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# Cold, thermal and oscillator closure of the atomic chain

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**Abstract**

We consider a simple microscopic model for a solid body and study the problematic nature of micro/macro transitions. The microscopic model describes the solid body by a many particle system that develops according to NEWTONs equations of motion.

We discuss various initial value problems that lead to the propagation of waves. The initial value problems are solved directly from the microscopic equations of motion. Additionally these equations serve to establish macroscopic field equations.

The macroscopic field equations consist of conservation laws, which follow rigorously from the microscopic equations, and of closure relations which are completely determined by the distributions of the microscopic motion. In particular we consider three kinds of closure relations which correspond to three different kinds of equilibrium.

It turns out that closure relations cannot be given appropriately without relating them to the initial conditions, and that closure relations might change during the temporal development of the initial data, because the body undergoes several transitions between different states of local equilibrium. In those examples that we have considered, the macroscopic variables mass density and temperature do not constitute an unique kind of microscopic motion.

# 1 Introduction

A thermodynamic process in a given body is described in thermodynamics by means of an initial- and boundary value problem for a system of partial differential equations. Usually such a system is established as follows: There are equations of universal character, i.e. they are valid for any material. Among these equations the conservation laws of mass, momentum and energy are particularly important. The universal equations are supplemented by so called constitutive equations, which relate the basic variables to those quantities which appear in the universal equations but are no basic variables.

The constitutive equations represent the closure of the open scheme of universal equations and therefore these are often called closure relations. Usually the closure relations are not related to the initial and boundary data, but are exclusively related to the considered material. The name constitutive equations is due to this reason.

In this study we show by means of a simple example that the choice of the appropriate closure relations might be intimately influenced by the initial and boundary data, a fact, which is in contrast to common belief. Furthermore it may even happen that the temporal development of the initial data requires a change of the adequate closure relations during the thermodynamic process.

For the demonstration of this statement we consider an atomic chain in one dimension as a simple model for a solid body. On the micro scale we describe the microscopic motion of the individual atoms by NEWTONs equations of motion. We solve these equations exclusively for macroscopic initial data, these are those that effect only macroscopic portions of the chain. How these data can be used for the microscopic preparation in order to solve NEWTONs equations will be explained in sections 8.1, 9.2 and 9.5. We restrict our interest to initial data that lead to the propagation of waves. Initial data which initiate diffusion like motion will be studied in a forthcoming paper.

In order to derive the field equations we start from NEWTONs equations and show that they imply macroscopic equations of balance. All appearing quantities can be represented by microscopic representations. In these representations the macroscopic quantities like the mass-, momentum-, energy density, pressure and heat flux are written as mean values in time and space in terms of the so called window function. From the macroscopic point of view the window function should be so small that its support is concentrated around the point $(t, x)$, where we want to compute the macroscopic fields, whereas from the microscopic point of view the support of the window function should contain enough particle trajectories in order to guarantee stochastical convergence to the macroscopic fields and to obtain closure relations.

Thus the equations of balance become field equations by closure relations that result from a macroscopic limit. The macroscopic state of the solid body will be described by three fields in time and space, viz. mass density $\rho\,(t, x)$, velocity $v\,(t, x)$ and temperature $T\,(t, x)$, and we consider these quantities as the basic variables. We study pure initial value problems for $\rho\,(0, x)$, $v\,(0, x)$ and $T\,(0, x)$.

The closure relations that we are interested in may be classified as follows:

(i) *Cold Closure*: The thermal motion, i.e. stochastic vibrations of the atoms, is completely ignored here.

(ii) *Thermal Closure*: There is thermal motion of displacements and velocities of the atoms, which are both completely uncorrelated. This case is well known to thermodynamicists. Their closure relations rely often on the assumption of a unique local thermal equilibrium.

(iii) *Oscillator Closure*: There is thermal motion of displacements of two particle oscillators. The corresponding velocities are determined by the microscopic equations of motion and are thus correlated to the displacements. This kind of closure serves to illustrate that in general there is no unique thermal equilibrium. The oscillator closure is by no means artificial. The described oscillator motion can be created by quite usual macroscopic initial data.

All three closure relations lead on the macroscopic scale to symmetric hyperbolic systems. To each system we indicate an entropy function that is also defined in terms of microscopic quantities. However, the entropy is not calculated here from BOLTZMANNs famous formula which relates the entropy to the number of micro states that can realize a given macro state. Instead we ground the entropy on the PFAFFian form between energy, pressure, density and temperature. All these quantities have simple uniquely determined microscopic representations and induce uniquely a microscopic representation of the entropy.

In particular the *oscillator closure* will thus lead to an entropy that is a rigorous consequence of NEWTONs microscopic equations of motion.

The study is organized as follows: The sections 2 to 6 deal with a many particle system which consists of $N$ structureless atoms whose dynamics is described by NEWTONs equations of motion. These are supplemented by pairwise interaction potentials.

The microscale is related to the macro scale by the so called window function which is defined in section 3. The window function maps the microscopic trajectories to a macroscopic point in time and space, and it is the central quantity that enables the calculation of marcoscopic mean values of microscopic observables with respect to time and space.

In section 4 and 5 we define a general class of mean values and in particular the basic quantities mass-, momentum- and energy density. General equations of balance and especially the conservation laws will then be established and in turn we may identify the corresponding fluxes.

In section 6 we formulate the general closure problem and additionally we identify the velocity dependent parts of the constitutive quantities.

In sections 7.1 and 7.2 we reduce the obtained results to the one dimensional atomic chain as a simple model for a one dimensional solid body.

The section 7.3 is of great importance. Here we introduce different time and space scales for the microscale and the macroscale, respectively. The microscopic time and space units are related to properties of the pair potentials. The units of macroscopic time and space regions result from a given scaling parameter which is the same for time and space and is proportional to the particle number $N$. This guarantees that wave speeds become independent of $N$ and restricts the study to pure wave prpagation. Furthermore this kind of scaling induces macroscopic fields which become also independent of $N$ if only $N$ is sufficiently large.

In the last three sections we introduce the three different closure assumptions and study their appropriateness. In section 8 we start with the *cold closure* that ignores complety thermal motion. We show that one can formulate RIEMANNian initial data so that the resulting macroscopic system, which considers only the mass density and the velocity as variables, agrees in some sense with the direct solution of the microscopic equations. However, it will also turn out that a temperature field develops and must thus be taken into account.

At the beginning of section 9 we introduce the temperature as the mean kinetic energy of the thermal motion. Hereafter we define global thermal equilibrium, and prepare the atomic chain according to that definition. The resulting distribution function will then be used to establish the *thermal closure*, which assumes in addition local thermal equilbrium. Then we consider in section 9.5 and 9.6 an other RIEMANNian initial value problem in order to demonstrate that the assumption of local thermal equilibrium is in general not realized by the microscopic motion. Instead we observe that the distances and velocities of the atoms are distributed by the so called oscillator motion, which is discussed in detail in section 10.

In section 10 we verify that it is possible to generate by quite natural initial data a kind of oscillator motion, where the $N$ atoms move with the same frequency in $N/2$ oscillators. This kind of motion constitutes a second equilibrium which can be realized by the same values of mass density and temperature that we used to create thermal motion. The corresponding distribution functions then serve to establish the *oscillator closure*.

Next we consider a further RIEMANNian initial value problem which deviates only slightly from the one that has served to motivate the *oscillator closure*, and in fact the temporal development of the macroscopic fields looks similar as before. However, from the known microscopic data we obtain new distribution functions which are neither pure thermal nor pure oscillator functions. Instead we observe a transition of pure thermal motion to some kind of oscillator motion. Nevertheless all these kind of motions constitute local equilibria.

This result is in contrast to the case of the BOLTZMANN gas, which has a unique equilibrium distribution, viz. the MAXWELLian. The analogue closure problem leads to the hyperbolic system of EULER equations. This system was studied and solved in [1] and [2].

It is due to the presence of permanent strong interaction forces between the atoms that the solid behaves different and cannot be described macroscopically by a single hyperbolic system. The thermal- and the oscillator motion yield two possible examples.

In a series of papers, [3], [4], [5] and [6], Masaru Sugiyama and collaborators report on a serious and careful study on the same subject. However, their procedure and intention is quite different from ours. Sugiyama starts also from NEWTONs equations for the one dimensional atomic chain and their pairwise interaction potential is qualitatively the same as that we have used. But the closure problem is solved in Sugiyamas studies in a completely different way.

Note that we derive rigorously from NEWTONs equations the macroscopic conservation laws and the corresponding microscopic representations of macroscopic quantities. In the next step we introduce the various closure relations. On the contrary, Sugiyama and collaborators considered one single closure relation, which was given by a distribution function of GAUSSian type for $N$ independent atoms. This function is used to reduce the problem of dealing with $N$ coupled NEWTON equations to a system of only five coupled equations for those five unknowns that appear in the GAUSSian type distribution function as macroscopic parameters.

## 2 Newtonian Dynamics of Structureless Particles

We consider a body consisting of $N$ structureless atoms. These are called particles from now on. All particles have the same mass $m$, and they are indexed by small greek letters $\alpha, \beta, ... \in \{1, 2, .., N\}$. At time $t \geq 0$ the particles are located at positions $\mathbf{x}^{\alpha}(t)$ and they have velocities $\dot{\mathbf{x}}^{\alpha}(t)$.

At any time $t$ the microstate of the body, $\gamma_N$, is completely described by the $6N$ positions and velocities

$$\gamma_N(t) = \left(\mathbf{x}^1(t), \dot{\mathbf{x}}^1(t), ...., \mathbf{x}^N(t), \dot{\mathbf{x}}^N(t)\right). \tag{1}$$

The dynamics of the microstate is determined by NEWTONs equations of motion

$$m\ddot{x}_i^{\alpha} = G_i^{\alpha} + \sum_{\beta=1}^{N} K_i^{\alpha\beta} \tag{2}$$

A particle $\alpha$ is subjected to a total force $K_i^{\alpha}$ which is decomposed into the external force $G_i^{\alpha}$ and the interaction force $K_i^{\alpha\beta}$ between $\alpha$ and any other particles $\beta$. The external force may include the inertial forces. In this study we consider only interaction forces that can be derived from a pair potential $\varphi: \mathbb{R}_0^+ \to \mathbb{R}$. In particular we choose a potential function of the so called Lennard-Jones type, which will be used for numerical examples later on:

$$\varphi(r) = \frac{1}{8}\frac{1}{r^4} - \frac{1}{4}\frac{1}{r^2}. \tag{3}$$

Thus the interaction force has for $\alpha \neq \beta$ the explicit form

$$K_i^{\alpha\beta} = -\frac{\partial\varphi\left(\left|\mathbf{r}^{\alpha\beta}\right|\right)}{\partial x_i^{\alpha}} = \varphi'(|\mathbf{x}^{\beta} - \mathbf{x}^{\alpha}|)\frac{x_i^{\beta} - x_i^{\alpha}}{|\mathbf{x}^{\beta} - \mathbf{x}^{\alpha}|}, \tag{4}$$

where $\mathbf{r}^{\alpha\beta} = \mathbf{x}^{\beta} - \mathbf{x}^{\alpha}$. Obviously (4) satisfies NEWTONs third law, *actio* = *reactio*:

$$K_i^{\alpha\beta} = -K_i^{\beta\alpha}. \tag{5}$$

Therefore we **define** in addition $K_i^{\alpha\alpha} = 0$.

## 3 The Window Function

We shall introduce now the window function $\chi(t, \mathbf{x})$, which relates the microscale to the macroscale. The function $\chi$ opens in space time by its finite support a window to the microscopic positions and velocities of the particles. Later on we shall establish the micro macro transition, where we choose the supp($\chi$) so that the window contains infinitely many particle worldlines from a microscopic viewpoint. However, from a macroscopic viewpoint supp($\chi$) shrinks to a single point in space time. In the next section the window function will be used to define macroscopic quantities at time $t$ and space point $\mathbf{x}$.

We provide the window function with the following properties:

(i) $\chi : \mathbb{R}^4 \to \mathbb{R}$ is continuous differentiable with $\chi\left(t, \mathbf{x}\right) \geq 0$.

(ii) $\mathrm{supp}(\chi) \subset (0, \infty) \times \mathbb{R}^3$.

(iii) $\int\limits_{-\infty}^{+\infty} \chi\left(t, \mathbf{x}\right)\, dt\, d^3\mathbf{x} \;=\; 1.$

We shall choose the support of the window function macroscopically small, but microscopically very large so that the window contains still an enormous number of microscopic trajectories. This is necessary in order to pass to the three thermodynamic limits which will be considered in sections 8, 9 and 10.

