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The Maximum Entropy Principle Revisited

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Abstract

We study the effect of the *Maximum Entropy Principle* (MEP) on the thermodynamic behaviour of gases. The MEP relies on the kinetic theory of gases and yields the local constitutive equations of *Extended Thermodynamics*.

There are two extreme cases on the scale of the kinetic theory: Dominance of particle interactions and free flight. In its current form the MEP gives the phase density that maximizes the entropy at each instant of time. This is appropriate in case of dominant particle interaction but it is not adequate for free flight. Here we introduce a modified MEP that is capable to link both extreme cases.

To illustrate the way the modified MEP works, we consider an example which leads in the case of dominant particle interactions to the EULER equations. In addition there results a representation theorem that contains the global solutions of the EULER equations with all shock interactions for arbitrary large variations of the initial data.

1 Extended Thermodynamics Versus Kinetic Theory

1.0 Introduction

Extended Thermodynamics was established in 1966 by I. Müller in order to remove the paradoxes of heat conduction and shear pulses in viscous materials [8]. The theory was brought into its present form by I. Müller and I Shi Liu [6] in 1983. In the same year T. Ruggeri showed that the equations of Extended Thermodynamics (ET) constitute a quasilinear symmetric hyperbolic system with a convex extension [10].

Up to now the closure problem of ET was solved by means of the phenomenological entropy principle. However, it turned out that the MEP may serve to link the closure problem to the underlying kinetic or microscopic theory. The fact that the MEP implies the phenomenological entropy principle was first shown by W. Dreyer in 1987 [4].

In 1996 G. Boillat and T Ruggeri generalized and improved Dreyer's reasonings [2].

The strategy of ET in cases of high Mach numbers and/or high frequencies of disturbances was studied by W. Weiss in 1990 [11] and [16].

The same subject was investigated by C.D. Levermore in 1995 who relies also on the MEP. However, he suggested to consider the nonlinear closure also with respect to those variables which vanish in equilibrium. This was not considered before [5].

Some other modern kinetic schemes bear a resemblance to the current study. These were studied independently of ET by B.Pertame in [12], [13],[14] mainly for the Euler system and, relying on ET, by C.D. Levermore [5] and by P. Le Tallec , J.P. Perlat [15] for higher order moment systems. Regarding the MEP up to now the kinetic schemes as well as ET only consider the limit $\tau_{ME} \to 0$, where τ_{ME} is the free-flight time interval.

1.1 A Survey on Extended Thermodynamics

Extended Thermodynamics (ET) is a field theory for the description of thermodynamic processes. The scheme of ET consists of the following postulates (i) - (v):

(i) *The state of a body at any time t is completely determined by M volume densities u_A (with M multiindices A) which are given at every point $\mathbf{x}$ of the body.*

The functions $u_A(t, \mathbf{x})$ are the basic variables of ET. Among them there are the mass density ρ, the momentum density ρv_k, the energy density ρe and so on. Sometimes it is useful to replace some of these by other variables which are not volume densities, like the velocity or the temperature.

(ii) *The field equations for the variables u_A rely on equations of balance which read*

$$\begin{aligned} \frac{\partial u_A}{\partial t} + \frac{\partial F_{Ak}}{\partial x_k} &= P_A \qquad \textit{in regular points,} && (1.1) \\ -V_s [\![u_A]\!] + [\![F_{Ak}]\!] N_k &= 0 \qquad \textit{on singular surfaces.} && (1.2) \end{aligned}$$

N_k denote the components of the normal vector and V_s is the normal speed of the singular surface. The double brackets denote the jumps across the singular surface. The equations (1.1), (1.2) become field equations for the variables after they are supplemented by constitutive equations for the fluxes F_{Ak} and the productions P_A. The constitutive equations relate F_{Ak} and P_A to the variables in a material dependent manner.

(iii)$_1$ *In ET it is assumed that the constitutive equations are local in the variables:*

$$F_{Ak} = \tilde{F}_{Ak}(u_B), \quad P_A = \tilde{P}_A(u_B). \qquad (1.3)$$

A solution of (1.1), (1.2) and (1.3) is called *thermodynamic process.*

(iii)$_2$ *A solution of (1.1), (1.2) and (1.3) with $P_A = 0$ is an equilibrium process.*

(iv) *The field equations must be independent of an observer in the following sense:*

(iv)$_1$ *The combinations*

$$\frac{\partial u_A}{\partial t} + \frac{\partial F_{Ak}}{\partial x_k} - P_A$$

must form tensors with respect to GALILEIAN *transformations.*

(iv)$_2$ *Those parts of* $\tilde{F}_{Ak}$ *and* $\tilde{P}_A$ *that are tensors with respect to* GALILEIAN *transformations must have the same form in every* GALILEIAN *system.*

A discussion and evaluation of this principle can be found in [7], [9].

A further restriction of the constitutive functions arises from the entropy principle

(v)$_1$ *There exist an entropy density h, an entropy flux* Φ_k *and an entropy production* σ which are given by local *constitutive functions*

$$h = \tilde{h}(u_B), \quad \Phi_k = \tilde{\Phi}_k(u_B), \quad \sigma = \tilde{\sigma}(u_B) \tag{1.4}$$

so that for thermodynamic processes

$$\frac{\partial h}{\partial t} + \frac{\partial \Phi_k}{\partial x_k} = \sigma \geq 0, \quad -V_s[\![h]\!] + [\![\Phi_k]\!]N_k := \sigma_s \geq 0 \tag{1.5}$$

holds in regular points and on singular surfaces, respectively.

The equality sign of $(1.5)_1$ holds in an equilibrium process, while the equality sign in $(1.5)_2$ defines the property of ideal walls, that are, for example, realized in contact surfaces of thermometers.

(v)$_2$ *The equations (1.5) form scalars with respect to* GALILEIAN *transformation. The entropy density and the entropy productions are scalars and the flux* Φ_k *contains a contribution* φ_k *that is a vector with respect to* GALILEIAN *transformation. The functions* $\tilde{h}, \tilde{\varphi}_k$ *and* $\tilde{\sigma}$ *must have the same form in every* GALILEIAN *frame.*

(v)$_3$ *In case that the energy density* ρe *is among the variables* u_A*, and when* ρs *denotes the equilibrium part of the entropy density, then the quantity*

$$T := \left(\frac{\partial \rho s}{\partial \rho e}\right)^{-1} \tag{1.6}$$

is the absolute temperature.

(v)$_5$ *The matrix of second derivatives of* $\tilde{h}$ *with respect to the variables* u_A *must be negative definite.*

These restrictions lead to quite explicit constitutive functions. For ideal gases they are so restrictive that they completely determine the fluxes F_{Ak}.

In general, the restrictions guarantee that the resulting system of field equations is of symmetric hyperbolic type with a convex extension, see the excellent textbook by Müller & Ruggeri [9].

1.2 Survey on Kinetic Theory

We consider a monatomic gas at "high" temperature and "low" number density of atoms so that it can be described by the phase density $f(t, \mathbf{x}, \mathbf{c})$ which gives the number density of atoms in the neighbourhood $d\mathbf{x}d\mathbf{c}$ of the phase space point $(\mathbf{x}, \mathbf{c}) :=$ (position, velocity) at time t. The phase density obeys the BOLTZMANN equation

$$\frac{\partial f}{\partial t} + c_k \frac{\partial f}{\partial x_k} = S(f). \tag{1.7}$$

S denotes the collision operator. One of its possible explicit forms will be given in section 2.1.

We form moments of f that we may identify with the variables u_A and the fluxes F_{Ak} as follows:

$$u_A(t, \mathbf{x}) = m \int c_A f(t, \mathbf{x}, \mathbf{c}) d^3\mathbf{c}, \;\; F_{Ak}(t, \mathbf{x}) = m \int c_A c_k f(t, \mathbf{x}, \mathbf{c}) d^3\mathbf{c}. \tag{1.8}$$

m denotes the atomic mass and c_A abbreviates the tensorial product $c_{i_1} c_{i_2} \ldots c_{i_M}$ and c_A is put equal to 1 for $A = 0$. The $\mathbf{c}$ integrations ranges from $-\infty$ to $+\infty$. When we furthermore define the productions P_A according to

$$P_A(t, \mathbf{x}) = m \int c_A S(f) d^3\mathbf{c},$$

it becomes obvious that the equations of balance (1.1) result from the BOLTZMANN equation. In ET these appear as postulates.

