.

7 Numerical examples

The results of the proceeding sections will be illustrated by two numerical examples. For simplicity we set $\tau_R = \infty$, so that from a 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 as a pure wave phenomenon. Furthermore we assume that the phase density does not depend on x_2. In order to simulate interesting effects, we consider the following macroscopical initial data for the energy density e^0 and the momentum densities $\mathbf{p}^0$ (cf. figure 1 for the energy density).

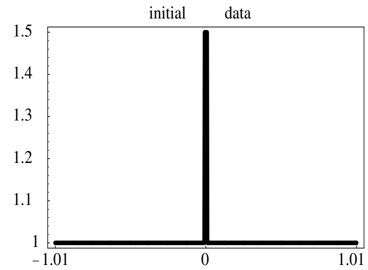

Figure 1: Initial energy pulse

$$e^0(\mathbf{x}) = \begin{cases} 1.5 & \text{if} \quad |x_1| \leq 0.01 \\ 1.0 & \text{if} \quad |x_1| > 0.01 \end{cases}, \quad \mathbf{p}^0(\mathbf{x}) = 0. \tag{95}$$

On the microscopic level we assume, that the phonon gas is initially in equilibrium, i.e.

$$\varphi^0 = \Theta_R \varphi^0. \tag{96}$$

Furthermore, the DEBYE speed c_D is set to 0.5.

All figures corresponding to the kinetic equation (36) and to its moment systems (84) are calculated by means of the kinetic schemes (76)-(77) and (89)-(90), respectively. Obviously, a suitable discretization with respect to $\mathbf{x}$ and $\mathbf{n}$ was chosen. In order to calculate the MEP projectors Θ_M we solved the nonlinear optimization problem 4.2 for the corresponding LAGRANGE multipliers by a gradient method.

The first example concerns the evolution of the initial energy pulse (95) according to the kinetic equation and for different values of τ_N.

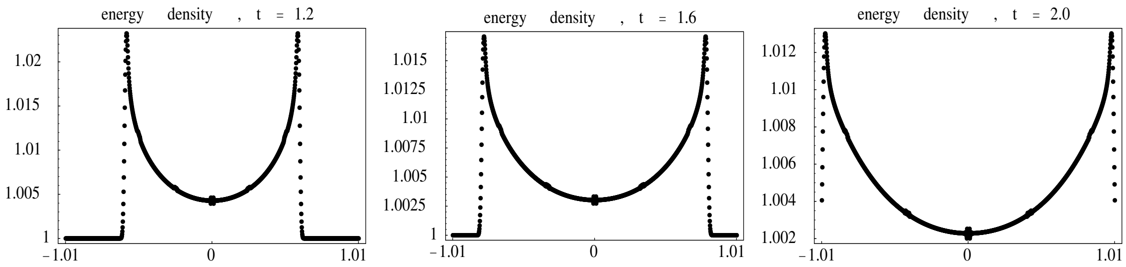

Figure 2: Example 1. Evolution of the energy pulse for $\tau_N = 2.0$

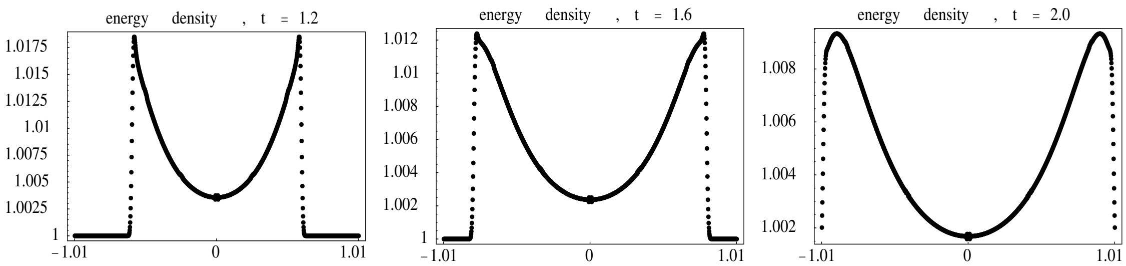

Figure 3: Example 1. Evolution of the energy pulse for $\tau_N = 1.0$

The Figures 2-4 show the spatial dependence of the energy density at different times. They correspond to $\tau_N = 2.$, $\tau_N = 1.$ and $\tau_N = 0.5$, respectively. According to [10] we can interpret the results as follows. For large values of τ_N, as in Figure 2, the pulse is ballistic and its fronts move with the DEBYE speed c_D to the left and to the right, respectively. Figure 4 illustrates the case of small τ_N. Here, the shape of the pulse is characteristic for the so called second sound, that propagates with a speed less than c_D (in our 2D case about $0.7c_D$). In Figure 3 we observe a transition