For each particle index $\alpha$ we define

$$\chi_\alpha\left(\vartheta, t, \mathbf{x}\right) = \chi\left(\vartheta - t, \mathbf{x}^\alpha\left(\vartheta\right) - \mathbf{x}\right) \tag{6}$$

in order to formulate the following Lemma, which yields the complete information for the derivation of the conservation and balance laws:

**Lemma:**

(i) The partial derivative of $\chi_\alpha$ with respect to $t$ can be written as

$$\frac{\partial \chi_\alpha}{\partial t}\left(\vartheta, t, \mathbf{x}\right) = -\frac{\partial \chi_\alpha}{\partial \vartheta}\left(\vartheta, t, \mathbf{x}\right) - \frac{\partial \chi_\alpha}{\partial x_k}\left(\vartheta, t, \mathbf{x}\right) \dot{x}_k^\alpha(\vartheta), \tag{7}$$

(ii) The difference of two window functions with different particle index has the *divergence* form

$$\begin{aligned} &\chi_\alpha\left(\vartheta, t, \mathbf{x}\right) - \chi_\beta\left(\vartheta, t, \mathbf{x}\right) = \\ &\frac{\partial}{\partial x_k}\left(\left(x_k^\beta - x_k^\alpha\right) \int\limits_0^1 \chi\left(\vartheta - t, \mathbf{x}^\alpha\left(\vartheta\right) - \mathbf{x} + \mu\left(\mathbf{x}^\beta - \mathbf{x}^\alpha\right)\right) d\mu\right) \end{aligned} \tag{8}$$

The **proof** of (i) follows immediately from the given definition of $\chi_\alpha\left(\vartheta, t, \mathbf{x}\right)$, and the **proof** of (ii) starts with the identity

$$\begin{aligned} &\chi\left(\vartheta - t, \mathbf{x}^\alpha\left(\vartheta\right) - \mathbf{x}\right) - \chi\left(\vartheta - t, \mathbf{x}^\beta\left(\vartheta\right) - \mathbf{x}\right) = \\ &-\int\limits_0^1 \frac{\partial}{\partial \mu} \chi\left(\vartheta - t, \mathbf{x}^\alpha\left(\vartheta\right) - \mathbf{x} + \mu\left(\mathbf{x}^\beta - \mathbf{x}^\alpha\right)\right) d\mu. \end{aligned} \tag{9}$$

According to the chain rule we can transform the $\mu$ derivative into the divergence derivative that occurs in (ii). ■

# 4 The General Equations of Balance

Recall that the micro state of a body is given by the list $\gamma_N$ of $6N$ positions and velocities. For the description of the macro state of the body we need a reduced list $\Gamma_{N_M}$ of variables, with $N_M \ll N$ . The most important case is the list $\Gamma_5$ which contains the five macroscopic variables mass density $\rho$, momentum density $\rho\mathbf{v}$ and energy density $\rho e$. These are formed at time $t$ and at the space point $\mathbf{x}$ by the **definitions**

$$\begin{aligned}
\rho(t,\mathbf{x}) &= \int_0^\infty \sum_{\alpha=1}^N m\,\chi_\alpha(\vartheta,t,\mathbf{x})\,d\vartheta, \\
\rho v_i(t,\mathbf{x}) &= \int_0^\infty \sum_{\alpha=1}^N m\,\dot{x}_i^\alpha(\vartheta)\,\chi_\alpha(\vartheta,t,\mathbf{x})\,d\vartheta, \\
\rho e(t,\mathbf{x}) &= \int_0^\infty \sum_{\alpha=1}^N \left(\frac{m}{2}\dot{x}_i^\alpha(\vartheta)\,\dot{x}_i^\alpha(\vartheta) + \frac{1}{2}\sum_{\beta=1}^N \varphi\left(\left|\mathbf{r}^{\alpha\beta}(\vartheta)\right|\right)\right)\chi_\alpha(\vartheta,t,\mathbf{x})\,d\vartheta.
\end{aligned} \tag{10}$$

The right hand sides of (10) define volume densities of additive quantities, i.e. the total mass, the total momentum and the total energy of the body can be represented by volume integrals of the mass density, the momentum density and the energy density, respectively. The definitions of these densities are very natural: A window, which is located at $(t,\mathbf{x})$, is considered, and the number density of particle trajectories within this window is multiplied with the mass $m$, the momentum $m\dot{x}_i^\alpha$ and the energy $\frac{m}{2}\dot{x}_i^\alpha\dot{x}_i^\alpha + \frac{1}{2}\varphi\left(\left|\mathbf{r}^{\alpha\beta}\right|\right)$ of a single particle, respectively.

Field equations for volume densities as variables rely on equations of balance which we shall derive next. In order to exhibit the general structure and the microscopic origin of the equations of balance, it is useful to generalize first the definition (10) and to formulate their generic structure. From (10) we read off the generic form

$$\begin{aligned}
&u_A(t,\mathbf{x}) = \\
&\int_0^\infty \sum_{\alpha=1}^N \left(O_A^\alpha(\vartheta) + \sum_{\beta=1}^N O_A^{\alpha\beta}(\vartheta)\right)\chi_\alpha(\vartheta,t,\mathbf{x})\,d\vartheta, \qquad (A = 0,1,2....,N_M - 1)\,.
\end{aligned} \tag{11}$$

The quantities $O_A^\alpha$ and $O_A^{\alpha\beta}$ denote microscopic one- and two- particle observables, respectively.

| | $O_A^\alpha$ | $O_A^{\alpha\beta}$ |
|---|---|---|
| $A=0$, Mass | $m$ | $0$ |
| $A=1,2,3$, Momentum | $m\dot{x}_i^\alpha$ | $0$ |
| $A=4$, Energy | $\frac{m}{2}\dot{x}_i^\alpha\dot{x}_i^\alpha$ | $\frac{1}{2}\varphi_{\alpha\beta}$ |

(12)

We have introduced the abbreviation $\varphi_{\alpha\beta} = \varphi\left(|\mathbf{r}_{\alpha\beta}|\right)$ for $\beta \neq \alpha$ and $\varphi_{\alpha\alpha} = 0$ in this table. We shall now use the generic form (11) to establish general equations of balance for the quantities $u_A$. In this study we consider only microscopic observables that may have the following dependencies

$$O_A^\alpha(\vartheta) = \tilde{O}_A^\alpha\left(\dot{\mathbf{x}}^\alpha(\vartheta)\right), \qquad O_A^{\alpha\beta}(\vartheta) = \tilde{O}_A^{\alpha\beta}\left(\mathbf{r}^{\alpha\beta}(\vartheta), \dot{\mathbf{x}}^\alpha(\vartheta), \dot{\mathbf{x}}^\beta(\vartheta)\right), \tag{13}$$

i.e. the one particle observable $O_A^\alpha$ can at most depend on the velocity, while the two particle observable $O_A^{\alpha\beta}$ may depend on the velocities of the particles $\alpha$ and $\beta$ and on their relative distance.

Next we show that to each volume density $u_A$ $(A = 0, 1, 2..., N_M - 1)$ there correspond fluxes $f_{Ak}$, productions $S_A$ and supplies $Z_A$, so that among them the following equations of balance hold:

$$\frac{\partial u_A}{\partial t} + \frac{\partial f_{Ak}}{\partial x_k} = S_A + Z_A. \tag{14}$$

We start from (11), and differentiate $u_A(t, \mathbf{x})$ at constant $\mathbf{x}$ with respect to time $t$ to obtain

$$\frac{\partial u_A(t,\mathbf{x})}{\partial t} = \int_0^\infty \sum_{\alpha=1}^N \left(O_A^\alpha(\vartheta) + \sum_{\beta=1}^N O_A^{\alpha\beta}(\vartheta)\right) \frac{\partial \chi_\alpha(\vartheta, t, \mathbf{x})}{\partial t}\, d\vartheta. \tag{15}$$

The derivative of the window function is replaced by (7). Hereafter a partial integration with respect to time $\vartheta$ is carried out, and after some rearrangements there results

$$\begin{aligned} \frac{\partial u_A(t,\mathbf{x})}{\partial t} \quad &+ \quad \frac{\partial}{\partial x_k}\left(\int_0^\infty \sum_{\alpha=1}^N \left(O_A^\alpha(\vartheta) + \sum_{\beta=1}^N O_A^{\alpha\beta}(\vartheta)\right) \dot{x}_k^\alpha(\vartheta)\, \chi_\alpha(\vartheta, t, \mathbf{x})\, d\vartheta\right) = \\ &\int_0^\infty \sum_{\alpha=1}^N \left(\frac{d\, O_A^\alpha(\vartheta)}{d\,\vartheta} + \sum_{\beta=1}^N \frac{d\, O_A^{\alpha\beta}(\vartheta)}{d\,\vartheta}\right) \chi_\alpha(\vartheta, t, \mathbf{x})\, d\vartheta. \end{aligned} \tag{16}$$

The expression under the divergence gives already the first contribution to the flux $f_{Ak}$ we are looking for. Next we apply, according to (13), the chain rule to the $\vartheta$ derivatives on the right hand side. For this purpose we define to each volume density $u_A$ $(A = 0, 1, 2..., N_M - 1)$ a corresponding $N \times N$ matrix $\mathbf{M_A}$ with components $((M_A^{\alpha\beta}))$ which are formed by the microscopic observables according to

$$M_A^{\alpha\beta} = \frac{\partial \tilde{O}_A^{\alpha\beta}}{\partial r_j^{\alpha\beta}} \dot{r}_j^{\alpha\beta} + \frac{1}{m} \frac{\partial \tilde{O}_A^\alpha}{\partial \dot{x}_j^\alpha} K_j^{\alpha\beta} + \frac{1}{m} \sum_{\gamma=1}^N \left(\frac{\partial \tilde{O}_A^{\alpha\beta}}{\partial \dot{x}_j^\alpha} K_j^{\alpha\gamma} + \frac{\partial \tilde{O}_A^{\alpha\beta}}{\partial \dot{x}_j^\beta} K_j^{\beta\gamma}\right). \tag{17}$$

The definition of $\mathbf{M_A}$ is only unique in those cases which have zero productions. We have defined $\mathbf{M_A}$ so that the observables $O_A^\alpha(\vartheta) + \sum\limits_{\beta=1}^N O_A^{\alpha\beta}(\vartheta)$ remain as a whole.

By $M_A^{[\alpha\beta]}$ and $M_A^{(\alpha\beta)}$ we denote the antisymmetric and symmetric part of $\mathbf{M_A}$, respectively. We obtain from (16):

$$\frac{\partial u_A(t,\mathbf{x})}{\partial t}+\frac{\partial}{\partial x_k}\left(\int\limits_0^\infty\sum_{\alpha=1}^N\left(O_A^\alpha(\vartheta)+\sum_{\beta=1}^N O_A^{\alpha\beta}(\vartheta)\right)\dot{x}_k^\alpha(\vartheta)\,\chi_\alpha(\vartheta,t,\mathbf{x})\;d\vartheta\right)=$$
$$\int\limits_0^\infty\sum_{\alpha=1}^N\sum_{\beta=1}M_A^{[\alpha\beta]}(\vartheta)\,\chi_\alpha(\vartheta,t,\mathbf{x})\;d\vartheta+\int\limits_0^\infty\sum_{\alpha=1}^N\sum_{\beta=1}^N M_A^{(\alpha\beta)}(\vartheta)\,\chi_\alpha(\vartheta,t,\mathbf{x})\;d\vartheta \tag{18}$$
$$+\int\limits_0^\infty\frac{1}{m}\sum_{\alpha=1}^N\left(\frac{\partial\tilde{O}_A^\alpha}{\partial\dot{x}_j^\alpha}G_j^\alpha+\sum_{\beta=1}^N\left(\frac{\partial\tilde{O}_A^{\alpha\beta}}{\partial\dot{x}_j^\alpha}G_j^\alpha+\frac{\partial\tilde{O}_A^{\alpha\beta}}{\partial\dot{x}_j^\beta}G_j^\beta\right)\right)\chi_\alpha(\vartheta,t,\mathbf{x})\;d\vartheta.$$

The first expression on the right hand side contains the antisymmetric part of the matrix $M_A$ and can be written as a divergence, because we can apply the second part of the Lemma from section 3 to the identity

$$\sum_{\alpha=1}^N\sum_{\beta=1}^N M_A^{[\alpha\beta]}(\vartheta)\,\chi_\alpha(\vartheta,t,\mathbf{x})=\frac{1}{2}\sum_{\alpha=1}^N\sum_{\beta=1}^N M_A^{[\alpha\beta]}(\vartheta)\left(\chi_\alpha(\vartheta,t,\mathbf{x})-\chi_\beta(\vartheta,t,\mathbf{x})\right). \tag{19}$$

Thus finally we end up with the following

**Proposition:**
(i) If we define the fluxes, productions and supplies according to

$$f_{Ak}(t,\mathbf{x})=\int\limits_0^\infty\left(\sum_{\alpha=1}^N\left(O_A^\alpha(\vartheta)+\sum_{\beta=1}^N O_A^{\alpha\beta}(\vartheta)\right)\dot{x}_k^\alpha(\vartheta)\,\chi_\alpha(\vartheta,t,\mathbf{x})-\right.$$
$$\left.\frac{1}{2}\sum_{\alpha,\beta=1}^N M_A^{[\alpha\beta]}(\vartheta)\,r_k^{\alpha\beta}(\vartheta)\int\limits_0^1\chi\left(\vartheta-t,\mathbf{x}^\alpha(\vartheta)-\mathbf{x}+\mu\mathbf{r}^{\alpha\beta}(\vartheta)\right)d\mu\right)d\vartheta,$$
$$S_A(t,\mathbf{x})=\int\limits_0^\infty\sum_{\alpha=1}^N\sum_{\beta}M_A^{(\alpha\beta)}(\vartheta)\,\chi_\alpha(\vartheta,t,\mathbf{x})\;d\vartheta, \tag{20}$$
$$Z_A(t,\mathbf{x})=\int\limits_0^\infty\frac{1}{m}\sum_{\alpha=1}^N\left(\frac{\partial\tilde{O}_A^\alpha}{\partial\dot{x}_j^\alpha}G_j^\alpha+\sum_{\beta=1}^N\left(\frac{\partial\tilde{O}_A^{\alpha\beta}}{\partial\dot{x}_j^\alpha}G_j^\alpha+\frac{\partial\tilde{O}_A^{\alpha\beta}}{\partial\dot{x}_j^\beta}G_j^\beta\right)\right)\chi_\alpha(\vartheta,t,\mathbf{x})\;d\vartheta,$$

then the following equations of balance are satisfied:

$$\frac{\partial u_A}{\partial t}+\frac{\partial f_{Ak}}{\partial x_k}=S_A+Z_A. \tag{21}$$

(ii) The macroscopic influence of the external forces $\mathbf{G}^\alpha$ is represented by the supplies $Z_A$, while the interaction forces $\mathbf{K}^{\alpha\beta}$ contribute to the fluxes $\mathbf{f}_A$ as well as to the productions $S_A$.

(iii)The antisymmetric part $M_A^{[\alpha\beta]}$ of the matrix $\mathbf{M}_A$, which is given in (17), will contribute to the fluxes, while the productions are exclusively formed by the symmetric part $M_A^{(\alpha\beta)}$. ■

Note that the fields $u_A(t,\mathbf{x})$ and $f_{Ak}(t,\mathbf{x})$, and also $S_A(t,\mathbf{x})$ and $Z_A(t,\mathbf{x})$, are continuous differentiable according to their definition via the window function. For that reason we can also establish global equations of balance. We consider a fixed volume $V$ and obtain from (21) by integration and a subsequent application of GAUSSs Theorem

$$\frac{d}{dt}\int\limits_V u_A(t,\mathbf{x})\,d^3x = -\oint\limits_{\partial V} f_{Ak}(t,\mathbf{x})\,da_k + \int\limits_V \left(S_A(t,\mathbf{x}) + Z_A(t,\mathbf{x})\right)d^3x. \tag{22}$$

Later on, after having carried out the closure of the system (21), the fields $u_A(t,\mathbf{x})$, $f_{Ak}(t,\mathbf{x})$, $S_A(t,\mathbf{x})$ and $Z_A(t,\mathbf{x})$ will be equipped with additional thermodynamic properties and consequently may become discontinuous. When this happens we shall assume that the global equation (22) is more fundamental than the system (21). Thus we shall still rely on the global equations of balance (22) and seek for weak solutions.

## 5 The Conservation Laws of Mass, Momentum and Energy

In the last section we started with the microscopic representations of the macroscopic volume densities of mass, momentum and energy. After that we generalized these representations to a general class of volume densities and derived the corresponding equations of balance. This procedure allowed the identification of general fluxes, productions and supplies.

