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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 Newton's equations of motion.

We discuss various Riemannian 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 of mass density and temperature do not constitute a unique kind of microscopic motion in equilibrium.

1. Introduction

1.1. Scope of this study

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 not basic variables.

The constitutive equations represent the closure of the open scheme of universal equations. Thus, constitutive equations 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 notion 'constitutive equation' 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 microscale we describe the microscopic motion of the individual atoms by Newton's equations of motion. We solve these equations exclusively for macroscopic Riemannian initial data. However, to solve Newton's equations we need microscopic initial data. How these data can be prepared will be explained in sections 8.1, 9.2 and 9.5. We restrict our interest to Riemannian initial data that lead to the propagation of waves. Initial data which initiate diffusion-like motion will be studied in a forthcoming paper.

The derivation of field equations must be split into two steps. In a first step we start from Newton's equations and show that they imply macroscopic equations of balance. In these equations there appear macroscopic quantities like mass-, momentum-, energy density, pressure and heat flux, and these 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.

In this study we consider the fields of mass density $\rho(t, x)$, velocity $v(t, x)$ and temperature $T(t, x)$ as the basic variables. We study pure initial value problems with Riemannian initial data for $\rho(0, x)$, $v(0, x)$ and $T(0, x)$.

In a second step we supplement the equations of balance by closure relations which relate the basic fields to the energy density $\rho e(t, x)$, the pressure tensor $p_{ik}(t, x)$ and to the heat flux $q_k(t, x)$.

We consider three kinds of possible microscopic motions that lead in turn to three different classes of closure relations:

(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 often rely 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.

It is important to consider all three kinds of microscopic motions, because they might appear simultaneously in arbitrary large regions of space and time. Moreover, the three kinds of microscopic motions realize three different kinds of equilibria. Next we shall discuss these facts in detail.

After solving Newton's equations of motion for various given Riemannian initial data we observed a quite surprising scaling behaviour of the resulting global solution. If the particle number N is sufficiently large, then the solution does not change when we inflate the space x and the time t according to λx and λt with an arbitrary, positive scaling factor λ. Later on we shall choose the scaling factor λ proportional to N, because this choice will be proved of physical importance.

Before we discuss an important consequence of the scaling behaviour of a Riemann solution, we give a new definition of the notion local equilibrium. Usually a material at the macroscopic space–time point (t, x) is said to be in local equilibrium if the macrostate of the material at that point is completely given by a distribution function of the microscopic motion which has only the quantities ρ, v and T as parameters.

We prefer here a different definition†: an atomic chain at the macroscopic space–time point (t, x) is said to be in local equilibrium if its microscopic motion, which is described by a distribution function in the close vicinity of (t, x), can also be established globally independent of space and time and is globally described by the same distribution function. In addition, we require that arbitrary small disturbances of the microscopic motion do not lead to a change of the distribution function.

Note that the new definition of local equilibrium does not contain any reference to the quantities ρ, v and T. In particular, it is not assumed that the characterization of an equilibrium distribution function is given by a finite set of variables.

The processes that we consider in this study show that both definitions are not equivalent.

We proceed with the discussion of the consequences of the scaling behaviour of the Riemann solution. When we combine the scaling behaviour with the new definition of local equilibrium we are led to conclude that all three kinds of closure, namely *cold closure, thermal closure* and *oscillator closure*, constitute local equilibria. Moreover, it is due to the observed scaling behaviour of the Riemann solution of Newton's equations of motion that these allow only solutions that constitute local equilibria. Nevertheless, we will observe that the considered closure relations are only sufficient for special Riemannian initial data. If this happens, it is now obvious that an improvement of the macroscopic system to describe the development of the initial data cannot be obtained by considering closure relations that take care of more variables as ρ, v and T.

Next we characterize the mathematical and thermodynamical structure of the considered macroscopic systems. All three closure relations lead to symmetric hyperbolic systems. For each system we identify an entropy function that is also defined in terms of microscopic quantities. However, the entropy is not calculated here from Boltzmann's famous formula which relates the entropy to the number of microstates that can realize a given macrostate. 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 in the three cases uniquely a microscopic representation of the entropy.

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

1.2. The organization of the paper

Sections 2–6 deal with a many-particle system which consists of N structureless atoms whose dynamics is described by Newton's equations of motion. These are supplemented by pairwise interaction potentials.

The microscale is related to the macroscale 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 macroscopic mean values of microscopic observables with respect to time and space.

In sections 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 given definition requires that there are no forces of gravity.

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 propagation. Furthermore, this kind of scaling induces macroscopic fields which also become independent of N if N is sufficiently large.

In sections 8–10 we introduce the three different closure assumptions and study their appropriateness. In section 8 we start with the *cold closure* that ignores 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 thus must 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. In sections 9.5 and 9.6 we consider another 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 by quite natural initial data it is possible to generate 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 serve to establish the *oscillator closure*.

Next we consider a further Riemannian initial value problem which deviates only slightly from the one that served to motivate the *oscillator closure*, and in fact the temporal development of the macroscopic fields looks similar. 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 from 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, namely the Maxwellian. The analogue closure problem leads to the hyperbolic system of Euler equations. This system was studied and solved in [1, 2].

It is due to the presence of permanent strong interaction forces between the atoms that the solid behaves differently 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 [3–6] 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 also starts from Newton's 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 completely differently.

Note that we derive rigorously from Newton's equations the macroscopic conservation laws and the corresponding microscopic representations of macroscopic quantities. In the next step we introduce the various closure relations. By contrast, Sugiyama and co-workers considered only one closure relation, which was given by a distribution function of Gaussian type for N independent atoms. This function was 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 $\alpha, \beta, \ldots \in \{1, 2, \ldots, N\}$. At time $t \geqslant 0$ the particles are located at positions $x^\alpha(t)$ and they have velocities $\dot{x}^\alpha(t)$.

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

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

The dynamics of the microstate is determined by Newton's equations of motion

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

A particle α is subjected to a total force K_i^α which is decomposed into the external force G_i^α and the interaction force $K_i^{\alpha\beta}$ between α and any other particles β. 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

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

where $r^{\alpha\beta} = x^\beta - x^\alpha$. Obviously (4) satisfies Newton's 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 now introduce the window function $\chi(t, x)$, which relates the microscale to the macroscale. The function χ 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(χ) so that the window contains infinitely many particle worldlines from a microscopic viewpoint. However, from a macroscopic viewpoint supp(χ) 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 x.

We provide the window function with the following properties:

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

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

(iii) $\int_{-\infty}^{+\infty} \chi(t, x) \, dt \, d^3x = 1$.

We shall choose the support of the window function macroscopically small, but microscopically very large so that the window still contains an enormous number of

microscopic trajectories. This is necessary in order to pass to the three thermodynamic limits which will be considered in sections 8–10.

For each particle index α we define

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

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 χ_α with respect to t can be written as*

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

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

$$\chi_\alpha(\vartheta, t, \boldsymbol{x}) - \chi_\beta(\vartheta, t, \boldsymbol{x}) = \frac{\partial}{\partial x_k}\left((x_k^\beta - x_k^\alpha)\int_0^1 \chi(\vartheta - t, \boldsymbol{x}^\alpha(\vartheta) - \boldsymbol{x} + \mu(\boldsymbol{x}^\beta - \boldsymbol{x}^\alpha))\,\mathrm{d}\mu\right). \tag{8}$$

Proof. The proof of (i) follows immediately from the given definition of $\chi_\alpha(\vartheta, t, \boldsymbol{x})$, and the proof of (ii) starts with the identity

$$\chi(\vartheta - t, \boldsymbol{x}^\alpha(\vartheta) - \boldsymbol{x}) - \chi(\vartheta - t, \boldsymbol{x}^\beta(\vartheta) - \boldsymbol{x})$$
$$= -\int_0^1 \frac{\partial}{\partial \mu}\chi(\vartheta - t, \boldsymbol{x}^\alpha(\vartheta) - \boldsymbol{x} + \mu(\boldsymbol{x}^\beta - \boldsymbol{x}^\alpha))\,\mathrm{d}\mu. \tag{9}$$

According to the chain rule we can transform the μ derivative into the divergence derivative that occurs in (ii). □

4. The general equations of balance

Recall that the microstate of a body is given by the list γ_N of $6N$ positions and velocities. For the description of the macrostate of the body we need a reduced list Γ_{N_M} of variables, with $N_M \ll N$. The most important case is the list Γ_5 which contains the five macroscopic variables mass density ρ, momentum density $\rho\boldsymbol{v}$ and energy density ρe. These are formed at time t and at the space point $\boldsymbol{x}$ by the definitions

$$\rho(t, \boldsymbol{x}) = \int_0^\infty \sum_{\alpha=1}^N m\chi_\alpha(\vartheta, t, \boldsymbol{x})\,\mathrm{d}\vartheta$$

$$\rho v_i(t, \boldsymbol{x}) = \int_0^\infty \sum_{\alpha=1}^N m\dot{x}_i^\alpha(\vartheta)\chi_\alpha(\vartheta, t, \boldsymbol{x})\,\mathrm{d}\vartheta \tag{10}$$

$$\rho e(t, \boldsymbol{x}) = \int_0^\infty \sum_{\alpha=1}^N \left(\frac{m}{2}\dot{x}_i^\alpha(\vartheta)\dot{x}_i^\alpha(\vartheta) + \frac{1}{2}\sum_{\beta=1}^N \varphi(|r^{\alpha\beta}(\vartheta)|)\right)\chi_\alpha(\vartheta, t, \boldsymbol{x})\,\mathrm{d}\vartheta.$$

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 $(t, \boldsymbol{x})$, 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 $\frac{m}{2}\dot{x}_i^\alpha\dot{x}_i^\alpha + \frac{1}{2}\varphi(|r^{\alpha\beta}|)$ of a single particle, respectively.

Table 1.