The entropy inequality (1.5) may likewise be considered as a consequence of the BOLTZMANN equation.

To achieve this we define entropy density, entropy flux and entropy production as

$$\begin{aligned} h(t, \mathbf{x}) &= -k \int f(t, \mathbf{x}, \mathbf{c}) \ln \left(\frac{1}{y} f(t, \mathbf{x}, \mathbf{c}) \right) d^3\mathbf{c}, \\ \Phi_k(t, \mathbf{x}) &= -k \int c_k f(t, \mathbf{x}, \mathbf{c}) \ln \left(\frac{1}{y} f(t, \mathbf{x}, \mathbf{c}) \right) d^3\mathbf{c}, \\ \sigma(t, \mathbf{x}) &= -k \int S(f(t, \mathbf{x}, \mathbf{c})) \ln \left(\frac{1}{y} f(t, \mathbf{x}, \mathbf{c}) \right) d^3\mathbf{c}. \end{aligned} \tag{1.9}$$

k is BOLTZMANN'S constant and $y = \frac{m^3}{h}$, where h denotes PLANCK'S constant. Obviously (1.7) implies $(1.5)_1$. The proof that $\sigma \geq 0$ can be found in [9].

We have thus partially derived the laws of ET from a kinetic point of view.

However, the most important feature of ET is still missing, viz. the local constitutive equations

$$F_{Ak} = \tilde{F}_{Ak}(u_B), \quad S_A = \tilde{S}_A(u_B), \quad h = \tilde{h}(u_B), \quad \Phi_k = \tilde{\Phi}_k(u_B). \tag{1.10}$$

The kinetic analogue to the assumption (1.10) of ET is a phase density whose dependence on t and $\mathbf{x}$ is implicit through a dependence on $u_B(t, \mathbf{x})$:

$$f(t, \mathbf{x}, \mathbf{c}) = w(u_B(t, \mathbf{x}), \mathbf{c}).$$

If w were known we would use the definitions (1.9) in order to calculate the constitutive functions (1.10).

1.3 The Maximum Entropy Principle

The Maximum Entropy Principle (MEP) yields a phase density w that implies constitutive functions (1.10) so that the resulting system of field equation is of symmetric hyperbolic type with a convex extension.

According to the MEP the phase density w maximizes the entropy density h under the constraints of prescribed values of $u_A = m \int d\mathbf{c} c_A f$.

We take care of these constraints by LAGRANGE multiplies Λ_A, which are functions of u_A but not of $\mathbf{c}$, so that we can maximize the expression

$$-k \int f \ln \left(\frac{1}{y} f \right) d^3\mathbf{c} - \sum_{A=1}^{M} \Lambda_A \left(m \int c_A f d^3\mathbf{c} - u_A \right)$$

without constraints.

The resulting phase density reads

$$w(u_B, \mathbf{c}) = \hat{w}(\Lambda_B, \mathbf{c}) = y \cdot \exp \left[-1 - \frac{m}{k} \sum_{B=1}^{M} \Lambda_B c_B \right].$$

Thus we may obtain the equations

$$u_A = \hat{u}_A(\Lambda_B),\ F_{Ak} = \hat{F}_{Ak}(\Lambda_B),\ S_A = \hat{S}_A(\Lambda_B),\ h = \hat{h}(\Lambda_B),\ \Phi_k = \hat{\Phi}_k(\Lambda_B).$$

The equations $u_A = \hat{u}_A(\Lambda_B)$ must be inverted to give $\Lambda_A = \tilde{\Lambda}_A(u_B)$, which are used to eliminate the LAGRANGE multiplies from all other functions.

It is shown in [4], [9] and [2] that there holds

$$\frac{\partial u_A}{\partial \Lambda_B} = \frac{\partial u_B}{\partial \Lambda_A} \text{ -- neg. def.}, \quad \frac{\partial f_{Ak}}{\partial \Lambda_B} = \frac{\partial f_{Bk}}{\partial \Lambda_A}, \quad \frac{\partial^2 h}{\partial \Lambda_A \partial \Lambda_B} \text{ -- neg. def.}$$

whereby the symmetric hyperbolic character of the field equations is established.

1.4 The Strategy of Extended Thermodynamics

The first fourteen moments of the phase density have an easy physical interpretation. For $c_A = (1, c_i, \frac{1}{2}\mathbf{c}^2)$ we obtain $u_A = (\rho, \rho v_i, \rho e)$, i.e. the mass density, the momentum density and the energy density. v_i and e denote the velocity and the specific energy, respectively.

The corresponding balance equations for these variables are conservation laws, $S_A = 0$, and they contain the fluxes $F_{Ak} = (\rho v_k, P_{ik}, Q_k)$. These give the mass flux, the momentum flux and the energy flux. Momentum flux and energy flux can be decomposed as

$$\begin{aligned} P_{ik} &= \rho v_i v_k + p_{ik} = \rho v_i v_k + p\delta_{ik} + p_{<ik>}, \\ Q_k &= \rho e v_k + p_{ik} v_i + q_k = \left(\rho u + p + \frac{\rho}{2} v^2\right) v_k + p_{<ik>} v_i + q_k. \end{aligned}$$

p_{ik} is the pressure tensor which can be decomposed further into pressure p and pressure deviator $p_{<ik>}$. u denotes the internal energy and q is the heat flux. If we would stop here, that is we would describe the thermodynamic state by the first five moments as variables, then the resulting phase density that maximizes the entropy would be the MAXWELLIAN

$$f_M(t, \mathbf{x}, \mathbf{c}) = w_M(u_B(t, \mathbf{x}), \mathbf{c}) = \frac{\rho}{m} \sqrt{\frac{m}{2\pi k T}}^3 \exp\left(-\frac{m}{2kT}(\mathbf{c} - \mathbf{v})^2\right). \qquad (1.11)$$

Note that the temperature T appears here due to postulate (1.6) which yields $u = \frac{3}{2}\frac{k}{m}T$.

It follows that $p_{<ik>} = 0$, $q_i = 0$ and we end up with the EULER equations. Their explicit form is given in section 3.3.

Next we describe the strategy of ET:

When it turns out that a thermodynamic process which is described by the EULER equations does not agree with experimental data, the set of variables will be *extended.*

Instead of $u_A = (\rho, \rho v_i, \rho e)$ we choose $u_A = (\rho, \rho v_i, \rho e, P_{ij}, Q_i)$ as variables. These describe a thermodynamic state by thirteen independent[1] variables.

The corresponding fluxes and productions are

$$F_{Ak} = (\rho v_k, P_{ik}, Q_k, M_{ijk}, N_{ik}), \quad S_A(0, 0_i, 0, S_{<ij>}, S_i).$$

The resulting phase density that maximizes the entropy is equivalent to GRADS phase density $w_G(u_A(t, \mathbf{x}), \mathbf{c})$ up to terms quadratic in $p_{<ij>}$ and q_i, see [9].

w_G relates the unknown fluxes M_{ijk} and N_{ik} and productions $S_{<ij>}$ and S_i to the variables u_B.

The thirteen field equations constitute again a symmetric hyperbolic system which includes the NAVIER STOKES FOURIER theory in an approximative manner. We refer again the reader to [9] for the details.

If this system also does not describe a thermodynamic process satisfactory, then more moments as variables must be taken into account.

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[1] Note that $\rho e = \frac{3}{2} P_{ii}$ holds for ideal gases.

A careful study by W. Weiss [11] reveals that the number of variables quickly and dramatically exceeds $N = 13$.

In the next two chapters we develop a new idea that may eventually be capable to stay with 13 variables even for high Mach numbers and far from equilibrium.

2 The Maximum Entropy Principle Revisited

2.1 Physical Foundations

Three characteristic lengths control the properties of gases. These are

$$l_C = d, \qquad l_R = \frac{m}{\pi d^2}\frac{1}{\rho}, \qquad l_G = \frac{1}{\max\left(\frac{|grad_x f|}{f}\right)} \approx \frac{1}{\max\left(\frac{|grad_x \rho|}{\rho}\right)}. \tag{2.1}$$

A mean sound speed $c_0 = \sqrt{\frac{k}{m}T_0}$ may serve to define the corresponding characteristic times

$$\tau_C = \frac{1}{c_0} l_C, \qquad \tau_R = \frac{1}{c_0} l_R, \qquad \tau_G = \frac{1}{c_0} l_G. \tag{2.2}$$

d is the atomic diameter and m denotes the atomic mass. l_C, l_R and l_G are called interaction length, relaxation length and gradient length, respectively.