In this section we write down the special microscopic representations which are necessary in order to describe the conservation of mass, momentum and energy. To this end we read off from Table (12) the generating microscopic observables $\tilde{O}_A^\alpha$ and $\tilde{O}_A^{\alpha\beta}$ for $A = 0,1,2,3,4$ and insert these into the expressions (20).

All productions $S_A$ turn out to be zero. For that reason mass, momentum and energy are called conserved quantities and their equations of balance are called conservation laws.

As it was mentioned before, the external forces may include the gravitational force and the inertial forces like centrifugal force and CORIOLIS force. After having understood their appearance in the general equations of balance. We will not study these forces in detail. Thus we assume $\mathbf{G}^\alpha = 0$, which implies vanishing momentum and energy supplies. Furthermore there is obviously no mass supply.

The mass flux $f_{0k}$ is equal to the momentum densitiy $\rho v_k$. The momentum flux $f_{ik}$

and the energy flux $f_{4k}$ are denoted by $P_{ik}$ and $Q_k$, respectively. They read

$$P_{ik}\left(t,\mathbf{x}\right)=\int\limits_0^\infty d\vartheta\Big(\sum_{\alpha=1}^{N} m\,\dot{x}_i^\alpha\left(\vartheta\right)\dot{x}_k^\alpha\left(\vartheta\right)\chi_\alpha\left(\vartheta,t,\mathbf{x}\right)-$$

$$\frac{1}{2}\sum_{\alpha,\beta=1}^{N}K_i^{\alpha\beta}\left(\vartheta\right)r_k^{\alpha\beta}\left(\vartheta\right)\int\limits_0^1\chi\left(\vartheta-t,\mathbf{x}^\alpha\left(\vartheta\right)-\mathbf{x}+\mu\mathbf{r}^{\alpha\beta}\left(\vartheta\right)\right)d\mu\Big)\,, \tag{23}$$

$$Q_k\left(t,\mathbf{x}\right)=\int\limits_0^\infty d\vartheta\Big(\sum_{\alpha=1}^{N}\Big(\frac{m}{2}\dot{x}_j^\alpha\left(\vartheta\right)\dot{x}_j^\alpha\left(\vartheta\right)+\frac{1}{2}\sum_{\beta=1}^{N}\varphi\left(|\mathbf{r}^{\alpha\beta}(\vartheta)|\right)\Big)\dot{x}_k^\alpha\left(\vartheta\right)\chi_\alpha\left(\vartheta,t,\mathbf{x}\right)-$$

$$\tag{24}$$

$$\frac{1}{4}\sum_{\alpha,\beta=1}^{N}K_j^{\alpha\beta}\left(\vartheta\right)\Big(\dot{x}_j^\alpha\left(\vartheta\right)+\dot{x}_j^\beta\left(\vartheta\right)\Big)r_k^{\alpha\beta}\left(\vartheta\right)\int\limits_0^1\chi\Big(\vartheta-t,\mathbf{x}^\alpha\left(\vartheta\right)-\mathbf{x}+\mu\mathbf{r}^{\alpha\beta}\left(\vartheta\right)\Big)d\mu\Big)\,.$$

With these representations the conservation laws read

$$\frac{\partial\rho}{\partial t}+\frac{\partial\rho v_k}{\partial x_k}=0,\qquad\frac{\partial\rho v_i}{\partial t}+\frac{\partial P_{ik}}{\partial x_k}=0,\qquad\frac{\partial\rho e}{\partial t}+\frac{\partial Q_k}{\partial x_k}=0. \tag{25}$$

In this study we do not consider more general cases than the five conservation laws, for which we shall discuss now the closure problem.

# 6 The General Closure Problem

We describe the macro state of a body by the first five volume densities $\rho$, $\rho\mathbf{v}$ and $\rho e$. These quantities are considered as the basic variables of the macroscopic continuum theory, and we seek for a closed set of five field equations. These rely on the five conservation laws (25).

The general closure problem consists of finding relations that relate the fluxes $P_{ik}$ and $Q_k$ in a material dependent manner to the basic variables. However, these relations include also universal parts, namely those that depend on the velocity $\mathbf{v}$. We can identify these parts by replacing the microscopic velocities $\dot{\mathbf{x}}^\alpha$ by so called excess (or thermal) velocities $\mathbf{C}^\alpha$, which are defined as

$$C_i^\alpha\left(\vartheta,t,\mathbf{x}\right)=\dot{x}_i^\alpha\left(\vartheta\right)-v_i\left(t,\mathbf{x}\right). \tag{26}$$

Hereby the energy density and the fluxes decompose into velocity dependent parts and into parts which are invariant with respect to GALILEIian transformations:

$$\rho e=\frac{\rho}{2}\mathbf{v}^2+\rho u,\qquad P_{ik}=\rho v_i v_k+p_{ik},\qquad Q_k=\Big(\Big(\frac{\rho}{2}\mathbf{v}^2+\rho u\Big)\delta_{ik}+p_{ik}\Big)v_i+q_k. \tag{27}$$

The newly introduced quantities $\rho u$, $p_{ik}$ and $q_k$ are called internal energy density, pressure tensor and heat flux, respectively. They are defined as follows

$$\begin{aligned}\rho u\left(t,\mathbf{x}\right) = &\int_0^\infty \sum_{\alpha=1}^{N}\left(\frac{m}{2}C_i^\alpha\left(\vartheta,t,\mathbf{x}\right)C_i^\alpha\left(\vartheta,t,\mathbf{x}\right)+\right.\\ &\left.\frac{1}{2}\sum_{\beta=1}^{N}\varphi\left(\left|\mathbf{r}^{\alpha\beta}(\vartheta)\right|\right)\right)\chi_\alpha\left(\vartheta,t,\mathbf{x}\right)d\vartheta,\end{aligned} \tag{28}$$

$$\begin{aligned}p_{ik}\left(t,\mathbf{x}\right) = &\int_0^\infty \left(\sum_{\alpha=1}^{N} mC_i^\alpha\left(\vartheta,t,\mathbf{x}\right)C_k^\alpha\left(\vartheta,t,\mathbf{x}\right)\chi_\alpha\left(\vartheta,t,\mathbf{x}\right)-\right.\\ &\left.\frac{1}{2}\sum_{\alpha,\beta=1}^{N}K_i^{\alpha\beta}\left(\vartheta\right)r_k^{\alpha\beta}\left(\vartheta\right)\int_0^1\chi\left(\vartheta-t,\mathbf{x}^\alpha\left(\vartheta\right)-\mathbf{x}+\mu\mathbf{r}^{\alpha\beta}\left(\vartheta\right)\right)\,d\mu\right)d\vartheta,\end{aligned} \tag{29}$$

$$\begin{aligned}&q_k\left(t,\mathbf{x}\right) =\\ &\int_0^\infty\left(\sum_{\alpha=1}^{N}\left(\frac{m}{2}C_j^\alpha\left(\vartheta,t,\mathbf{x}\right)C_j^\alpha\left(\vartheta,t,\mathbf{x}\right)+\frac{1}{2}\sum_{\beta=1}^{N}\varphi\left(\left|\mathbf{r}^{\alpha\beta}(\vartheta)\right|\right)\right)C_k^\alpha\left(\vartheta,t,\mathbf{x}\right)\chi_\alpha\left(\vartheta,t,\mathbf{x}\right)\right.\\ &\quad-\frac{1}{4}\sum_{\alpha,\beta=1}^{N}K_j^{\alpha\beta}\left(\vartheta\right)\left(C_j^\alpha\left(\vartheta,t,\mathbf{x}\right)+C_j^\beta\left(\vartheta,t,\mathbf{x}\right)\right)r_k^{\alpha\beta}\left(\vartheta\right)\times\\ &\quad\left.\int_0^1\chi\left(\vartheta-t,\mathbf{x}^\alpha\left(\vartheta\right)-\mathbf{x}+\mu\mathbf{r}^{\alpha\beta}\left(\vartheta\right)\right)\,d\mu\right)d\vartheta\,.\end{aligned} \tag{30}$$

Now we can reformulate the general closure problem as follows: Instead of $\rho$, $\rho\mathbf{v}$ and $\rho e$ we consider $\rho$, $\mathbf{v}$ and $u$ as basic variables and the new closure problem consists of finding relations that relate the pressure tensor $p_{ik}$ and the heat flux $q_k$ in a material dependent manner to the new basic variables.

The main objective of the next sections will be a comprehensive study of the closure problem for a simple body: The one dimensional atomic chain. This example serves to illustrate that there is a very close relation of the closure problem to the initial value problem of the resulting field equations. It will turn out that one cannot solve the closure problem appropriately without paying attention to the kind of initial data for which the field equations are intended to be solved.

# 7 The One Dimensional Atomic Chain

## 7.1 Newtons Dynamics

The one dimensional atomic chain consists of $N$ atoms with mass $m = 1$ and with positions at time $\vartheta$,

$$\{x^1(\vartheta), x^2(\vartheta), ...., x^{N-1}(\vartheta), x^N(\vartheta)\}, \tag{31}$$

along one single direction. The positions of the $1^{th}$ and of the $N^{th}$ atom are fixed and given by

$$x^1(\vartheta) = 0, \qquad x^N(\vartheta) = L. \tag{32}$$

The other atoms move according to pairwise nearest neighbour interaction. We recall the pair potential given in (3):

$$\varphi(r_\alpha) = \frac{1}{8}\frac{1}{r_\alpha^4} - \frac{1}{4}\frac{1}{r_\alpha^2}, \qquad \text{with} \qquad r_\alpha = x^{\alpha+1} - x^\alpha, \qquad \alpha = 1, 2, 3, ..., N-1. \tag{33}$$

The numbers in the pair potential are choosen so that $\varphi'(1) = 0$ and $\varphi''(1) = 1$.

We do not consider external forces, and NEWTONs equations of motion thus read

$$\ddot{x}^\alpha(\vartheta) = \varphi'(r_\alpha(\vartheta)) - \varphi'(r_{\alpha-1}(\vartheta)), \qquad \alpha = 2, 3, ..., N-1. \tag{34}$$

From a microscopic viewpoint the initial conditions for the system (34) are given by the initial locations

$$\{x^1(0) = 0, x^2(0) = x_0^2, ...., x^{N-1}(0) = x_0^{N-1}, x^N(0) = L\}, \tag{35}$$

and by the initial velocities

$$\{\dot{x}^1(0) = 0, \dot{x}^2(0) = \dot{x}_0^2, ...., \dot{x}^{N-1}(0) = \dot{x}_0^{N-1}, \dot{x}^N(0) = 0\}. \tag{36}$$

of all atoms.

From a macroscopic viewpoint, however, such a detailed description is not possible. Macroscopically we can only prescribe initial values for the macroscopic variables, viz. $\rho(0,x)$, $v(0,x)$ and $u(0,x)$. The relations between the microscopic and the macroscopic initial value problem will be discussed in detail in sections 8.1, 9.2 and 9.5.

## 7.2 Conservation Laws For The One Dimensional Atomic Chain

The general results regarding the conservation laws will now be reduced to the one-dimensional atomic chain. We start from the general results (25) and (24) and specialize to one space dimension. Hereafter we incorporate the restriction to nearest neighbour interaction to the microscopic representations (28), (29) and (24) and end up with the result:

(i) The conservation laws for mass, momentum and energy in one space dimension read

$$\begin{aligned}
&\frac{\partial \rho}{\partial t}+\frac{\partial \rho v}{\partial x}=0, \\
&\frac{\partial \rho v}{\partial t}+\frac{\partial}{\partial x}\left(\rho v^{2}+p\right)=0, \\
&\frac{\partial \rho\left(\frac{1}{2} v^{2}+u\right)}{\partial t}+\frac{\partial}{\partial x}\left(\rho\left(\frac{1}{2} v^{2}+u+\frac{p}{\rho}\right) v+q\right)=0.
\end{aligned} \tag{37}$$

(ii) For nearest neighbour interaction the microscopic representations are given by

$$\begin{aligned}
\rho(t, x) &= \int_{0}^{\infty} \sum_{\alpha=1}^{N} \chi_{\alpha}(\vartheta, t, x)\, d\vartheta, \\
\rho v(t, \mathbf{x}) &= \int_{0}^{\infty} \sum_{\alpha=1}^{N} \dot{x}^{\alpha}(\vartheta)\, \chi_{\alpha}(\vartheta, t, \mathbf{x})\, d\vartheta, \\
\rho u(t, \mathbf{x}) &= \int_{0}^{\infty} \sum_{\alpha=1}^{N}\left(\frac{1}{2} C^{\alpha}(\vartheta, t, \mathbf{x})^{2}+\varphi\left(r_{\alpha}(\vartheta)\right)\right) \chi_{\alpha}(\vartheta, t, \mathbf{x})\, d\vartheta,
\end{aligned} \tag{38}$$

for the basic variables, and by

$$\begin{aligned}
p(t, x) = & \int_{0}^{\infty} \sum_{\alpha=1}^{N}\Bigg(C^{\alpha}(\vartheta, t, x)^{2}\, \chi_{\alpha}(\vartheta, t, \mathbf{x})- \\
& \qquad \varphi^{\prime}\left(r_{\alpha}(\vartheta)\right) r_{\alpha}(\vartheta) \int_{0}^{1} \chi\left(\vartheta-t, x^{\alpha}(\vartheta)-x+\mu r_{\alpha}(\vartheta)\right) d\mu\Bigg) d\vartheta, \\
q(t, x) = & \int_{0}^{\infty} \sum_{\alpha=1}^{N}\Bigg(\left(\frac{1}{2} C^{\alpha}(\vartheta, t, x)^{2}+\varphi\left(r_{\alpha}(\vartheta)\right)\right) C^{\alpha}(\vartheta, t, x)\, \chi_{\alpha}(\vartheta, t, x)- \\
& \qquad \frac{1}{2} \varphi^{\prime}\left(r_{\alpha}(\vartheta)\right) r_{\alpha}(\vartheta)\, C^{\alpha}(\vartheta, t, x) \int_{0}^{1} \chi\left(\vartheta-t, x^{\alpha}(\vartheta)-x+\mu r_{\alpha}(\vartheta)\right) d\mu\Bigg) d\vartheta.
\end{aligned} \tag{39}$$

for the pressure and the heat flux.

## 7.3 Macroscopic versus Microscopic Scaling of Time and Space

All microscopic calculations use space and time units as follows: The microscopic space unit is choosen so that $\varphi'(1) = 0$ and the microscopic time unit is choosen so that $\varphi''(1) = 1$.