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

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 first generalize definitions (10) and to formulate their generic structure. From (10) we read off the generic form

$$u_A(t, \boldsymbol{x}) = \int_0^\infty \sum_{\alpha=1}^N \left(O_A^\alpha(\vartheta) + \sum_{\beta=1}^N O_A^{\alpha\beta}(\vartheta) \right) \chi_\alpha(\vartheta, t, \boldsymbol{x}) \, d\vartheta \qquad (A = 0, 1, 2, \ldots, N_M - 1).$$

(11)

The quantities O_A^α and $O_A^{\alpha\beta}$ denote microscopic one- and two-particle observables, respectively: see table 1, where we have introduced the abbreviation $\varphi_{\alpha\beta} = \varphi(|r_{\alpha\beta}|)$ for $\beta \neq \alpha$ and $\varphi_{\alpha\alpha} = 0$. We shall now use the generic form (11) to establish general equations of balance for the quantities u_A. In this paper we consider only microscopic observables that may have the following dependences:

$$O_A^\alpha(\vartheta) = \tilde{O}_A^\alpha(\dot{\boldsymbol{x}}^\alpha(\vartheta)) \qquad O_A^{\alpha\beta}(\vartheta) = \tilde{O}_A^{\alpha\beta}(r^{\alpha\beta}(\vartheta), \dot{\boldsymbol{x}}^\alpha(\vartheta), \dot{\boldsymbol{x}}^\beta(\vartheta)) \qquad (12)$$

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

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

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

(13)

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

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

(14)

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

$$\frac{\partial u_A(t, \boldsymbol{x})}{\partial t} + \frac{\partial}{\partial x_k} \left(\int_0^\infty \sum_{\alpha=1}^N \left(O_A^\alpha(\vartheta) + \sum_{\beta=1}^N O_A^{\alpha\beta}(\vartheta) \right) \dot{x}_k^\alpha(\vartheta) \chi_\alpha(\vartheta, t, \boldsymbol{x}) \, d\vartheta \right)$$

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

(15)

The expression under the divergence already gives the first contribution to the flux f_{Ak} we are looking for. Next we apply, according to (12), the chain rule to the ϑ derivatives on the right-hand side. For this purpose we define for each volume density u_A ($A = 0, 1, 2, \ldots, N_M - 1$)

a corresponding $N \times N$ matrix M_A with components $((M_A^{\alpha\beta}))$ which are formed by the microscopic observables according to

$$M_A^{\alpha\beta} = \frac{\partial \tilde{O}_A^{\alpha\beta}}{\partial r_j^{\alpha\beta}} \dot{r}_j^{\alpha\beta} + \frac{1}{m} \frac{\partial \tilde{O}_A^{\alpha}}{\partial \dot{x}_j^{\alpha}} K_j^{\alpha\beta} + \frac{1}{m} \sum_{\gamma=1}^{N} \left(\frac{\partial \tilde{O}_A^{\alpha\beta}}{\partial \dot{x}_j^{\alpha}} K_j^{\alpha\gamma} + \frac{\partial \tilde{O}_A^{\alpha\beta}}{\partial \dot{x}_j^{\beta}} K_j^{\beta\gamma} \right). \quad (16)$$

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

By $M_A^{[\alpha\beta]}$ and $M_A^{(\alpha\beta)}$ we denote the antisymmetric and symmetric part of M_A, respectively. We obtain from (15):

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

$$= \int_0^{\infty} \sum_{\alpha=1}^{N} \sum_{\beta=1}^{N} M_A^{[\alpha\beta]}(\vartheta) \chi_{\alpha}(\vartheta, t, x) \, d\vartheta + \int_0^{\infty} \sum_{\alpha=1}^{N} \sum_{\beta=1}^{N} M_A^{(\alpha\beta)}(\vartheta) \chi_{\alpha}(\vartheta, t, x) \, d\vartheta$$

$$+ \int_0^{\infty} \frac{1}{m} \sum_{\alpha=1}^{N} \left(\frac{\partial \tilde{O}_A^{\alpha}}{\partial \dot{x}_j^{\alpha}} G_j^{\alpha} + \sum_{\beta=1}^{N} \left(\frac{\partial \tilde{O}_A^{\alpha\beta}}{\partial \dot{x}_j^{\alpha}} G_j^{\alpha} + \frac{\partial \tilde{O}_A^{\alpha\beta}}{\partial \dot{x}_j^{\beta}} G_j^{\beta} \right) \right) \chi_{\alpha}(\vartheta, t, x) \, d\vartheta. \quad (17)$$

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:

$$\sum_{\alpha=1}^{N} \sum_{\beta=1}^{N} M_A^{[\alpha\beta]}(\vartheta) \chi_{\alpha}(\vartheta, t, x) = \tfrac{1}{2} \sum_{\alpha=1}^{N} \sum_{\beta=1}^{N} M_A^{[\alpha\beta]}(\vartheta)(\chi_{\alpha}(\vartheta, t, x) - \chi_{\beta}(\vartheta, t, x)). \quad (18)$$

Thus finally we end up with the following proposition.

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

$$f_{Ak}(t, x) = \int_0^{\infty} \left(\sum_{\alpha=1}^{N} \left(O_A^{\alpha}(\vartheta) + \sum_{\beta=1}^{N} O_A^{\alpha\beta}(\vartheta) \right) \dot{x}_k^{\alpha}(\vartheta) \chi_{\alpha}(\vartheta, t, x) \tfrac{1}{2} \sum_{\alpha,\beta=1}^{N} M_A^{[\alpha\beta]}(\vartheta) r_k^{\alpha\beta}(\vartheta) \right.$$

$$\times \left. \int_0^{1} \chi(\vartheta - t, x^{\alpha}(\vartheta) - x + \mu r^{\alpha\beta}(\vartheta)) \, d\mu \right) d\vartheta$$

$$S_A(t, x) = \int_0^{\infty} \sum_{\alpha=1}^{N} \sum_{\beta} M_A^{(\alpha\beta)}(\vartheta) \chi_{\alpha}(\vartheta, t, x) \, d\vartheta$$

$$Z_A(t, x) = \int_0^{\infty} \frac{1}{m} \sum_{\alpha=1}^{N} \left(\frac{\partial \tilde{O}_A^{\alpha}}{\partial \dot{x}_j^{\alpha}} G_j^{\alpha} + \sum_{\beta=1}^{N} \left(\frac{\partial \tilde{O}_A^{\alpha\beta}}{\partial \dot{x}_j^{\alpha}} G_j^{\alpha} + \frac{\partial \tilde{O}_A^{\alpha\beta}}{\partial \dot{x}_j^{\beta}} G_j^{\beta} \right) \right) \chi_{\alpha}(\vartheta, t, x) \, d\vartheta$$

$$(19)$$

then the following equations of balance are satisfied:

$$\frac{\partial u_A}{\partial t} + \frac{\partial f_{Ak}}{\partial x_k} = S_A + Z_A. \quad (20)$$

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

(iii) The antisymmetric part $M_A^{[\alpha\beta]}$ of the matrix M_A, which is given in (16), will contribute to the fluxes, while the productions are exclusively formed by the symmetric part $M_A^{(\alpha\beta)}$.

Note that the fields $u_A(t, x)$ and $f_{Ak}(t, x)$, and also $S_A(t, x)$ and $Z_A(t, x)$, 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 (20) by integration and a subsequent application of Gauss's theorem

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_V u_A(t, \boldsymbol{x}) \, \mathrm{d}^3 x = -\oint_{\partial V} f_{Ak}(t, \boldsymbol{x}) \, \mathrm{d}a_k + \int_V (S_A(t, \boldsymbol{x}) + Z_A(t, \boldsymbol{x})) \, \mathrm{d}^3 x. \tag{21}$$

Later, after having carried out the closure of the system (20), the fields $u_A(t, \boldsymbol{x})$, $f_{Ak}(t, \boldsymbol{x})$, $S_A(t, \boldsymbol{x})$ and $Z_A(t, \boldsymbol{x})$ will be equipped with additional thermodynamic properties and consequently may become discontinuous. When this happens we shall assume that the global equation (21) is more fundamental than the system (20). Thus we shall still rely on the global equations of balance (21) 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 1 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 expressions (19).

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

The mass flux f_{0k} is equal to the momentum density ρv_k. The momentum flux f_{ik} and the energy flux f_{4k} are denoted by P_{ik} and Q_k, respectively:

$$\begin{aligned}
P_{ik}(t, \boldsymbol{x}) = \int_0^\infty \mathrm{d}\vartheta \Bigg(& \sum_{\alpha=1}^N m \dot{x}_i^\alpha(\vartheta) \dot{x}_k^\alpha(\vartheta) \chi_\alpha(\vartheta, t, \boldsymbol{x}) \\
& - \frac{1}{2} \sum_{\alpha,\beta=1}^N K_i^{\alpha\beta}(\vartheta) r_k^{\alpha\beta}(\vartheta) \int_0^1 \chi(\vartheta - t, \boldsymbol{x}^\alpha(\vartheta) - \boldsymbol{x} + \mu \boldsymbol{r}^{\alpha\beta}(\vartheta)) \, \mathrm{d}\mu \Bigg)
\end{aligned} \tag{22}$$

$$\begin{aligned}
Q_k(t, \boldsymbol{x}) = \int_0^\infty \mathrm{d}\vartheta \Bigg(& \sum_{\alpha=1}^N \left(\frac{m}{2} \dot{x}_j^\alpha(\vartheta) \dot{x}_j^\alpha(\vartheta) + \frac{1}{2} \sum_{\beta=1}^N \varphi(|r^{\alpha\beta}(\vartheta)|) \right) \dot{x}_k^\alpha(\vartheta) \chi_\alpha(\vartheta, t, \boldsymbol{x}) \\
& - \frac{1}{4} \sum_{\alpha,\beta=1}^N K_j^{\alpha\beta}(\vartheta)(\dot{x}_j^\alpha(\vartheta) + \dot{x}_j^\beta(\vartheta)) r_k^{\alpha\beta}(\vartheta) \\
& \times \int_0^1 \chi(\vartheta - t, \boldsymbol{x}^\alpha(\vartheta) - \boldsymbol{x} + \mu \boldsymbol{r}^{\alpha\beta}(\vartheta)) \, \mathrm{d}\mu \Bigg).
\end{aligned} \tag{23}$$

With these representations the conservation laws are

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho v_k}{\partial x_k} = 0 \qquad \frac{\partial \rho v_i}{\partial t} + \frac{\partial P_{ik}}{\partial x_k} = 0 \qquad \frac{\partial \rho e}{\partial t} + \frac{\partial Q_k}{\partial x_k} = 0. \tag{24}$$

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

6. The general closure problem

We describe the macrostate of a body by the first five volume densities ρ, $\rho \boldsymbol{v}$ and ρe. 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 (24).