The length l_C gives the magnitude of the interaction radius. The relaxation length l_R determines the mean free path, which is the mean distance between two collisions. The gradient length l_G is a measure for the extension of macroscopic inhomogeneities, and may for example be given by the extension of the gas container or by the thickness of a shock wave.

For an easy discussion we rewrite the BOLTZMANN equation (1.7) in space coordinates relative to l_G and with an explicit but simplified expression for the production of collisions that is called KROOKs model:

$$\frac{\partial f}{\partial t} = -\frac{1}{\tau_G}\frac{c}{c_0}\left(\frac{c_k}{c}\frac{\partial f}{\partial x_k}\right) - \frac{1}{\tau_R}\left(f - f_M\right). \tag{2.3}$$

The evolution of the phase density due to free flight of the atoms is given by the first term of the rhs of (2.3). The second term takes into account the interaction of atoms in a very simple manner: It describes the relaxation of a given phase density to a MAXWELLIAN.

The validity of the Boltzmann equation relies on two inequalities that compare the collision time τ_C, which does not appear in (2.3) explicitely, with the gradient time τ_G and the relaxation time τ_R, viz.

$$\tau_C \ll \tau_R \qquad \textit{and} \qquad \tau_C \ll \tau_G. \tag{2.4}$$

Next we discuss the relations between τ_R and $\tau_G \frac{c_0}{c} \approx \tau_G \left(\frac{v}{c_0} + 1 \right)^{-1} = \tau_G \left(M_a + 1 \right)^{-1}$. Here v denotes the magnitude of the macroscopic velocity and $M_a = \frac{v}{c_0}$ is a mean MACH number. There are three ranges that lead to quite different macroscopic behaviour of the gas. For a discussion of these ranges we start at a time t where the fields $u_A(t, \mathbf{x})$ are assumed to be given, so that we can use them to determine the phase density at time t by maximizing the entropy.

Range I: $\tau_R \ll \tau_G \left(M_a + 1 \right)^{-1}$

In this range there is initially a fast relaxation. In all points of the gas the phase density approaches the local MAXWELLIAN w_M. Only after $f = w_M$ is locally reached, the gradient term in (2.3) starts to become important and determines the future development.

Under these conditions the gas can be described by the first few moments of the phase density as macroscopic variables u_A. For the extreme case of the inequality $\tau_R \ll \tau_G \left(M_a + 1 \right)^{-1}$we are justified to use $f = w_M$ at all times, and the macroscopic behaviour of the gas is then described by the EULER equations.

Note that here the gas looses very quickly the knowledge of the actual phase density that was realized at the former time t.

Range II: $\tau_R \gg \tau_G \left(M_a + 1 \right)^{-1}$

In this range we can first of all ignore the relaxation term in (2.3). The gas develops by free flight of its atoms and the knowledge on the initial phase density is conserved. Here many moments of the phase density are needed as variables u_A for a proper description of the macroscopic behaviour of the gas.

Range III: τ_R comparable with $\tau_G \left(M_a + 1 \right)^{-1}$

Both mechanisms of the rhs of (2.3) act simultanuously. Macroscopically this is realized by the appearance of heat conduction and viscosity.

If we approach this case starting from range I , then a proper macroscopic description is given by *Extended Thermodynamics* with thirteen fields which include the NAVIER STOKES FOURIER Therory in an approximative manner. This is carefully described in [9].

For increasing ratio $\tau_G \left(M_a + 1 \right)^{-1} / \tau_R$ an inreasing number of moments of f as macroscopic variables u_A must be included. On the macroscale the large quasilinear hyperbolic systems come thus into play.

However, if we approach range III starting from range II, then a proper description of macroscopic processes within the framework of *Extended Thermodynamics* is not possible anymore.

We shall now introduce a modification of the *Maximum Entropy Principle* that allows in all three ranges the description of macroscopic processes with only a few moments as variables.

As before we start at a time t, where the macrostate of the gas is given by a finite number of moments as variables $u_A (A = 1, 2, ..., N)$. We are looking for a solution of the Boltzmann equation (2.3) at time $t + \tau$ which is given at time t by $f(t, \mathbf{x}, \mathbf{c}) = w(u_A(t, \mathbf{x}), \mathbf{c})$. w is obtained by maximizing the entropy under the constraints of given $u_A(t, \mathbf{x})$.

This task is already partially solved by the representation

$$f(t+\tau, \mathbf{x}, \mathbf{c}) = w(u_A(t, \mathbf{x} - \mathbf{c}\tau), \mathbf{c}) + \frac{1}{\tau_R} \int_t^{t+\tau} \left[w_M(u_A(\vartheta, \mathbf{x} - \mathbf{c}(t+\tau-\vartheta)), \mathbf{c}) - f(\vartheta, \mathbf{x} - \mathbf{c}(t+\tau-\vartheta), \mathbf{c}) \right] d\vartheta \tag{2.5}$$

The first term of the rhs is due to free flight, while the second term takes care of the collisions. As a first approximation we replace the actual phase density under the time integral by that function that was obtained by maximization of entropy at time t. The resulting representation is thus evolutionary and reads

$$f(t+\tau, \mathbf{x}, \mathbf{c}) = w(u_A(t, \mathbf{x} - \mathbf{c}\tau), \mathbf{c}) + \frac{1}{\tau_R} \int_t^{t+\tau} (w_M - w) \left(u_A(\vartheta, \mathbf{x} - \mathbf{c}(t+\tau-\vartheta)), \mathbf{c} \right) d\vartheta. \tag{2.6}$$

Now the crucial argument will be given:

We follow the course of time by using (2.6) only up to the time $t + \tau_{ME}$, i.e. within the range $0 \leq \tau \leq \tau_{ME}$. We call τ_{ME} the time of *maximizing entropy.* At time τ_{ME} we calculate $u_A(t + \tau_{ME}, \mathbf{x})$ according to

$$u_A(t + \tau_{ME}, \mathbf{x}) = \int c_A f(t + \tau_{ME}, \mathbf{x}, \mathbf{c}) d^3\mathbf{c}. \tag{2.7}$$

and maximize the entropy again, however now for given $u_A(t + \tau_{ME}, \mathbf{x})$.

This procedure annihilates the knowledge on the former initial condition at time t. Thus entropy is created and the procedure of maximizing entropy has the same effect as the collision integral of the BOLTZMANN equation has.

By the appropriate choice of τ_{ME}, i.e. the appropriate sequence of subsequent maximizations of entropy, we are able to control for a fixed number of moments as variables whether we describe range I, II or III.

If we choose, for example, the first thirteen moments as variables, then the limit $\tau_{ME} \to 0$ yields the classical version of *Extended Thermodynamics* with 13 variables. Note that the limit $\tau_{ME} \to 0$ means that a finite time interval contains infinitely many maximizations.

On the other hand, if one realizes within the classical *Extended Thermodynamics* that 13 variables are not sufficient for a given process, the number of variables will be increased. Here the same effect is obtained by reducing the number of maximizations which leads from the collision controlled region to the region where the free flight becomes more and more important.

Next we shall illustrate these ideas for the simple case where the thermodynamic state is described by the first 5 moments of the phase density. The phase density that follows from the *Maximum Entropy Principle* is simply the *Maxwellian* w_M, and in the limit $\tau_{ME} \to 0$ there results the EULER equations. This case may serve to exhibit the subtle details of the whole procedure and gives as a most important result in addition a *global explicit weak solution of the Euler equations for arbitrary initial data of bounded variation.*

2.2 A new representation theorem for the initial value problem of the Euler system

According to the above presented reasonings we shall now formulate the iterated scheme for the mass density ρ, the velocity $\mathbf{v}$ and temperature T. To initialize the scheme we start with

- Bounded and integrable initial data for $\mathbf{x} \in \mathbb{R}^3$:
  $\rho(0,\mathbf{x}) = \rho_0(\mathbf{x}) \geq \epsilon > 0, \quad \mathbf{v}(0,\mathbf{x}) = \mathbf{v}_0(\mathbf{x}), \quad T(0,\mathbf{x}) = T_0(\mathbf{x}) \geq \delta > 0.$
- A fixed time $\tau_{ME} > 0$ of free flight, so that at equidistant times
  $t_n = n \cdot \tau_{ME}$, $(n = 0, 1, 2, ...)$, the maximization of entropy takes place.