In these units the total length $L$ of the chain is thus proportional to the particle number $N$, and due to $\varphi''(1) = 1$ the duration of the microscopic process under consideration, $t_F$, must also be a large number.

In order to avoid these large numbers in the representations of the macroscopic fields, where many particles are involved, we use macroscopic time and space units and introduce a positive scaling factor according to

$$t_F = \lambda \tilde{t}_F, \qquad L = \lambda \tilde{L}. \tag{40}$$

In macroscopic units the total length of the chain and the duration of the process are denoted $\tilde{L}$ and $\tilde{t}_F$, respectively. For convenience we choose in the numerical examples $\tilde{t}_F = 1$.

This scaling corresponds to a coordinate transformation. Let $t$ and $x$ denote the microscopic time and space coordinates and $\tilde{t}$ and $\tilde{x}$ the corresponding macroscopic coordinates. Then we write

$$\tilde{t} = \frac{1}{\lambda} t, \qquad \tilde{x} = \frac{1}{\lambda} x. \tag{41}$$

However, later on we shall suppress the tilde symbol above the macroscopic quantities.

Regarding the visualization the advantage of this convention of the results is obvious. In addition there is a fundamental reason for this type of scaling, which in fact relies on the following **observation**:

Later on we shall consider various macroscopic RIEMANN initial value problems with a single jump at, say $x = 0$. These will be solved on the microscale subsequently for an increasing number $N$ of particles. The given kind of scaling leads then to convergence to the macroscopic fields in the limit $N \to \infty$, i.e. the macroscopic fields become independent of $N$ for sufficiently large $N$. In addition the macroscopic fields turn out to be invariant with respect to the scaling transformation (41):

$$u_A(t, x) = u_A(\lambda t, \lambda x). \tag{42}$$

We conclude that the macroscopic fields depend only on the ratio $\frac{x}{t}$.

In section 10.5 we shall discuss the consequences of this important observation.

Note that time and space are scaled here with the same factor $\lambda$. This implies, that microscopic wave speeds do not depend on the particle number $N$. Actually this restricts us to consider only wave phenomena but no diffusion in the macroscopic limit $N \to \infty$. Diffusion phenomena would require different time and space scalings.

# 8 The Cold Closure

## 8.1 Macroscopic Initial Data and Preparation of the Atomic Chain

In the first example we study the following macroscopic initial value problem: We describe the macrostate of a chain with $N$ particles and with fixed length $L$ by only two variables, viz. the mass density $\rho\,(t,x)$ and the velocity $v\,(t,x)$. The initial data are

$$\rho\,(0,x)=\left\{\begin{array}{ccc}\rho_l & & x\leq\frac{L}{2}\\ & \text{for} & \\ \rho_r & & x>\frac{L}{2}\end{array}\right.,\qquad v\,(0,x)=\left\{\begin{array}{ccc}v_l & & x\leq\frac{L}{2}\\ & \text{for} & \\ v_r & & x>\frac{L}{2}\end{array}\right.. \tag{43}$$

Obviously these data are not sufficient to solve an initial value problem for the $N-2$ equations of motion (34). Thus there arises the question how to prepare the initial data of the atomic chain.

Let be $N_l$ and $N_r$ the number of atoms which are initially left and right from $L/2$, respectively. We may calculate these quantities for given $N$, $\rho_l$ and $\rho_r$ according to the simple equations

$$L=2\frac{N-1}{\rho_l+\rho_r},\qquad N_l+N_r=N-1,\qquad \frac{N_l}{\rho_l}+\frac{N_r}{\rho_r}=L. \tag{44}$$

The first equation, $(44)_1$, represents the length of the chain by $(N-1)$ intervals × the mean lenght $2/\left(\rho_l+\rho_r\right)$ of an interval. $(44)_2$ decomposes the number of intervals, and $(44)_3$ decomposes the lenght $L$ into its left and right part, where $\frac{L}{2}=\frac{N_l}{\rho_l}=\frac{N_r}{\rho_r}$.

**Assumption:** The initial data for the atomic chain are given as follows:

$$x_0^\alpha=\left\{\begin{array}{ccc}\frac{1}{\rho_l}\left(\alpha-1\right) & & \alpha=1,2,...,N_l\\ & \text{for} & \\ \frac{1}{\rho_l}N_l+\frac{1}{\rho_r}\left(\alpha-N_l-1\right) & & \alpha=N_l+1,...,N,\end{array}\right.$$
$$\dot{x}_0^\alpha=\left\{\begin{array}{ccc}v_l & & \alpha=1,2,...,N_l\\ & \text{for} & \\ v_r & & \alpha=N_l+1,...,N\,.\end{array}\right. \tag{45}$$

We have thus assumed that the atoms have initially constant distances on the left and on the right part of the chain. In addition they have constant velocities on each side. This corresponds to zero temperature of the chain at time $t=0$.

## 8.2 Calculation of the Macroscopic Fields by Solving Newtons Equations

We solve now the $N-2$ equations of motion (34) with $N=35000$ and use the obtained data to calculate the macroscopic fields mass densitiy $\rho\,(t,x)$ and velocity

$v(t,x)$ according to the microscopic representations $(38)_{1,2}$ . The Figure 1 depicts the space time diagramm of the mass density for $0 \leq t \leq 1$ and $0 \leq x \leq 4$ with the scaling factor $\lambda = 7413$.

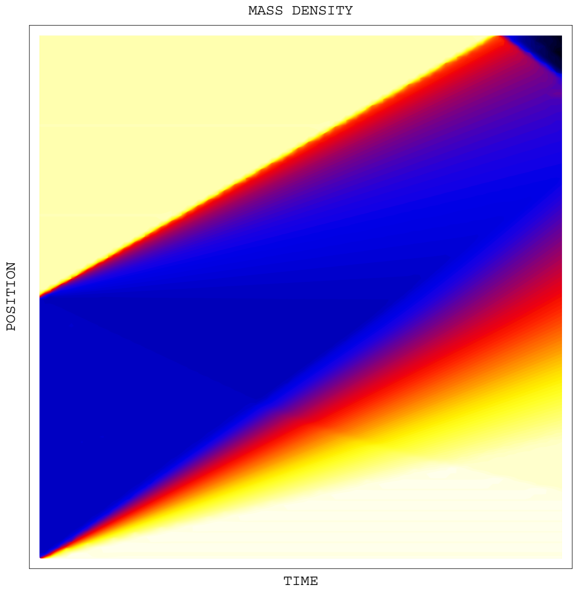

Fig. 1: Space time diagram of the mass density according to NEWTONs equations.

The initial data are $\rho_l = 1.36$, $\rho_r = 1.00$, $v_l = 0.53$, $v_r = 0.00$. These data results from the evaluation of macroscopic Rankine-Hugoniot conditions which will be discussed in section 8.5.

We observe that the initial discontinuity at $x = 2$ initiates a propagating shock like structure right up to the right boundary, where a reflection took place.

A more detailed description of the temporal development of this shock like structure will be given in section 8.4.

The rarefaction wave that enters the diagram from below will not interest us here. It results from the interaction of the chain with the lower boundary.

## 8.3 Cold Closure and Field Equations

In the last section we have calculated the fields of mass density and velocity for a macroscopic initial value problem from the solution of the $N-2$ microscopic equations of motion. In this section we are interested in the same initial value problem, but we use now a macroscopic system of two field equations for the mass density and for the velocity.

This system relies on the two conservation laws $(37)_{1,2}$. If $\Omega$ is any convex set in space time with piecewise smooth, positive oriented boundary $\partial\Omega$, then the conservation law for mass and momentum may be written down in integral form

$$\begin{aligned} &\oint\limits_{\partial\Omega} (\rho dx - \rho v dt) = 0, \\ &\oint\limits_{\partial\Omega} \left(\rho v dx - \left(\rho v^2 + p\right) dt\right) = 0\,, \end{aligned} \tag{46}$$

and must be supplemented by a constitutive law that relates the pressure in $(46)_2$ to the variables. This is achieved by the **assumption:**

Within the support of the window function at the space time point $(t,x)$ we calculate the pressure from the microscopic representation (39) by setting

$$r_\alpha = \frac{1}{\rho\,(t,x)}, \qquad \text{and} \qquad \dot{x}^\alpha = v\,(t,x) \qquad \text{for} \qquad x^\alpha \in \operatorname{supp}\,(\chi(t,x))\,. \quad (47)$$

We call the assumption (47) the *cold closure*, because thermal vibrations of the atoms are completely ignored here.

The evaluation of $(39)_1$ for the *cold closure* assumption implies

$$p = -\varphi'\left(\frac{1}{\rho}\right). \tag{48}$$

If we replace the pressure $p$ in (46) by $-\varphi'\left(\frac{1}{\rho}\right)$, we obtain the weak form of a closed macroscopic system, which leads in regular points to the differential form

$$\frac{\partial\rho}{\partial t} + \frac{\partial\rho v}{\partial x} = 0, \qquad \frac{\partial\rho v}{\partial t} + \frac{\partial}{\partial x}\left(\rho v^2 - \varphi'\left(\frac{1}{\rho}\right)\right) = 0, \tag{49}$$

and across a shock front to the Rankine Hugoniot jump conditions

$$-V_S\,[[\rho]] + [[\rho v]] = 0, \qquad -V_S\,[[\rho v]] + \left[\left[\rho v^2 - \varphi'\left(\frac{1}{\rho}\right)\right]\right] = 0. \tag{50}$$

In equation (50) $[[a]] = a_r - a_l$ denotes the jump of any field $a = a(x)$, and $V_S$ is the shock velocity.

Note that the fields in $(37)_{1,2}$, which depend on the window function and the micro trajectories $x^\alpha(t)$, are continuous differentiable. However, after having replaced the exact microscopic representation of the pressure by the constitutive law (48), the resulting field equations may have regular as well as discontinuous solutions, and both are described by (46).

In order to obtain the condition for hyperbolicity and the characteristic speeds of the system (49), we write it in the form

$$\frac{\partial\rho}{\partial t} + v\frac{\partial\rho}{\partial x} + \rho\frac{\partial v}{\partial x} = 0\ , \qquad \frac{\partial v}{\partial t} + \frac{1}{\rho^3}\varphi''(\frac{1}{\rho})\frac{\partial\rho}{\partial x} + v\frac{\partial v}{\partial x} = 0. \tag{51}$$

There results immediately the characteristic speeds

$$\lambda_{1,2} = v \pm \frac{1}{\rho}\sqrt{\varphi''(\frac{1}{\rho})}, \tag{52}$$

and the condition for hyperbolicity is $\varphi''(\frac{1}{\rho}) > 0$, i.e. $\rho > \sqrt{\frac{3}{5}}$ for the function $\varphi$ given in (3). Note that this function satisfies $\varphi''(1) = 1$, a condition which leads for $\rho = 1$ and $v = 0$ to the characteristic speeds $\lambda_{1,2} = \pm 1$.

## 8.4 Properties of the Field Equations

The system (49) and (50) represents a closed system of field equations for weak solutions of the initial value problem from the above. This sytem is obviously of hyperbolic type in the region $\varphi'' > 0$.

Next we study the role of the conservation law $(37)_3$ of the energy. In particular we have to answer the important question, whether the *cold closure* eventually contradicts the energy conservation, because, due to (47) the energy density $\rho e$ and the energy flux $Q$ become also functions of $\rho$ and $v$, so that the conservation law $(37)_3$ yields a third equation for the two unknown fields $\rho\,(t,x)$ and $v\,(t,x)$, viz.

$$\begin{gathered}\frac{\partial \rho \hat{e}\,(\rho,\rho v)}{\partial t}+\frac{\partial \hat{Q}\,(\rho,\rho v)}{\partial x}=0,\ \text{with}\\ \hat{e}\,(\rho,\rho v)=\left(\frac{v^2}{2}+\varphi\left(\frac{1}{\rho}\right)\right),\quad \hat{Q}\,(\rho,\rho v)=\left(\rho\hat{e}\,(\rho,\rho v)-\varphi'\left(\frac{1}{\rho}\right)\right)v.\end{gathered}\tag{53}$$

However, this establishes by no means a contradiction, because there is the following

**Proposition:** (i) There exist so called LAGRANGE multipiers $\Lambda^\rho$ and $\Lambda^{\rho v}$ so that the conservation law of the energy can be written as a linear combination of the two other conservation laws:

$$\frac{\partial \hat{e}\,(\rho,\rho v)}{\partial t}+\frac{\partial \hat{Q}\,(\rho,\rho v)}{\partial x}=\Lambda^\rho\left(\frac{\partial\rho}{\partial t}+\frac{\partial\rho v}{\partial x}\right)+\Lambda^{\rho v}\left(\frac{\partial\rho v}{\partial t}+\frac{\partial}{\partial x}\left(\rho v^2-\varphi'\left(\frac{1}{\rho}\right)\right)\right).\tag{54}$$

In regular points the right hand side of (54) vanishes and thus any solution of (49), (50) satisfies in addition the energy equation (53).

(ii) If $\varphi''\left(\frac{1}{\rho}\right)>0$ holds, the matrix of second derivatives of the function $\rho\hat{e}\,(\rho,\rho v)$ is positive definite.

(iii) Consequently, the system (49) is of symmetric hyperbolic type and has the energy as a convex extension.

**Proof:** We start from $(53)_{2,3}$ and form the left hand side of equation (54). After some rearrangements we obtain (54) with the identifications

$$\Lambda^\rho=-\frac{1}{2}v^2+\varphi\left(\frac{1}{\rho}\right)-\frac{1}{\rho}\varphi'\left(\frac{1}{\rho}\right),\qquad \Lambda^{\rho v}=v.\tag{55}$$

Next we form the matrix of second derivatives of the function $\hat{e}\,(\rho,\rho v)$. There results

$$\begin{pmatrix}\frac{1}{\rho^3}\left(\rho^2v^2+\varphi''\left(\frac{1}{\rho}\right)\right) & -\frac{1}{\rho}v\\ -\frac{1}{\rho}v & \frac{1}{\rho}\end{pmatrix}\tag{56}$$

and this is positive definite if $\varphi''\left(\frac{1}{\rho}\right)>0$.