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 also include universal parts, namely those that depend on the velocity $\boldsymbol{v}$. We can identify these parts by replacing the microscopic velocities $\dot{x}^\alpha$ by so-called excess (or thermal) velocities $\boldsymbol{C}^\alpha$, which are defined as

$$C_i^\alpha(\vartheta, t, \boldsymbol{x}) = \dot{x}_i^\alpha(\vartheta) - v_i(t, \boldsymbol{x}). \tag{25}$$

In this way, the energy density and the fluxes decompose into velocity-dependent parts and into parts which are invariant with respect to Galilean transformations:

$$\rho e = \frac{\rho}{2} v^2 + \rho u \qquad P_{ik} = \rho v_i v_k + p_{ik} \qquad Q_k = \left(\left(\frac{\rho}{2} v^2 + \rho u \right) \delta_{ik} + p_{ik} \right) v_i + q_k. \tag{26}$$

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

$$\rho u(t, \boldsymbol{x}) = \int_0^\infty \sum_{\alpha=1}^N \left(\frac{m}{2} C_i^\alpha(\vartheta, t, \boldsymbol{x}) C_i^\alpha(\vartheta, t, \boldsymbol{x}) + \frac{1}{2} \sum_{\beta=1}^N \varphi(|r^{\alpha\beta}(\vartheta)|) \right) \chi_\alpha(\vartheta, t, \boldsymbol{x}) \, d\vartheta \tag{27}$$

$$p_{ik}(t, \boldsymbol{x}) = \int_0^\infty \left(\sum_{\alpha=1}^N m C_i^\alpha(\vartheta, t, \boldsymbol{x}) C_k^\alpha(\vartheta, t, \boldsymbol{x}) \chi_\alpha(\vartheta, t, \boldsymbol{x}) \right.$$
$$\left. - \frac{1}{2} \sum_{\alpha,\beta=1}^N K_i^{\alpha\beta}(\vartheta) r_k^{\alpha\beta}(\vartheta) \int_0^1 \chi(\vartheta - t, \boldsymbol{x}^\alpha(\vartheta) - \boldsymbol{x} + \mu r^{\alpha\beta}(\vartheta)) \, d\mu \right) d\vartheta \tag{28}$$

$$q_k(t, \boldsymbol{x}) = \int_0^\infty \left(\sum_{\alpha=1}^N \left(\frac{m}{2} C_j^\alpha(\vartheta, t, \boldsymbol{x}) C_j^\alpha(\vartheta, t, \boldsymbol{x}) + \frac{1}{2} \sum_{\beta=1}^N \varphi(|r^{\alpha\beta}(\vartheta)|) \right) \right.$$
$$\times C_k^\alpha(\vartheta, t, \boldsymbol{x}) \chi_\alpha(\vartheta, t, \boldsymbol{x})$$
$$- \frac{1}{4} \sum_{\alpha,\beta=1}^N K_j^{\alpha\beta}(\vartheta)(C_j^\alpha(\vartheta, t, \boldsymbol{x}) + C_j^\beta(\vartheta, t, \boldsymbol{x})) r_k^{\alpha\beta}(\vartheta)$$
$$\left. \times \int_0^1 \chi(\vartheta - t, \boldsymbol{x}^\alpha(\vartheta) - \boldsymbol{x} + \mu r^{\alpha\beta}(\vartheta)) \, d\mu \right) d\vartheta. \tag{29}$$

Now we can reformulate the general closure problem. Instead of ρ, $\rho \boldsymbol{v}$ and ρe we consider ρ, $\boldsymbol{v}$ 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 is 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. Newton's dynamics

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

$$\{x^1(\vartheta), x^2(\vartheta), \ldots, x^{N-1}(\vartheta), x^N(\vartheta)\} \tag{30}$$

along one direction. The positions of the first and of the Nth atom are fixed and given by

$$x^1(\vartheta) = 0 \qquad x^N(\vartheta) = L. \tag{31}$$

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

$$\varphi(r_\alpha) = \frac{1}{8}\frac{1}{r_\alpha^4} - \frac{1}{4}\frac{1}{r_\alpha^2} \qquad \text{with} \quad r_\alpha = x^{\alpha+1} - x^\alpha \qquad \alpha = 1, 2, 3, \ldots, N-1. \tag{32}$$

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

We do not consider external forces, and Newton's equations of motion thus read

$$\ddot{x}^\alpha(\vartheta) = \varphi'(r_\alpha(\vartheta)) - \varphi'(r_{\alpha-1}(\vartheta)) \qquad \alpha = 2, 3, \ldots, N-1. \tag{33}$$

From a microscopic viewpoint the initial conditions for system (33) are given by the initial locations

$$\{x^1(0) = 0, x^2(0) = x_0^2, \ldots, x^{N-1}(0) = x_0^{N-1}, x^N(0) = L\} \tag{34}$$

and by the initial velocities

$$\{\dot{x}^1(0) = 0, \dot{x}^2(0) = \dot{x}_0^2, \ldots, \dot{x}^{N-1}(0) = \dot{x}_0^{N-1}, \dot{x}^N(0) = 0\} \tag{35}$$

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, namely $\rho(0, x)$, $v(0, x)$ 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 (23) and (24) and specialize to one space dimension. Hereafter we incorporate the restriction to nearest neighbour interaction to the microscopic representations (23), (27) and (28) and end up with the following result.

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

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho v}{\partial x} = 0 \tag{36a}$$

$$\frac{\partial \rho v}{\partial t} + \frac{\partial}{\partial x}(\rho v^2 + p) = 0 \tag{36b}$$

$$\frac{\partial \rho(\frac{1}{2}v^2 + u)}{\partial t} + \frac{\partial}{\partial x}\left(\rho\left(\frac{1}{2}v^2 + u + \frac{p}{\rho}\right)v + q\right) = 0. \tag{36c}$$

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

$$\rho(t, x) = \int_0^\infty \sum_{\alpha=1}^N \chi_\alpha(\vartheta, t, x)\, d\vartheta \tag{37a}$$

$$\rho v(t, \boldsymbol{x}) = \int_0^\infty \sum_{\alpha=1}^N \dot{x}^\alpha(\vartheta) \chi_\alpha(\vartheta, t, \boldsymbol{x}) \, \mathrm{d}\vartheta \tag{37b}$$

$$\rho u(t, \boldsymbol{x}) = \int_0^\infty \sum_{\alpha=1}^N (\tfrac{1}{2} C^\alpha(\vartheta, t, \boldsymbol{x})^2 + \varphi(r_\alpha(\vartheta))) \chi_\alpha(\vartheta, t, \boldsymbol{x}) \, \mathrm{d}\vartheta \tag{37c}$$

for the basic variables, and by

$$p(t, x) = \int_0^\infty \sum_{\alpha=1}^N \Bigg(C^\alpha(\vartheta, t, x)^2 \chi_\alpha(\vartheta, t, \boldsymbol{x})$$
$$-\varphi'(r_\alpha(\vartheta)) r_\alpha(\vartheta) \int_0^1 \chi(\vartheta - t, x^\alpha(\vartheta) - x + \mu r_\alpha(\vartheta)) \, \mathrm{d}\mu \Bigg) \mathrm{d}\vartheta \tag{38a}$$

$$q(t, x) = \int_0^\infty \sum_{\alpha=1}^N \Bigg((\tfrac{1}{2} C^\alpha(\vartheta, t, x)^2 + \varphi(r_\alpha(\vartheta))) C^\alpha(\vartheta, t, x) \chi_\alpha(\vartheta, t, x)$$
$$-\tfrac{1}{2} \varphi'(r_\alpha(\vartheta)) r_\alpha(\vartheta) C^\alpha(\vartheta, t, x)$$
$$\times \int_0^1 \chi(\vartheta - t, x^\alpha(\vartheta) - x + \mu r_\alpha(\vartheta)) \, \mathrm{d}\mu \Bigg) \mathrm{d}\vartheta \tag{38b}$$

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 chosen so that $\varphi'(1) = 0$ and the microscopic time unit is chosen 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

$$t_F = \lambda \tilde{t}_F \qquad L = \lambda \tilde{L}. \tag{39}$$

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

$$\tilde{t} = \frac{1}{\lambda} t \qquad \tilde{x} = \frac{1}{\lambda} x. \tag{40}$$

Later, 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, we shall consider various macroscopic Riemann initial value problems with a single jump at, say, $x = 0$. These will be subsequently solved on the microscale for an increasing number N of particles. The given kind of scaling then leads 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 (40):

$$u_A(t, x) = u_A(\lambda t, \lambda x). \tag{41}$$

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 λ. This implies that microscopic wave speeds do not depend on the particle number N. Actually, this restricts us to consider only wave phenomena but not diffusion in the macroscopic limit $N \rightarrow \infty$. 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, namely the mass density $\rho(t, x)$ and the velocity $v(t, x)$. The initial data are

$$\rho(0, x) = \begin{cases} \rho_l & \text{for} \quad x \leqslant \frac{L}{2} \\ \rho_r & \text{for} \quad x > \frac{L}{2} \end{cases} \qquad v(0, x) = \begin{cases} v_l & \text{for} \quad x \leqslant \frac{L}{2} \\ v_r & \text{for} \quad x > \frac{L}{2}. \end{cases} \tag{42}$$

Obviously these data are not sufficient to solve an initial value problem for the $N-2$ equations of motion (33). Thus, there arises the question how to prepare the initial data of the atomic chain.