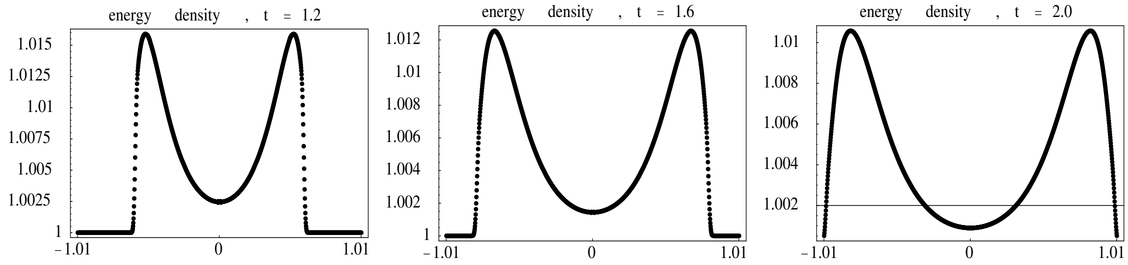

Figure 4: Example 1. Evolution of the energy pulse for $\tau_N = 0.5$

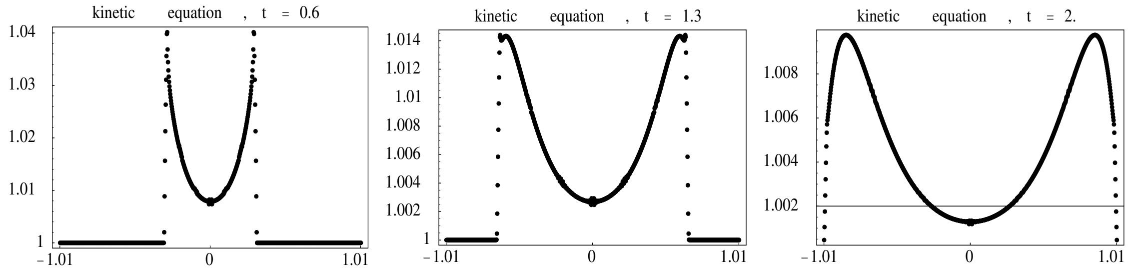

Figure 5: Example 2. Evolution of the energy pulse according to the kinetic equation

regime. The pulse starts as a ballistic pulse. After about 1.6 time units it changes its shape and becomes second sound. The second example illustrates the relationship between solutions of the kinetic equation and solutions of the moment systems. The initial data are again given by (95), the relaxation time τ_N is set to 0.7. The energy density corresponding to a solution of the CAUCHY problem of the kinetic equation is depicted in Figure 5, whereas the Figures 6-9 show the evolution of the initial energy pulse according to various moment systems. The moment systems are denoted as follows. The moment system of order s corresponds to a vector of moment weights $\vec{m}_s$ containing all tensors with respect to the components of $\mathbf{n}$ up to order s, namely

$$\vec{m}_s(\mathbf{n}) = \Big(1,\, n_1,\, n_2,\, n_1^2,\, n_1 n_2,\, n_2^2,\, ...\Big)^T \tag{97}$$

Note, that not all components of $\vec{m}_s$ are linear independent. In particular, we find, that only $2s+1$ components of $\vec{m}_s$ are linear independent. The Figures 6 and 7 reveal, that moment systems with a small number of moments produce quite bad approximations. However, the results become better if the number of moments is increased. Finally, we have a good correspondence of the kinetic equation and of the moment system of order 40 in Figure 9. Furthermore, the Figures 6-9 exhibit, how the number of appearing waves increases with the order of the moment system.