The third part of the proposition relies on

$$\Lambda^{\rho} = \frac{\partial \rho \hat{e}\left(\rho, \rho v\right)}{\partial \rho}, \qquad \Lambda^{\rho v} = \frac{\partial \rho \hat{e}\left(\rho, \rho v\right)}{\partial \rho v}, \tag{57}$$

and these relations follow immediately from (54). The convexity of $\hat{e}\left(\rho, \rho v\right)$ guarantees that we may change the variables from $u_A = (\rho, \rho v)$ to $u'_A = (\Lambda^{\rho}, \Lambda^{\rho v})$, $A = 0, 1$. Let be

$$e' = \rho e - \Lambda^{\rho} \rho - \Lambda^{\rho v} \rho v, \qquad Q' = Q - \Lambda^{\rho} \rho v - \Lambda^{\rho v} \left(\rho v^2 - \varphi'\left(\frac{1}{\rho}\right)\right), \tag{58}$$

which implies

$$\rho = -\frac{\partial e'}{\partial \Lambda^{\rho}}, \qquad \rho v = -\frac{\partial e'}{\partial \Lambda^{\rho v}}, \qquad \rho v = -\frac{\partial Q'}{\partial \Lambda^{\rho}}, \qquad \rho v^2 - \varphi'\left(\frac{1}{\rho}\right) = -\frac{\partial Q'}{\partial \Lambda^{\rho v}}. \tag{59}$$

From these equations we conclude that the system of field equations (49) can be written as

$$\sum_{B=0}^{1} \left( \frac{\partial^2 e'}{\partial u'_A \partial u'_B} \frac{\partial u'_B}{\partial t} + \frac{\partial^2 Q'}{\partial u'_A \partial u'_B} \frac{\partial u'_B}{\partial x} \right) = 0. \tag{60}$$

The convexity of $\hat{e}\left(\rho, \rho v\right)$ implies the convexity of its LEGENDRE transform $e'\left(\Lambda^{\rho}, \Lambda^{\rho v}\right)$, which proves that (60) is the symmetric hyperbolic form of the original system (49). The reader is refered to the poineering work by Friedrichs and Lax [FL]. ■

This last result motivates the introduction of the entropy even for the *cold closure* which is properly a purely mechanical case. We choose the entropy density $\rho h = -\rho e$, which is in agreement with modern thermodynamics, where the negative of the convex extension of the system of field equations is always called entropy. For details we refer the reader to the interesting study of this subject [8] by G. Boillat and T. Ruggeri.

## 8.5 Rankine Hugoniot Conditions and Shock Selection Criterium

The purpose of this section is the evaluation of the RANKINE HUGONIOT conditions for the RIEMANNian initial data (43). Furthermore we shall establish the entropy balance across the initial discontinuity as a shock selection criterium.

We fix the fields right from the shock to be $\rho_r = 1$ and $v_r = 0$. The fields on the left hand side are denoted as $\rho_l = \rho$ and $v_l = v$, and we choose the density $\rho$ as the shock parameter. Then the RANKINE HUGONIOT conditions (50) yield

$$V_S^2 = -\frac{\varphi'\left(\frac{1}{\rho}\right)}{\left(1 - \frac{1}{\rho}\right)} > 0 \quad \text{for } \rho > 0, \quad \text{and} \qquad v = \left(1 - \frac{1}{\rho}\right) V_S. \tag{61}$$

In order to single out the unphysical solutions of (61) we consider the entropy condition. It requires a positive entropy production $\sigma_S$ across a discontinuity. From the observation that here the entropy density is equal to the negative of the energy density we conclude from the known energy jump that the entropy production is given by

$$\sigma_S = V_S[[\rho\left(\frac{v^2}{2}+\varphi\left(\frac{1}{\rho}\right)\right)]] - [[\left(\rho\hat{e}\left(\rho,\rho v\right)-\varphi'\left(\frac{1}{\rho}\right)\right)v]] \geq 0. \tag{62}$$

It can be shown from (62) that only compressive shocks, i.e. $\rho > 1$, are allowed.

In the next subsection we will compare the prediction of a single shock due to (61), (62) with the solution of the RIEMANN problem due to NEWTONs equations.

## 8.6 Comparison of the Results

A solution of (61), that satisfies the entropy condition (62), is given by

$$\rho_l = 1.36,\ \ \rho_r = 1.00,\ \ v_l = 0.53,\ \ v_r = 0.0 \text{ and } V_S = 2.0 \tag{63}$$

This predicts a single shock, starting at $t = 0$, $x = \frac{L}{2}$, which should properly end up in the upper right corner from Figure 1. Recall that Figure 1 in section 8.2, which was solved from the microscopic equations of motion, relies on the same initial data for $\rho$ and $v$.

We conclude that the *cold closure* exhibits some shortcomings:

(i) The microscopic equations of motion predicts for the Riemann problem no single shock solution, and furthermore the shock like structure, which results from NEWTONs equations reaches the boundary earlier as it is predicted by $V_S = 2$.

(ii) The macroscopic *cold closure* equations predicts energy production across the shock, which is in contrast to the microscopic equations of motion.

The reason for these shortcomings might be the neglection of the development of thermal motion in the *cold closure* assumption.

# 9 The Thermal Closure

## 9.1 Thermal Motion, Temperature and Distribution Function

In the last section we have identified one reason for failure of the applicability of the *cold closure* to the considered initial value problem: We ignored the development of the stochastic thermal motion. These will be taken into account now.

We start with the introduction of the macroscopic temperature field $T(t,x)$ and define this quantity by the kinetic energy of the excess motion of the particles:

$$\frac{\rho}{2}T(t,x)=\int\limits_{0}^{\infty}\sum_{\alpha=1}^{N}\frac{1}{2}C^{\alpha}(\vartheta,t,\mathbf{x})^{2}\,\chi_{\alpha}(\vartheta,t,\mathbf{x})\;d\vartheta. \tag{64}$$

Note that the *cold closure* assumes $C^{\alpha}(\vartheta,t,\mathbf{x})=\dot{x}^{\alpha}(\vartheta)-v(t,x)\equiv 0$, and thus forbids the generation of thermal motion. This is obviously an artificial assumption and explains the difference of the microscopic result to the Rankine Hugoniot prediction of the last section. From now on we include the temperature in the list of macroscopic variables.

We **define** *thermal motion* by two **assumptions**:

(i) The distribution of distances and velocities are completey uncorrelated, so that their common distribution has the probability density $G:\quad \mathbb{R}_0^+\times\mathbb{R}\to\mathbb{R}_0^+$ where $G(r,c)\geq 0$ is the product of two propability densities $F:\mathbb{R}_0^+\to\mathbb{R}_0^+$ and $f:\mathbb{R}\to\mathbb{R}_0^+$:

$$G(r,c)=F(r)\,f(c)\,,\qquad \int\limits_{0}^{\infty}F(r)\;dr=1,\qquad \int\limits_{-\infty}^{\infty}f(c)\;dc=1\,. \tag{65}$$

(ii) The velocities $c$ are assumed to be distributed by the GAUSSian density

$$f_G(\beta,c)=\sqrt{\frac{\beta}{2\pi}}\exp\left(-\beta\frac{c^2}{2}\right). \tag{66}$$

Later on we will see by solving Newtons equations in equilibrium that for a fixed temperature $T$, the function $f$ is realized by $f(c)=f_G(\beta,c)$, where $\beta$ is the inverse temperature $\frac{1}{T}$. This notation is often used in thermodynamics.

(iii) The distances $r$ are assumed to be distributed by the function

$$\begin{aligned}\hat{F}(\alpha,\beta,r)&=\frac{1}{z(\alpha,\beta)}\exp\left(-\alpha r-\beta\varphi(r)\right),\quad\text{with}\\ z(\alpha,\beta)&=\int\limits_{0}^{\infty}\exp\left(-\alpha r-\beta\varphi(r)\right)\,dr.\end{aligned} \tag{67}$$

The quantity $\alpha$ is determined by the mean distance of two neighbouring particles

$$\frac{1}{\rho}=\bar{r}(\alpha,\beta)=\int\limits_{0}^{\infty}r\hat{F}(\alpha,\beta,r)\;dr. \tag{68}$$

Later on we will see by solving Newtons equations in equilibrium that for fixed density $\rho$ and temperature $T$ the function $\hat{F}$ is realized by $F(r)=\hat{F}(\alpha,\frac{1}{T},r)$.

In addition to (68) we also define the mean potential energy, which will be used next:

$$\bar{\varphi}\left(\alpha,\beta\right)=\int\limits_{0}^{\infty}\varphi\left(r\right)\hat{F}\left(\alpha,\beta,r\right)\,dr. \tag{69}$$

The assumptions (i),(ii) and (iii) are in accordance with the *Maximum Entropy Principle* and hold when the atomic chain is in thermal equilibrium. Regarding the *Maximum Entropy Principle* we refer the reader to the detailed discussions by W. Dreyer [9] and G. Boillat & T. Ruggeri [10].

## 9.2 Preparation of the Atomic Chain in Thermal Equilibrium

In thermal equilibrium the macrostate of the atomic chain is completely determined by three constant values of mass density $\rho > 0$, velocity $v$ and temperature $T$. Now we prepare microscopic initial data for an atomic chain, consisting of $N$ particles, for given values of $\rho$, $v$ and $T$. The length of the chain is $L = (N-1)/\rho$.

The preparation procedure is devided into three steps:

(i) We start with a configuration where all positions of the atoms are distributed equidistantly according to the given density $\rho$ and where the mean velocity $v$ of the particles is zero:

$$y_0^\gamma = (\gamma-1)/\rho\,, \qquad \dot{y}_0^\gamma = C^\gamma\ ,\ \gamma = 1,2,...,N. \tag{70}$$

Here the stochastic excess velocities $C^\gamma$ are GAUSSian distributed for $1 < \gamma < N$ with mean velocity $< C^\gamma >= 0$ and mean square $T' =< (C^\gamma)^2 >$. $T'$ is determined by the obvious equation that uses the mean potential energy given in (69):

$$\frac{1}{2}T' + \varphi(\frac{1}{\rho}) = \frac{1}{2}T + \bar{\varphi}(\alpha,\frac{1}{T})\ . \tag{71}$$

The parameter $\alpha$ has to be determined here by (68) for given $\rho$ and $T$. The atoms at $y_0^0 = 0$ and $y_0^N = 0$ are constrained to zero velocities.

(ii) In a second step we solve the microscopic equations of motion for these initial data. The condition (71) are choosen so that after some time $t_0 > 0$ the positions of the atoms are additionally distributed according to the thermal distribution of distances (67). There result new positions $y^\gamma(t_0)$ and velocities $\dot{y}^\gamma(t_0)$, $\gamma = 1,...,N$.

(iii) In a third step we define the desired initial data by

$$x_0^\gamma = y^\gamma(t_0)\,, \qquad \dot{x}_0^\gamma = \dot{y}^\gamma(t_0) + v\ . \tag{72}$$

## 9.3 Calculation of Distribution Functions by Solving Newtons Equations and Comparison with the Analytical Formulae

By solving Newtons equations for the global data $\alpha = 17.12$ and $\beta = 0.94$, so that $\rho(\alpha, \beta) = 2.0$ and $T = 1.06$, we may determine the distributions of velocities and distances. These are depicted in Figure 2 by the dots. The solid lines in Figure 2 represent the analytical functions (66) and (67), respectively. We observe a perfect agreement between the empirical microscopic distributions and the analytical functions.

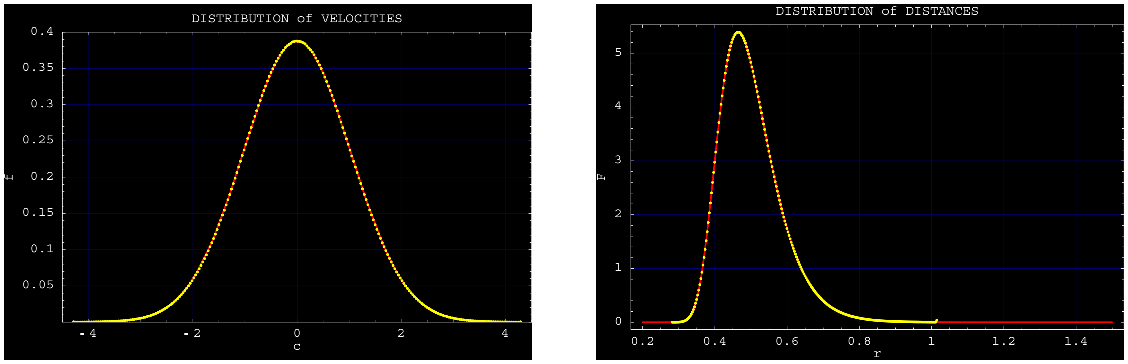

Fig. 2 Distribution of velocities and distances, comparison of microscopic data and analytical results.

## 9.4 Thermal Closure and Field Equations

The agreement that we have found in the last section serves as a motivation to replace the *cold closure* by the *thermal closure*. We shall **assume** now that the distribution functions of global equilibrium are also realized locally at any space time point. Thus we describe the macrostate of the atomic chain by the three variables $\rho$, $v$ and $T$.

The system of field equations relies on the three conservation laws (37), which we write down in the one dimensional integral form

$$\begin{aligned}
&\oint_{\partial\Omega} (\rho dx - \rho v dt) = 0, \\
&\oint_{\partial\Omega} \left(\rho v dx - \left(\rho v^2 + p\right) dt\right) = 0, \\
&\oint_{\partial\Omega} \left(\left(\frac{\rho}{2} v^2 + \rho u\right) dx - \left(\frac{\rho}{2} v^2 + \rho u + p\right) v dt\right) = 0\,.
\end{aligned} \tag{73}$$

Here $\Omega$ is a convex set in space time with piecewise smooth, positive oriented boundary $\partial\Omega$.

These equations must be supplemented by constitutive laws that relate the pressure, the internal energy and the heat flux to the variables. This is achieved by the **ansatz:**

$$\begin{aligned}
\frac{1}{\rho} &= \int\limits_0^\infty r\hat{F}\left(\alpha,\beta,r\right)\,dr = \hat{r}\left(\alpha,\beta\right), \\
T &= \int\limits_{-\infty}^\infty c^2 f_G\left(\beta,c\right)\,dc = \frac{1}{\beta}, \\
p &= \rho T - \rho\int\limits_0^\infty r\varphi'\left(r\right)\hat{F}\left(\alpha,\beta,r\right)\,dr = \frac{\alpha}{\beta}, \qquad (74) \\
u &= \frac{1}{2}T + \int\limits_0^\infty \varphi\left(r\right)\hat{F}\left(\alpha,\beta,r\right)\,dr = \frac{1}{2}T + \bar{\varphi}\left(\alpha,\beta\right) = \hat{u}\left(\alpha,\beta\right), \\
q &= 0.
\end{aligned}$$

The list (74) defines the *thermal closure* with $f_G\left(\beta,c\right)$ and $\hat{F}\left(\alpha,\beta,r\right)$ given by (66) and (67), respectively. In each line the first equality results from the evaluation of the microscopic representations (38) and (39). The nonconvective part of the energy flux $q$ is zero because the used distribution functions assumes local equilibrium. The second equality in each line introduces some useful abbreviations that will be used in the following. Furthermore the pressure integral was subjected to a partial integration. The remaining integrals must be evaluated numerically.