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

$$L = 2\frac{N-1}{\rho_l + \rho_r} \tag{43a}$$

$$N_l + N_r = N - 1 \tag{43b}$$

$$\frac{N_l}{\rho_l} + \frac{N_r}{\rho_r} = L. \tag{43c}$$

Equation, (43a), represents the length of the chain by $(N-1)$ intervals $\times$ the mean length $2/(\rho_l + \rho_r)$ of an interval. (43b) decomposes the number of intervals, and (43c) decomposes the length 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:

$$x_0^\alpha = \begin{cases} \dfrac{1}{\rho_l}(\alpha - 1) & \text{for} \quad \alpha = 1, 2, \ldots, N_l \\ \dfrac{1}{\rho_l}N_l + \dfrac{1}{\rho_r}(\alpha - N_l - 1) & \text{for} \quad \alpha = N_l + 1, \ldots, N \end{cases}$$
$$\dot{x}_0^\alpha = \begin{cases} v_l & \text{for} \quad \alpha = 1, 2, \ldots, N_l \\ v_r & \text{for} \quad \alpha = N_l + 1, \ldots, N. \end{cases} \tag{44}$$

We have thus assumed that the atoms have initially constant distances on the left and right parts 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 Newton's equations

We now solve the $N - 2$ equations of motion (33) with $N = 35\,000$ and use the obtained data to calculate the macroscopic fields mass density $\rho(t, x)$ and velocity $v(t, x)$ according to the microscopic representations (37a), (37b). Figure 1 depicts the space–time diagram of the mass density for $0 \leqslant t \leqslant 1$ and $0 \leqslant x \leqslant 4$ with the scaling factor $\lambda = 7413$.
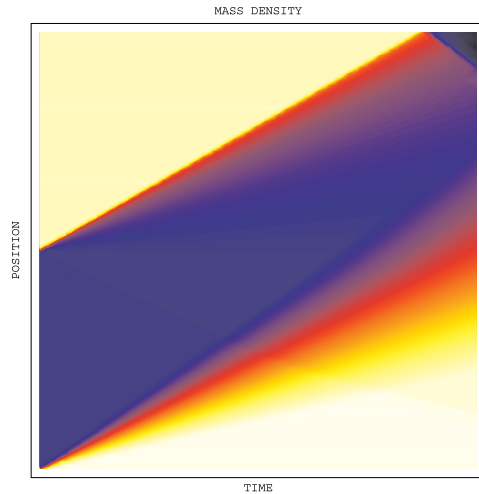
MASS DENSITY

POSITION

TIME

Figure 1. Space–time diagram of the mass density according to Newton's equations.

The initial data are $\rho_l = 1.36$, $\rho_r = 1.00$, $v_l = 0.53$, $v_r = 0.00$. These data result 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 (36*a*), (36*b*). If Ω is any convex set in space–time with piecewise smooth, positive oriented boundary $\partial\Omega$, then the conservation laws for mass and momentum may be written in integral form:

$$\oint_{\partial\Omega} (\rho\,\mathrm{d}x - \rho v\,\mathrm{d}t) = 0 \tag{45a}$$

$$\oint_{\partial\Omega} (\rho v\,\mathrm{d}x - (\rho v^2 + p)\,\mathrm{d}t) = 0 \tag{45b}$$

and must be supplemented by a constitutive law that relates the pressure in (45*b*) to the variables. We obtain this law if we supplement the microscopic equations of motion by an assumption regarding the distribution of distances r_α and velocities $\dot{x}^\alpha$ of microscopic particles of the chain.

Assumption. Within the support of the window function at the space–time point (t, x) we calculate the pressure from the microscopic representation (38) by setting

$$r_\alpha = \frac{1}{\rho(t, x)} \qquad \text{and} \qquad \dot{x}^\alpha = v(t, x) \qquad \text{for} \quad x^\alpha \in \mathrm{supp}(\chi(t, x)). \tag{46}$$

We call assumption (46) the *cold closure*, because thermal vibrations of the atoms are completely ignored here.

Note that we are able to judge the *cold closure* by solving the microscopic equations of motion. Later, we will do this for special cases.

The evaluation of (38a) for the *cold closure* assumption implies

$$p = -\varphi'\left(\frac{1}{\rho}\right). \tag{47}$$

If we replace the pressure p in (45) by $-\varphi'(\frac{1}{\rho})$, we obtain the weak form of a closed macroscopic system, which leads in regular points to the differential form

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho v}{\partial x} = 0 \qquad \frac{\partial \rho v}{\partial t} + \frac{\partial}{\partial x}\left(\rho v^2 - \varphi'\left(\frac{1}{\rho}\right)\right) = 0 \tag{48}$$

and across a shock front to the Rankine–Hugoniot jump conditions

$$-V_S[[\rho]] + [[\rho v]] = 0 \qquad -V_S[[\rho v]] + \left[\left[\rho v^2 - \varphi'\left(\frac{1}{\rho}\right)\right]\right] = 0. \tag{49}$$

In equation (49) $[[a]] = a_r - a_l$ denotes the jump of any field $a = a(x)$, and V_S is the shock velocity.

Note that the fields in (36a), (36b), which depend on the window function and the microtrajectories $x^\alpha(t)$, are continuous differentiable. However, after having replaced the exact microscopic representation of the pressure by the constitutive law (47), the resulting field equations may have regular as well as discontinuous solutions, and both are described by (45).

In order to obtain the condition for hyperbolicity and the characteristic speeds of system (48), we write it in the form

$$\frac{\partial \rho}{\partial t} + v\frac{\partial \rho}{\partial x} + \rho\frac{\partial v}{\partial x} = 0 \qquad \frac{\partial v}{\partial t} + \frac{1}{\rho^3}\varphi''\left(\frac{1}{\rho}\right)\frac{\partial \rho}{\partial x} + v\frac{\partial v}{\partial x} = 0. \tag{50}$$

There immediately results the characteristic speeds

$$\lambda_{1,2} = v \pm \frac{1}{\rho}\sqrt{\varphi''\left(\frac{1}{\rho}\right)} \tag{51}$$

and the condition for hyperbolicity is $\varphi''(\frac{1}{\rho}) > 0$, i.e. $\rho > \sqrt{\frac{3}{5}}$ for the function φ 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 (48) and (49) represents a closed system of field equations for weak solutions of the initial value problem above. This system is obviously of hyperbolic type in the region $\varphi'' > 0$.

Next we study the role of the conservation law (36c) of the energy. In particular, we have to answer the important question, whether the *cold closure* eventually contradicts the energy conservation, because, due to (46), the energy density ρe and the energy flux Q become also functions of ρ and v, so that the conservation law (36c) yields a third equation for the two unknown fields $\rho(t, x)$ and $v(t, x)$, namely

$$\frac{\partial \rho \hat{e}(\rho, \rho v)}{\partial t} + \frac{\partial \hat{Q}(\rho, \rho v)}{\partial x} = 0 \tag{52a}$$

with

$$\hat{e}(\rho, \rho v) = \left(\frac{v^2}{2} + \varphi \left(\frac{1}{\rho} \right) \right) \qquad \hat{Q}(\rho, \rho v) = \left(\rho \hat{e}(\rho, \rho v) - \varphi' \left(\frac{1}{\rho} \right) \right) v. \qquad (52b)$$

This is by no means a contradiction, because there is the following proposition.

Proposition. *(i) There exist so-called Lagrange multipiers Λ^ρ 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:*

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

$$(53)$$

In regular points the right-hand side of (53) vanishes and thus any solution of (48), (49) satisfies, in addition, the energy equation (52).

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

   (iii) Consequently, system (48) is of symmetric hyperbolic type and has the energy as a convex extension.

Proof. We start from (52*b*) and from the left-hand side of equation (53). After some rearrangements we obtain (53) with the identifications

$$\Lambda^\rho = -\frac{1}{2} v^2 + \varphi \left(\frac{1}{\rho} \right) - \frac{1}{\rho} \varphi' \left(\frac{1}{\rho} \right) \qquad \Lambda^{\rho v} = v. \qquad (54)$$

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

$$\begin{pmatrix} \frac{1}{\rho^3} (\rho^2 v^2 + \varphi''(\frac{1}{\rho})) & -\frac{1}{\rho} v \\ -\frac{1}{\rho} v & \frac{1}{\rho} \end{pmatrix} \qquad (55)$$

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

   The third part of the proposition relies on

$$\Lambda^\rho = \frac{\partial \rho \hat{e}(\rho, \rho v)}{\partial \rho} \qquad \Lambda^{\rho v} = \frac{\partial \rho \hat{e}(\rho, \rho v)}{\partial \rho v} \qquad (56)$$

and these relations follow immediately from (53). The convexity of $\hat{e}(\rho, \rho v)$ 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

$$e' = \rho e - \Lambda^\rho \rho - \Lambda^{\rho v} \rho v \qquad Q' = Q - \Lambda^\rho \rho v - \Lambda^{\rho v} \left(\rho v^2 - \varphi' \left(\frac{1}{\rho} \right) \right) \qquad (57)$$

which implies

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

From these equations we conclude that the system of field equations (48) can be written as

$$\sum_{B=0}^{1} \left(\frac{\partial^2 e'}{\partial u'_A \partial u'_B} \frac{\partial u'_B}{\partial t} + \frac{\partial^2 Q'}{\partial u'_A \partial u'_B} \frac{\partial u'_B}{\partial x} \right) = 0. \qquad (59)$$

The convexity of $\hat{e}(\rho, \rho v)$ implies the convexity of its Legendre transform $e'(\Lambda^\rho, \Lambda^{\rho v})$, which proves that (59) is the symmetric hyperbolic form of the original system (48). The reader is referred to the pioneering work by Friedrichs and Lax [7]. $\qquad \square$

   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 Boillat and Ruggeri.

8.5. Rankine–Hugoniot conditions and shock selection criterion

The purpose of this section is the evaluation of the Rankine–Hugoniot conditions for the Riemannian initial data (42). Furthermore, we shall establish the entropy balance across the initial discontinuity as a shock selection criterion.