For simplicity we shall later on set the particle mass m, Boltzmann‘s constant k and y equal to 1. The iterated scheme for the variables density ρ, velocity $\mathbf{v}$ and temperature T reads within the time interval $0 < \tau \leq \tau_{ME}$:

$$\begin{aligned} \rho(t_n+\tau,\mathbf{x}) &= \int_{-\infty}^{\infty} f_n(\mathbf{x}-\tau\mathbf{c},\mathbf{c})\, d^3\mathbf{c} \\ (\rho v_i)(t_n+\tau,\mathbf{x}) &= \int_{-\infty}^{\infty} c_i f_n(\mathbf{x}-\tau\mathbf{c},\mathbf{c})\, d^3\mathbf{c} \\ (\frac{1}{2}\rho v^2 + \frac{3}{2}\rho T)(t_n+\tau,\mathbf{x}) &= \int_{-\infty}^{\infty} \frac{1}{2}c^2 f_n(\mathbf{x}-\tau\mathbf{c},\mathbf{c})\, d^3\mathbf{c} \end{aligned} \tag{2.8}$$

Here $f_n(\mathbf{y},\mathbf{c}) = w_M(u_B(t_n,\mathbf{y}),\mathbf{c})$ is the three-dimensional MAXWELLIAN phase density :

$$f_n(\mathbf{y},\mathbf{c}) = \frac{\rho(t_n,\mathbf{y})}{(2\pi T(t_n,\mathbf{y}))^{3/2}} \cdot \exp(-\frac{(\mathbf{c}-\mathbf{v})^2}{2T(t_n,\mathbf{y})}) \tag{2.9}$$

This scheme can be brought into compact generic form, if we recall the abbreviations

$$\mathbf{c_A} = \begin{cases} 1 & , \quad A = 0 \\ c_i & , \quad A = i = 1,2,3 \\ \frac{1}{2}c^2 & , \quad A = 4 \end{cases} \tag{2.10}$$

Then the variables u_A and fluxes F_{Ak} read

$$\begin{aligned} u_A(t_n+\tau,\mathbf{x}) &= \int_{-\infty}^{\infty} \mathbf{c_A} f_n(\mathbf{x}-\tau\mathbf{c},\mathbf{c})\ d^3\mathbf{c} \\ F_{Ak}(t_n+\tau,\mathbf{x}) &= \int_{-\infty}^{\infty} \mathbf{c_A} c_k f_n(\mathbf{x}-\tau\mathbf{c},\mathbf{c})\ d^3\mathbf{c} \end{aligned} \tag{2.11}$$

Note that $u_0=\rho$, $u_i=\rho v_i\,(i=1,2,3)$ and $u_4=\frac{1}{2}\rho v^2+\frac{3}{2}T$.

The entropy density h and entropy flux Φ_k are

$$\begin{aligned} h(t_n+\tau,\mathbf{x}) &= -\int_{-\infty}^{\infty} (f_n ln f_n)(\mathbf{x}-\tau\mathbf{c},\mathbf{c})\ d^3\mathbf{c} \\ \Phi_k(t_n+\tau,\mathbf{x}) &= -\int_{-\infty}^{\infty} c_k (f_n ln f_n)(\mathbf{x}-\tau\mathbf{c},\mathbf{c})\ d^3\mathbf{c}\ . \end{aligned} \tag{2.12}$$

For $\tau=0$, w_M is the phase density that was obtained by maximizing the entropy at time t_n for given constraints $u_A(t_n,\mathbf{x})$. When the time $t_{n+1}=t_n+\tau_{ME}$ is reached there will be the next maximization of entropy under the new constraints $u_A(t_{n+1},\mathbf{x})$.

Within the range $0<\tau<\tau_{ME}$ the phase density solves the collision free Boltzmann equation.

Proposition 2.1. *Let* $0<\tau<\tau_{ME}$ *and* $n=0,1,2,....$

The fields $u_A(t_n+\tau,\mathbf{x})$, $F_{Ak}(t_n+\tau,\mathbf{x})$ *and all of its derivatives in space and time are smooth, and they satisfy the conservation laws*

$$\frac{\partial u_A}{\partial \tau}(t_n+\tau,\mathbf{x})+\frac{\partial F_{Ak}}{\partial x_k}(t_n+\tau,\mathbf{x})=0.$$

Remark: Note that these equations do not constitute a *local* quasilinear hyperbolic system for the variables u_A, because the fluxes F_{Ak} at time $t_n+\tau$ and position $\mathbf{x}$ depend on the whole field $u_A(\cdot,t)$ at time t.

Sketch of the proof: If we substitute $\mathbf{c}$ by $\mathbf{y}=\mathbf{x}-\tau\mathbf{c}$ in (2.11) and regard $f_n(\mathbf{y},\mathbf{c})=w_M(u_B(t_n,\mathbf{y}),\mathbf{c})$ we obtain

$$\begin{aligned} u_A(t_n+\tau,\mathbf{x}) &= \frac{1}{\tau^3}\int c_A w_M\left(u_B(t_n,\mathbf{y}),\frac{\mathbf{x}-\mathbf{y}}{\tau}\right) d^3\mathbf{y} \quad \text{and} \\ F_{Ak}(t_n+\tau,\mathbf{x}) &= \frac{1}{\tau^3}\int c_A \frac{x_k-y_k}{\tau} w_M\left(u_B(t_n,\mathbf{y}),\frac{\mathbf{x}-\mathbf{y}}{\tau}\right) d^3\mathbf{y} \end{aligned}$$

with $c_A=\left(1,\frac{x_i-y_i}{\tau},\frac{(\mathbf{x}-\mathbf{y})^2}{2\tau^2}\right)$. In these integrals the u_B's do not depend on $\mathbf{x}$ and τ. We have thus shown the smoothness of u_A, F_{Ak} and of all its derivatives with respect to τ and $\mathbf{x}$.

In order to prove the conservation form for these variables and fluxes we rely again on the expressions (2.11). There holds due to the chain rule:

$$\begin{aligned}
\partial_\tau u_A(t_n+\tau,\mathbf{x}) &= \int_{-\infty}^{\infty} \mathbf{c_A}\partial_\tau f_n(\mathbf{x}-\tau\mathbf{c},\mathbf{c})\ d^3\mathbf{c} \\
&= \int_{-\infty}^{\infty} \mathbf{c_A}\partial_{x_k} f_n(\mathbf{x}-\tau\mathbf{c},\mathbf{c})(-c_k)\ d^3\mathbf{c} \\
&= -\partial_{x_k}\int_{-\infty}^{\infty} \mathbf{c_A} c_k f_n(\mathbf{x}-\tau\mathbf{c},\mathbf{c})\ d^3\mathbf{c} \\
&= -\partial_{x_k} F_{Ak}(t_n+\tau,\mathbf{x}).
\end{aligned}$$

Proposition 2.2. *Let $\Omega \subset \mathbb{R}_0^+ \times \mathbb{R}^3$ be any bounded convex region in space and time. By $d\vec{o}$ we denote a positive oriented boundary element of $\partial\Omega$. The representations (2.11) have the following properties:*

(i) *In the limit $\tau_{ME} \to 0$ the volume densities u_A, fluxes F_{Ak}, the entropy density h and entropy flux Φ_k become local functions of the variables ρ, v_i and T, viz.*

$$u_A = \begin{pmatrix} \rho \\ \rho v_i \\ \rho\frac{v^2}{2}+\frac{3}{2}\rho T \end{pmatrix}, \quad F_{Ak} = \begin{pmatrix} \rho v_k \\ \rho v_i v_k + \rho T\delta_{ik} \\ \rho\left(\frac{v^2}{2}+\frac{5}{2}T\right)v_k \end{pmatrix}$$

$$h = \tfrac{3}{2}\rho\ln\left(T\rho^{-\frac{2}{3}}\right), \qquad \Phi_k = hv_k.$$

(ii) *For $\tau_{ME} > 0$ as well as in the* EULER*ian limit $\tau_{ME} \to 0$ we obtain the following weak formulation, which takes discontinuities into account:*

$$\int_{\partial\Omega} (u_A, F_{Ak})\, d\vec{o} = 0. \tag{2.13}$$

(iii) *In regular points the regular form of the* EULER *equations are satisfied for $\tau_{ME} \to 0$.*

(iv) *The following entropy inequality is satisfied for $\tau_{ME} > 0$ as well as in the* EULER*ian limit $\tau_{ME} \to 0$:*

$$\int_{\partial\Omega} (h, \Phi_k) d\vec{o} \geq 0. \tag{2.14}$$

The brackets (u_A, F_{Ak}) and (h, Φ_k) denote four-vectors in time (first position) and space (last three positions).