We have thus established a closed system of field equations for the variables $\rho$, $v$ and $T$ or alternatively for the variables $\alpha, \beta$ and $v$. The system consists of the conservation laws (73) and of the constitutive equations (74).

After having closed the system of conservation laws, the integral form (73) takes care of discontinuous shock solutions. This is in analogy to the *cold closure*. The system of differential equations (37) result from its weak form (73), that additionally yields the shock conditions: Let be $(\rho, v, T)$ and $(\rho', v', T')$ the constant states left and right, respectively, to a shock front with velocity $V_S$. By applying a GALILEIian transformation it is always possible to assume $v' = 0$ without loss of generality. Then we obtain after some rearrangements the following RANKINE HUGONIOT shock conditions:

$$\begin{aligned}
V_S &= \frac{v}{1-\frac{\rho'}{\rho}}\,, \\
v^2 &= \left(\frac{1}{\rho'}-\frac{1}{\rho}\right)\left(p-p'\right)\,, \qquad (75) \\
0 &= 2\left(u'-u\right) + \left(\frac{1}{\rho'}-\frac{1}{\rho}\right)\left(p+p'\right)\,.
\end{aligned}$$

We proceed to establish the properties of the field equations and to find a shock selection criterion. To this end we shall prove first that it is possible to define a specific entropy $h(\rho, T)$, which satisfies the so called Gibbs relation between $u(\rho, T)$, $p(\rho, T)$ and $T > 0$ :

$$dh = \frac{1}{T} du + \frac{1}{T} p d\left(\frac{1}{\rho}\right), \tag{76}$$

The Gibbs relation imply an integrability condition which guarantees that the right hand side of (76) is indeed an integrable differential form:

$$\frac{\partial u}{\partial\left(\frac{1}{\rho}\right)} = T\frac{\partial p}{\partial T} - p, \tag{77}$$

In order to check (76) we write down the following relations for the mass density and the internal energy, and use the function $z(\alpha, \beta) = \int\limits_0^\infty \exp(-\alpha r - \beta\varphi(r))\, dr$ which was introduced in (67):

$$\frac{1}{\rho} = -\frac{\partial \ln\left(\frac{z(\alpha,\beta)}{\sqrt{\beta}}\right)}{\partial\alpha} \quad \text{and} \quad u = -\frac{\partial \ln\left(\frac{z(\alpha,\beta)}{\sqrt{\beta}}\right)}{\partial\beta}. \tag{78}$$

Consequently with $p = \alpha/\beta$ we may form the following differential form, which depends on $\alpha$ and $\beta$;

$$\beta\left(du + pd\left(\frac{1}{\rho}\right)\right) = d\left(\beta u + \frac{\alpha}{\rho} + \ln\left(\frac{z(\alpha, \beta)}{\sqrt{\beta}}\right)\right). \tag{79}$$

This proves (76) and identifies the specific entropy:

$$h = \beta u + \frac{\alpha}{\rho} + \ln\left(\frac{z(\alpha, \beta)}{\sqrt{\beta}}\right). \tag{80}$$

Note that it is possible to prove the integrability condition (77) directly from the *thermal closure* assumption (74) without any knowledge about the entropy density $h$ in (80).

Finally we determine the condition which leads to a hyperbolic system that can be brought additionally into the symmetric hyperbolic form.

This can be achieved by replacing the specific internal energy density $u$ by the energy density $e = \rho(u + v^2/2)$ and after some simple rearrangements we obtain:

$$\begin{aligned} &d(\rho h) = \Lambda^\rho d\rho + \Lambda^{\rho v} d(\rho v) + \Lambda^e de, \quad \text{with} \\ &\Lambda^\rho = -\left(u - Th + \frac{p}{\rho} - \frac{v^2}{2}\right), \quad \Lambda^{\rho v} = -\frac{v}{T}, \quad \Lambda^e = \frac{1}{T}. \end{aligned} \tag{81}$$

Hereafter we prove the identity

$$d(\rho h v) = \Lambda^\rho d(\rho v) + \Lambda^{\rho v} d\left(\rho v^2 + p\right) + \Lambda^e d\left(\rho\left(u + v^2/2\right)v + pv\right). \tag{82}$$

Finally we establish the conditions for convexity of $-\rho h\left(\rho, \rho v, \rho e\right)$, i.e. with $u_A = \left(\rho, \rho v, \rho e\right)$. Convexity means that the matrix $\frac{\partial^2(\rho h)}{\partial u_A \partial u_B}$ is negative definit. Let $\Omega \subset \mathbb{R}_0^+ \times \mathbb{R}_0^+$ be any convex region in the $(\alpha, \beta)$ state space. If the Legendre transform $h'(\alpha, \beta) = \ln\left(z(\alpha, \beta)/\sqrt{\beta}\right)$ of the entropy density is concave in $\Omega$, then to each $(\alpha, \beta) \in \Omega$ there corresponds a unique pair $(\rho, T)$ that satisfies $\beta = \frac{1}{T}$ and the equation (68), and guarantees additionally the negative definiteness of the matrix $\frac{\partial^2(\rho h)}{\partial u_A \partial u_B}$.

These results have the important consequence that

$$\begin{aligned}\frac{\partial \rho h}{\partial t} + \frac{\partial \rho h v}{\partial x} =& \Lambda^\rho \left(\frac{\partial \rho}{\partial t} + \frac{\partial \rho v}{\partial x}\right) + \Lambda^{\rho v}\left(\frac{\partial \rho v}{\partial t} + \frac{\partial}{\partial x}\left(\rho v^2 + p\right)\right) + \\ & \Lambda^e \left(\frac{\partial e}{\partial t} + \frac{\partial}{\partial x}\left(\rho\left(u + v^2/2\right)v + pv\right)\right)\end{aligned} \tag{83}$$

holds, so that the field equations have a convex extension and can be brought into the symmetric hyperbolic form.

## 9.5 Riemannian Initial Data and Preparation of the Atomic Chain

In the next example we study the following macroscopic initial value problem: We describe the macrostate of the chain with $N$ particles and with fixed length $L$ by three variables, viz. the mass density $\rho\left(t, x\right)$, the velocity $v\left(t, x\right)$ and the temperaure $T\left(t, x\right)$. The initial data are

$$\rho\left(0, x\right) = \left\{\begin{array}{l} \rho_l \\ \\ \rho_r \end{array}\right. , \quad v\left(0, x\right) = \left\{\begin{array}{l} v_l \\ \\ v_r \end{array}\right. , \quad T\left(0, x\right) = \left\{\begin{array}{l} T_l \\ \\ T_r \end{array}\right. , \quad \text{for} \quad \begin{array}{l} x \leq \frac{L}{2} \\ \\ x > \frac{L}{2}. \end{array} \tag{84}$$

These data are also not sufficient to solve an initial value problem for the $N-2$ equations of motion (34). Thus again there arises the question how to prepare the initial data of the atomic chain:

At first we consider the atomic chain to be composed of two half chains of length $L/2$ with $N_l$ and $N_r$ particles, respectively, where $N_l$, $N_r$ and $L$ are given by (44). Each half chain is assumed to be in thermal equilibrium at its individual densities $\rho_l$, $\rho_r$ and at its individual temperatures $T_l$, $T_r$. The independent preparation of thermal equilibrium for each half chain was already described in detail in section 9.2.

Finally we bring both half chains in contact.

## 9.6 Failure of the Thermal Closure

We choose the initial data $\rho_l = 1.5$, $\rho_r = 1.0$, $v_l = v_r = 0$, $T_l = T_r = 0$, i.e. we start with two cold chains, and solve *Newton*s equations for $N = 35000$ particles.

We choose the scaling factor $\lambda = 2800$ and calulate from the obtained data at time $t = 1.0$ the fields of density and temperature. The results are depicted in Figure 3.

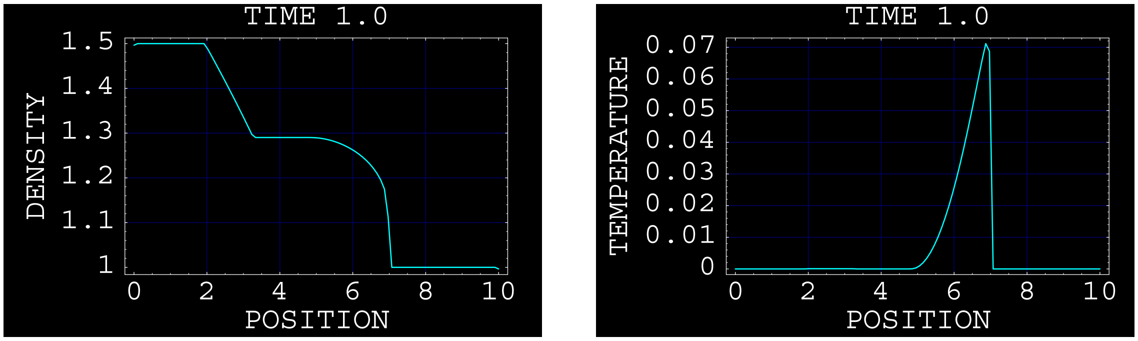

Fig. 3 Density and temperature according to NEWTONs equations for RIEMANNian initial data.

The density exhibits the development of a shock like structure and of two weak discontinuities. Furthermore we observe that at the position where the density forms the shock like structure, the temperatures apparently develops a shock which is accompanied by a tail. In the region of the weak discontinuities there is no development of the temperature, i.e. the atomic chain remains cold and is thus completely determined by the *cold closure* in that region.

Next we ask whether the chain has established local thermal equilibrium, at least in the vicinity of the shock. We answer this question by using the data that we have obtained from the solution of NEWTONs equations, and we calculate the distribution of distances.
The Figure 4 shows the surprising result.

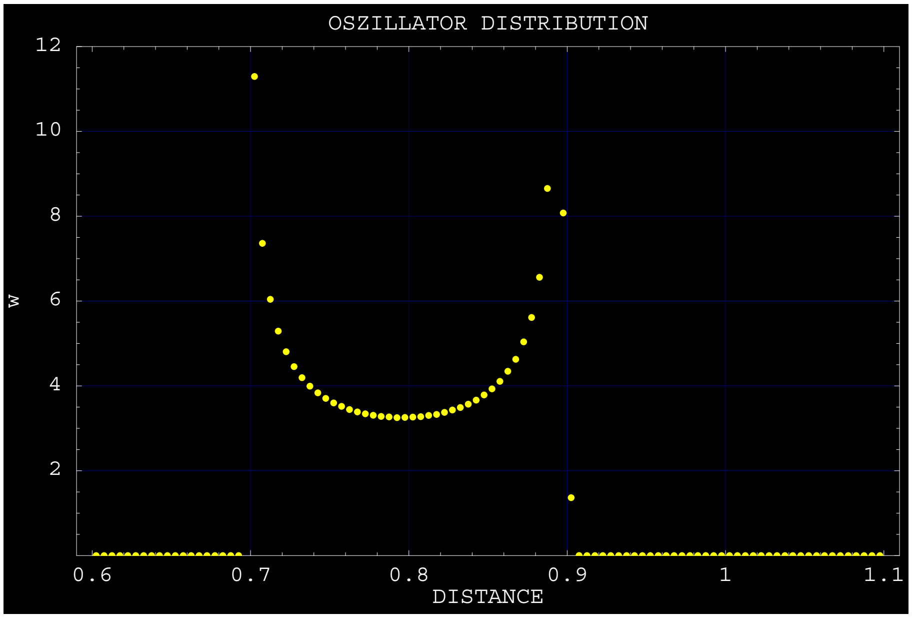

Fig. 4 Distribution of distances according to NEWTONs equations at time $t = 1.0$ and at position $x = 6.1$.

The distribution which is depicted in Figure 4 results at time $t = 1$ and at position $x = 6.1$. Properly we should expect a graph which has qualitatively the shape of the equilibrium distribution from Figure 2. However, there results a distribution with a complete different behaviour.

We conclude that the *thermal closure* fails to describe the macroscopic behaviour of the atomic chain. Next we shall explain this fact and the indication *oscillator distribution* in detail.

# 10 The Oscillator Closure

## 10.1 Oscillator Motion, Temperature and Distribution Function

A careful study of the microscopic motion of the atomic chain has revealed that the *thermal closure* cannot predict appropriately the development of the RIEMANNian initial data of the last example. Recall that *thermal motion* as it was defined in section 9.1. is indicated by a stochastic change of postions and velocities, so that both quantities are uncorrelated.

In the current case a detailed study of the microscopic motion shows that the thermal motion of the $N$ atoms is generated by $N/2$ oscillators of the following type:

In general the atomic chain consists at any time $t$ of $N-1$ different distances between the particles, i.e. for fixed particle number $\alpha$ we have

$$\{..., r_{\alpha-3}(t), r_{\alpha-2}(t), r_{\alpha-1}(t), r_{\alpha}(t), r_{\alpha+1}(t), r_{\alpha+2}(t), r_{\alpha+3}(t), ...\}. \tag{85}$$

However, at the considered temperatures only two different distances $r(t)$ and $s(t)$ have appeared alternatively, so that the microscopic motion is of the kind

$$\{..., s(t), r(t), s(t), r(t), s(t), r(t), s(t), ...\}. \tag{86}$$

Furthermore $r(t)$ and $s(t)$ are restricted by the condition

$$r(t) + s(t) = \frac{2}{\rho}. \tag{87}$$

We conclude that there is only one representative equation of motion for the oscillator motion, viz.

$$\ddot{r}(t) = 2\left(\varphi'\left(\frac{2}{\rho} - r(t)\right) - \varphi'(r(t))\right). \tag{88}$$

Instead of $r$ we use sometimes for convenience the quantity $x = (1/\rho - r)/2$ which measures the displacement from the mean distance. Note that the mass density is a constant on the atomic scale, i.e. within the support of the window function. Thus we can write

$$\ddot{x}\left(t\right)=\varphi'\left(\frac{1}{\rho}-2x\left(t\right)\right)-\varphi'\left(\frac{1}{\rho}+2x\left(t\right)\right). \tag{89}$$

Without loss of generality we solve this equation for the initial displacement $x\left(0\right)=0$ and for a given positive initial velocity $\dot{x}\left(0\right)$.