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 ρ as the shock parameter. Then the Rankine–Hugoniot conditions (49) yield

$$V_S^2 = -\frac{\varphi'(\frac{1}{\rho})}{(1 - \frac{1}{\rho})} > 0 \qquad \text{for} \quad \rho > 0 \qquad \text{and} \qquad v = \left(1 - \frac{1}{\rho}\right) V_S. \tag{60}$$

In order to single out the unphysical solutions of (60) we consider the entropy condition. It requires a positive entropy production σ_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

$$\sigma_S = V_S \left[\!\!\left[\rho\left(\frac{v^2}{2} + \varphi\left(\frac{1}{\rho}\right)\right)\right]\!\!\right] - \left[\!\!\left[\left(\rho\hat{e}(\rho, \rho v) - \varphi'\left(\frac{1}{\rho}\right)\right)v\right]\!\!\right] \geqslant 0. \tag{61}$$

It can be shown from (61) that only compressive shocks, i.e. $\rho > 1$, are allowed.

In the next section we compare the prediction of a single shock due to (60), (61) with the solution of the Riemann problem due to Newton's equations.

8.6. Comparison of the results

A solution of (60), that satisfies the entropy condition (61), is given by

$$\rho_l = 1.36 \qquad \rho_r = 1.00 \qquad v_l = 0.53 \qquad v_r = 0.0 \qquad \text{and} \qquad V_S = 2.0. \tag{62}$$

This predicts a single shock, starting at $t = 0$, $x = \frac{L}{2}$, which should properly end up in the upper right corner of 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 ρ 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 Newton's equations reaches the boundary earlier, as 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 neglect 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 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. This 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:

$$\frac{\rho}{2} T(t, x) = \int_0^\infty \sum_{\alpha=1}^N \tfrac{1}{2} C^\alpha(\vartheta, t, \boldsymbol{x})^2 \chi_\alpha(\vartheta, t, \boldsymbol{x}) \, d\vartheta. \tag{63}$$

Note that the *cold closure* assumes $C^\alpha(\vartheta, t, x) = \dot{x}^\alpha(\vartheta) - v(t, x) \equiv 0$, 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 the three following assumptions.

Assumptions.

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

$$G(r, c) = F(r) f(c) \qquad \int_0^\infty F(r) \, dr = 1 \qquad \int_{-\infty}^\infty f(c) \, dc = 1. \tag{64}$$

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

$$f_G(\beta, c) = \sqrt{\frac{\beta}{2\pi}} \exp\left(-\beta \frac{c^2}{2}\right). \tag{65}$$

Later, we will see by solving Newton's equations in equilibrium that for a fixed temperature T, the function f is realized by $f(c) = f_G(\beta, c)$, where β 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

$$\hat{F}(\alpha, \beta, r) = \frac{1}{z(\alpha, \beta)} \exp(-\alpha r - \beta \varphi(r))$$
$$\text{with} \quad z(\alpha, \beta) = \int_0^\infty \exp(-\alpha r - \beta \varphi(r)) \, dr. \tag{66}$$

The quantity α is determined by the mean distance of two neighbouring particles

$$\frac{1}{\rho} = \bar{r}(\alpha, \beta) = \int_0^\infty r \hat{F}(\alpha, \beta, r) \, dr. \tag{67}$$

Later on we will see by solving Newton's equations in equilibrium that for fixed density ρ and temperature T the function $\hat{F}$ is realized by $F(r) = \hat{F}(\alpha, \frac{1}{T}, r)$.

In addition to (67) we also define the mean potential energy, which will be used next:

$$\bar{\varphi}(\alpha, \beta) = \int_0^\infty \varphi(r) \hat{F}(\alpha, \beta, r) \, dr. \tag{68}$$

Assumptions (i)–(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 Dreyer [9] and Boillat and 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 ρ, v and T. The length of the chain is $L = (N - 1)/\rho$.

The preparation procedure is divided into three steps.

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

$$y_0^\gamma = (\gamma - 1)/\rho \qquad \dot{y}_0^\gamma = C^\gamma \qquad \gamma = 1, 2, \ldots, N. \tag{69}$$

Here the stochastic excess velocities C^γ are Gaussian distributed for $1 < \gamma < N$ with mean velocity $\langle C^\gamma \rangle = 0$ and mean square $T' = \langle (C^\gamma)^2 \rangle$. T' is determined by the obvious equation that uses the mean potential energy given in (68):

$$\frac{1}{2}T' + \varphi\left(\frac{1}{\rho}\right) = \frac{1}{2}T + \bar{\varphi}\left(\alpha, \frac{1}{T}\right). \tag{70}$$

The parameter α has to be determined here by (67) for given ρ 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. Condition (70) is chosen so that after some time $t_0 > 0$ the positions of the atoms are additionally distributed according to the thermal distribution of distances (66). There result new positions $y^\gamma(t_0)$ and velocities $\dot{y}^\gamma(t_0)$, $\gamma = 1, \ldots, N$.

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

$$x_0^\gamma = y^\gamma(t_0) \qquad \dot{x}_0^\gamma = \dot{y}^\gamma(t_0) + v. \tag{71}$$

9.3. Calculation of distribution functions by solving Newton's equations and comparison with the analytical formulae

By solving Newton's 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 curves in figure 2 represent the analytical functions (65) and (66), respectively. We observe a perfect agreement between the empirical microscopic distributions and the analytical functions. We consider a total chain with $N = 10\,000$ particles, $\lambda = 5000$, $0 \leqslant x \leqslant 1$, $0 \leqslant t \leqslant 1$.

### 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 now assume 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 ρ, v and T.

The system of field equations relies on the three conservation laws (36), which we write in the one-dimensional integral form:

$$\oint_{\partial\Omega} (\rho \, dx - \rho v \, dt) = 0$$

$$\oint_{\partial\Omega} (\rho v \, dx - (\rho v^2 + p) \, dt) = 0 \tag{72}$$

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

Here Ω 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. We obtain this law if we supplement the microscopic equations of motion by an assumption regarding the distribution of distances r_α and velocities $\dot{x}^\alpha$ of microscopic particles of the chain. Here we assume that the distances
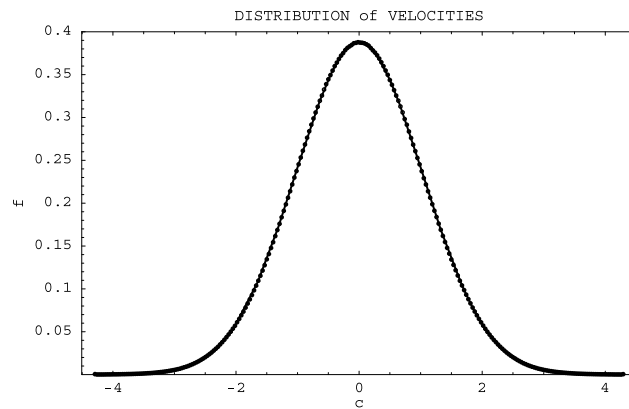
(a)
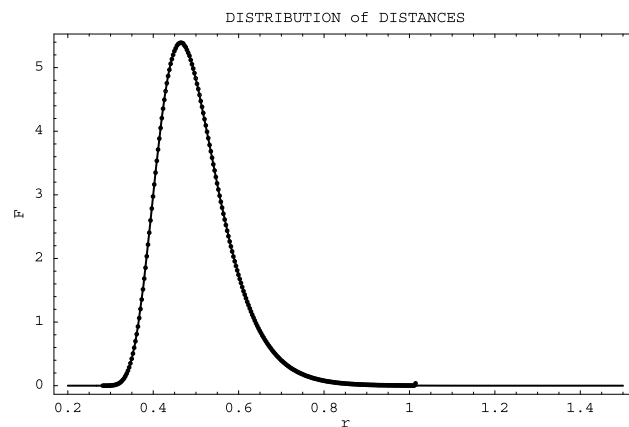
(b)

Figure 2. Distribution of velocities (*a*) and distances (*b*), comparison of microscopic data and analytical results.

and velocities are distributed according to the thermal motion which we have introduced just before. It follows that

$$\frac{1}{\rho} = \int_0^\infty r \hat{F}(\alpha, \beta, r) \, dr = \hat{r}(\alpha, \beta) \tag{73a}$$

$$T = \int_{-\infty}^\infty c^2 f_G(\beta, c) \, dc = \frac{1}{\beta} \tag{73b}$$

$$p = \rho T - \rho \int_0^\infty r \varphi'(r) \hat{F}(\alpha, \beta, r) \, dr = \frac{\alpha}{\beta} \tag{73c}$$

$$u = \tfrac{1}{2}T + \int_0^\infty \varphi(r) \hat{F}(\alpha, \beta, r) \, dr = \tfrac{1}{2}T + \bar{\varphi}(\alpha, \beta) = \hat{u}(\alpha, \beta) \tag{73d}$$

$$q = 0. \tag{73e}$$

Equations (73) define the *thermal closure* with $f_G(\beta, c)$ and $\hat{F}(\alpha, \beta, r)$ given by (65) and (66), respectively. In each line the first equality results from the evaluation of the microscopic

representations (37) and (38). The nonconvective part of the energy flux q is zero because the distribution functions used assume 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 ρ, v and T, or alternatively for the variables α, β and v. The system consists of the conservation laws (72) and of the constitutive equations (73).