Remarks

(1) The limit $\tau_{ME} \to 0$ means that a thermodynamic process is realized by an infinite number of maximizations within a time intervall Δt.

(2) Each maximization increases the entropy, and for this reason the maximization of entropy simulates the interaction of the microscopic particles of the gas.

(3) In singular points of a shock curve with velocity v_s, which may appear in the limit $\tau_{ME} \to 0$, the RANKINE-HUGONIOT equations

$$-v_s[\![u_A]\!] + [\![F_{Ak}]\!]N_k = 0$$

hold. In addition, there is a positiv entropy production according to

$$\sigma_s = -v_s[\![h]\!] + [\![\Phi_k]\!]N_k \geq 0.$$

Sketch of the proof:
(i): In the limit $\tau_{ME} \to 0$ the fields $u_A = u_A(t, \mathbf{x})$ do not depend on $\mathbf{c}$ anymore, i.e. they are constants regarding the $\mathbf{c}$-integrations. Using this fact, we obtain by a straightforward calculation the representations given in (i). The convergence can be proved in the L_1-norm. Regarding the proposition (ii) + (iii) it is sufficient to prove the weak form $\int_{\partial\Omega}(u_A, F_{Ak})d\vec{o} = 0$ for $\tau_{ME} > 0$. The EULERian limit $\tau_{ME} \to 0$ can be obtained by means of proposition 2.2 (i).

Let be $\tau_{ME} > 0$:

In this case the time axis is devided by the maximization times $0 = t_0 < t_1 < t_2 < \cdots$, so that the convex domain Ω can be decomposed into the subdomains

$$\begin{cases} \Omega_0 & = \left\{(\delta, \mathbf{x}) \in \Omega \middle|\, 0 \leq \delta \leq \frac{t_0+t_1}{2}\right\}, \\ \Omega_n & = \left\{(\delta, \mathbf{x}) \in \Omega \middle|\, \frac{t_{n-1}+t_n}{2} \leq \delta \leq \frac{t_n+t_{n+1}}{2}\right\} (n = 1, 2, 3, \ldots). \end{cases} \tag{2.15}$$

Since $\int_{\partial\Omega}(u_A, F_{Ak})d\vec{o} = \sum_{n\geq 0}\int_{\partial\Omega_n}(u_A, F_{Ak})d\vec{o}$, it is sufficient to assume without loss of generality that the time range

$$\Theta_\Omega = \left\{t \geq 0 \middle|\, \exists x \in \mathbb{R}^3 : (t, \mathbf{x}) \in \Omega\right\}$$

of Ω contains at most one maximization time t.

Then for ε out of the range $0 < \varepsilon < \frac{1}{2}\tau_{ME}$ we define a further decomposition of each $\Omega_n, n \geq 1$, into three parts:

$$\begin{cases} \Omega^\varepsilon_{n,L} & = \{(\delta, \mathbf{x}) \in \Omega_n |\, \delta \leq t_n - \varepsilon\}, \\ \Omega^\varepsilon_{n,M} & = \{(\delta, \mathbf{x}) \in \Omega_n |\, t_n - \varepsilon \leq \delta \leq t_n + \varepsilon\}, \\ \Omega^\varepsilon_{n,R} & = \{(\delta, \mathbf{x}) \in \Omega_n |\, \delta \geq t_n + \varepsilon\}. \end{cases} \tag{2.16}$$

These decompositions are visualized in the following two graphs:

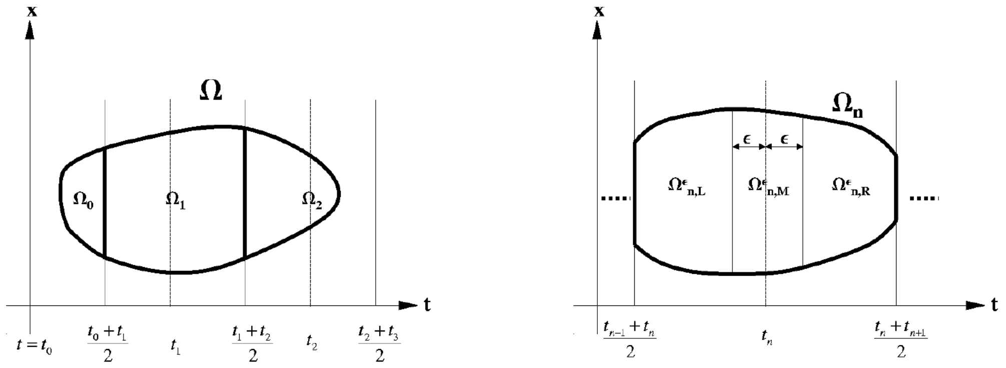

Figure 2.1: The decompositions of Ω and Ω_n.

We obtain

$$\int\limits_{\partial\Omega_n} (u_A, F_{Ak}) d\vec{o} = \int\limits_{\partial\Omega^\varepsilon_{n,L}} (u_A, F_{Ak}) d\vec{o} + \int\limits_{\partial\Omega^\varepsilon_{n,R}} (u_A, F_{Ak}) d\vec{o} + \int\limits_{\partial\Omega^\varepsilon_{n,M}} (u_A, F_{Ak}) d\vec{o},$$

and proceed to show that the first two integrals on the right-hand side must vanish:

The fields $u_A(t, \mathbf{x})$ and $F_{Ak}(t, \mathbf{x})$ are smooth in the domains $\Omega^\varepsilon_{n,L}$, $\Omega^\varepsilon_{n,R}$. For both domains we thus can apply the GAUSSian Divergence Theorem to the conservation law $\partial_t u_A + \partial_{x_k} F_{Ak} = 0$ resulting from the first proposition in order to get

$$\int\limits_{\partial\Omega^\varepsilon_{n,L}} (u_A, F_{Ak}) d\vec{o} = \int\limits_{\partial\Omega^\varepsilon_{n,R}} (u_A, F_{Ak}) d\vec{o} = 0.$$

This implies

$$\begin{aligned} \int\limits_{\partial\Omega_n} (u_A, F_{Ak}) d\vec{o} &= \int\limits_{\partial\Omega^\varepsilon_{n,M}} (u_A, F_{Ak}) d\vec{o} = \lim_{\varepsilon\to 0} \int\limits_{\partial\Omega^\varepsilon_{n,M}} (u_A, F_{Ak}) d\vec{o} \\ &= \int_{\Omega^*_n} \left\{ \int c_A \left[f_n(\mathbf{x}, \mathbf{c}) - f_{n-1}(\mathbf{x} - \tau_{ME}\mathbf{c}, \mathbf{c}) \right] d^3\mathbf{c} \right\} d^3\mathbf{x}, \end{aligned}$$

where $\Omega^*_n = \{\mathbf{x} \in \mathbb{R}^3 | (t_n, \mathbf{x}) \in \Omega\}$. t_{n-1} is the maximization time that preceeds the maximization time t_n. The MAXWELLian f_n has to be read off from (2.9).

The last integral expression vanishes for $c_A = \left(1, c_i, \frac{1}{2}\mathbf{c}^2\right)$ due to

$$\int c_A f_n(\mathbf{x}, \mathbf{c}) d^3\mathbf{c} = \int c_A f_{n-1}(\mathbf{x} - \tau_{ME}\mathbf{c}, \mathbf{c}) d^3\mathbf{c} \tag{2.17}$$

which expresses the constraints that were used for the maximization procedure. We have thus established that the weak form (2.13) for a general convex domain

Ω is implied by the representations (2.11). In particular (2.13) holds also in the EULERian limit $\tau_{ME} \to 0$.

In each regular point $(t, \mathbf{x})$ we can now apply the GAUSSian Divergence Theorem to (2.13) in the EULERian limit in order to get the proposition (iii).