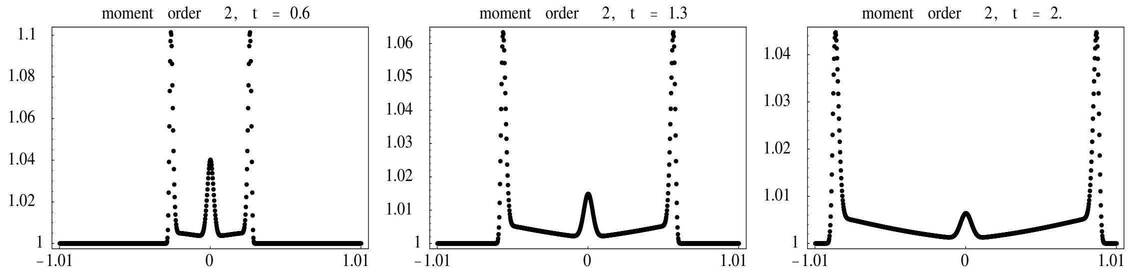

Figure 6: Example 2. Evolution of the energy pulse according to the moment system of order 2

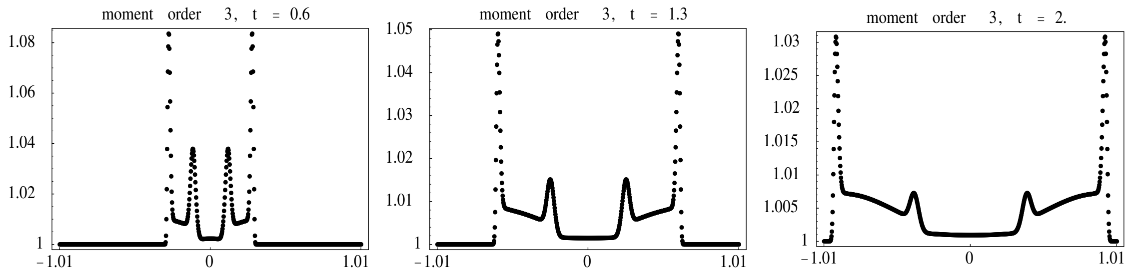

Figure 7: Example 2. Evolution of the energy pulse according to the moment system of order 3

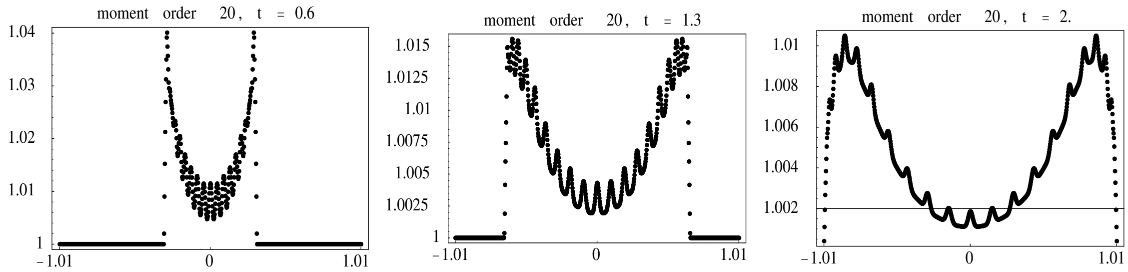

Figure 8: Example 2. Evolution of the energy pulse according to the moment system of order 20

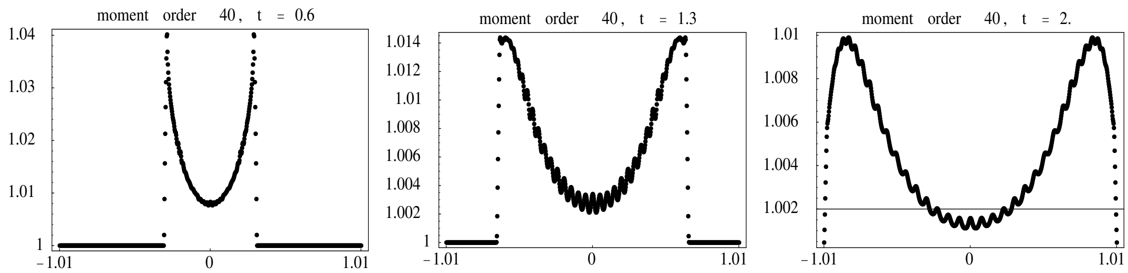

Figure 9: Example 2. Evolution of the energy pulse according to the moment system of order 40

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