After having closed the system of conservation laws, the integral form (72) takes care of discontinuous shock solutions. This is in analogy to the *cold closure*. The system of differential equations (36) results from its weak form (72), that additionally yields the shock conditions: let (ρ, v, T) and (ρ', v', T') be the constant states left and right, respectively, to a shock front with velocity V_S. By applying a Galilean transformation it is always possible to assume $v' = 0$ without loss of generality. Then we obtain, after some rearrangement, the following Rankine–Hugoniot shock conditions:

$$
\begin{aligned}
V_S &= \frac{v}{1 - \frac{\rho'}{\rho}} \\
v^2 &= \left(\frac{1}{\rho'} - \frac{1}{\rho} \right) (p - p') \\
0 &= 2(u' - u) + \left(\frac{1}{\rho'} - \frac{1}{\rho} \right) (p + p').
\end{aligned}
\tag{74}
$$

We proceed to establish the properties of the field equations and to find a shock selection criterion. To this end we shall first prove 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 $T > 0$:

$$
\mathrm{d}h = \frac{1}{T}\,\mathrm{d}u + \frac{1}{T} p\,\mathrm{d}\left(\frac{1}{\rho} \right).
\tag{75}
$$

The Gibbs relation implies an integrability condition which guarantees that the right-hand side of (75) is indeed an integrable differential form:

$$
\frac{\partial u}{\partial(\frac{1}{\rho})} = T \frac{\partial p}{\partial T} - p.
\tag{76}
$$

In order to check (75) we write the following relations for the mass density and the internal energy, and use the function $z(\alpha, \beta) = \int_0^\infty \exp(-\alpha r - \beta\varphi(r))\,\mathrm{d}r$ which was introduced in (66):

$$
\frac{1}{\rho} = -\frac{\partial \ln(\frac{z(\alpha,\beta)}{\sqrt{\beta}})}{\partial \alpha}
\qquad \text{and} \qquad
u = -\frac{\partial \ln(\frac{z(\alpha,\beta)}{\sqrt{\beta}})}{\partial \beta}.
\tag{77}
$$

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

$$
\beta \left(\mathrm{d}u + p\,\mathrm{d}\left(\frac{1}{\rho} \right) \right) = \mathrm{d}\left(\beta u + \frac{\alpha}{\rho} + \ln\left(\frac{z(\alpha,\beta)}{\sqrt{\beta}} \right) \right).
\tag{78}
$$

This proves (75) and identifies the specific entropy:

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

Note that it is possible to prove the integrability condition (76) directly from the *thermal closure* assumption (73) without any knowledge about the entropy density h in (79).

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:

$$d(\rho h) = \Lambda^\rho \, d\rho + \Lambda^{\rho v} \, d(\rho v) + \Lambda^e \, de \qquad \text{with}$$

$$\Lambda^\rho = -\left(u - Th + \frac{p}{\rho} - \frac{v^2}{2}\right) \qquad \Lambda^{\rho v} = -\frac{v}{T} \qquad \Lambda^e = \frac{1}{T}. \tag{80}$$

Hereafter we prove the identity

$$d(\rho h v) = \Lambda^\rho \, d(\rho v) + \Lambda^{\rho v} \, d(\rho v^2 + p) + \Lambda^e \, d(\rho(u + v^2/2)v + pv). \tag{81}$$

Finally we establish the conditions for convexity of $-\rho h(\rho, \rho v, \rho e)$, i.e. with $u_A = (\rho, \rho v, \rho e)$. Convexity means that the matrix $\frac{\partial^2 (\rho h)}{\partial u_A \partial u_B}$ is negative definite. Let $\Omega \subset \mathbb{R}_0^+ \times \mathbb{R}_0^+$ be any convex region in the (α, β) state space. If the Legendre transform $h'(\alpha, \beta) = \ln(z(\alpha, \beta)/\sqrt{\beta})$ of the entropy density is concave in Ω, then to each $(\alpha, \beta) \in \Omega$ there corresponds a unique pair (ρ, T) that satisfies $\beta = \frac{1}{T}$ and the equation (67), 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

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho h v}{\partial x} = \Lambda^\rho \left(\frac{\partial \rho}{\partial t} + \frac{\partial \rho v}{\partial x}\right) + \Lambda^{\rho v} \left(\frac{\partial \rho v}{\partial t} + \frac{\partial}{\partial x}(\rho v^2 + p)\right)$$

$$+ \Lambda^e \left(\frac{\partial e}{\partial t} + \frac{\partial}{\partial x}(\rho(u + v^2/2)v + pv)\right) \tag{82}$$

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, namely the mass density $\rho(t, x)$, the velocity $v(t, x)$ and the temperaure $T(t, x)$. The initial data are

$$\rho(0, x) = \begin{cases} \rho_l \\ \rho_r \end{cases} \qquad v(0, x) = \begin{cases} v_l \\ v_r \end{cases} \qquad T(0, x) = \begin{cases} T_l & \text{for} \quad x \leqslant \frac{L}{2} \\ T_r & \text{for} \quad x > \frac{L}{2}. \end{cases} \tag{83}$$

These data are also not sufficient to solve an initial value problem for the $N - 2$ equations of motion (33). Thus, there again arises the question of 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 (43). Each half-chain is assumed to be in thermal equilibrium at its individual densities ρ_l, ρ_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 $N = 35\,000$ particles. We choose the scaling
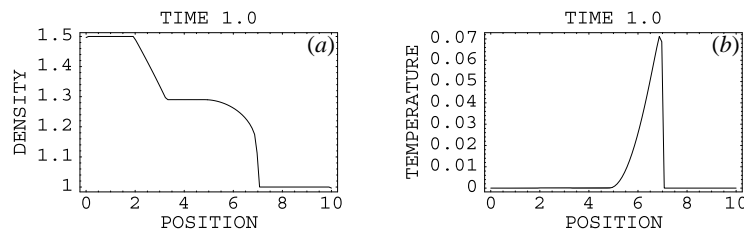
Figure 3. Density (*a*) and temperature (*b*) according to Newton's equation for Riemannian initial data.
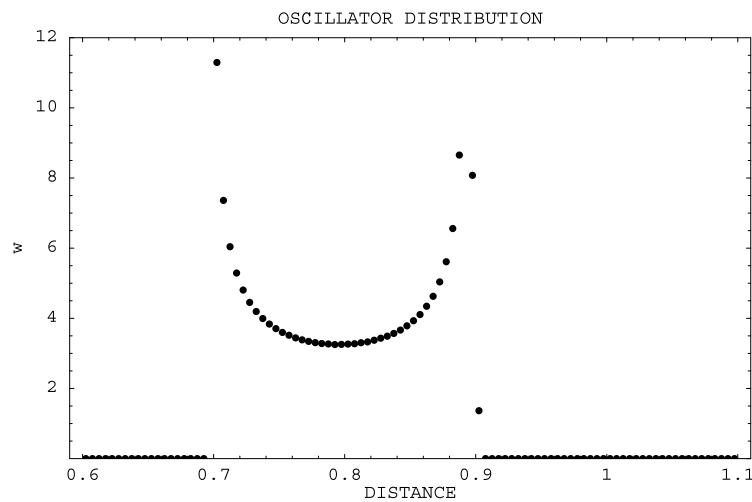

Figure 4. Distribution of distances according to Newton's equations at time $t = 1.0$ and at position $x = 6.1$.

factor $\lambda = 2800$ and calculate from the obtained data at time $t = 1.0$ the fields of density and temperature. The results are depicted in figure 3.

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 temperature 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 Newton's equations, and we calculate the distribution of distances. Figure 4 shows the surprising result.

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 appropriately predict the development of the Riemannian initial data of the last example. Recall that *thermal motion*, as 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 α we have

$$\{\ldots, r_{\alpha-3}(t), r_{\alpha-2}(t), r_{\alpha-1}(t), r_\alpha(t), r_{\alpha+1}(t), r_{\alpha+2}(t), r_{\alpha+3}(t), \ldots\}. \tag{84}$$

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

$$\{\ldots, s(t), r(t), s(t), r(t), s(t), r(t), s(t), \ldots\}. \tag{85}$$

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

$$r(t) + s(t) = \frac{2}{\rho}. \tag{86}$$

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

$$\ddot{r}(t) = 2\left(\varphi'\left(\frac{2}{\rho} - r(t)\right) - \varphi'(r(t))\right). \tag{87}$$

Instead of r we sometimes use 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

$$\ddot{x}(t) = \varphi'\left(\frac{1}{\rho} - 2x(t)\right) - \varphi'\left(\frac{1}{\rho} + 2x(t)\right). \tag{88}$$

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

Before we proceed, we note that equations (86)–(88) imply that the velocities of the two particles which constitute the oscillator, say $\dot{x}_{\alpha+1}(t)$ and $\dot{x}_\alpha(t)$, are restricted according to $\dot{x}_{\alpha+1}(t) = -\dot{x}_\alpha(t)$. This fact will become important when we evaluate the microscopic representations of the macroscopic fields.

The first integral of (88) reads $\dot{x}(t) = \pm\sqrt{e_0 - \varphi(\frac{1}{\rho} - 2x(t)) - \varphi(\frac{1}{\rho} + 2x(t))}$, where e_0 is the integration constant. The oscillator moves between its minimal and maximal distances r_- and r_+, which are restricted by

$$r_- + r_+ = \frac{2}{\rho}. \tag{89}$$

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

$$\dot{x}(t) = \pm\sqrt{\varphi(r_+) + \varphi(r_-) - \varphi(r(t)) - \varphi\left(\frac{2}{\rho} - r(t)\right)}. \tag{90}$$

Due to (90) the mean value of $\dot{x}(t)$ in time is zero, and we shall define the r-dependent positive part of the excess velocity:

$$C(r_-, r_+, r) = \sqrt{\varphi(r_+) + \varphi(r_-) - \varphi(r) - \varphi(r_- + r_+ - r)}. \tag{91}$$

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

To this end we define the duration of a half-period of the oscillator motion where $\dot{x}(t) \geqslant 0$:

$$t_*(r_-, r_+) = \int_{r_-}^{r_+} \frac{\mathrm{d}r}{\sqrt{\varphi(r_+) + \varphi(r_-) - \varphi(r) - \varphi(r_- + r_+ - r)}} > 0. \tag{92}$$

The integral exists in the convex region of φ, 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 $w(r_-, r_+, r)$ on the interval (r_-, r_+) according to

$$w(r_-, r_+, r) = \frac{1}{t_*(r_-, r_+)\sqrt{\varphi(r_+) + \varphi(r_-) - \varphi(r) - \varphi(r_- + r_+ - r)}}$$
$$\text{with} \quad \int_{r_-}^{r_+} w(r_-, r_+, r)\,\mathrm{d}r = 1. \tag{93}$$

Note that $w(r_-, r_+, r)\,\mathrm{d}r$ gives the probabilty of finding at any time t the distance r within the infinitesimal interval $[r, r + \mathrm{d}r]$. From (93) there results the important symmetry condition

$$w(r_-, r_+, r) = w(r_-, r_+, r_- + r_+ - r). \tag{94}$$

The distribution function $w(r_-, r_+, r)$ 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:

$$T = \frac{1}{t_*(r_-, r_+)} \int_0^{t_*(r_-, r_+)} \dot{x}(t)^2\,\mathrm{d}t = \frac{1}{t_*(r_-, r_+)} \int_{r_-}^{r_+} C(r_-, r_+, r)\,\mathrm{d}r. \tag{95}$$

This definition is analogous to the corresponding definition (73b) for the thermal closure.