Regarding the proposition (iv) which states the existence of the entropy inequality (2.14), we start the proof again with the decompositions (2.15) and (2.16) of Ω. Since $\int_{\partial\Omega}(h, \Phi_k)d\vec{o} = \sum_{n\geq 0}\int_{\partial\Omega_n}(h, \Phi_k)d\vec{o}$, it is sufficient to prove $\int_{\partial\Omega_n}(h, \Phi_k)d\vec{o} \geq 0$ for each n:

We obtain

$$\int_{\partial\Omega_n}(h, \Phi_k)d\vec{o} = \int_{\partial\Omega^\varepsilon_{n,L}}(h, \Phi_k)d\vec{o} + \int_{\partial\Omega^\varepsilon_{n,R}}(h, \Phi_k)d\vec{o} + \int_{\partial\Omega^\varepsilon_{n,M}}(h, \Phi_k)d\vec{o} \qquad (2.18)$$

and shall show that the first two integrals on the right hand side vanish:

The entropy-function $h(t, \mathbf{x})$ and the entropy-flux $\Phi_k(t, \mathbf{x})$ are smooth fields in the domain $\Omega^\varepsilon_{n,R}$, because according to (2.12) we have for $(t, \mathbf{x}) \in \Omega^\varepsilon_{n,R}$

$$\begin{aligned} h(t, \mathbf{x}) &= -\int (f_n \ln f_n)(\mathbf{x} - (t - t_n)\mathbf{c}, \mathbf{c})d^3\mathbf{c}, \\ \Phi_k(t, \mathbf{x}) &= -\int c_k(f_n \ln f_n)(\mathbf{x} - (t - t_n)\mathbf{c}, \mathbf{c})d^3\mathbf{c}. \end{aligned}$$

In this domain we obtain due to the chain rule:

$$\partial_t h(t, \mathbf{x}) = -\partial_{x_k}\Phi_k(t, \mathbf{x}). \qquad (2.19)$$

This implies $\int_{\partial\Omega^\varepsilon_{n,R}}(h, \Phi_k)d\vec{o} = 0$, and $\int_{\partial\Omega^\varepsilon_{n,L}}(h, \Phi_k)d\vec{o} = 0$ can likewise be obtained.

For every sufficiently small $\varepsilon > 0$ there holds

$$\begin{aligned} \int\limits_{\partial\Omega_n}(h, \Phi_k)d\vec{o} &= \lim_{\varepsilon\to 0}\int\limits_{\partial\Omega^\varepsilon_{n,M}}(h, \Phi_k)d\vec{o} \qquad (2.20) \\ = \int\limits_{\Omega^*_n}&\left\{\int [-(f_n \ln f_n)(\mathbf{x}, \mathbf{c}) + (f_{n-1}\ln f_{n-1})(\mathbf{x} - \tau_{ME}\mathbf{c}, \mathbf{c})]\, d^3\mathbf{c}\right\} d^3\mathbf{x}, \end{aligned}$$

where $\Omega^*_n = \{\mathbf{x} \in \mathbb{R}^3 | (t_n, \mathbf{x}) \in \Omega\}$, and $t_{n-1} < t_n$ is the maximization time that preceeds t_n.

Next we shall show that the integral (2.20) is non-negative. To this we need the following

Lemma 2.1. *For $u, v > 0$ we have*

$$v \ln v - u \ln u = [\ln u + 1](v - u) + R(u, v) \qquad (2.21)$$

with the function $R(u, v) := v[\ln v - \ln u] - (v - u) \geq 0$.

Proof of Lemma 2.1. Due to TAYLORs formula there is a $\xi > 0$ between $u, v > 0$ such that

$$v \ln v = u \ln u + (\ln u + 1)(v - u) + \frac{1}{2\xi}(v - u)^2. \tag{2.22}$$

We conclude $R(u, v) = \frac{1}{2\xi}(v - u)^2 \geq 0$.

Now we apply Lemma 2.1. to $u = f_n(\mathbf{x}, \mathbf{c})$, $v = f_{n-1}(\mathbf{x} - \tau_{ME}\mathbf{c}, \mathbf{c})$:

$$\begin{aligned}
&\int \left[-(f_n \ln f_n)(\mathbf{x}, \mathbf{c}) + (f_{n-1} \ln f_{n-1})(\mathbf{x} - \tau_{ME}\mathbf{c}, \mathbf{c})\right] d^3\mathbf{c} \\
= \; & -\int \left[1 + \ln f_n(\mathbf{x}, \mathbf{c})\right] \left[f_n(\mathbf{x}, \mathbf{c}) - f_{n-1}(\mathbf{x} - \tau_{ME}\mathbf{c}, \mathbf{c})\right] d^3\mathbf{c} \\
& + \int R(f_n(\mathbf{x}, \mathbf{c}), f_{n-1}(\mathbf{x} - \tau_{ME}\mathbf{c}, \mathbf{c})) d^3\mathbf{c}.
\end{aligned} \tag{2.23}$$

The second integral is non-negative and the first one vanishes for the following reasons: $[1 + \ln f_n(\mathbf{x}, \mathbf{c})]$ is a quadratic polynomial in $\mathbf{c}$, containing only c_i and $\mathbf{c}^2$, and for $c_A = \left(1, c_i, \frac{1}{2}\mathbf{c}^2\right)$ there follows due to (2.17)

$$0 = \int c_A \left[f_n(\mathbf{x}, \mathbf{c}) - f_{n-1}(\mathbf{x} - \tau_{ME}\mathbf{c}, \mathbf{c})\right] d^3\mathbf{c}. \tag{2.24}$$

For $\tau_{ME} > 0$ we have thus established the entropy inequality (2.14). It is due to proposition 2.2 (i) that this inequality is also valid in the EULERian limit, where shocks may appear. ■

3 Some Initial Value Problems

The thermodynamic state in the neighbourhood of the EULERIAN limit is best suited to illustrate the mechanism of maximizing the entropy after subsequent non zero time intervals. To this we use the representations

$$\begin{aligned}
u_A(t + \tau, \mathbf{x}) &= m \int c_A w_M(u_B(t, \mathbf{x} - \mathbf{c}\tau), \mathbf{c}) d^3\mathbf{c} \\
F_{Ak}(t + \tau, \mathbf{x}) &= m \int c_A c_k w_M(u_B(t, \mathbf{x} - \mathbf{c}\tau), \mathbf{c}) d^3\mathbf{c}
\end{aligned} \tag{3.1}$$

and solve some selected macroscopic one-dimensional initial value problems. (3.1) is only a different notation for (2.11), where $f_n(\mathbf{y}, \mathbf{c}) = w_M(u_B(t_n, \mathbf{y}), \mathbf{c})$ is just the Maxwellian phase-density. Both notations are useful for different purposes.

3.1 Evaluation of the Representations in One Space Dimension

In order to solve the initial value problem for the EULER equations in one space dimension we choose a fixed $\tau = \tau_{ME} > 0$ and define the equidistant times $t_n = n\tau_{ME}$ $(n = 0, 1, 2, \ldots)$.

For given fields $\rho_n(\cdot) = \rho(t_n, \cdot)$, $v_n(\cdot) = v(t_n, \cdot)$, $T_n(\cdot) = T(t_n, \cdot)$ at time t_n, starting with the initial data ρ_0, v_0, T_0 given at time $t = 0$, these fields are obtained at time t_{n+1} according to the scheme

$$\left.\begin{aligned} \rho_{n+1}(x) &= \int_{-\infty}^{+\infty} f_n(x - c\tau, c)dc \\ (\rho v)_{n+1}(x) &= \int_{-\infty}^{+\infty} c f_n(x - c\tau, c)dc \\ (\rho(3T + v^2))_{n+1}(x) &= \int_{-\infty}^{+\infty} (c^2 + 2T_n(x - c\tau)) f_n(x - c\tau, c)dc. \end{aligned}\right\} \tag{3.2}$$

Here the phase density $f_n(y, c)$ is given by

$$f_n(y, c) = \frac{\rho_n(y)}{\sqrt{2\pi T_n(y)}} \exp\left[-\frac{(c - v_n(y))^2}{2T_n(y)}\right]. \tag{3.3}$$

This scheme can be obtained from the representations (3.1) by integrating over c_2 and c_3. For $\tau \to 0$ it solves the weak EULER equations as it will be described in section 3.3.