Before we proceed, we note that the equations (87), (88) and (89) imply that the velocities of the two particles which constitute the oscillator, say $\dot{x}_{\alpha+1}\left(t\right)$ and $\dot{x}_{\alpha}\left(t\right)$, are restricted according to $\dot{x}_{\alpha+1}\left(t\right)=-\dot{x}_{\alpha}\left(t\right)$. This fact will become important when we evaluate the microscopic representations of the macroscopic fields.

The first integral of (89) reads $\dot{x}\left(t\right)=\pm\sqrt{e_0-\varphi\left(\frac{1}{\rho}-2x\left(t\right)\right)-\varphi\left(\frac{1}{\rho}+2x\left(t\right)\right)}$,where $e_0$ is the integration constant. The oscillator moves between its minimal and maximal distances $r_-$ and $r_+$, which are restricted by

$$r_-+r_+=\frac{2}{\rho}. \tag{90}$$

Finally we choose the integration constant $e_0=\varphi\left(r_-\right)+\varphi\left(r_+\right)$. The representation of $\dot{x}\left(t\right)$ that we shall use further on is now given by

$$\dot{x}\left(t\right)=\pm\sqrt{\varphi\left(r_+\right)+\varphi\left(r_-\right)-\varphi\left(r\left(t\right)\right)-\varphi\left(\frac{2}{\rho}-r\left(t\right)\right)}. \tag{91}$$

Due to (91) the mean value of $\dot{x}(t)$ in time is zero, and we shall define the r-dependent positive part of the excess velocity:

$$C(r_-,r_+,r)=\sqrt{\varphi\left(r_+\right)+\varphi\left(r_-\right)-\varphi\left(r\right)-\varphi\left(r_-+r_+-r\right)}. \tag{92}$$

It is important to recognize that the only microscopic variable which is left, is the distance $r$. Thus we can construct now a distribution function that only takes care for the distribution of possible values of $r$.

To this we **define** the duration of a half period of the oscillator motion where $\dot{x}\left(t\right)\geq 0$:

$$t_*\left(r_-,r_+\right)=\int\limits_{r_-}^{r_+}\frac{dr}{\sqrt{\varphi\left(r_+\right)+\varphi\left(r_-\right)-\varphi\left(r\right)-\varphi\left(r_-+r_+-r\right)}}>0. \tag{93}$$

The integral exists in the convex region of $\varphi$, because there the integrand approaches $1/\sqrt{(r-r_-)(\varphi'(r_+)-\varphi'(r_-))}$ and $1/\sqrt{(r_+-r)(\varphi'(r_+)-\varphi'(r_-))}$, respectively, in the limits $r\to r_-$ and $r\to r_+$.

Next we define a function $w\left(r_{-}, r_{+}, r\right)$ on the interval $\left(r_{-}, r_{+}\right)$ according to

$$
\begin{aligned}
& w\left(r_{-}, r_{+}, r\right)=\frac{1}{t_{*}\left(r_{-}, r_{+}\right) \sqrt{\varphi\left(r_{+}\right)+\varphi\left(r_{-}\right)-\varphi(r)-\varphi\left(r_{-}+r_{+}-r\right)}}, \\
& \text{with} \quad \int_{r_{-}}^{r_{+}} w\left(r_{-}, r_{+}, r\right) d r=1
\end{aligned} \tag{94}
$$

Note that $w\left(r_{-}, r_{+}, r\right) d r$ gives the the probabilty to find at any time $t$ the distance $r$ within the infinitesimal interval $[r, r+d r]$. From (94) there results the important symmetry condition

$$
w\left(r_{-}, r_{+}, r\right)=w\left(r_{-}, r_{+}, r_{-}+r_{+}-r\right), \tag{95}
$$

The distribution function $w\left(r_{-}, r_{+}, r\right)$ will be used in section 10.3 to establish the *oscillator closure*. However, already here we shall introduce the temperature of the oscillator motion as follows

$$
T=\frac{1}{t_{*}\left(r_{-}, r_{+}\right)} \int_{0}^{t_{*}\left(r_{-}, r_{+}\right)} \dot{x}(t)^{2} d t=\frac{1}{t_{*}\left(r_{-}, r_{+}\right)} \int_{r_{-}}^{r_{+}} \frac{d r}{w\left(r_{-}, r_{+}, r\right)}. \tag{96}
$$

This definition is analogue to the corresponding definition $(74)_2$ for the thermal closure.

## 10.2 Realization of the Oscillator Distribution by Newtons Equations

In section 9.6 we considered Riemannian initial data with zero temperature which lead for later times in some region to a temperature field. The distribution function in that region is called oscillator distribution and is displayed in Figure 4.

The statistical parameters to that curve are $\rho(t=1, x=6.1)=1.25$ and $T(t=1, x=6.1)=0.033$. Now we may use these data in order to calculate $r_{-}=0.70$ and $r_{+}=0.90$ from (90) and (96). The solid line in Figure 5 represents the analytical expression (94), and for a comparison with the corresponding distribution that was calculated from NEWTONs equations, we have put the data from Figure 4 once more as dots.

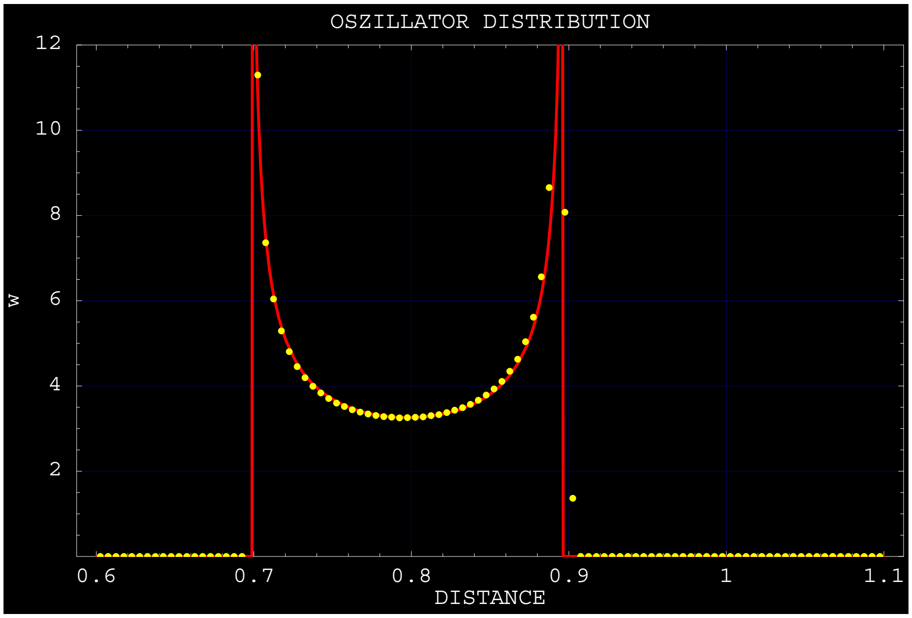

Fig. 5 Distribution of distances, comparison of microscopic data and analytical results.

We state complete agreement between both procedures.

Consequently we conclude that a given pair $(\rho, T)$ does not constitute a unique equillibrium, because we know from section 9.2 that a pair $(\rho, T)$ may be realized by the classical *thermal motion*, while here we have learned that the same pair could also be realized by the oscillator motion.

## 10.3 Oscillator Closure and Field Equations

We consider again the macroscopic system of the three conservation laws

$$\begin{aligned}
&\oint_{\partial\Omega} (\rho dx - \rho v dt) = 0, \\
&\oint_{\partial\Omega} \left(\rho v dx - \left(\rho v^2 + p\right) dt\right) = 0, \\
&\oint_{\partial\Omega} \left(\left(\frac{\rho}{2} v^2 + \rho u\right) dx - \left(\frac{\rho}{2} v^2 + \rho u + p\right) v dt\right) = 0\,.
\end{aligned} \tag{97}$$

which must be supplemented by constitutive laws that relate the pressure, the internal energy and the heat flux to the basic variables $\rho$ and $T$ . Note that the constitutive laws cannot depend on the other basic variable $v$.

In the list of variables we replace now $\rho$ and $T$ by $r_-$ and $r_+$ , because these latter quantities appear explicitely in the distribution function $w\,(r_-, r_+, r)$. Consequently we write down the mass density, the pressure, the internal energy, the temperature and the heat flux as functions of $r_-$ and $r_+$.

This is achieved by the closure **ansatz:**

$$
\begin{aligned}
\frac{1}{\rho} &= \int_{r_-}^{r_+} r w\left(r_-, r_+, r\right) \, dr = \frac{1}{2}\left(r_- + r_+\right), \\
T &= \int_{r_-}^{r_+} C^2 w\left(r_-, r_+, r\right) \, dr = \frac{1}{t_*} \int_{r_-}^{r_+} \sqrt{\varphi\left(r_+\right) + \varphi\left(r_-\right) - \varphi\left(r\right) - \varphi\left(r_- + r_+ - r\right)} \, dr, \\
p &= \rho \int_{r_-}^{r_+} \left(C^2 - r\varphi'\left(r\right)\right) w\left(r_-, r_+, r\right) \, dr \qquad (98) \\
&= -\frac{1}{t_*} \int_{r_-}^{r_+} \frac{\varphi'\left(r\right) \, dr}{\sqrt{\varphi\left(r_+\right) + \varphi\left(r_-\right) - \varphi\left(r\right) - \varphi\left(r_- + r_+ - r\right)}}, \\
u &= \int_{r_-}^{r_+} \left(\frac{1}{2}C^2 + \varphi\left(r\right)\right) w\left(r_-, r_+, r\right) \, dr = \frac{1}{2}\left(\varphi\left(r_-\right) + \varphi\left(r_+\right)\right), \\
q &= 0.
\end{aligned}
$$

The list (98) defines the *oscillator closure* with $t_*(r_-, r_+)$, $w\left(r_-, r_+, r\right)$ and $C\left(r_-, r_+, r\right)$ given by (93), (94) and (92), respectively. In each line the first equality results from the evaluation of the microscopic representations (38) and (39) with the oscillator distribution function. The nonconvective part of the energy flux, $q$, is zero because the individual particle velocities of an oscillator cancel each other. The second equality in each line results from some simple manipulations of the integrals. The remaining integrals must be evaluated numerically.

We have thus established a closed system of field equations for the variables $\rho$, $v$ and $T$ or alternatively for the variables $r_-, r_+$ and $v$. The system consists of the conservation laws (97) and of the constitutive equations (98). Using the closure conditions (98) we are able to derive from (97) the differential form (37) of the conservation laws as well as the Rankine Hugoniot conditions (75), which are also valid here.

## 10.4 Properties of the Field Equations

Recall that the *oscillator closure* assumes randomly distributed distances between the particles of the chain. However, in contrast to the *thermal closure*, their velocities are determined from Newton s law for given distances. Nevertheless, even in this case there holds the Gibbs equation

$$
T dh = du + p d\left(\frac{1}{\rho}\right). \qquad (99)
$$

This fact will be proved in the following, and an explicit expression for the specific entropy $h$ will be given. The subsequent reasoning that leads to the symmetric hyperbolic form of the system (97) and (98) runs along the same lines as it was carried out for the *thermal closure* and will therefore be skipped.

**Proposition:** (i) In the convex region $\varphi''(r) > 0$ there holds the integrability condition between the functions density $\rho\left(r_{-}, r_{+}\right)$, temperature $T\left(r_{-}, r_{+}\right)$, pressure $p\left(r_{-}, r_{+}\right)$ and internal energy $u\left(r_{-}, r_{+}\right)$, which are defined in (98), viz.

$$\frac{\partial}{\partial r_{-}}\left(\frac{1}{T}\left(\frac{\partial u}{\partial r_{+}}+\frac{1}{2} p\right)\right)=\frac{\partial}{\partial r_{+}}\left(\frac{1}{T}\left(\frac{\partial u}{\partial r_{-}}+\frac{1}{2} p\right)\right). \tag{100}$$

(ii) The condition (100) implies the existence of the specific entropy function $h\left(r_{-}, r_{+}\right)$ according to

$$\frac{\partial h}{\partial r_{-}}=\frac{1}{T}\left(\frac{\partial u}{\partial r_{-}}+\frac{1}{2} p\right), \quad \frac{\partial h}{\partial r_{+}}=\frac{1}{T}\left(\frac{\partial u}{\partial r_{+}}+\frac{1}{2} p\right), \tag{101}$$

which yields after integration

$$h\left(r_{-}, r_{+}\right)=\ln \left(\int_{r_{-}}^{r_{+}} \sqrt{\varphi\left(r_{+}\right)+\varphi\left(r_{-}\right)-\varphi(r)-\varphi\left(r_{-}+r_{+}-r\right)}\; d r\right). \tag{102}$$

**Proof:** (100) is the integrabily condition for (99). By introducing the functions $p_0\left(r_{-}, r_{+}\right)=t_*\left(r_{-}, r_{+}\right) p\left(r_{-}, r_{+}\right)$ and $T_0\left(r_{-}, r_{+}\right)=t_*\left(r_{-}, r_{+}\right) T\left(r_{-}, r_{+}\right)$, and with (98) $_4$, we may write down (100) in its equivalent form

$$\begin{aligned}
&\frac{\partial p_0}{\partial r_{+}}-\frac{\partial p_0}{\partial r_{-}}= \\
&\varphi'\left(r_{+}\right) \frac{\partial t_*}{\partial r_{-}}-\varphi'\left(r_{-}\right) \frac{\partial t_*}{\partial r_{+}}+\frac{1}{T}\left(\left(\varphi'\left(r_{-}\right)+p\right) \frac{\partial T_0}{\partial r_{+}}-\left(\varphi'\left(r_{+}\right)+p\right) \frac{\partial T_0}{\partial r_{-}}\right).
\end{aligned} \tag{103}$$

Next we calculate the identities

$$\frac{\partial T_0}{\partial r_{-}}=\frac{t_*}{2}\left(\varphi'\left(r_{-}\right)+p\right), \quad \frac{\partial T_0}{\partial r_{+}}=\frac{t_*}{2}\left(\varphi'\left(r_{+}\right)+p\right), \tag{104}$$

and introduce these in (103), which reduces to

$$\frac{\partial}{\partial r_{+}}\left(p_0+\varphi'\left(r_{-}\right) t_*\right)=\frac{\partial}{\partial r_{-}}\left(p_0+\varphi'\left(r_{+}\right) t_*\right). \tag{105}$$

If we use again the identities (104), we can write down the condition (105) in the form

$$\frac{\partial^2 T_0}{\partial r_{-} \partial r_{+}}=\frac{\partial^2 T_0}{\partial r_{+} \partial r_{-}}. \tag{106}$$