10.2. Realization of the oscillator distribution by Newton's 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 (89) and (95). The solid curve in figure 5 represents the analytical expression (93), and for a comparison with the corresponding distribution that was calculated from Newton's equations, we have put the data from figure 4 once more as dots.

We find complete agreement between both procedures.

Consequently, we conclude that a given pair (ρ, T) does not constitute a unique equilibrium, because we know from section 9.2 that a pair (ρ, T) may be realized by the classical *thermal motion*, while here we have learned that the same pair can also be realized by the oscillator motion.
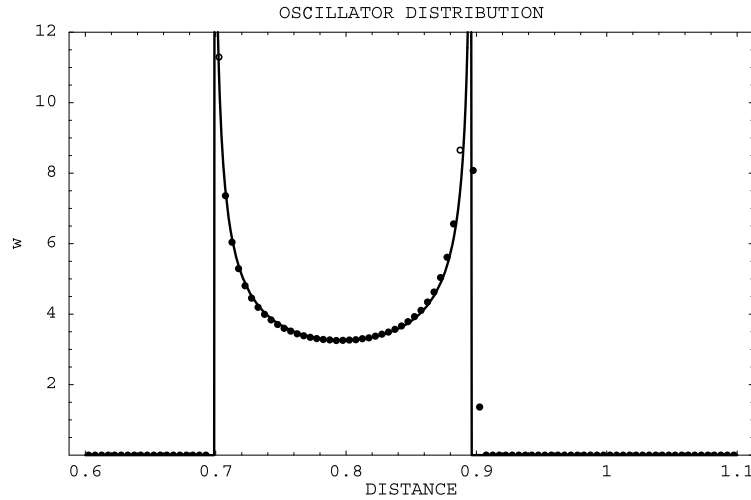
Figure 5. Distribution of distances, comparison of microscopic data and analytical results.

10.3. Oscillator closure and field equations

We consider again the macroscopic system of the three conservation laws

$$\oint_{\partial\Omega} (\rho\,\mathrm{d}x - \rho v\,\mathrm{d}t) = 0$$

$$\oint_{\partial\Omega} (\rho v\,\mathrm{d}x - (\rho v^2 + p)\,\mathrm{d}t) = 0 \tag{96}$$

$$\oint_{\partial\Omega} \left(\left(\frac{\rho}{2}v^2 + \rho u\right)\mathrm{d}x - \left(\frac{\rho}{2}v^2 + \rho u + p\right) v\,\mathrm{d}t \right) = 0$$

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

We obtain the constitutive laws if we supplement the microscopic equations of motion by an assumption regarding the distribution of distances r_α and velocities $\dot{x}^\alpha$ of microscopic particles of the chain. Here we assume that the distances and velocities are distributed according to the *oscillator motion* which we have introduced just before.

In the list of variables we replace ρ and T by r_- and r_+, because these latter quantities appear explicitly 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:

$$\frac{1}{\rho} = \int_{r_-}^{r_+} r\,w(r_-, r_+, r)\,\mathrm{d}r = \tfrac{1}{2}(r_- + r_+) \tag{97a}$$

$$T = \int_{r_-}^{r_+} C^2 w(r_-, r_+, r)\,\mathrm{d}r = \frac{1}{t_*} \int_{r_-}^{r_+} \sqrt{\varphi(r_+) + \varphi(r_-) - \varphi(r) - \varphi(r_- + r_+ - r)}\,\mathrm{d}r \tag{97b}$$

$$p = \rho \int_{r_-}^{r_+} (C^2 - r\varphi'(r))w(r_-, r_+, r)\,\mathrm{d}r$$

$$= -\frac{1}{t_*} \int_{r_-}^{r_+} \frac{\varphi'(r)\,\mathrm{d}r}{\sqrt{\varphi(r_+) + \varphi(r_-) - \varphi(r) - \varphi(r_- + r_+ - r)}} \tag{97c}$$

$$u = \int_{r_-}^{r_+} (\tfrac{1}{2}C^2 + \varphi(r))w(r_-, r_+, r)\,\mathrm{d}r = \tfrac{1}{2}(\varphi(r_-) + \varphi(r_+)) \tag{97d}$$

$$q = 0. \tag{97e}$$

The list (97) defines the *oscillator closure* with $t_*(r_-, r_+)$, $w(r_-, r_+, r)$ and $C(r_-, r_+, r)$ given by (92), (93) and (91), respectively. In each line the first equality results from the evaluation of the microscopic representations (37) and (38) 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 ρ, v and T or alternatively for the variables r_-, r_+ and v. The system consists of the conservation laws (96) and of the constitutive equations (97). Using the closure conditions (97) we are able to derive from (96) the differential form (36) of the conservation laws as well as the Rankine–Hugoniot conditions (74), 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

$$T\,\mathrm{d}h = \mathrm{d}u + p\,\mathrm{d}\left(\frac{1}{\rho}\right). \tag{98}$$

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 (96) and (97) runs along the same lines as 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 $\rho(r_-, r_+)$, temperature $T(r_-, r_+)$, pressure $p(r_-, r_+)$ and internal energy $u(r_-, r_+)$, which are defined in (97):*

$$\frac{\partial}{\partial r_-}\left(\frac{1}{T}\left(\frac{\partial u}{\partial r_+} + \frac{1}{2}p\right)\right) = \frac{\partial}{\partial r_+}\left(\frac{1}{T}\left(\frac{\partial u}{\partial r_-} + \frac{1}{2}p\right)\right). \tag{99}$$

(ii) The condition (99) implies the existence of the specific entropy function $h(r_-, r_+)$ according to

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

which yields after integration

$$h(r_-, r_+) = \ln\left(\int_{r_-}^{r_+} \sqrt{\varphi(r_+) + \varphi(r_-) - \varphi(r) - \varphi(r_- + r_+ - r)}\,\mathrm{d}r\right). \tag{101}$$

Proof. (99) is the integrabily condition for (98). By introducing the functions $p_0(r_-, r_+) = t_*(r_-, r_+)p(r_-, r_+)$ and $T_0(r_-, r_+) = t_*(r_-, r_+)T(r_-, r_+)$, and with (97d), we may write (99)

in its equivalent form

$$\frac{\partial p_0}{\partial r_+} - \frac{\partial p_0}{\partial r_-} = \varphi'(r_+)\frac{\partial t_*}{\partial r_-} - \varphi'(r_-)\frac{\partial t_*}{\partial r_+} + \frac{1}{T}\left((\varphi'(r_-) + p)\frac{\partial T_0}{\partial r_+} - (\varphi'(r_+) + p)\frac{\partial T_0}{\partial r_-}\right). \quad (102)$$

Next we calculate the identities

$$\frac{\partial T_0}{\partial r_-} = \frac{t_*}{2}(\varphi'(r_-) + p) \qquad \frac{\partial T_0}{\partial r_+} = \frac{t_*}{2}(\varphi'(r_+) + p) \qquad (103)$$

and introduce these in (102), which reduces to

$$\frac{\partial}{\partial r_+}(p_0 + \varphi'(r_-)t_*) = \frac{\partial}{\partial r_-}(p_0 + \varphi'(r_+)t_*). \quad (104)$$

If we again use the identities (103), we can write condition (104) in the form

$$\frac{\partial^2 T_0}{\partial r_- \partial r_+} = \frac{\partial^2 T_0}{\partial r_+ \partial r_-}. \quad (105)$$

It 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 condition (104) by direct substitution:

$$\frac{\partial t_*}{\partial r_+} = \frac{+t_*}{r_+ - r_-} - \frac{1}{2}\int_{r_-}^{r_+} \frac{\varphi'(r_+) - \varphi'(r)\frac{r - r_-}{r_+ - r_-} - \varphi'(r_- + r_+ - r)\frac{r_+ - r}{r_+ - r_-}}{[\varphi(r_-) + \varphi(r_+) - \varphi(r) - \varphi(r_- + r_+ - r)]^{\frac{3}{2}}}\,\mathrm{d}r \quad (106a)$$

$$\frac{\partial t_*}{\partial r_-} = \frac{-t_*}{r_+ - r_-} - \frac{1}{2}\int_{r_-}^{r_+} \frac{\varphi'(r_-) - \varphi'(r)\frac{r_+ - r}{r_+ - r_-} - \varphi'(r_- + r_+ - r)\frac{r - r_-}{r_+ - r_-}}{[\varphi(r_-) + \varphi(r_+) - \varphi(r) - \varphi(r_- + r_+ - r)]^{\frac{3}{2}}}\,\mathrm{d}r \quad (106b)$$

$$\frac{\partial p_0}{\partial r_+} = -\frac{t_*}{r_+ - r_-}\cdot\varphi'(r_+)$$

$$+ \frac{1}{2}\int_{r_-}^{r_+} \frac{\varphi'(r_+)[\varphi'(r)\frac{r_+ - r}{r_+ - r_-} + \varphi'(r_- + r_+ - r)\frac{r - r_-}{r_+ - r_-}] - \varphi'(r)\varphi'(r_- + r_+ - r)}{[\varphi(r_-) + \varphi(r_+) - \varphi(r) - \varphi(r_- + r_+ - r)]^{\frac{3}{2}}}\,\mathrm{d}r$$

$$\frac{\partial p_0}{\partial r_-} = +\frac{t_*}{r_+ - r_-}\cdot\varphi'(r_-) \qquad (107)$$

$$+ \frac{1}{2}\int_{r_-}^{r_+} \frac{\varphi'(r_-)[\varphi'(r)\frac{r - r_-}{r_+ - r_-} + \varphi'(r_- + r_+ - r)\frac{r_+ - r}{r_+ - r_-}] - \varphi'(r)\varphi'(r_- + r_+ - r)}{[\varphi(r_-) + \varphi(r_+) - \varphi(r) - \varphi(r_- + r_+ - r)]^{\frac{3}{2}}}\,\mathrm{d}r.$$