3.2 From Free Flight to the Eulerian Limit

We consider a density distribution $\rho_0(x)$ at zero velocity and uniform temperature:

$$\rho(0, x) = \rho_0(x) = \begin{cases} 1 & |x| > 1 \\ 1.1 & |x| \le 1 \end{cases}, v(0, x) = v_0 = 0,\ T(0, x) = T_0 = 1.$$

We are interested in density distributions within the range $x \in [-5, 5]$ at time $t = 1.5$ for different maximizing entropy times τ_{ME}.

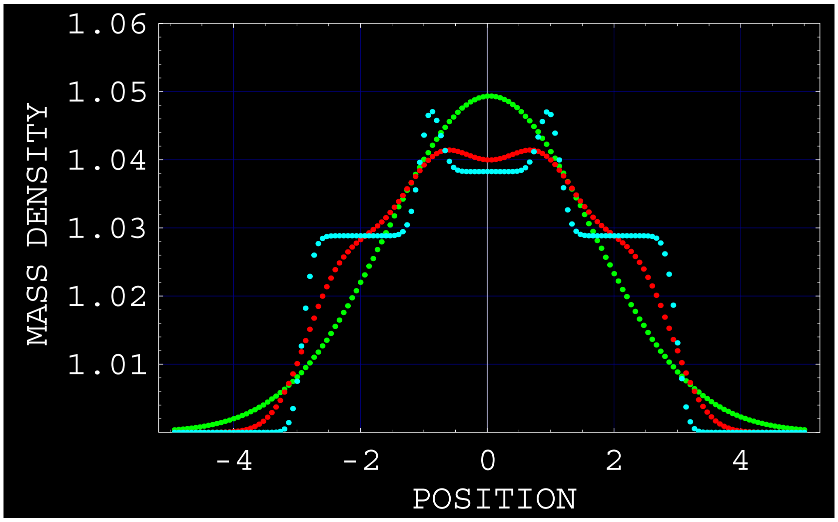

Figure 3.1: Density distributions for 1, 10, 100 maximizations

Figure 3.1 depicts three density distributions at $t = 1.5$. The diffusion like distribution results from pure free flight with only one maximization at the beginning.

The distribution that shows already the formation of moving fronts is obtained when we choose $\tau_{ME} = 0.15$, i.e. there are 10 maximizations within the time interval $[0, 1.5]$. When we decrease τ_{ME} further, the fronts become steeper, and this is exhibited by the third distribution that is obtained for $\tau_{ME} = 0, 015$. This is almost the EULERian limit.

The physical content of the EULERian limit is the overwhelming importance of collisions against free flight. A chosen $\tau_{ME} > 0$ thus determines which of both mechanisms has more influence on a thermodynamic process.

Thermodynamic processes with increasing importance of the free flight phenomena require within classical ET an increasing number of variables. Here the importance of free flight is taken into account by choosing the appropriate τ_{ME} for a fixed number of variables.

According to the indications from the above example we may hope that the modified Maximum Entropy Principle will eventually lead to a modified ET that need not to increase the number of variables above 14 for the description of processes far from equilibrium or with high Mach number, where free flight phenomena become important.

3.3 The EULERian Limit

There is another advantage of the modified Maximum Entropy Principle which relies on the resulting representations (3.2) – (3.3).

We consider now exclusively the EULERian limit $\tau_{ME} \to 0$ in order to illustrate the superpriority of the representations (3.2) – (3.3) against the use of difference schemes for the solution of an initial value problem of the EULER equations.

To this we choose as an extreme example discontinuous initial data so that in later times the interaction of a shock wave and a rarefaction wave will appear.

The determination of the initial data requires some knowledge of the weak form of the EULER equations. This will be given in the next section.

3.3.1 The Weak Form of the EULER equations

In one space dimension we are looking for $M = 3$ fields $u_A = \left(\rho, \rho v, \rho(u + \frac{v^2}{2})\right)^T$ which satisfy the *weak form of the* EULER *equations*:

$$\left.\begin{aligned} \int\limits_{\partial\Omega} \rho dx - (\rho v) dt = 0 \\ \int\limits_{\partial\Omega} (\rho v) dx - (\rho v^2 + p) dt = 0 \\ \int\limits_{\partial\Omega} \rho(u + \tfrac{v^2}{2}) dx - \rho v \left(u + \tfrac{v^2}{2} + \tfrac{p}{\rho}\right) dt = 0 \end{aligned}\right\} \tag{3.4}$$

Here $\Omega \subset \mathbb{R} \times \mathbb{R}_0^+$ is a convex set in space-time with piecewise smooth, positive oriented boundary. Note that this weak formulation takes discontinuities into account, since there are no longer derivatives of these fields.

In an ideal gas the pressure p, internal energy u and temperature T are related as follows:

$$u = \frac{3}{2}\frac{k}{m}T, \qquad p = \frac{2}{3}\rho u = \frac{k}{m}\rho T. \tag{3.5}$$

In the following we set $k = 1, m = 1$.

We consider *initial data* of bounded variation for ρ, v and T, which may have jumps:

$$\rho(0, x) = \rho_0(x), \qquad v(0, x) = v_0(x), \qquad T(0, x) = T_0(x). \tag{3.6}$$

It is well known that the weak formulation (3.4) implies EULER*s differential equations* in regular points:

$$\left.\begin{aligned} \rho_t + (\rho v)_x = 0 \\ (\rho v)_t + (\rho v^2 + p)_x = 0 \\ \left(\rho(u + \tfrac{v^2}{2})\right)_t + \left(\rho v \left(u + \tfrac{v^2}{2} + \tfrac{p}{\rho}\right)\right)_x = 0 \end{aligned}\right\} \tag{3.7}$$

If $x = x(t)$ is a shock-discontinuity of the weak solution (3.4) with speed $v_s = \dot{x}(t)$, $u_- = (\rho_-, v_-, T_-)$ the state left to the shock and $u_+ = (\rho_+, v_+, T_+)$ the state to the right, then (3.4) leads to the RANKINE-HUGONIOT *jump conditions:*

$$\left.\begin{aligned} v_s(\rho_+ - \rho_-) = \rho_+ v_+ - \rho_- v_-, \\ v_s(\rho_+ v_+ - \rho_- v_-) = (\rho_+ v_+^2 + p_+) - (\rho_- v_-^2 + p_-), \\ v_s \left[\rho_+ \left(u_+ + \tfrac{v_+^2}{2}\right) - \rho_- \left(u_- + \tfrac{v_-^2}{2}\right)\right] = \\ \rho_+ v_+ \left(u_+ + \tfrac{v_+^2}{2} + \tfrac{p_+}{\rho_+}\right) - \rho_- v_- \left(u_- + \tfrac{v_-^2}{2} + \tfrac{p_-}{\rho_-}\right) \end{aligned}\right\} \tag{3.8}$$

Furthermore we require that the weak solution of (3.4) must satisfy the following *entropy-inequality*

$$\int\limits_{\partial\Omega} h dx - \Phi dt \geq 0 \tag{3.9}$$

with positive oriented $\partial\Omega$, the entropy density h and the entropy flux Φ:

$$\left.\begin{aligned} h(\rho, v, u) &= \tfrac{3}{2}\rho \ln \tfrac{u}{\rho^{2/3}} \\ \Phi(\rho, v, u) &= v \cdot h(\rho, v, u) \end{aligned}\right\} \tag{3.10}$$

In singular points the local form of (3.9) reads

$$-v_s(h_+ - h_-) + (\Phi_+ - \Phi_-) \geq 0, \tag{3.11}$$

which must be satisfied at each shock curve of (3.4).
The solution that satisfies (3.8) and (3.11) is called *entropy shock.*

Now we give parameter representations for the single entropy shocks. For this purpose we choose the initial data as follows:

Let be $(\rho_0, v_0, T_0) \in \mathbb{R}^+ \times \mathbb{R} \times \mathbb{R}^+$ and define $p_0 := \rho_0 T_0$.