There remains to derive the not obvious existence and continuity of the $t_*$ and $p_0$ derivatives. Here we shall present their explicit form which may also serve to check the condition (105) by direct substitution:

$$\begin{aligned}
\frac{\partial t_*}{\partial r_+} &= \frac{+t_*}{r_+ - r_-} - \frac{1}{2}\int\limits_{r_-}^{r_+} \frac{\varphi'(r_+) - \varphi'(r)\frac{r-r_-}{r_+-r_-} - \varphi'(r_- + r_+ - r)\frac{r_+-r}{r_+-r_-}}{[\varphi(r_-) + \varphi(r_+) - \varphi(r) - \varphi(r_- + r_+ - r)]^{\frac{3}{2}}}\, dr\,, \\
\frac{\partial t_*}{\partial r_-} &= \frac{-t_*}{r_+ - r_-} - \frac{1}{2}\int\limits_{r_-}^{r_+} \frac{\varphi'(r_-) - \varphi'(r)\frac{r_+-r}{r_+-r_-} - \varphi'(r_- + r_+ - r)\frac{r-r_-}{r_+-r_-}}{[\varphi(r_-) + \varphi(r_+) - \varphi(r) - \varphi(r_- + r_+ - r)]^{\frac{3}{2}}}\, dr\,.
\end{aligned} \tag{107}$$

$$\begin{aligned}
\frac{\partial p_0}{\partial r_+} &= -\frac{t_*}{r_+ - r_-}\cdot\varphi'(r_+) \\
&\quad + \frac{1}{2}\int\limits_{r_-}^{r_+} \frac{\varphi'(r_+)\left[\varphi'(r)\frac{r_+-r}{r_+-r_-} + \varphi'(r_- + r_+ - r)\frac{r-r_-}{r_+-r_-}\right] - \varphi'(r)\,\varphi'(r_- + r_+ - r)}{[\varphi(r_-) + \varphi(r_+) - \varphi(r) - \varphi(r_- + r_+ - r)]^{\frac{3}{2}}}\, dr\,, \\
\frac{\partial p_0}{\partial r_-} &= +\frac{t_*}{r_+ - r_-}\cdot\varphi'(r_-) \\
&\quad + \frac{1}{2}\int\limits_{r_-}^{r_+} \frac{\varphi'(r_-)\left[\varphi'(r)\frac{r-r_-}{r_+-r_-} + \varphi'(r_- + r_+ - r)\frac{r_+-r}{r_+-r_-}\right] - \varphi'(r)\,\varphi'(r_- + r_+ - r)}{[\varphi(r_-) + \varphi(r_+) - \varphi(r) - \varphi(r_- + r_+ - r)]^{\frac{3}{2}}}\, dr\,.
\end{aligned} \tag{108}$$

These integrals exist in the convex region $\varphi''(r) > 0$, but they cannot be obtained by a simple differentiation rule, because there appear singularities with exponent $-3/2$ at $r = r_-$ and at $r = r_+$. Here we have calculated the partial derivatives by its definitions. For example $(107)_2$ may be obtained as follows: We start with

$$\frac{\partial t_*}{\partial r_-} = \lim_{\epsilon\to 0}\frac{1}{\epsilon}\left[t_*(r_- + \epsilon, r_+) - t_*(r_-, r_+)\right]\,, \tag{109}$$

and substitute the integral representation for $t_*(r_- + \epsilon, r_+)$ with the lower integration limit $r_- + \epsilon$ and the upper integration limit $r_+$ by the transformation

$$r \to r_- + (r_+ - r_-)\frac{r - r_- - \epsilon}{r_+ - r_- - \epsilon}\,. \tag{110}$$

Then in (109) both representations for $t_*(r_- + \epsilon, r_+)$ and $t_*(r_-, r_+)$ have the same integration limits $r_\pm$, and we can combine them to a single integral in order to pass to the limit $\epsilon \to 0$. The other representations may be obtained in the same way.

## 10.5 Transition from the Thermal Motion to the Oscillator Motion

Recall that we have considered in section 9.6 RIEMANNian initial data with zero temperature. For later times these data imply the development of a temperature field that was not constituted by thermal motion but by oscillator motion.

Now we consider initial RIEMANNian data with nonzero temperature. In particular we prepare both half chains so that they initially realize thermal motion with different temperatures. The data are $\rho_l = 1.5$, $\rho_r = 1.0$, $v_l = v_r = 0$, $T_l = 0.01$ and $T_r = 0.005$. The total chain consists of $N = 10000$ particles, and for the macroscopic representations we choose the scaling factor $\lambda = 800$.

These data are used now to solve *Newton*s equations, and to calculate at time $t = 1.0$ subsequently the temperature field as well as the distributions of the velocities and the distances at various positions. In the sequel we are going to discuss the surprising results which are depicted in Figures 6 and 7.

The upper left graph in Figures 6 and 7 shows the temperature field at time $t = 1.0$. The shape of the field is almost the same that we have obtained in Figure 3, where we started with zero temperature in both half chains. However, the microscopic motion behind the two temperature fields is completely different. The microscopic motion that induces the temperature field in Figure 3 is pure oscillator motion. On the contrary, the microscopic motion that induces the temperature field in this section is neither pure oscillator motion nor pure thermal motion but a mixing of both. This statement is exhibited by the other graphs of Figures 6 and 7. These depict at time $t = 1.0$ the distributions of velocities and distances, respectively, for five different positions along the $x$ coordinate.

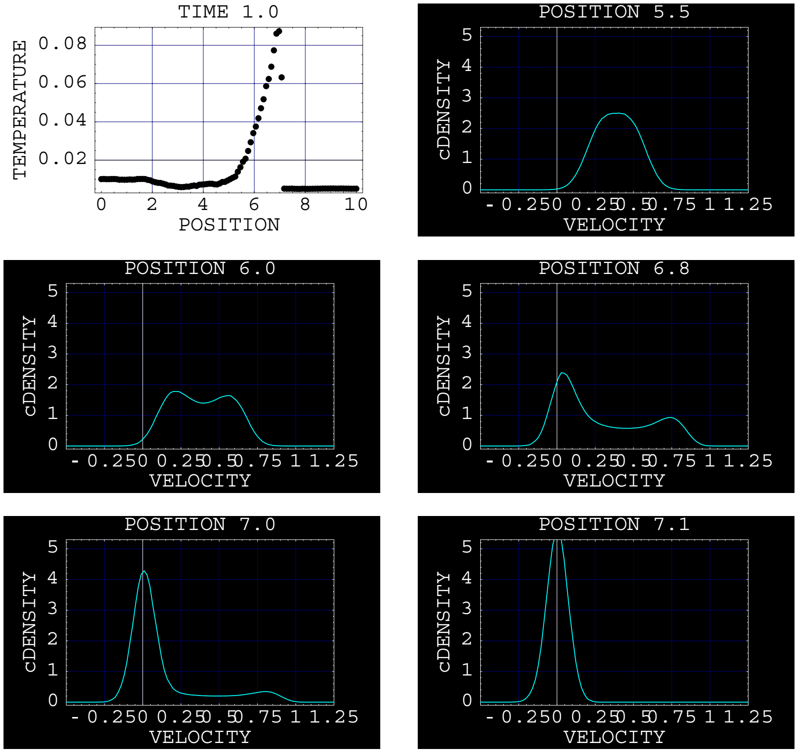

Fig. 6 Transition of the distributions of velocities for various positions within the temperature pulse.

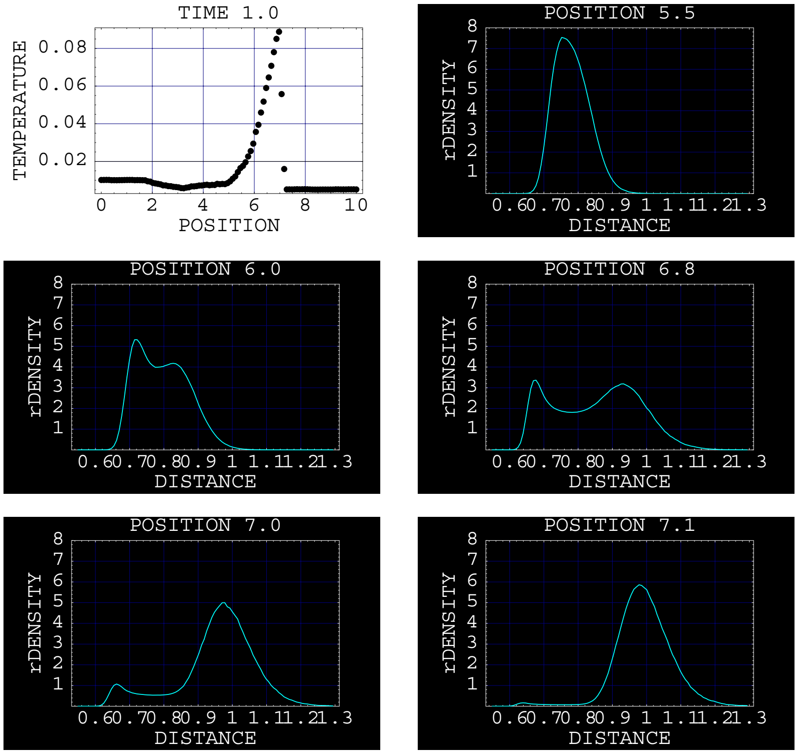

Fig. 7 Transition of distribution of distances for various positions within the temperature pulse.

We observe that the first and the last distribution functions, which are displayed in Figures 6 and 7, represent the thermal motion which is due to the thermal preparation of both half chains. The intermediate distribution functions exhibit some kind of transition between thermal and oscillator motion. In particular, the distribution of distances at position $x = 6.8$ causes a reminiscence to the pure oscillator distribution from Figure 5.

We conclude that in addition to the thermal and oscillator motion between the positions from $x = 5.5$ up to $x = 7.1$ there appear new kinds of microscopic motions that were not considered before. To all these different motions there correspond distribution functions, which represent different kinds of local equilibria. We shall illustrate now the consequences of this statement and start the discussion with a **definition**:

A given distribution function describes a *local equilibrium*, if it is possible to prepare the microstate of the chain so that the local distribution can also be realized globally independent of time and space in a total chain with an arbitrary large number of particles, and if this global solution is a stable equilibrium.

We pose and answer now two questions: Is this definition in accordance with conventional definitions of local equilibrium? And secondly, do the distribution functions from Figures 6 and 7 describe local equilbria?

Regarding the first question we point out that there is no unique definition of local equilibrium in the literature.

Often local equilibrium is defined by vanishing heat flux and vanishing pressure deviator. Sometimes this definition is replaced by the statement that a body is at $(t, x)$ in local equilibrium if it is sufficiently described by the prescription of density and temperature at this point.

Regarding the second question we have observed that according to our definition all the distribution functions which are depicted in Figures 6 and 7 describe local equilibria. This relies on the observation, see section 7.3, that the local microscopic motion as well as the macroscopic fields depend on time and space only via the ratio $\frac{x}{t}$, if $N$ is sufficiently large. This case will be considered now exclusively.

There is an interesting consequence of this observation which can be read off from Figure 8, which assumes without loss of generality the jump in the RIEMANNian initial data at $x = 0$.

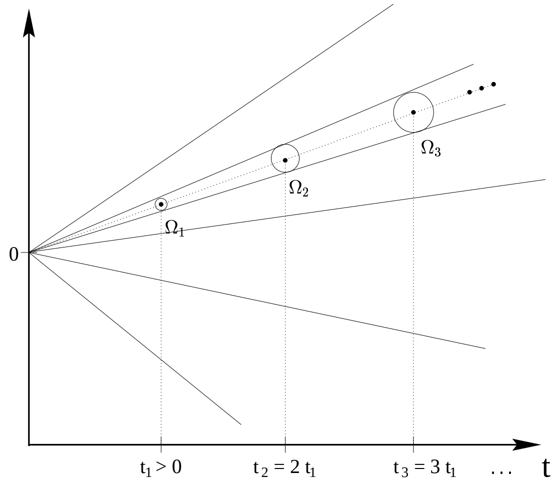

Fig. 8: The scaling invariance of the microscopic RIEMANN solution

We consider the infinite sequence of regions $\Omega_1$, $\Omega_2$, $\Omega_3$, ..., of increasing size. If the fields $u_A(x/t)$ do not change significantly in time and space within a small region, say $\Omega_1$, then the same is true in a macroscopically large region $\Omega_n$, with large $n$.

We describe now how a chain must be prepared in order to establish globally the local distributions at any point $(t_0, x_0)$. Around this point we choose a region, say $\Omega_1$, sufficiently small so that the microscopic motion within $\Omega_1$ does not change significantly.

Next we inflate $\Omega_1$ within the segment from Figure 8 in order to end up with a large region $\Omega_n$ from where we use the global data for the global construction of the distributions of velocities and distancies.

Recall that the microscopic motion in $\Omega_n$ is the same as in $\Omega_1$.

Finally we discuss an interesting consequence. We calculate the heat flux field at time 1.0. The result is shown in Figure 9. It is important to recall that the heat flux is zero for the pure thermal motion as well as for the pure oscillator motion. On the contrary, those microscopic motions that constitute the other local equilibria induce a nonzero macroscopic heat flux. However this does not mean, that the heat flux is proportional to the temperature gradient.

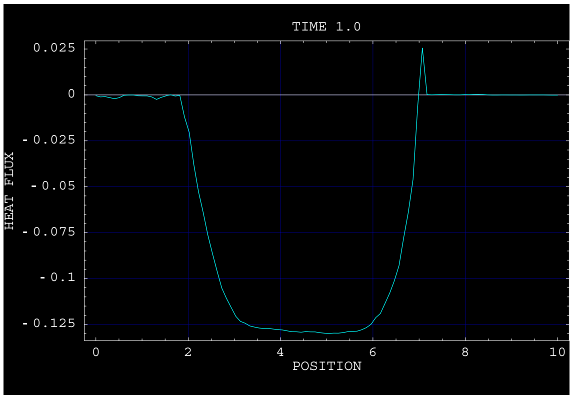

Fig. 9 Heat flux field at time $t = 1$.

This can be immediately observed from a comparison of Figure 9 with the corresponding temperature field from Figures 6 and 7. Moreover, obviously also the time and space dependence of the heat flux is given by the ratio $x/t$, and for that reason, the heat flux cannot be proportional to the temperature gradient.

Thus in the considered examples there is no accordance between our definition and the conventional definition of local equilibrium.

The conventional definition of local equilibrium assumes implicitely that the microscopic motion is uniquely determined by a finite number of macroscopic parameters like density and temperature.

This is not true in our examples, even then if we only consider pure thermal and pure oscillator motion.

Thus generally the appropriate closure changes within a given RIEMANN solution.

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