These integrals exist in the convex region $\varphi''(r) > 0$, but they cannot be obtained by a simple differentiation rule, because singularities with exponent $-\frac{3}{2}$ appear at $r = r_-$ and at $r = r_+$. Here we have calculated the partial derivatives by its definitions. For example, (106b) may be obtained as follows. We start with

$$\frac{\partial t_*}{\partial r_-} = \lim_{\epsilon \to 0}\frac{1}{\epsilon}[t_*(r_- + \epsilon, r_+) - t_*(r_-, r_+)] \quad (108)$$

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

$$r \to r_- + (r_+ - r_-)\frac{r - r_- - \epsilon}{r_+ - r_- - \epsilon}. \quad (109)$$

Then in (108) 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. $\square$
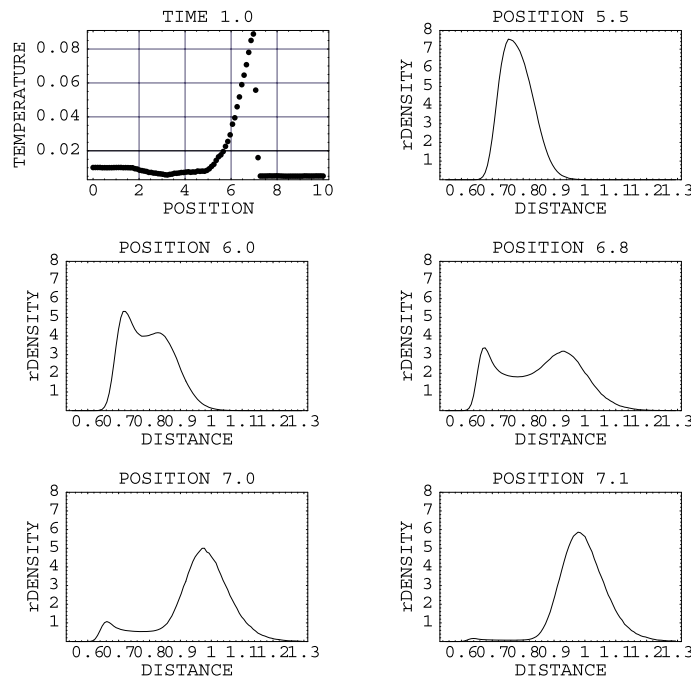
Figure 6. Transition of the distributions of velocities for various positions within the temperature pulse.

10.5. Transition from the thermal motion to the oscillator motion

Recall that in section 9.6 we considered 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 $N = 10\,000$ 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 $t = 1.0$ the temperature field as well as the distributions of the velocities and the distances at various positions. We now 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 as that we 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. By contrast, 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 borne out in 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.

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.
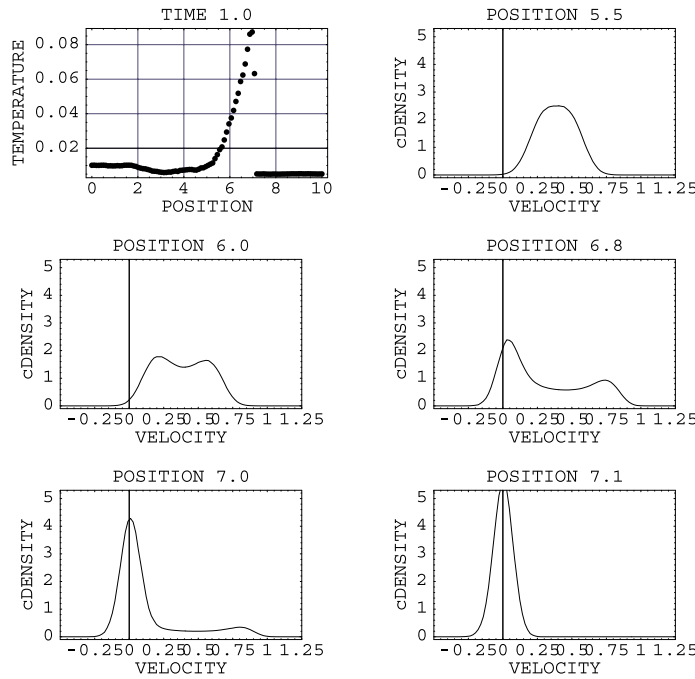
Figure 7. Transition of the distributions of distances for various positions within the temperature pulse.

The intermediate distribution functions exhibit some kind of transition between thermal and oscillator motion. In particular, the distribution of distances at position $x = 6.8$ is reminiscent of the pure oscillator distribution in 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 now illustrate the consequences of this statement, and start the discussion with a definition.

Definition. *An atomic chain at the macroscopic space–time point (t, x) is said to be in local equilibrium, if its microscopic motion, which is described by a distribution function in the close vicinity of (t, x), can also be established globally independent of space and time and is globally described by the same distribution function. In addition, we require that arbitrary small disturbances of the microscopic motion do not lead to a change of the distribution function.*

We now pose and answer 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: A material at the macroscopic space–time point (t, x) is said to be in local equilibrium, if the macrostate of the material at that point
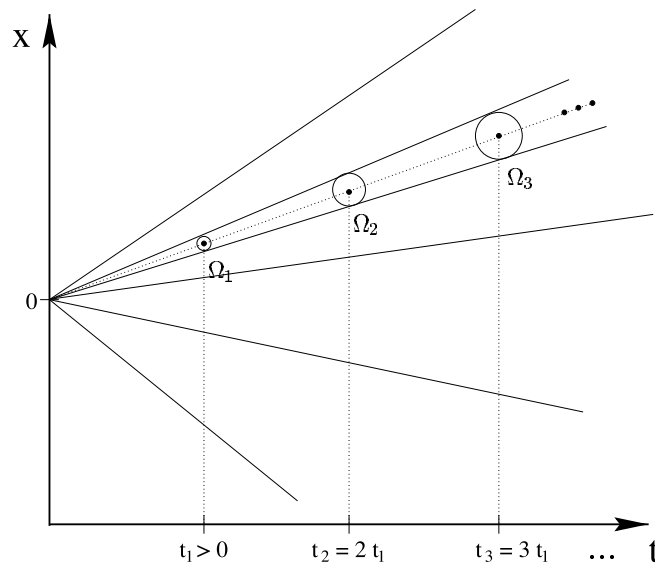
Figure 8. The scaling invariance of the microscopic Riemann solution.

is completely given by a distribution function of the microscopic motion which has only the quantities ρ, v and T as parameters.

Note that our definition of local equilibrium does not contain any reference to the quantities ρ, v and T. In particular it is not assumed that the characterization of an equilibrium distribution function is given by a finite set of variables.

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 x/t, if N is sufficiently large and if the jump is initially located at $x = 0$. 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 $x = 0$.

We consider the infinite sequence of regions Ω_1, Ω_2, Ω_3, ..., of increasing size. If the fields $u_A(x/t)$ do not change significantly in time and space within a small region, say Ω_1, then the same is true in a macroscopically large region Ω_n, with large n.

We now describe 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 Ω_1, sufficiently small so that the microscopic motion within Ω_1 does not change significantly.

Next we inflate Ω_1 within the segment from figure 8 in order to end up with a large region Ω_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 Ω_n is the same as in Ω_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. In contrast, 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.

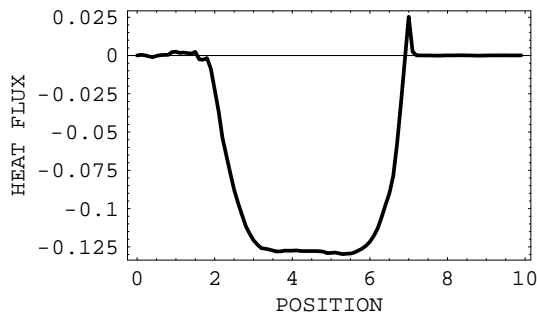This can be immediately observed from a comparison of figure 9 with the corresponding

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

temperature field from figures 6 and 7. Moreover, the time and space dependence of the heat flux is also obviously 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 implicitly 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 if we only consider pure thermal and pure oscillator motion.

Thus, generally the appropriate closure changes within a given Riemann solution.

11. Conclusions and perspectives

In this paper we have established a rigorous micro–macro transition for the atomic chain that serves as a simple model of a solid body.

The microscopic dynamics of the atomic chain is based on the Newtonian equations of motion for its microsopic particles.

The Newtonian equations imply macroscopic conservation laws and unique representations that uniquely link the thermodynamic quantities to the trajectories of the microscopic particles. This link is established by a window function of time and space.

The conservation laws become field equations for the thermodynamic variables if they are supplemented by macroscopic closure relations. For large particle numbers N and for given initial data the closure relations follow from the properties of the microscopic dynamics. The closure relations rely on two facts:

(1) We have only considered Riemannian initial data that lead exclusively to the propagation of waves. This special class of initial data imply macroscopic solutions of the microscopic dynamics that exhibit a special scaling behaviour admitting exclusively states of local equilibria.
(2) The corresponding statistical distributions of the atomic distances and velocities determine completely the microscopic motion and the form of the macroscopic field equations.

However, we could easily find initial data, such that their temporal development on the macroscale cannot be decribed by a single closure relation. If this happens, the macroscopic quantities cannot be calculated from macroscopic field equations; rather they can only be adequately calculated from their microscopic representations.

In fact, we have considered three different kinds of closure relations, and they are found to be realized in arbitrary large regions of space–time for given initial data.

The observed scaling behaviour, whereupon time and space are equally scaled by the particle number, results because we considered exlusively initial data that lead to the formation of wave motion on the macroscopic scale. In a further study we shall consider different initial data, that lead to diffusional motion on the macroscale. Preliminary studies have already shown, that initial contact discontinuities imply a scaling where time and space are treated differently with the particle number.

However, with respect to diffusional motion we must leave the restriction of one-dimensionality. Furthermore, we shall establish the micro–macro transition for a gaseous body. This is necessary because a gaseous body will not confront us with the problem of several kinds of microscopic equilibria, so that we can study the pure scaling behaviour without any interference with the non-uniqueness of local equilibria which we have met in the solid body.

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