We use the pressure p as a parameter which determines the strength of an entropy shock. (3.8) and (3.11) is ensolved by

$$\rho(p) = \rho_0 \frac{4p + p_0}{p + 4p_0} \tag{3.12}$$

$$v(p) = v_0 \pm \frac{\sqrt{3}(p - p_0)}{\sqrt{(4p + p_0)\rho_0}} \tag{3.13}$$

$$T(p) = \frac{p}{\rho(p)} \tag{3.14}$$

$$v_s(p) = v_0 + \frac{v(p) - v_0}{\rho(p) - \rho_0}\rho(p). \tag{3.15}$$

in the following way:

- The "+" sign in (3.13) and $p > p_0$ give the so called *3-shocks* with the constant state (ρ_0, v_0, T_0) on the right:

  $$(\rho_-, v_-, T_-) = (\rho(p), v(p), T(p)), \quad (\rho_+, v_+, T_+) = (\rho_0, v_0, T_0).$$

  These 3-shocks both satisfy the RANKINE-HUGONIOT conditions (3.8) as well as the entropy condition (3.11).

- The "-" sign in (3.13) and $p > p_0$ give the so called *1-shocks* with the constant state (ρ_0, v_0, T_0) on the left:

  $$(\rho_-, v_-, T_-) = (\rho_0, v_0, T_0), \quad (\rho_+, v_+, T_+) = (\rho(p), v(p), T(p)).$$

  These 1-shocks both satisfy the RANKINE-HUGONIOT conditions (3.8) as well as the entropy condition (3.11).

Now we define the *2-shocks*, that turn out to be *contact-discontinuities without entropy-production*:

To this alone we choose $\rho > 0$ instead of p as a parameter and set

$$(\rho_-, v_-, T_-) = (\rho_0, v_0, T_0), \quad (\rho_+, v_+, T_+) = \left(\rho, v_0, \frac{\rho_0 T_0}{\rho}\right).$$

These shocks satisfy the RANKINE-HUGONIOT- and entropy conditions.

Note that velocity and pressure are constant across a 2-shock. Here the shock-speed is $v_s = v_0$.

Remark. One can prove that the only shocks satisfying (3.8) and (3.11) are 1-, 2- and 3-shocks.

In addition to shock waves there may appear a pure rarefaction wave with the following initial data:

Let $(\rho_0, v_0, T_0) \in \mathbb{R}^+ \times \mathbb{R} \times \mathbb{R}^+$ be the initial state on one side and $p_0 = \rho_0 T_0$. Then we choose the initial state on the other side according to

$$\left.\begin{array}{rl} \rho_0 \left(\frac{p}{p_0}\right)^{\frac{3}{5}} & = \rho(p) \\ v_0 \pm \sqrt{\frac{15}{\rho_0}} \cdot p_0^{\frac{3}{10}} \left[p^{\frac{1}{5}} - p_0^{\frac{1}{5}}\right] & = v(p) \\ \frac{p}{\rho(p)} & = T(p) \end{array}\right\} \tag{3.16}$$

where $p > 0$ is the free pressure-parameter. The solution of the form $u_A = g_A\left(\frac{x}{t}\right)$ can be obtained from (3.16) which describes the integral curves of the vector field of right eigenvectors to the system (3.7).

These relations as well as the shock conditions can be found in [1] and [3].

3.3.2 Interaction of a Shock Wave with a Rarefaction Wave

In this section we study the interaction of a shock wave with a rarefaction wave according to the EULERian limit. To achieve this we choose Riemannian initial conditions as follows:

First of all we create a pure rarefaction wave at $x = 1$. To this we prescribe the state right to $x = 1$ as $\rho_+ = 1$, $v_+ = 0$, $T_+ = 1$, and calculate the state left to $x = 1$ by the equations (3.16) with $p = 32$. This state turned out to be $\rho_M = 8$, $v_M = -\sqrt{15}$, $T_M = 4$. Now we consider these data as the state right to a 3-shock starting at $x = -1$. The RANKINE-HUGONIOT conditions (3.12)–(3.15) are used to calculate the state left to $x = -1$ with $p = 88$. It comes out $\rho_- = 14.222$, $v_- = -2.123$, $T_- = 6.188$. The speed of the 3-shock reads $v_s = 0.127$.

The three graphs on the next page show the fields of mass density, velocity and temperature for the time interval $[0, 1]$, and the space coordinate x ranges from -2 to 2. The times of maximization are $t_n = \frac{n}{200}$, $n = 0, 1, \ldots, 200$. At time $t \approx 0.3$ the

3-shock encounters the rarefaction wave. The interaction between both leads to a complicated structure including an acceleration of the original 3-shock.

The extreme values for density, velocity and temerature read ρMin $= 0.7226$, ρMax $= 14.6517$, vMin $= -3.870$, vMax $= 1.8722$, TMin $= 1.0$ and TMax $= 6.2326$.

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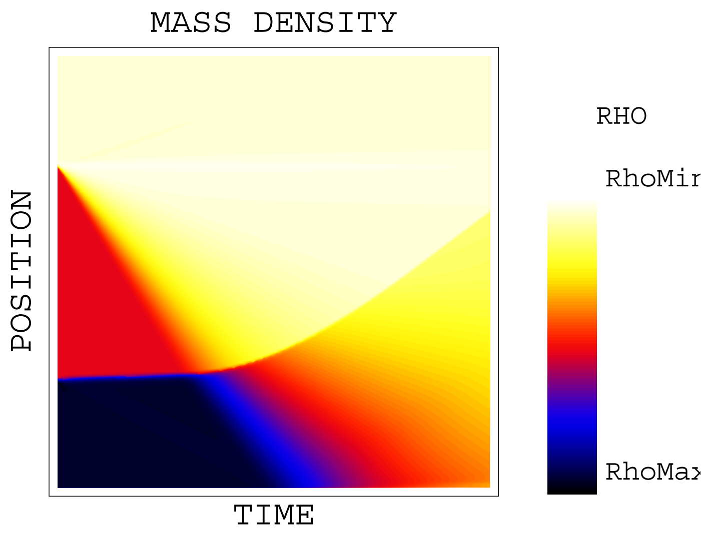
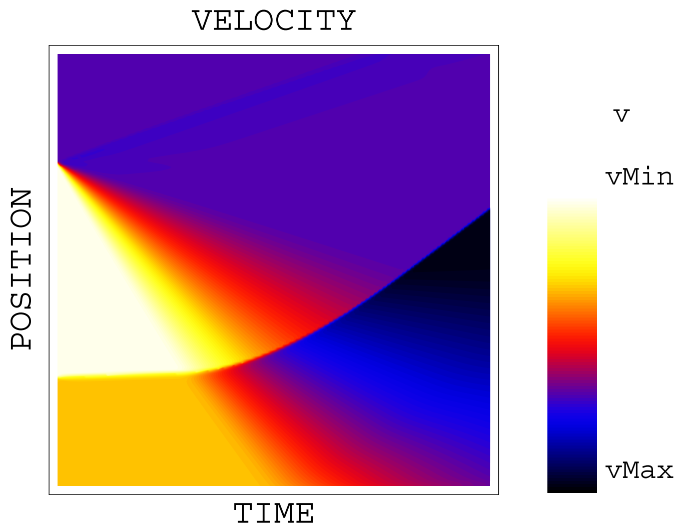
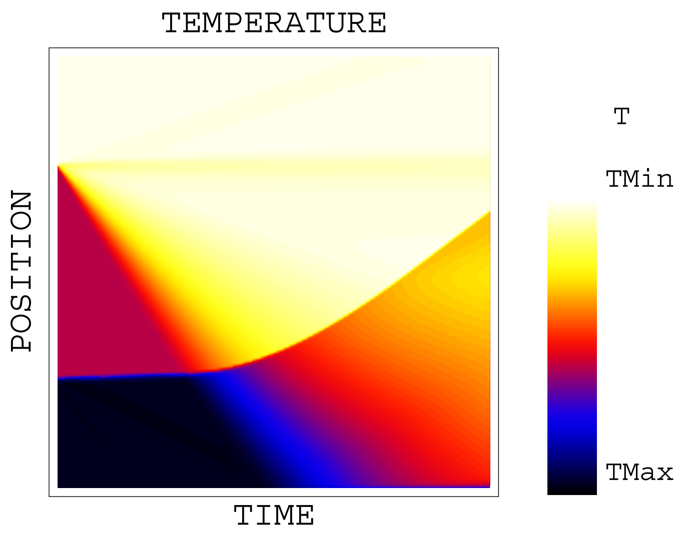

MASS DENSITY


VELOCITY


TEMPERATURE

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